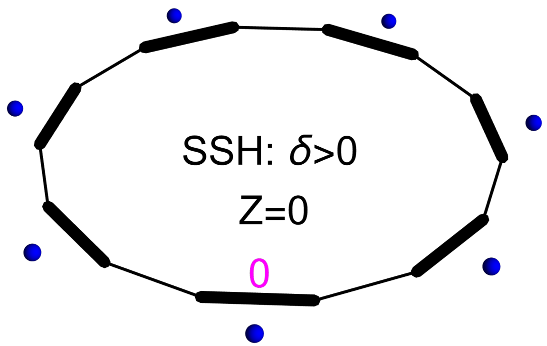
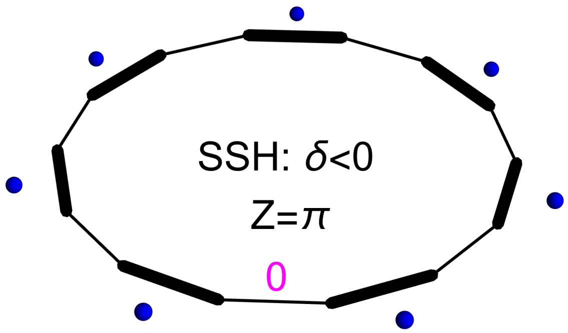
1D topological crystalline insulators

Jean-Noël Fuchs
LPTMC, CNRS and Sorbonne Université, Paris





δ = dimerization
Z = Zak phase

Review with J. Cayssol, J. Phys. Mater. 2021, arXiv:2012.11941
SSH & Shockley models with F. Piéchon, Phys. Rev. B 2021, arXiv:2106.03595

30’+10’

Collège de France 11/04/2025

Four messages/Outline

1) Two families of « topological phases of matter »

2) The Su-Schrieffer-Heeger chain is not a topological insulator

3) A small (but crucial) modification: s-p chain or Shockley model

4) Is the Kitaev/Majorana chain different from SSH?

1) Two families of gapped topological phases of matter

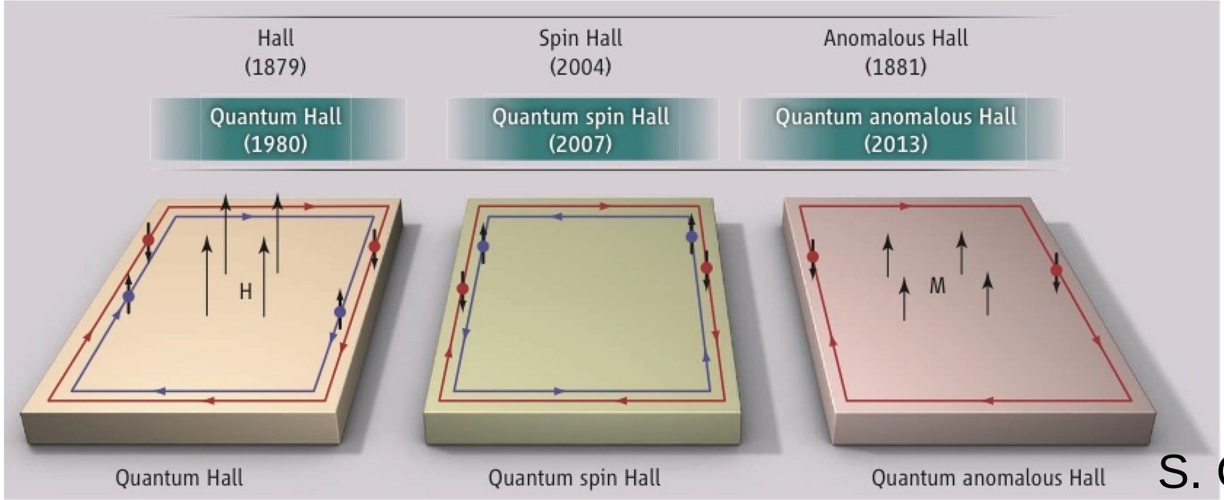
Integer topo phases (IQHE 1980)	Fractional topo phases (FQHE 1982)
Topo bands (Chern number) Berry phases	Topo groundstate degeneracy Anyons (fractionalized qps)
Short-range entanglement (not specific to quantum syst.)	Long-range entanglement (specific to quantum syst.)
Interactions not always needed	Interactions are crucial
Topological insulators Symmetry-protected topo phases (SPT)	Topological order Symmetry-enriched topo order (SET)
Thouless KNN 1982 Haldane 1983 $S = 1$ gapped AF chain Haldane 1988 Chern insulator Kane-Mele 2005 $\mathbb{Z}_2$ topo insulator	Laughlin 1983 fractional charges Wen 1990 topo order Kitaev 1997 toric code Levin-Wen 2005 string-nets

What is a topological insulator?

Bulk band insulator characterized by (measurable) topological invariant

Edges unavoidably host protected in-gap states (bulk-edge corresp.)

Intrinsic (2D Chern insulator with anomalous QHE, Haldane model 1988)
Or symmetry-protected (2D quantum spin Hall insulator, time-reversal symmetric, Z_2 invariant, Kane-Mele model 2005)



S. Oh, Science 2013

Textbook

2) Simplest example: SSH chain

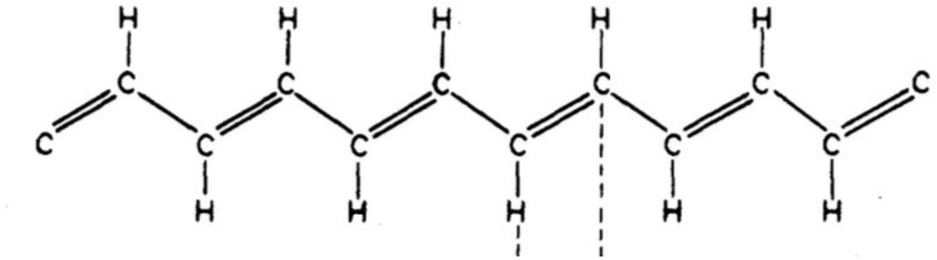
Dimerized tight-binding model (toy-model of trans-polyacetylene introduced to study domain wall solitons)

