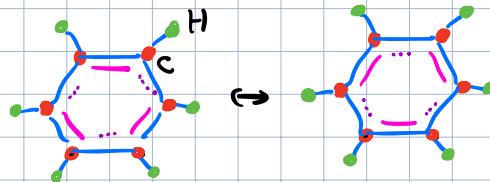


SSTH model is a model proposed to explain the physics of conducting polymers like polyacetylene. (Su, Schrieffer, Heeger, PRL 1979, PRB 1980)

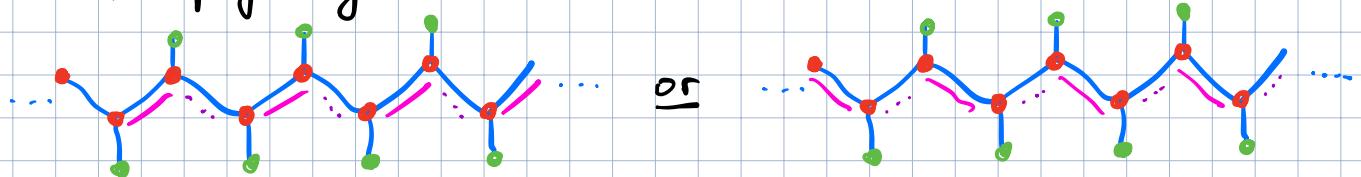
Recall the structure of benzene



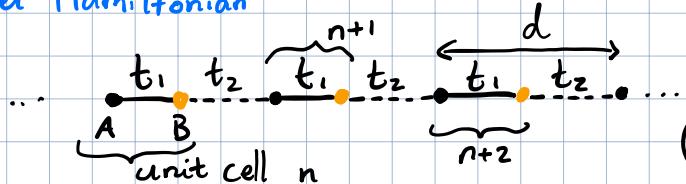
►  $sp^2$  hybridized bonds

►  $p^2$  extra electron forms "resonating valence bonds" (Pauling)

The model for polyacetylene is an extended version of benzene



\* 1D model Hamiltonian



Alternating hopping strengths arises from spontaneous dimerization

(Let us set lattice constant  $d=1$ )

$$\hat{H} = -t_1 \sum_n (C_{nA}^+ C_{nB} + C_{nB}^+ C_{nA}) - t_2 \sum_n (C_{n+1A}^+ C_{nB} + C_{nB}^+ C_{n+1A})$$

$$\text{Fourier transform: } C_{nk}^+ = \frac{1}{\sqrt{N}} \sum_k C_{kA}^+ e^{-ikn}$$

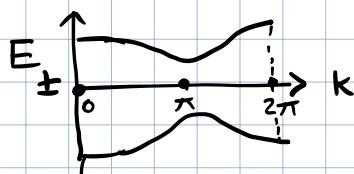
$$C_{nB}^+ = \frac{1}{\sqrt{N}} \sum_k C_{kB}^+ e^{-ikn}$$

$$\therefore \hat{H} = -t_1 \sum_k (C_{kA}^+ C_{kB} + C_{kB}^+ C_{kA}) - t_2 \sum_k (C_{kA}^+ C_{k+1B} e^{-ik} + C_{kB}^+ C_{k+1A} e^{ik})$$

$$\hat{H} = \sum_k \begin{pmatrix} C_{kA} \\ C_{kB} \end{pmatrix} \mathcal{H}_{\text{Bloch}}(k) \begin{pmatrix} C_{kA} \\ C_{kB} \end{pmatrix} \text{ where } \mathcal{H}_{\text{Bloch}}(k) \equiv \begin{pmatrix} 0 & -t_1 - t_2 e^{-ik} \\ -t_1 - t_2 e^{ik} & 0 \end{pmatrix}$$

