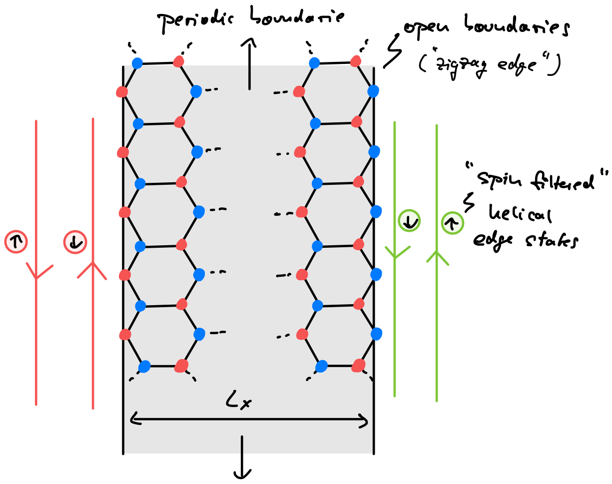
↓ Lecture 13 [30.05.25]

3.4. Edge modes

A particularly intriguing feature of phases with topological bands is the emergence of robust *edge modes* (the analogs of the chiral edge modes we encountered in quantum Hall systems, ← Section 1.6):

11 | ⊲ $\hat{H}_{\text{KM}}$ on a cylinder:

The system is therefore periodic in y-direction but has *boundaries* in x-direction.



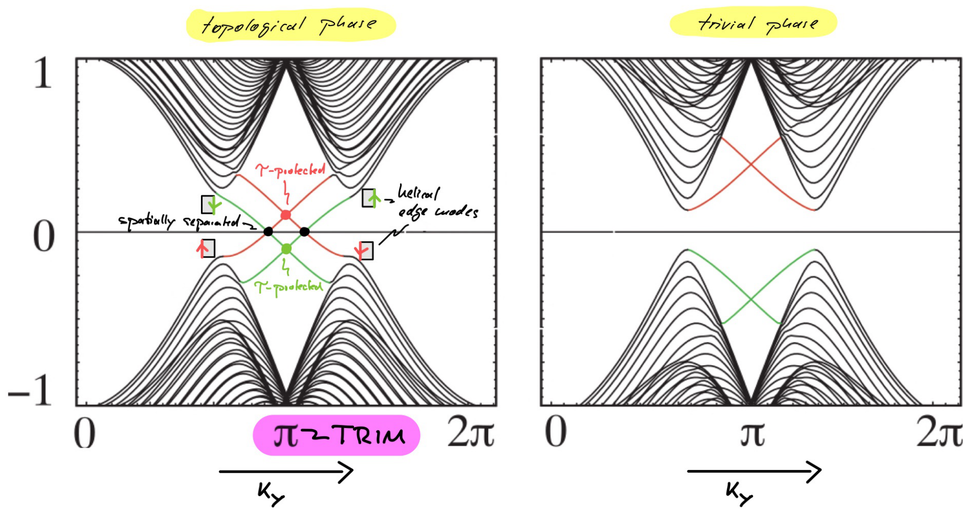
The type of boundary (“zigzag” vs. “armchair”) has no effect on the existence of the edge states but the spectrum below looks different for armchair boundaries.

→ Interpret strip as a 1D system with large, L_x-dependent unit cell

→ Fourier transform $\hat{H}_{\text{KM}}$ only in y-direction

→ 1D spectrum with $\mathcal{O}(L_x)$ bands labeled by y-momentum k_y

12 | Numerics → Edge modes:



This figure is taken from KANE and MELE’s original work [111].