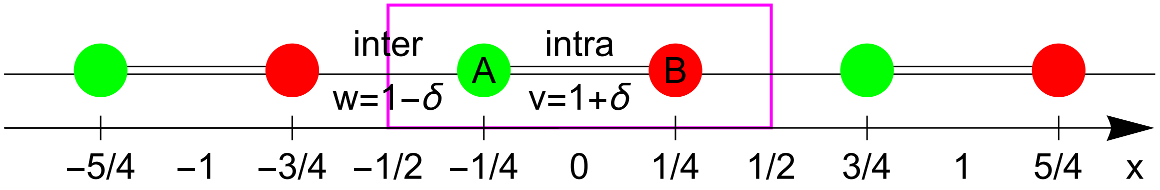
Bipartite, i.e. sublattice (or <u>chiral) symmetry</u>: A → A, B → -B

Topo invariant = winding number or Zak phase or polarization

Two different dimerizations (topo versus trivial) separated by a topo phase transition

Topological zero-energy edge modes (only for topo phase)





Su, Schrieffer, Heeger 1979

Textbook

Su Schrieffer Heeger Model

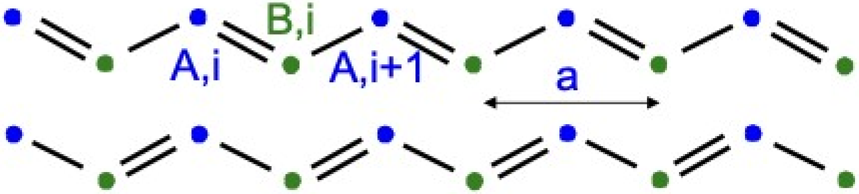
model for polyacetalene
simplest "two band" model

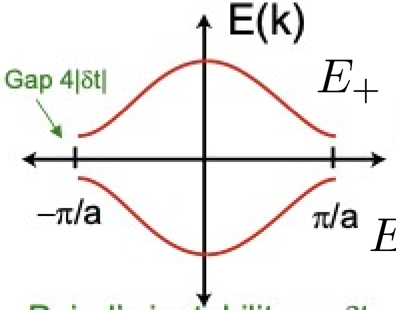
intra / inter

$$H = \sum_i (t+\delta t) c^\dagger_{Ai} c_{Bi} + (t-\delta t) c^\dagger_{Ai+1} c_{Bi} + h.c.$$

trivial phase $\delta t > 0$

topo phase $\delta t < 0$





$E_+ = +|\mathbf{d}(k)|$

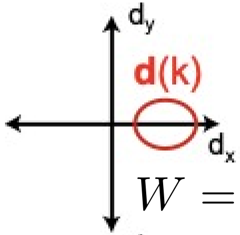
$E_- = -|\mathbf{d}(k)|$

$$H(k) = \mathbf{d}(k) \cdot \vec{\sigma}$$

$$d_x(k) = (t+\delta t) + (t-\delta t)\cos ka$$

$$d_y(k) = (t-\delta t)\sin ka$$

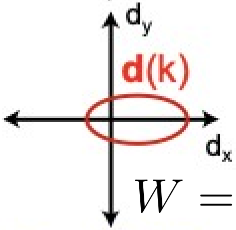
$$d_z(k) = 0$$



$W = 0$ Winding #

δt>0 : Berry phase 0 Zak phase

P = 0 Polarization



$W = 1$

δt<0 : Berry phase π

P = e/2

Provided symmetry requires $d_z(k)=0$, the states with δt>0 and δt<0 are topologically distinct.
Without the extra symmetry, all 1D band structures are topologically equivalent.