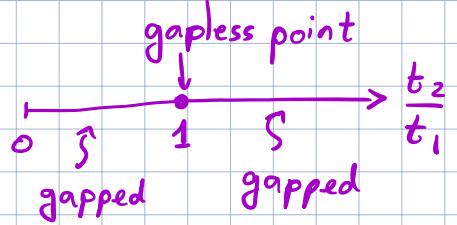
{More generally,  $\mathcal{H}_{\text{Bloch}} \equiv n \times n$  matrix for  $n$ - "orbitals"}

$$\text{Eigenvalues of } \mathcal{H}_{\text{Bloch}}(k): E_{\pm}(k) = \pm \left[ (t_1 + t_2 \cos k)^2 + (t_2 \sin k)^2 \right]^{1/2}$$



Let us set  $t_1, t_2 \geq 0$

Minimum gap at  $k=\pi$



Q: • Are both gapped phases the same or are they distinct?

- If they are 'same', Why are they separated by a transition?
- If they are distinct phases, what distinguishes them?

► Bulk distinction: geometric view  $2 \times 2$  Hermitian basis

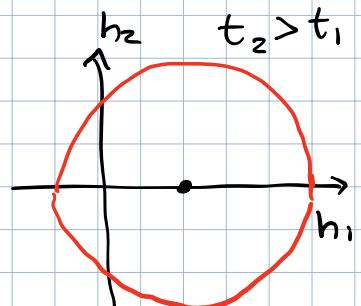
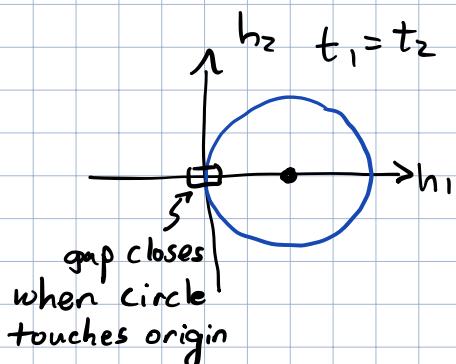
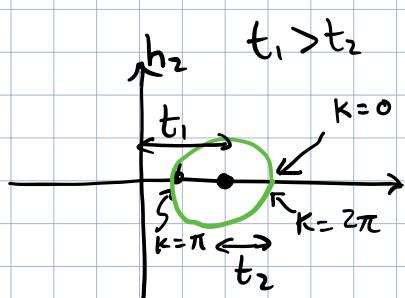
$$\text{Write } h_{\text{Bloch}}(k) = -h(k) \cdot \sigma_k$$

real coeff

$\sigma_k: \sigma_0, \sigma_1, \sigma_2, \sigma_3$   
 $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$$\text{Eigenvalues: } -h_0 \pm |\vec{h}| \quad \therefore \text{gap} = 2|\vec{h}(k)|$$

$$\left. \begin{array}{l} h_0 = h_3 = 0 \\ h_1 = t_1 + t_2 \cos k \\ h_2 = t_2 \sin k \end{array} \right\} (h_1 - t)^2 + h_2^2 = t_2^2 \quad \{\text{eqn for a circle in } h_1, h_2 \text{ plane}\}$$



\* Distinction between two insulators is in whether circle encloses the origin

\* Looks like a "yes" or "no" question  $\Rightarrow \mathbb{Z}_2$  invariant? (revisit below)

\* Looks like small deformations of "shape" (circle) shouldn't affect  $\Rightarrow$  topological protection

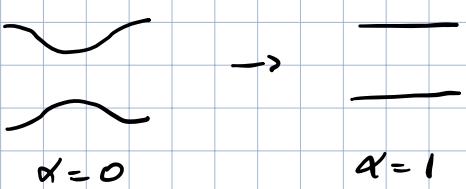
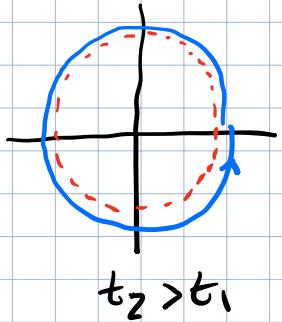
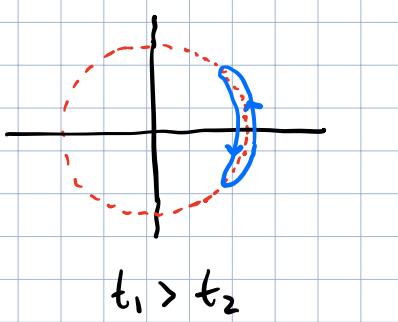
\* "Flattening the spectrum"

For cases where there is a gap (ie when  $t_1 \neq t_2$ ), we can define a modified Hamiltonian by smoothly "deforming" the SSH model Bloch Hamiltonian.