- Topological phase → Gapless edge modes
  - Robust (= no backscattering / gap opening) to TRS perturbations
  - The four band crossings of the edge modes are protected for two different reasons:
    - Black crossings: The crossing modes are localized on *opposite* edges of the strip. Gapping them out is therefore exponentially suppressed with the width L_x of the strip (gapped bulk!).
    - Colored crossings: The crossing modes live on the *same* edge of the sample (with opposite group velocity). Gapping them out is forbidden by *time-reversal symmetry* as these crossings happen at a TRIM ($k_y = \pi$) and are enforced by Kramers degeneracy. This is why the Kane-Mele topological insulator is an SPT phase: Disorder that *breaks* TRS can hybridize these edge modes and destroy the topological phase.
  - On each edge there is a right-propagating mode for one spin polarization and a left-propagating mode for the opposite spin polarization (for $\lambda_R = 0$, if spin is conserved).

    In the original plots above, it is actually $\lambda_R = 0.05 \neq 0$ so that spin conservation is broken. The breaking of spin-conservation is responsible for the ↓ *avoided crossings* that fuse the edge modes into the bulk bands (for $\lambda_R = 0$ the edge modes would *cross* the bulk modes, ➔ Problemset 6).
  - The edge modes are *helical* (not *chiral*) since the product of spin and momentum is constant on each edge.
- Trivial phase → No gapless edge modes

Details: ➔ Problemset 6

Notes:

- The two "stalactite-stalagmite" pairs in the above spectrum correspond to the 1D projections of the two (gapped) Dirac cones around $\boldsymbol{K}$ and $\boldsymbol{K}'$. The tips of these bulk bands are connected by the edge modes.
- For $\lambda_R = 0$ you can extract the edge modes of the ← *Haldane Chern insulator* by just looking at one of the two spin sectors (up or down, which determines the sign of the complex NNN hopping phase). Thus in the topological phase, the Haldane model supports *one* (then *chiral* [since spin does not exist]) edge mode on each boundary.

13 | Final Note on symmetries and names:

- As discussed, the KM model $\hat{H}_{\text{KM}}$ without Rashba SO coupling ($\lambda_R = 0$) can be thought of as two uncoupled, time-reversed copies of Haldane's Chern insulator. As such, the model features a particle conservation symmetry in each of the two spin sectors, i.e., its total symmetry is $U(1)_\uparrow \times U(1)_\downarrow$. By defining *charge* $n_c = n_\uparrow + n_\downarrow$ and *spin* $n_s = n_\uparrow - n_\downarrow$, one can reinterpret this symmetry as $U(1)_{\text{charge}} \times U(1)_{\text{spin}}$, where total charge (particle) conservation $U(1)_{\text{charge}}$ and total spin conservation $U(1)_{\text{spin}}$ hold separately. One can then introduce the usual charge current $\boldsymbol{J}_c = \boldsymbol{J}_\uparrow + \boldsymbol{J}_\downarrow$ and the ⁂ *spin current* $\boldsymbol{J}_s = (\hbar/2e)\left(\boldsymbol{J}_\uparrow - \boldsymbol{J}_\downarrow\right)$ and ask for the linear response of these quantities when an electric field is applied. This response is quantified by the usual charge Hall conductivity σ_{xy}^c (previously σ_{xy}) and its analogue, the ⁂ *spin Hall conductivity* σ_{xy}^s. Because the ground state of $\hat{H}_{\text{KM}}$ is given by two filled Chern bands with opposite Chern numbers $C = \pm 1$, the charge Hall conductivity vanishes identically: $\sigma_{xy}^c = 0$ (this follows from our general discussion in Section 1.4.2). By contrast, the spin Hall conductivity is non-zero and quantized at $\sigma_{xy}^s = e/2\pi = 2 \times (\hbar/2e) \times e^2/h$

(because there are two counterpropagating edge modes with opposite spin, coming from the two Chern bands with opposite Chern number). The phenomenon of a quantized spin Hall conductivity (and vanishing charge Hall conductivity) is called ⁂ *quantum spin Hall effect (QSHE)* and characterized by the combined symmetry $U(1)_{\text{charge}} \times U(1)_{\text{spin}}$.