Slide from C. Kane's Windsor Lecture in August 2010

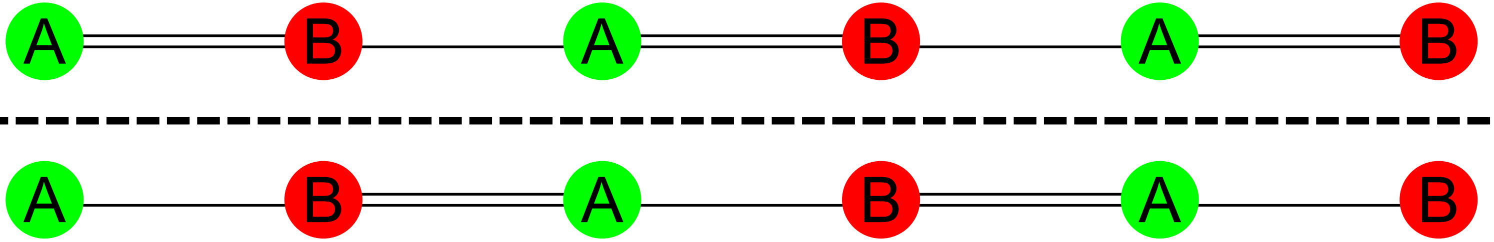
Textbook

Topological zero-energy end modes

Extreme cases ($\delta = \pm 1$) : weak bond is cut

triv: no ZM $\quad \delta > 0$

topo: 2 ZM $\quad \delta < 0$

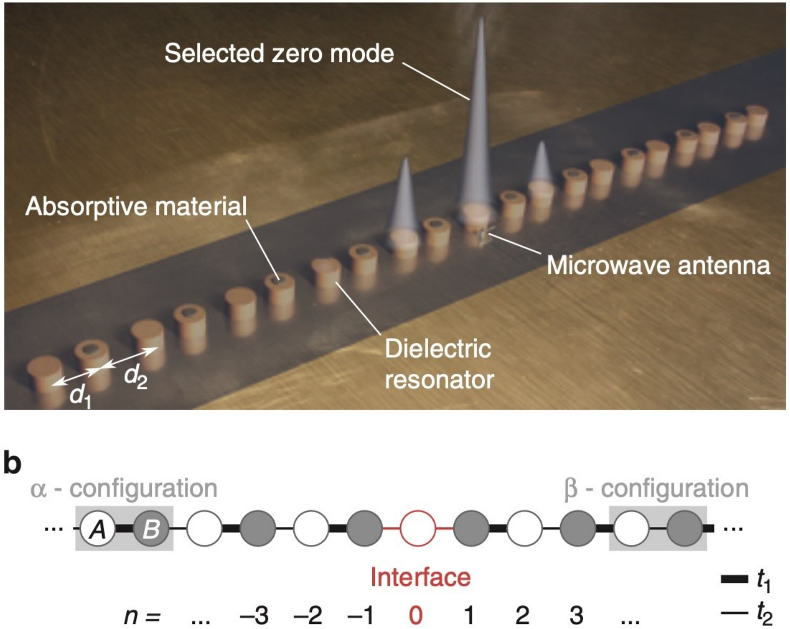


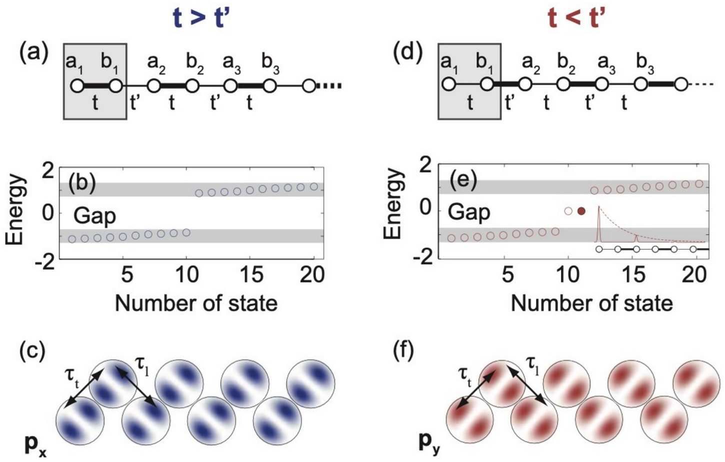
In general: exponential finite-size splitting of the "zero modes"

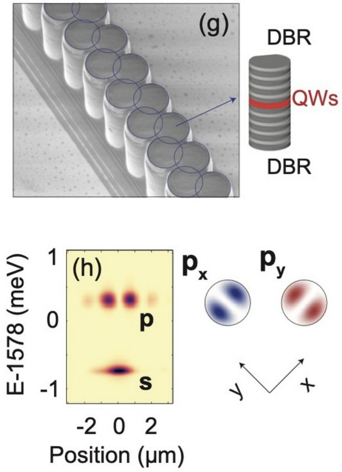
See J. Dalibard's 2018 CdF lectures

Experiments with the SSH chain

Cold atoms (BEC): I. Bloch's group 2013 → Zak phase difference
Microwaves: F. Mortessagne's group 2015 → defect-localized zero mode
Polaritons: J. Bloch and A. Amo's group 2017 → lasing in topo edge states
Rydberg atoms: A. Broaweys' group 2019 → hard-core bosons SPT