Let us set :  $\hat{n}(k) = \frac{\vec{h}(k)}{|\vec{h}(k)|}$

Consider  $H_{\text{Bloch}}(k, \alpha) = (1-\alpha) \vec{h}(k) \cdot \vec{\sigma} + \alpha \hat{n}(k) \cdot \vec{\sigma}$

When  $\alpha = 0$ ,  $H_{\text{Bloch}}(k, 0) = \vec{h}(k) \cdot \vec{\sigma}$  } As we tune  $\alpha : 0 \rightarrow 1$ ,  
 $\alpha = 1$ ,  $H_{\text{Bloch}}(k, 1) = \hat{n}(k) \cdot \vec{\sigma}$  } spectral gap does not close



\* For spectral flattened case, we can view the Bloch Hamiltonian

as a map from  $\{\text{circle}\}$   $\longrightarrow \{\text{circle}\}$   
 Brillouin Zone( $k$ )  $\hat{n}(k)$

\* Maps from  $S^1 \rightarrow S^1$  have topological invariant : Winding number  $\in \mathbb{Z}$

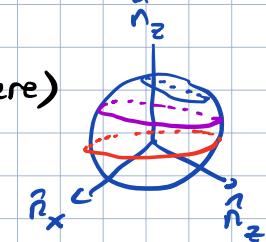
↪ "Homotopy theory" (David Mermin, RMP 1979 for gentle introduction)

↪ Look at loops and whether they can be "contracted" into one another  $\pi_1(S^1) = \mathbb{Z}$   
 closed loops in 1D BZ  $\hat{n}$  lives on circle

Q: We understand why 1D BZ is always a circle, but why does  $\hat{n}$  have to be on a circle? What can we add? why not  $h_0$  or  $h_3$ ?

► In one sense,  $h_0$  is "harmless"  $\because$  only shifts both bands up or down but can impact insulator vs metal.

►  $h_3$  has bigger impact  $\Rightarrow$  now  $\hat{n}$  lives on  $S^2$  (surface of sphere) and we can always contract loops without touching origin. Formally,  $\pi_1(S^2) = 0 \Rightarrow$  only trivial phase.



Q: Why  $\mathbb{Z}_2$ ? Earlier we said  $\mathbb{Z}_2$ : "Yes" or "No". what did we miss in SSH model? Why did we only find two phases?

\* Answer to both questions arises from asking what "deformations" are allowed in a general setting.

► Impose symmetries  $\rightarrow$  rule out  $h_0, h_3$

► Consider most general  $\mathcal{H}$  consistent with symmetries  $\rightarrow$  generalized SSH models

\* What symmetries can we impose? Motivation from Random matrix theory & generalization due to AZ, 1997

- ↳ Time reversal ( $T$ ):  $U \cdot K$
  - ↳ Charge conjugation ( $C$ ): particle-hole & Unitary
  - ↳ Chiral symmetry ( $S = C \cdot T$ )
- } symmetries
- ↳ 10-fold way to classify different phases

\* How do different symmetries act on operators & numbers

►  $T$ :  $C_n \rightarrow U_T C_n$      "n" includes spin index  
 $i \rightarrow -i$       $\Rightarrow U_T$  includes spin reversal