- It was a remarkable insight by Kane and Mele [111] that the two phases of the "Quantum Spin Hall effect in Graphene" [110] remained topologically distinct (via the Pfaffian index) *even without spin conservation* ($\lambda_R \neq 0$) – time-reversal symmetry is sufficient! This phase, protected by charge conservation $U(1)_{\text{charge}}$ and time-reversal symmetry $\mathbb{Z}_4^T$ [recall that $\tilde{T}_U^2 = -\mathbb{1}$ is equivalent to $\mathcal{T}_U^2 = (-1)^{\hat{N}_c}$, Section 2.1.2], and characterized by the Paffian $\mathbb{Z}_2$ index, is the *topological insulator (TI)* phase. Since spin conservation $U(1)_{\text{spin}}$ is generally broken in this phase, it is *not* characterized by a quantized spin Hall conductivity (= quantum spin Hall effect). One can indeed check that adding either TRS breaking terms *or* superconducting terms to the KM Hamiltonian $\hat{H}_{\text{KM}}$ on a cylinder *gaps out* the edge modes, indicating that the topological insulator is protected by TRS *and* charge conservation symmetry [94].

Thus, the *topological insulator (TI)* and the *quantum spin Hall (QSH) phase* are *different* symmetry-protected topological phases, and the KM model happens to realize both for $\lambda_R = 0$ [35]. [Remember (Section 0.5) that the classification of SPT phases depends on our choice of protecting symmetry!]

In the context of this (modern) terminology, the title of Kane and Mele's original paper "$\mathbb{Z}_2$ Topological Order and the Quantum Spin Hall Effect" [111] is confusing for two reasons: First, the paper is mostly about the topological insulator phase – and not the quantum spin Hall effect. The authors event point this out explicitly: *"The QSH phase is not generally characterized by a quantized spin Hall conductivity."* In addition, their notion of "topological order" does not match the modern terminology of "long-range entanglement." That is, Kane and Mele's topological insulator is the paradigmatic example of a *topological phase* that is *not* topologically ordered but *symmetry protected*.

3.5. ‡ Experiments

- The possibility to observe the quantum spin Hall effect (via a quantized ← *spin Hall conductance* that requires spin conservation, i.e., $\lambda_R = 0$) was predicted by BERNEVIG *et al.* in 2006 [118] and experimentally confirmed by KÖNIG *et al.* in 2007 [119] in so called ↑ HgTe *quantum wells* (HgTe = Mercury-Telluride).
- The alloy $Bi_{1-x}Sb_x$ (BiSb = Bismuth-Antimony) was predicted to be a (strong) topological insulator (in three dimensions) by FU and KANE in 2007 [97] which was experimentally confirmed by HSIEH *et al.* in 2008 [120].
- Following these first discoveries, many more materials were identified as topological insulators. For an extensive review including experimental results (before 2011) see QI and ZHANG [121].

Closing remarks for Chapters 1 to 3

We have now discussed two topological indices to label topological phases in two dimensions:

- The (first) *Chern number* classifies two-dimensional chiral topological phases (IQHE, QWZ model, Haldane model); we discussed these models in Chapters 1 and 2.
  - The Chern number *cannot* be generalized to three dimensions!
    (There are generalizations to *even* dimensions, though [122].)
  - For non-zero Chern numbers, time-reversal symmetry must be *broken*.
  - Phases of non-interacting fermions in bands with non-zero Chern numbers are examples of the ← *invertible topological orders* introduced in Section 0.5 [35].
- The $\mathbb{Z}_2$ *Pfaffian index* classifies symmetry-protected topological (SPT) phases in two dimensions (Kane-Mele topological insulator); we discussed this model in Chapter 3.
  - The Pfaffian index *can* be generalized to three dimensions and allows for the characterization of three-dimensional topological insulators [96, 100, 123].
  - For the Pfaffian index to be well-defined, time-reversal symmetry must be *preserved*.
  - The Kane-Mele topological insulator is a ← *short-range entangled* phase protected by time-reversal symmetry (and particle number/charge conservation) [35].