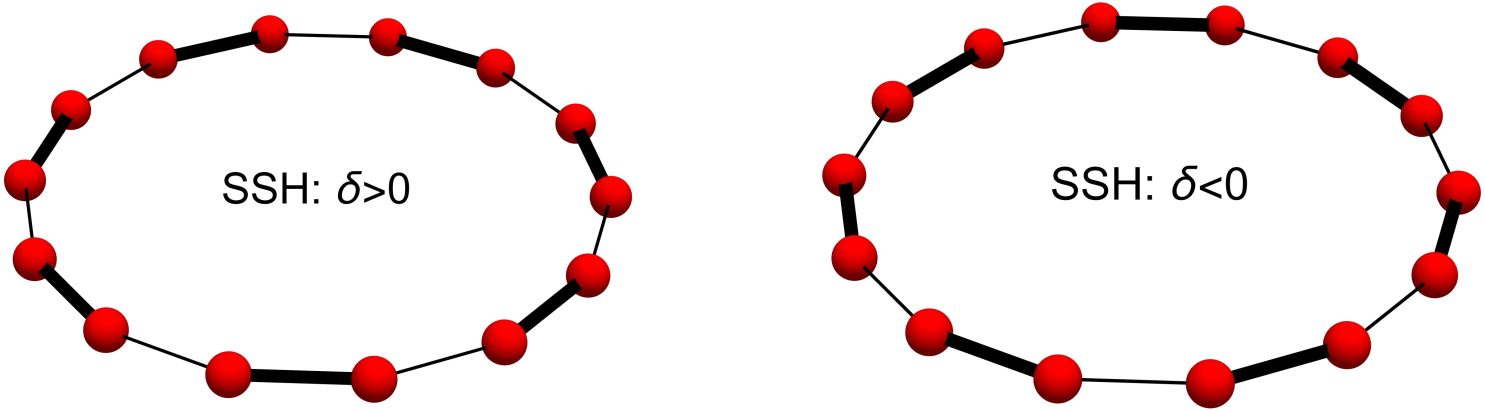






~~Textbook~~

Ring: 2 dimerizations are identical

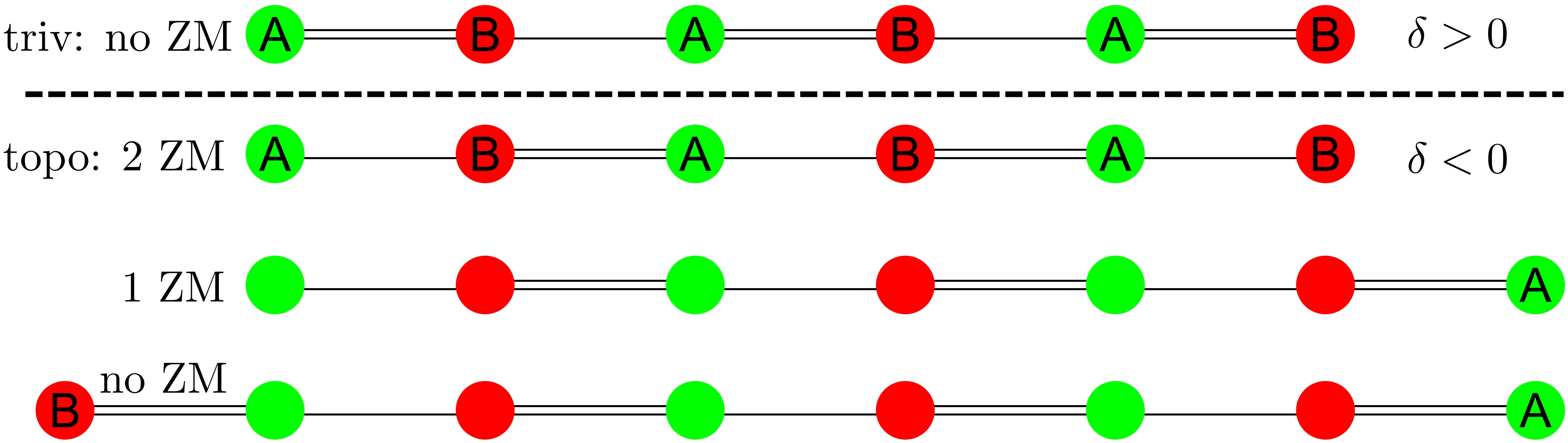


Related by half a unit cell translation.
Peierls instability: ------------ → -=-=-=-= versus =-=-=-=-
Two different groundstates of a spontaneous Z_2 symmetry breaking.
<u>Other example:</u> antiferromagnetic Ising chain
...↑↓↑↓↑↓↑↓… versus ...↓↑↓↑↓↑↓↑…
Both groundstates represent the same antiferromagnetic phase.

~~Textbook~~

Adding 2 sites changes “trivial” into “topo” without breaking sym.

ZM = zero mode localized on one edge



Nature of bulk phase can not depend on surface effects.

Ring : number of zero modes depends on the position of the cut.

Zak, Wannier and polarization

~~Textbook~~

Zak phase (0 or π) is not really different for the 2 dimerizations...
= peculiar Berry phase, non-contractible Brillouin zone cycle, gauge-inv.
~ Wannier (or band) center = average position in unit cell for the occupied band (choice of position origin, modulo 1): $Z = 2\pi\langle x\rangle_-$

Measurable quantity = electric polarization = electronic part + ionic part:

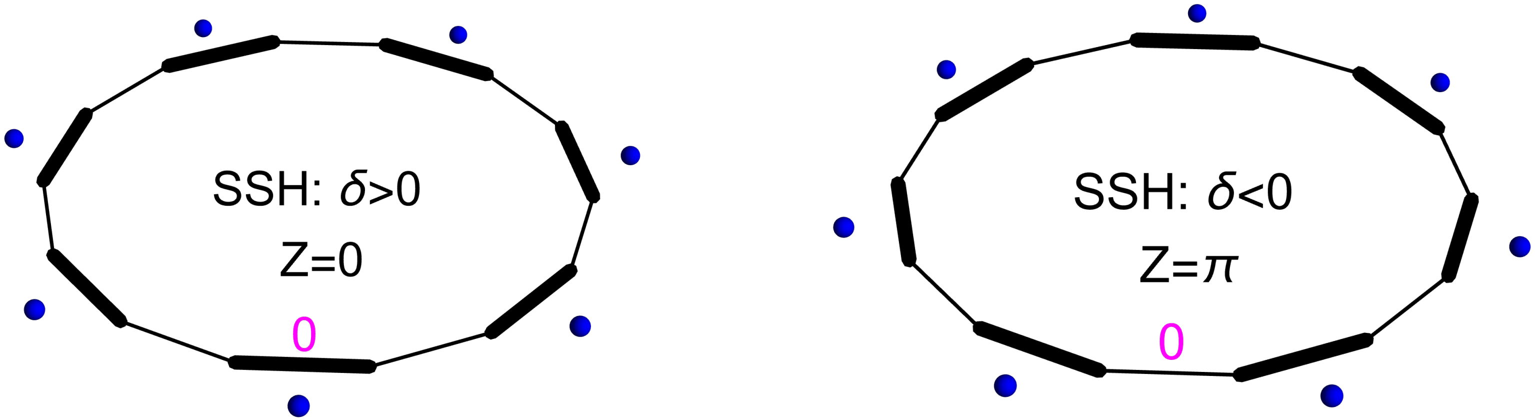
$$P = -\langle x\rangle_- + \sum_j \frac{1}{2}x_j = -\langle x\rangle_- + \bar{x} \text{ mod. } \frac{1}{2}$$

1 (spinless) electron per unit cell, charge = -1
Half filling, 2 identical sites per unit cell, ion charge = +1/2
Unit cell choice (translation invariance): polarization « quantum » P_q = ½

Inversion symmetry: P → -P = P modulo P_q
P = 0 or $P_q/2$: two classes of inversion-symmetric insulators (Z_2)

Zak 1989 ; King-Smith & Vanderbilt 93 ; Resta 92 & 94

~~Textbook~~ SSH: Zak phase & polarization



Origin on inversion center, also such that $\bar{x} = 0 \bmod 1/2$

Wannier centers always on strong bonds: $\langle x_- \rangle = 0$ or $1/2 \bmod 1$