• Antiunitary

site internal

Let us construct Fourier transform (set  $n = l, \alpha$ )

$$C_k = \frac{1}{\sqrt{N}} \sum_l \bar{e}^{ikl} C_n$$

$$\therefore C_k \mapsto \frac{1}{\sqrt{N}} \sum_l e^{ikl} U_T C_n = U_T C_{-k}$$

$$H = \sum_k C_k^+ \mathcal{H}(k) C_k \xrightarrow{T} \sum_k C_{-k}^+ U_T^+ \mathcal{H}^*(-k) U_T C_{-k}$$

$$= \sum_k C_k^+ U_T^+ \mathcal{H}^*(-k) U_T C_k \quad \therefore \mathcal{H}(k) \mapsto U_T^+ \mathcal{H}^*(-k) U_T$$

Is SSH Hamiltonian  $T$ -invariant?

$$\mathcal{H}(k) = -\vec{h}(k) \cdot \vec{\sigma} = -h_0(k) \sigma_0$$

Spinless  $\Rightarrow$  we can ignore  $U_T$

$$\begin{aligned} \therefore \mathcal{H}(k) &\mapsto -h_1(-k) \sigma_1 - h_2(-k) \sigma_2^* - h_3(-k) \sigma_3 - h_0(-k) \sigma_0 \\ &= -h_1(-k) \sigma_1 + h_2(-k) \sigma_2 - h_3(-k) \sigma_3 - h_0(-k) \sigma_0 \end{aligned}$$

$\therefore T$ -invariance  $\Rightarrow h_0, h_1, h_3$ : even func<sup>n</sup> of  $k$  &  $h_2$ : odd func<sup>n</sup> of  $k$

►  $C:$   $i \mapsto i$   
 $C_n \mapsto U_c^* C_n^+$

$$C_k \mapsto \sum_l e^{ikl} U_T^* C_l^+$$

$$\therefore C_k \mapsto U_c^* C_{-k}^+ \quad H \mapsto C_{-k} U_c^T \mathcal{H}(k) U_c^* C_{-k}^+$$

$$\begin{aligned} \therefore H &\mapsto \sum_k C_{-ka} (U_c^T)_{\alpha\beta} \mathcal{H}_{\beta\mu}(k) (U_c^*)_{\mu\nu} C_{-k\nu}^+ \\ &= \sum_k (\delta_{\alpha\nu} - C_{-k\nu}^+ C_{-ka}) (U_c^T)_{\alpha\beta} \mathcal{H}_{\beta\mu}(k) (U_c^*)_{\mu\nu} \\ &= \sum_k T_r \mathcal{H}(k) - \sum_k C_{-ka}^+ C_{k\nu} U_{\nu\beta}^T \mathcal{H}_{\beta\mu}(-k) U_{\mu a}^* \\ &= \sum_k T_r \mathcal{H}(k) - \sum_k C_{-ka}^+ C_{k\nu} (U_{\nu\mu}^T)^* \mathcal{H}_{\mu\beta}^*(-k) (U_{\beta a})_{\rho\nu} \end{aligned} \quad \left. \begin{array}{l} \text{C-Symmetry} \Rightarrow \\ \bullet \text{Tr } \mathcal{H}(k) = 0 \\ \bullet \mathcal{H}(k) \mapsto -U_c^+ \mathcal{H}^*(-k) U_c \end{array} \right\}$$

►  $S:$   $i \mapsto -i$ ,  $C_n \mapsto U_s C_n^+$ ,  $C_k \mapsto U_s C_k^+$  (check)

$$\begin{aligned} H &\mapsto \sum_k C_{ka} (U_s^T)_{\alpha\beta} \mathcal{H}_{\beta\mu}^*(k) (U_s)_{\mu\nu} C_{k\nu}^+ = \sum_k (\delta_{\alpha\nu} - C_{k\nu}^+ C_{ka}) U_{\alpha\beta}^+ \mathcal{H}_{\beta\mu}^* U_{\mu\nu} \\ &= \sum_k T_r \mathcal{H}(k) - \sum_k C_{ka}^+ C_{k\nu} (U_s^*)_{\alpha\mu}^+ \mathcal{H}_{\mu\beta} U_{\beta\nu}^* \quad \therefore \mathcal{H}(k) \mapsto -(U_s^*)^+ \mathcal{H}(k) U_s^* \end{aligned}$$