We now turn to topological phases of non-interacting fermions in *one* dimension …

4. Topological Insulators in 1D: The Su-Schrieffer-Heeger Chain

After our study of two-dimensional systems with topological band structures in Chapters 1 to 3, we now turn to *one-dimensional* systems (still with non-interacting fermions). We will introduce the paradigmatic Su-Schrieffer-Heeger chain and identify a new topological invariant to characterize its quantum phases. However, as a preliminary step, we must introduce a new symmetry (beyond time-reversal symmetry) called *sublattice symmetry* …

4.1. Preliminaries: Sublattice symmetry

1 | Reminder: (Symmetries we already know.)

In the following, $\hat{H}$ denotes a non-interacting many-body Hamiltonian on (fermionic) Fock space and H its single-particle counterpart.

- *Unitary symmetry* $\mathcal{U}$:

$$\mathcal{U}i\mathcal{U}^{-1} = +i \quad \text{and} \quad \mathcal{U}c_i\mathcal{U}^{-1} = \sum_j U_{ij}^\dagger c_j \tag{4.1a}$$

$$\left[\hat{H},\mathcal{U}\right] = 0 \quad \Leftrightarrow \quad UHU^\dagger = H \quad \Leftrightarrow \quad [H,U] = 0 \tag{4.1b}$$

- *Time-reversal symmetry* $\mathcal{T}_U$: [← Section 2.1.2]

$$\mathcal{T}_U i\mathcal{T}_U^{-1} = -i \quad \text{and} \quad \mathcal{T}_U c_i\mathcal{T}_U^{-1} = \sum_j U_{ij}^\dagger c_j \tag{4.2a}$$

$$\left[\hat{H},\mathcal{T}_U\right] = 0 \quad \Leftrightarrow \quad UH^*U^\dagger \triangleq H \quad \Leftrightarrow \quad [H,\underbrace{U\mathcal{K}}_{T_U}] = 0 \tag{4.2b}$$

Note that both U and $U\mathcal{K}$ are valid *symmetries* on the single-particle Hilbert space (i.e., they commute with the Hamiltonian H), in accordance with *Wigner's theorem* (➔ Problemset 1).

2 | Other symmetry types (?):

Having the (classes of) symmetries Eqs. (4.1) and (4.2) in mind, are there other types of symmetries that one can realize on a fermionic Fock space?

- ⊲ Unitary like $\mathcal{U}$ but with $c_i \leftrightarrow c_i^\dagger$:

$$\mathcal{C}_U i\mathcal{C}_U^{-1} = +i \quad \text{and} \quad \mathcal{C}_U c_i\mathcal{C}_U^{-1} = \sum_j U_{ij}^{*\dagger} c_j^\dagger \tag{4.3a}$$

$$\left[\hat{H},\mathcal{C}_U\right] = 0 \quad \Leftrightarrow \quad UH^*U^\dagger \triangleq -H \quad \Leftrightarrow \quad \{H,\underbrace{U\mathcal{K}}_{C_U}\} = 0 \tag{4.3b}$$

¡! Note that H *anticommutes* with C_U: $\{\bullet, \bullet\} = 0$
(The complex conjugate in U_{ij}^* is conventional and not crucial.)