$$Z = 2\pi \langle x \rangle_- = 0 \text{ or } \pi \bmod 2\pi$$

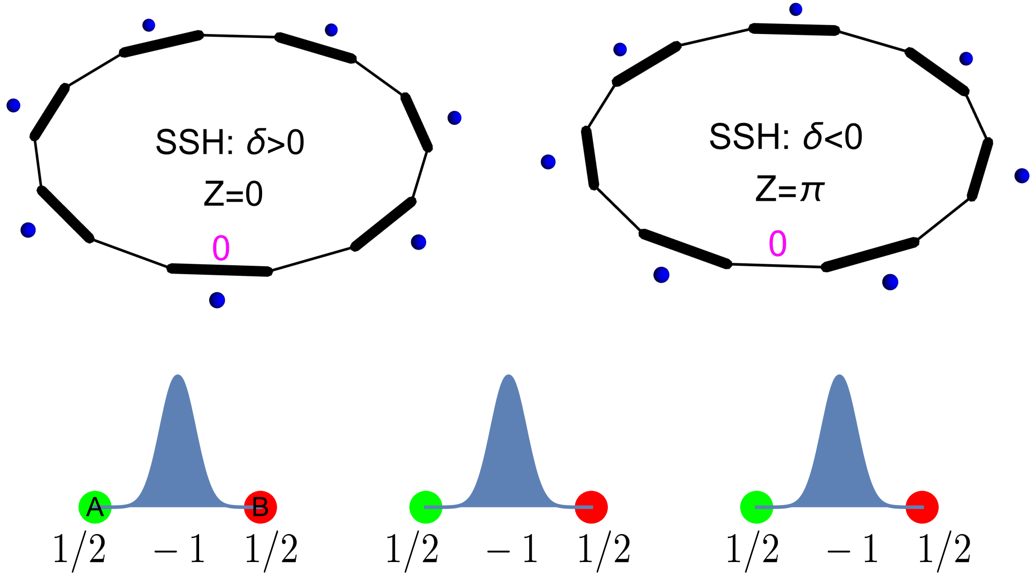
$$P = -\langle x \rangle_- + \bar{x} \bmod \frac{1}{2}$$

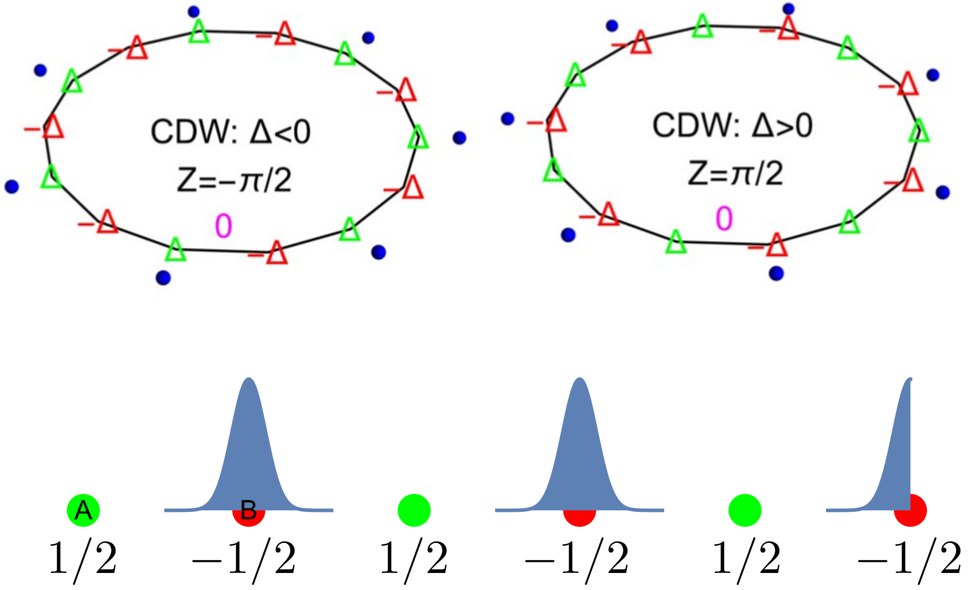
$$P = 0 \bmod \tfrac{1}{2}, \forall \delta \neq 0 \text{ , as if } Z = 0 \bmod \pi$$

~~Textbook~~ Inversion-symmetric band insulators

SSH (<u>bond inversion</u>): $P = 0$

CDW (<u>site inversion</u>): $P = \frac{P_q}{2}$





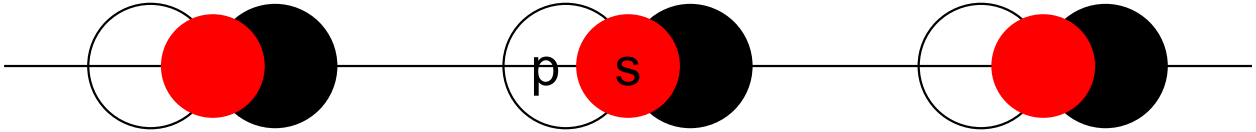
molecular insulator
non-polar dimers

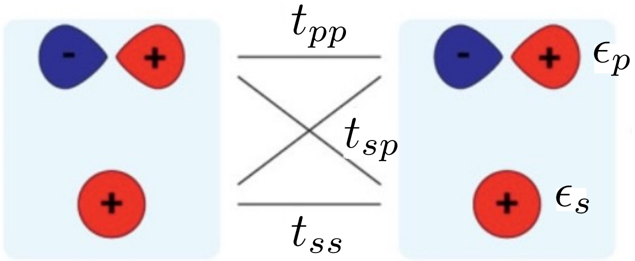
ionic insulator
1D rock salt Na^{+} Cl^{-}

3) Shockley model

Coupled s and p bands in 1D (1 site/unit cell, mixed inversion symmetry)

Inversion symmetry: s orbital even; p orbital odd





$$H(k) = \begin{pmatrix} \epsilon_s + 2t_{ss}\cos k & -i2t_{sp}\sin k \\ i2t_{sp}\sin k & \epsilon_p + 2t_{pp}\cos k \end{pmatrix}$$

Chiral limit: $\epsilon_s = -\epsilon_p < 0$ and $t_{ss} = -t_{pp} < 0$

$$\delta\epsilon = \epsilon_p - \epsilon_s = 2\epsilon_p > 0 \text{ and } 2\delta t = 2(t_{pp} - t_{ss}) = 4t_{pp} > 0$$

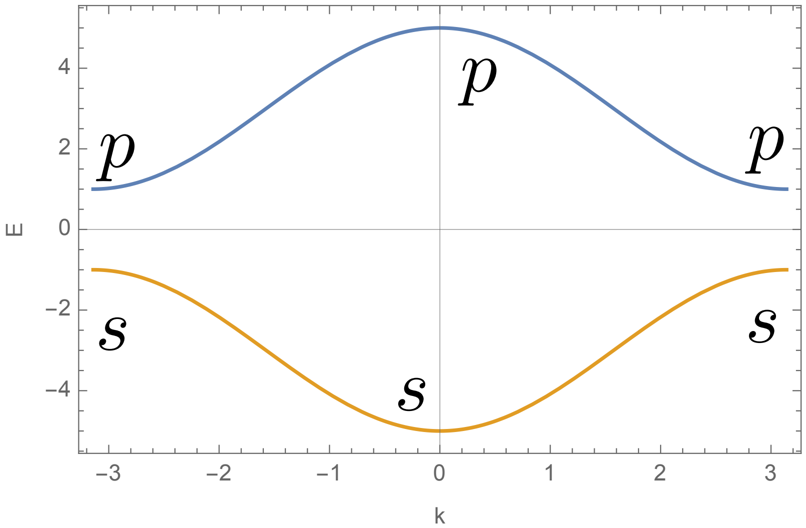
energy separation between orbitals — bandwidth