• For SSH model, let us demand "chiral symmetry" or "sublattice" symmetry

In our case, let us choose:

$$\begin{aligned} C_{nA} &\mapsto C_{nA}^+, \quad C_{nB} \mapsto -C_{nB}^+, \quad i \mapsto -i \\ \therefore C_{kA} &\mapsto C_{kA}^+, \quad C_{kB} \mapsto -C_{kB}^+, \quad i \mapsto -i \Rightarrow \left\{ \begin{array}{l} U_s = \sigma_3 \\ -\sigma_3 \mathcal{H} \sigma_3 = \mathcal{H} \\ 2 \text{Tr } \mathcal{H} = 0 \end{array} \right\} \Rightarrow h_0 = h_3 = 0 \end{aligned}$$

► Note: if we demand C-symmetry, can add  $[h_0(k) \cdot \sigma_3]$   $\Rightarrow \mathbb{Z}_2$  classification

## ► Edge distinction

\* Consider open chains with finite # unit cells

{ strong  $t_1$  phase }



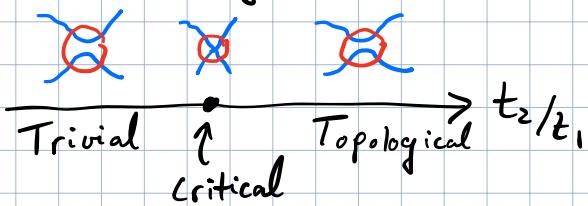
{ strong  $t_2$  phase }



\* Field theoretic view: Jackiw, Rebbi

With  $S$  symmetry  $\rightarrow \epsilon = 0$   
 $\& L \rightarrow \infty$ . Can't add  $C_{LA}^+ C_{LA}$

Useful as toy model to think about QFTs.



Near gapless critical point, we can zoom in near  $\epsilon = 0$  &  $k = \pi$  & write a continuum theory

Let us call  $t_1 \equiv t$ , and fix  $t_2/t_1 = 1 + m$  where  $m=0$  is critical point.  
 $m < 0 \Rightarrow$  trivial &  $m > 0 \Rightarrow$  topological.

Setting  $k = \pi + k_x$ , we get  $e^{ik} = e^{i(\pi + k_x)} = -e^{ik_x} \approx -(1 + ik_x)$

$$\therefore \mathcal{H}_{\text{Bloch}} = \begin{pmatrix} 0 & -t, -t_2 e^{ik} \\ -t, -t_2 e^{ik} & 0 \end{pmatrix} \approx \begin{pmatrix} 0 & -t + t(1+m)(1-ik_x) \\ -t + t(1+m)(1+ik_x) & 0 \end{pmatrix}$$

$$\mathcal{H}_{\text{Bloch}} \approx t(K_x \sigma_2 + m \sigma_1)$$

$$\hookrightarrow \text{dispersion} = \pm t \sqrt{m^2 + k_x^2}$$

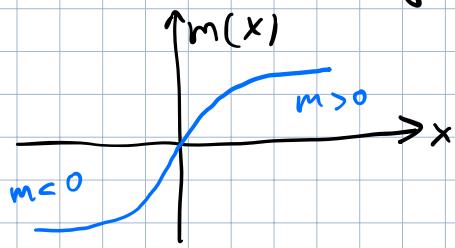
$m \equiv \text{mass}$

We can go to real space & write this as

$$\mathcal{H}_{\text{Bloch}} = t (-i \sigma_2 \partial_x + m \sigma_1)$$

"Emergent relativity"

To make a domain wall between trivial & topological, we can let  $m \equiv m(x)$ . Try to solve the Dirac equation for zero energy state (motivated by pictorial viewpoint)



$$\begin{aligned} -i \sigma_2 \partial_x \Psi + m(x) \sigma_1 \Psi &= 0 \\ \therefore -i \partial_x \Psi - i m(x) \sigma_3 \Psi &= 0 \\ \therefore \partial_x \Psi &= -m(x) \sigma_3 \Psi \end{aligned}$$