→ $\mathcal{C}_U$: ⁂ *Particle-hole symmetry (PHS)*

→ *Future lectures* on topological *superconductors*

- ∢ Antiunitary like $\mathcal{T}_U$ but with $c_i \leftrightarrow c_i^\dagger$:

$$\mathcal{S}_U\, i\, \mathcal{S}_U^{-1} = -i \quad \text{and} \quad \mathcal{S}_U\, c_i\, \mathcal{S}_U^{-1} = \sum_j U_{ij}^{*\dagger} c_j^\dagger \tag{4.4a}$$

$$\left[\hat{H}, \mathcal{S}_U\right] = 0 \quad \Leftrightarrow \quad UHU^\dagger \triangleq -H \quad \Leftrightarrow \quad \{H, \underbrace{U}_{S_U}\} = 0 \tag{4.4b}$$

¡! Note that H *anticommutes* with S_U ($\{\bullet, \bullet\} = 0$) but also that there is *no* complex conjugation on the single-particle level, i.e., $S_U = U$ is a *unitary* operator. (The complex conjugate in U_{ij}^* is again conventional and not crucial.)

→ $\mathcal{S}_U$: ⁂ *Chiral- or Sublattice symmetry (SLS)*

Here we stick to the term "sublattice symmetry" (SLS).

But why should we call $\mathcal{S}_U$ "sublattice symmetry" in the first place?
→ *Next point* below …

Note: The same arguments used for time-reversal symmetry (← Section 2.1.2) lead to

$$\{H, U\} = 0 \quad \Rightarrow \quad \left[H, U^2\right] = 0 \quad \xRightarrow{H \text{ generic}} \quad U^2 = e^{i\varphi}\mathbb{1} \tag{4.5}$$

→ Redefine $\tilde{U} = e^{-i\varphi/2}U \to \tilde{U}^2 = +\mathbb{1} \to$ *w.l.o.g.* $U^2 = +\mathbb{1}$

→ In contrast to time-reversal, there are not two "types" of sublattice symmetry!

(This difference is due to the missing antiunitarity on the single-particle level.)

¡! Whereas $\mathcal{U}$ and $\mathcal{T}_U$ can be interpreted as symmetries both on Fock space and on the single-particle Hilbert space, particle-hole symmetry $\mathcal{C}_U$ and sublattice symmetry $\mathcal{S}_U$ are only symmetries on Fock space; on the single-particle Hilbert space they act as unitary and antiunitary ↑ *pseudosymmetries*, respectively (i.e., they *anti*commute with the single-particle Hamiltonian).

This should be not surprising since both include an exchange of particles with holes, so that they mix sectors of different particle numbers. Such an operation is intrinsic to the many-particle description in Fock space and cannot be sensibly defined (or interpreted) as a symmetry in a (first quantized) single-particle description.

3 | Why "sublattice symmetry"?

i | ∢ SP Hamiltonian H with $UHU^\dagger = -H$

→ Spectrum $\sigma(H) = \sigma(-H)$

→ Spectrum symmetric about $E = 0$

By contrast, TRS implied a symmetric spectrum about the energy axis: $E(k) = E(-k)$.

ii | Assume H is $2L \times 2L$-matrix →

$$\exists \text{ Unitary } M : \; MHM^\dagger = \begin{pmatrix} D & 0 \\ 0 & -D \end{pmatrix} \quad \text{with diagonal matrix } D. \tag{4.6}$$

→

$$(QM)H(QM)^\dagger = \begin{pmatrix} 0 & D \\ D & 0 \end{pmatrix} \quad \text{with} \quad Q = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & -\mathbb{1} \end{pmatrix} \tag{4.7}$$

To see this, remember that a Hadamard gate H transforms a σ^z Pauli matrix into a σ^x Pauli matrix under conjugation.

Note that QM is just a unitary basis transformation in the SP Hilbert space.

iii | This means that for a sublattice symmetric system, there exists a unitary transformation of modes $\tilde{c}_i = \sum_j \tilde{U}_{ij} c_j$ such that