Charges/u.c. : 1 electron (charge -1) and 1 ion (charge $+1$) $\rightarrow P_q = 1$

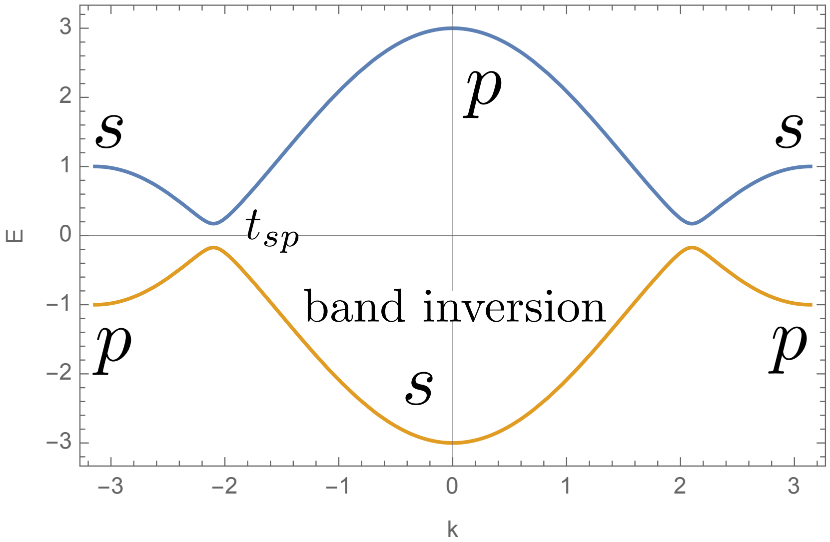
Shockley 1939; Vanderbilt & King-Smith 1993

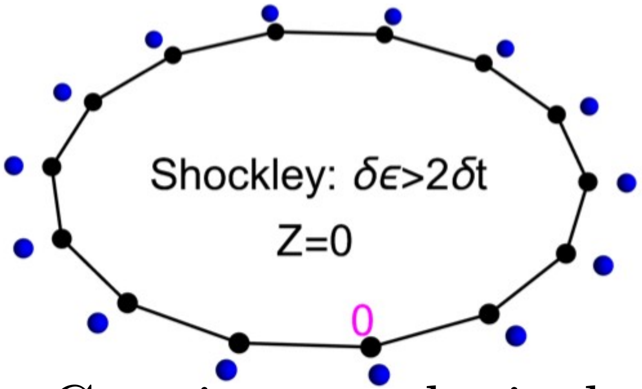
Shockley model

$\delta\epsilon > 2\delta t : P = 0, W = 0$



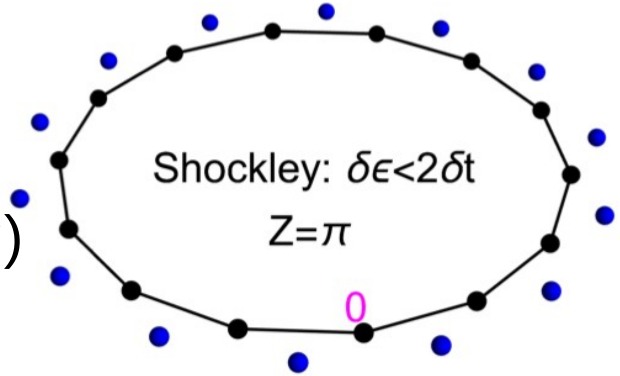
$\delta\epsilon < 2\delta t : P = P_q/2, W = 1$





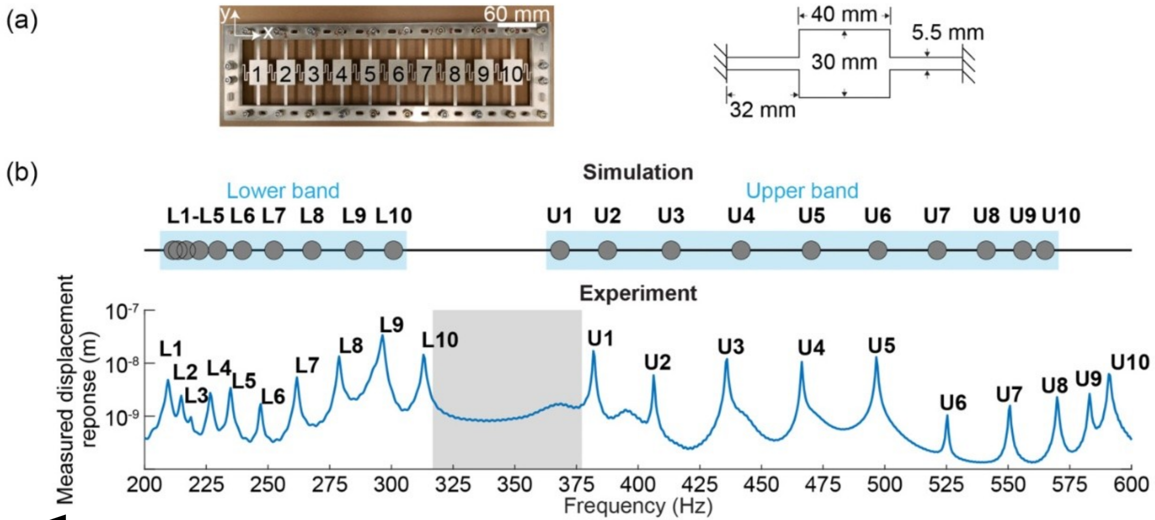
Atomic insulator (s bands)