2 component spinor

Let us pick basis states :  $\Phi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  &  $\Phi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$  so  $\sigma_3 \Phi_{\pm} = \pm \Phi_{\pm}$

Expand  $\Psi = a_+(x) \Phi_+ + a_-(x) \Phi_-$

$$\therefore (\partial_x a_+) \Phi_+ + (\partial_x a_-) \Phi_- = -m(x) a_+(x) \Phi_+ + m(x) a_-(x) \Phi_-$$

$$\therefore \begin{cases} \partial_x a_+ = -m(x) a_+ \Rightarrow a_+ = A_+ e^{-\int_0^x m(x') dx'} \\ \partial_x a_- = m(x) a_- \Rightarrow a_- = A_- e^{+\int_0^x m(x') dx'} \end{cases}$$

- Let  $x \rightarrow +\infty$  & profile   $\Rightarrow a_-$  diverges

$$\therefore A_- = 0$$

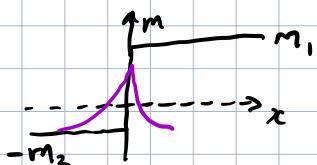
$$\therefore \Psi = A_+ e^{-\int_0^x m(x') dx'} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

- Let  $x \rightarrow +\infty$  & profile   $\Rightarrow a_+$  diverges

$$\therefore A_+ = 0$$

$$\therefore \Psi = A_- e^{\int_0^x m(x') dx'} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- We could pick specific profile, say



$$\Psi = \begin{pmatrix} 1 \\ 0 \end{pmatrix} * \begin{cases} A_+ e^{-m_1 x} & : x > 0 \\ A_+ e^{m_2 x} & : x < 0 \end{cases}$$

\* localized zero energy edge mode.

- General lessons:  $\Rightarrow$  Topological phase transition ~

Dirac mass changing sign as we tune parameters

$\Rightarrow$  Bulk topological phase ~ boundary localized "zero" modes.

\* Exercises:

[1] Consider a 1D chain with spin-polarized electrons at half-filling  $\langle n_i \rangle = 1/2$  coupled to phonons.

$$H = -t \sum_n (c_n^+ c_{n+1} + c_{n+1}^+ c_n) + g \sum_n \phi_n (c_n^+ c_{n+1} + c_{n+1}^+ c_n) + u \sum_n \phi_n^2 + \omega \sum_n \phi_n^4$$

Assuming a variational ansatz  $\phi_n = \phi(-1)^n$ , calculate the variational energy and minimize it with respect to  $\phi$ . What is the charge gap in the resulting insulator? Discuss what could happen if we dope this system with dilute electrons or holes.

[2] Consider a generalized SSH model with the Hamiltonian

$$H = -t_1 \sum_n (a_n^+ b_n + b_n^+ a_n) - t_2 \sum_n (b_n^+ a_{n+1} + h.c.) \\ - t_3 \sum_n (b_n^+ a_{n+2} + a_{n+2}^+ b_n)$$

- Go to momentum space and obtain  $\vec{h}(k)$ . Using a geometric picture or Winding #, explore the phase diagram with  $t_1=1$  & tuning  $t_2, t_3$ .
- Diagonalize Hamiltonian on finite chain and check edge modes in different phases. Give a simple pictorial view of edge modes.
- Can we add terms at the boundary to gap out edge modes? Imagine we are in class AIII which has chiral (S) symmetry only.

[3] Consider SSH model on semi-infinite chain with  $t_2 > t_1$

$$H = -t_1 \sum_{n=0}^{\infty} (a_n^+ b_n + b_n^+ a_n) - t_2 \sum_{n=0}^{\infty} (b_n^+ a_{n+1} + h.c.)$$

Construct lattice wavefunction of localized edge mode near left edge. How does wavefunction change as  $t_2 \rightarrow t_1$ ?