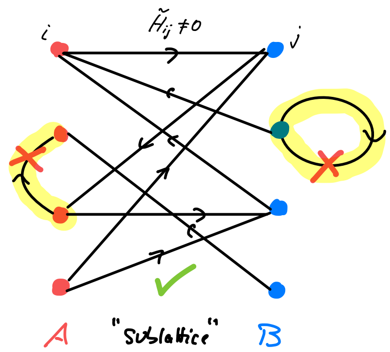
$$\hat{H} = \sum_{i,j} c_i^\dagger H_{ij} c_j \underset{w.l.o.g.}{\overset{\text{SLS}}{=}} \sum_{i,j} \tilde{c}_i^\dagger \tilde{H}_{ij} \tilde{c}_j \tag{4.8}$$

with block-off-diagonal SP Hamiltonian

$$\tilde{H} = \begin{pmatrix} 0 & h & \text{Hopping } A \mapsto B \\ h^\dagger & 0 & \text{Hopping } B \mapsto A \end{pmatrix} \tag{4.9}$$

The two subsets of modes A and B are referred to as "sublattices" even if a spatial lattice structure is missing.

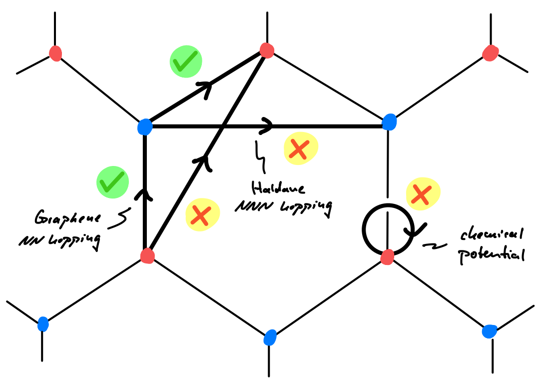
iv | $\tilde{H}$ couples only modes *between* the two "sublattices" A and B:



Often this sublattice structure is already visible in the real-space basis, i.e., a transformation to $\tilde{H}$ is not even necessary (SSH chain → *below*).

If one interprets $\tilde{H}$ as a (complex valued) adjacency matrix of a graph, the "sublattice symmetry" would be called ↑ *bipartiteness*. And indeed, it is well-known that a graph is bipartite if and only if the spectrum of its adjacency matrix is symmetric [124, Chapter 6.5].

v | Example: Graphene

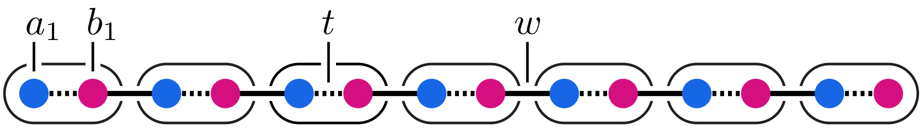


Note that a chemical potential $\mu \sum_i c_i^\dagger c_i$ can be interpreted as a hopping from site i to the same site; therefore it violates SLS.

4.2. The Su-Schrieffer-Heeger chain

- The *Su–Schrieffer–Heeger (SSH) chain* is a model of non-interacting, spinless fermions in one dimension that has been introduced by Su, Schrieffer and Heeger in 1979 [125] to describe soliton formation in polyacetylene (a linear chain of carbon atoms with alternating single and double bonds and one hydrogen atom bound to each carbon atom).
- In the context of topological phases, the model has become the example of choice to illustrate topological invariants and the emergence of robust edge modes [2] (which is why we study it).
- A detailed exposition of the SSH chain is given in the textbook by Asboth [2] but may also be found in almost any other textbook on topological insulators. There is also an introduction in my PhD thesis [126] (on which this section is based) with a quite detailed discussion of edge states in the appendices of Chapter 3.

1 | ⊲ 1D lattice with $2L$ sites grouped into L unit cells:



a_i, b_i: spinless fermion modes $(i = 1, \ldots, L)$

We can now define the ⁂ *SSH chain Hamiltonian*:

$$\hat{H}_{\text{SSH}} = t \underbrace{\sum_{i=1}^{L} (a_i^\dagger b_i + b_i^\dagger a_i)}_{\textit{Intra-site}\text{ hopping}} + w \underbrace{\sum_{i=1}^{L'} (b_i^\dagger a_{i+1} + a_{i+1}^\dagger b_i)}_{\textit{Inter-site}\text{ hopping}} \tag{4.10}$$

- $t, w \in \mathbb{R}$: alternating hopping amplitudes
- $L' = L - 1$ for OBC and $L' = L$ for PBC

  We will use both boundary types: Open boundaries (OBC) to study edge modes, and periodic boundaries (PBC) allow for Fourier transformation and definition of a topological index.