Covalent insulator (sp bonding)



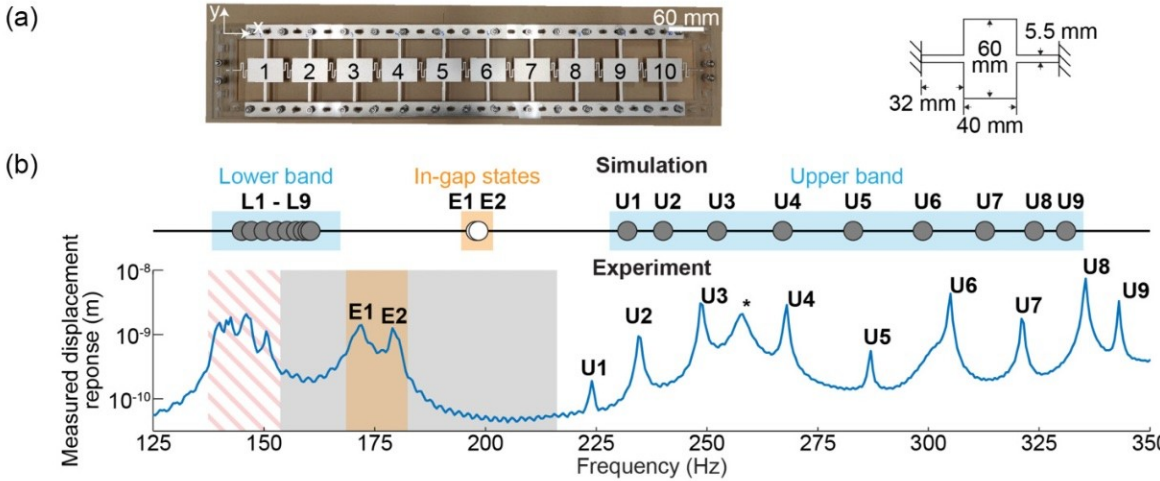
Genuine topological phase transition protected by inversion symmetry

Mechanical resonators chain



Trivial phase

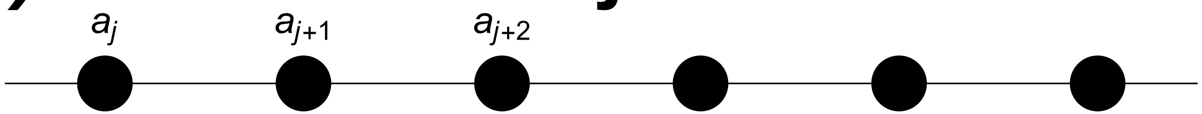
5 comments:
- In not mid
- Inv not chiral
- Splitting
- Indep length
- Not quantum



Topo phase
(2 in-gap states for any number of sites)

Gaurav Bahl’s group 2024

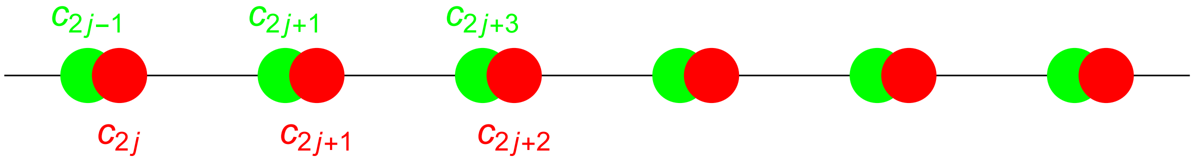
4) Kitaev/Majorana model



1D superconductor (BdG, mf)
Spinless complex fermions
p-wave pairing
Conserved fermionic parity

$$H_1 = \sum_j \Big[-w(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) - \mu \left(a_j^\dagger a_j - \frac{1}{2} \right) + \Delta a_j a_{j+1} + \Delta^* a_{j+1}^\dagger a_j^\dagger \Big] .$$

$$\{a_i, a_j^\dagger\} = \delta_{i,j}$$



1D Majorana chain
Dimerized hopping of real fermions
(like SSH?)
Conserved fermionic parity

intra inter

$$H_1 = \frac{i}{2} \sum_j [-\mu c_{2j-1} c_{2j} + 2w c_{2j} c_{2j+1}]$$

with $|\Delta| = w$

$$c_{2j-1} = a_j^\dagger + a_j$$
$$c_{2j} = i a_j^\dagger - i a_j$$

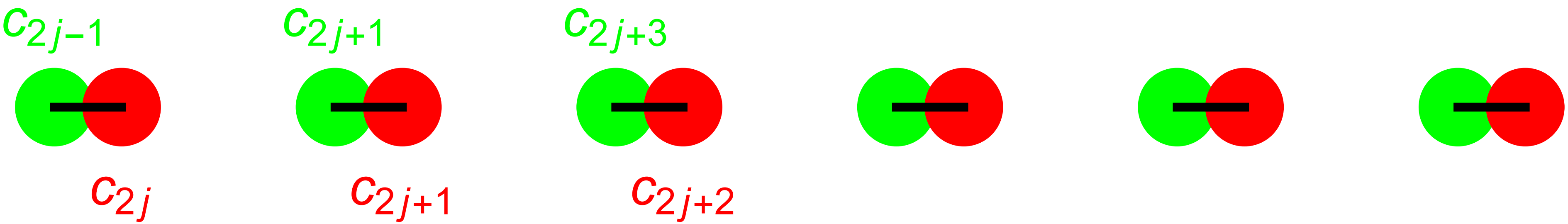
$$c_m^\dagger = c_m$$

Kitaev, Phys.-Usp. 44, 131 (2001)

Extreme cases

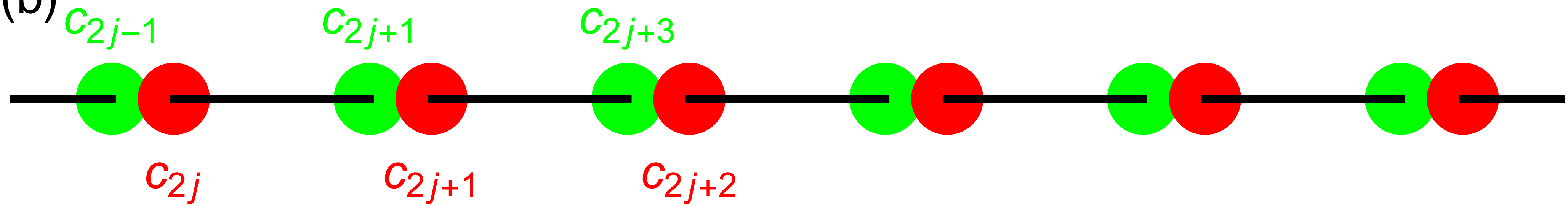
$$|\mu| > 2w = 0 \text{ (strong intra-site): trivial phase}$$

(a)



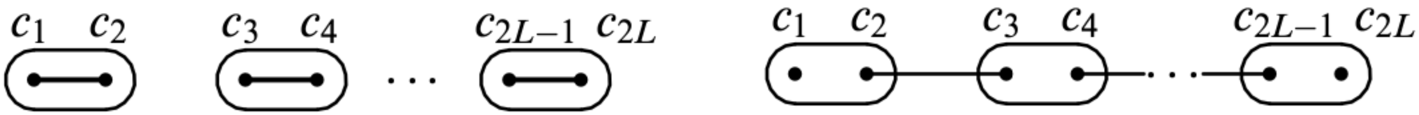
$$2w > \mu = 0 \text{ (strong inter-site): topo phase}$$

(b)



Kitaev, Phys.-Usp. 44, 131

Kitaev/Majorana model



	(a) $\|\mu\| > 2w$ (trivial phase)	(b) $\|\mu\| < 2w$ (topo)
OBC (Kitaev chain) edges equivalent to TFIM	unique GS even parity no edge mode	2-fold deg GS even/odd parity edge mode* occ/empty
PBC (Kitaev ring) no edges, global non-local order param.	unique GS even parity winding = 0	unique GS odd parity winding = 1
bulk no edges, local	"A subtle point is have the same	that both phases bulk properties."

*at 0 energy: 2 unpaired Majorana fermions = 1 complex fermion mode

From Kitaev's paper

These two cases represent two phases, or universality classes which exist in the model. A subtle point is that both phases have the same bulk properties. In fact, one phase can be transformed to the other (and vice versa) by mere permutation of Majorana operators,

$$c_m \mapsto c_{m+1} \,. \tag{10}$$

Such a local transformation (operator algebra automorphism) is usually considered as 'equivalence' in the study of lattice models‡. Yet the boundary properties of the two phases are clearly different: only the phase (b) has unpaired Majorana fermions at the ends of the chain. This is due to the fact that the operators c_{2j-1}, c_{2j} belong to one physical site while c_{2j}, c_{2j+1} do not. We may put it this way: one can not cut a physical site into two halves; if one could, both types of boundary states would be possible in both phases.

i.e. translation
by a/2

No unit cell choice
Two « orbitals »
belong to the same
site

Kitaev, Phys.-Usp. 44, 131 (2001)

Conclusion on inversion-symmetric insulators in 1D

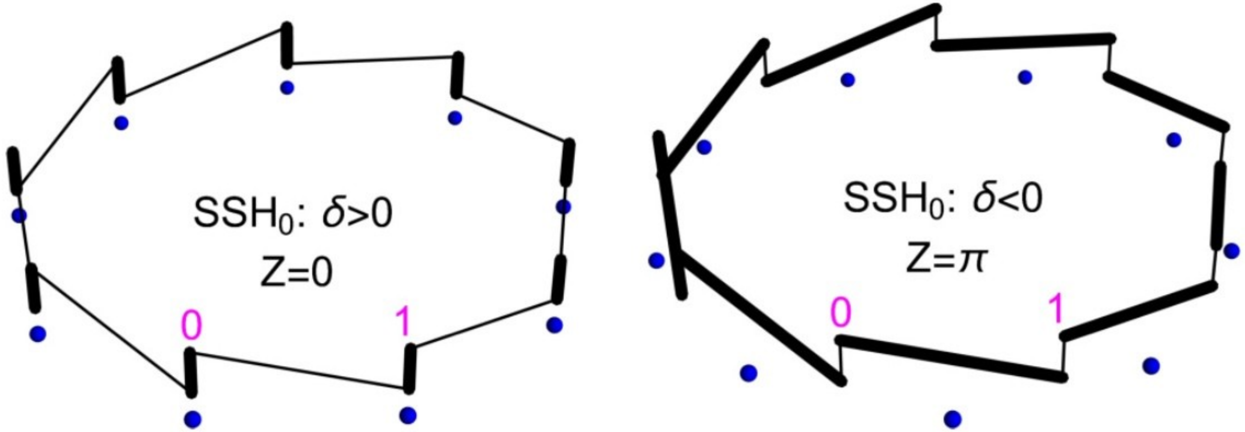
SSH	CDW	Shockley
single gapped phase	single gapped phase	two gapped phases
bond inversion	site inversion	mixed inversion
$P = 0 \bmod P_q$	$P = P_q/2 \bmod P_q$	$P = 0$ or $P_q/2 \bmod P_q$
molecular insulator	ionic insulator	atomic or covalent insulator

Intra > or < inter hopping does not matter (depends on choice of unit cell).
What matters is the electron position (Wannier center) with respect to the lattice.

Importance of <u>spatial embedding of the orbitals:</u> 2 orbitals per unit cell but at the same position or not.

Conclusion on Kitaev versus SSH

Kitaev ~ SSH_0 ~ chiral Shockley :
- two different gapped phases separated by topo phase transition
- particle-hole symmetry can not be broken. Conservation of fermionic parity Z_2.
- 2 “orbitals” per unit cell and at the *same* spatial location



SSH = $SSH_{1/2}$:
- *single* gapped phase
- polyacetylene has inversion but not chiral symmetry. SSH has chiral and inversion symmetry. Conservation of fermion number U(1).
- 2 orbitals per unit cell but at *different* spatial location

Thanks for your attention!