2 | Symmetries:

The SSH Hamiltonian (4.10) has several symmetries, not all crucial for the following discussion:

- Particle-number conservation/symmetry (PNS)
  This is an intrinsic symmetry of the class of quadratic fermion models without superconductivity; we cannot break it without leaving this class.
- Translation symmetry (TS)
  Translation symmetry is typically broken in real samples due to disorder.
- Sublattice symmetry (SLS):

$$\mathcal{S} i \mathcal{S}^{-1} := -i \quad \text{and} \quad \mathcal{S} a_i \mathcal{S}^{-1} := a_i^\dagger \quad \text{and} \quad \mathcal{S} b_i \mathcal{S}^{-1} := -b_i^\dagger \tag{4.11}$$

$\rightarrow [\hat{H}_{\text{SSH}}, \mathcal{S}] \stackrel{\circ}{=} 0$

Note that the minus sign $b_i \mapsto -b_i^\dagger$ is crucial for the commutation with the Hamiltonian!

The above definition is realized by the operator

$$\mathcal{S} \stackrel{\circ}{=} \prod_i (a_i^\dagger - a_i)(b_i^\dagger + b_i) \circ \mathcal{K} \tag{4.12}$$

Use $\{a_i, a_i^\dagger\} = 1$ and $a_i^2 = 0 = (a_i^\dagger)^2$ (and the same for b_i) to show this.

- Time-reversal symmetry (TRS):

$$\mathcal{T} i \mathcal{T}^{-1} := -i \quad \text{and} \quad \mathcal{T} a_i \mathcal{T}^{-1} := a_i \quad \text{and} \quad \mathcal{T} b_i \mathcal{T}^{-1} := b_i \tag{4.13}$$

$\rightarrow [\hat{H}_{\text{SSH}}, \mathcal{T}] \stackrel{\circ}{=} 0$

- Particle-hole symmetry (PHS):

$$\mathcal{C} i \mathcal{C}^{-1} := i \quad \text{and} \quad \mathcal{C} a_i \mathcal{C}^{-1} := a_i^\dagger \quad \text{and} \quad \mathcal{C} b_i \mathcal{C}^{-1} := -b_i^\dagger \tag{4.14}$$

$\rightarrow [\hat{H}_{\text{SSH}}, \mathcal{C}] \stackrel{\circ}{=} 0$

Are all these symmetries of the same importance to characterize the SSH chain?

3 | $\triangleleft$ "Generic" SSH chain:

$$\hat{H}'_{\text{SSH}} = \sum_{i=1}^{L} (t_i\, a_i^\dagger b_i + t_i^*\, b_i^\dagger a_i) + \sum_{i=1}^{L'} (w_i\, b_i^\dagger a_{i+1} + w_i^*\, a_{i+1}^\dagger b_i) \tag{4.15}$$

$t_i, w_i \in \mathbb{C}$: site-dependent & complex hopping amplitudes

$\stackrel{\circ}{\rightarrow}$ Preserved symmetries: PN & SLS

(Check that the complex hoppings destroy both TRS and PHS but not SLS.)

→ *Sublattice symmetry* is the natural symmetry of the SSH chain.

¡! For the analytical analysis below, we will still assume *translation invariance* so that we can Fourier transform the Hamiltonian. However, if one studies the model numerically, one can add translation-symmetry breaking perturbations to the Hamiltonian and verify that the features (in particular: the quantum phases) of the SSH chain are robust to SLS-symmetric disorder (→ *discussion of edge modes below*).