Seminar „Topological Insulators“

The Su-Schrieffer-Heeger model

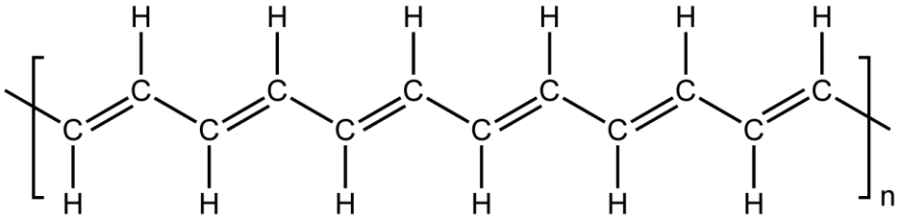
These slides are based on „A Short Course on Topological Insulators“ by J. K. Asbóth, L. Oroszlány, A. Pályi; arXiv:1509.02295v1

Outline

- Introduction and the Su-Schrieffer-Heeger (SSH) model
- SSH Hamiltonian
- Bulk Hamiltonian
- Edge states
- Chiral symmetry
- Number of edge states as topological invariant

Introduction and the Su-Schrieffer-Heeger (SSH) model

- Simplest one-dimensional case
- Su-Schrieffer-Heeger model for polyacetylene



trans-polyacetylene, (https://en.wikipedia.org/wiki/Polyacetylene#/media/File:Trans-(CH)n.png)

- Insulator in the bulk but conduction at the surface via conducting edge states
- Nontrivial topology of occupied bands is crucial
- Dimensionality and basic symmetries of an insulator determine if it can be a topological insulator

SSH Hamiltonian

- Noninteracting model, single-particle lattice Hamiltonian, zero of energy corresponding to the Fermi energy, $\hbar = 1$

Fig. 1.1 Geometry of the SSH model. Filled (empty) circles are sites on sublattice A (B), each hosting a single state. They are grouped into unit cells: the $n = 6$th cell is circled by a dotted line. Hopping amplitudes are staggered: intracell hopping v (thin lines) is different from intercell hopping w (thick lines). The left and right edge regions are indicated by blue and red shaded background.

- SSH-Model describes spinless fermions (electrons) hopping on a one-dimensional lattice with staggered hopping amplitudes

SSH Hamiltonian

- The dynamics of each electron is described by a single particle Hamiltonian

$$\hat{H} = v \sum_{m=1}^{N} \left(|m,B\rangle \langle m,A| + h.c. \right) + w \sum_{m=1}^{N-1} \left(|m+1,A\rangle \langle m,B| + h.c. \right)$$

- Study dynamics around ground state of SSH model at zero temperature and zero chemical poential
- For a chain consisting of N=4 unit cells

  the matrix of the Hamiltonian reads

$$H = \begin{pmatrix} 0 & v & 0 & 0 & 0 & 0 & 0 & 0 \\ v & 0 & w & 0 & 0 & 0 & 0 & 0 \\ 0 & w & 0 & v & 0 & 0 & 0 & 0 \\ 0 & 0 & v & 0 & w & 0 & 0 & 0 \\ 0 & 0 & 0 & w & 0 & v & 0 & 0 \\ 0 & 0 & 0 & 0 & v & 0 & w & 0 \\ 0 & 0 & 0 & 0 & 0 & w & 0 & v \\ 0 & 0 & 0 & 0 & 0 & 0 & v & 0 \end{pmatrix}$$

SSH Hamiltonian

- To emphasize the separation of external degrees of freedom (unit cell index m) and internal degrees of freedom (sublattice index) the following representation can be chosen:

  Use tensor product basis: $|m,\alpha\rangle \rightarrow |m\rangle \otimes |\alpha\rangle \in \mathscr{H}_{\text{external}} \otimes \mathscr{H}_{\text{internal}}$

  and the Pauli matrices: $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

  This leads to the Hamiltonian

$$\hat{H} = v \sum_{m=1}^{N} |m\rangle\langle m| \otimes \hat{\sigma}_x + w \sum_{m=1}^{N-1} \left(|m+1\rangle\langle m| \otimes \frac{\hat{\sigma}_x + i\hat{\sigma}_y}{2} + h.c. \right)$$

  Intracell hopping represented by intracell operator

  Intercell hopping represented by intercell operator

Bulk Hamiltonian

- Bulk: central part of the chain,
- Boudaries: the two ends or „edges“ of the chain
- In the thermodynamic limit N→∞ the bulk determines the most important properties
- Bulk should not depend on definition of the edges, therefore for simplicity periodic boundary conditions (Born-von Karman)

$$\hat{H}_{\text{bulk}} = \sum_{m=1}^{N} \left(v \left| m, B \right\rangle \left\langle m, A \right| + w \left| (m \bmod N) + 1, A \right\rangle \left\langle m, B \right| \right) + h.c.$$

with Eigenstates $\hat{H}_{\text{bulk}} \left| \Psi_n(k) \right\rangle = E_n(k) \left| \Psi_n(k) \right\rangle$

Bulk Hamiltonian

Derivation of the bulk momentum-space Hamiltonian

- Start with plane wave basis states for external degree of freedom

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{imk} |m\rangle \qquad \text{for } k \in \{\delta_k, 2\delta_k, \ldots, N\delta_k\} \quad \text{with } \delta_k = \frac{2\pi}{N}$$

- Bloch eigenstates can be found:

$$|\Psi_n(k)\rangle = |k\rangle \otimes |u_n(k)\rangle \qquad |u_n(k)\rangle = a_n(k)\,|A\rangle + b_n(k)\,|B\rangle$$

where $|u_n(k)\rangle \in \mathscr{H}_{\text{internal}}$ are the eigenstates of the bulk momentum-space Hamiltonian

$$\hat{H}(k) = \langle k|\, \hat{H}_{\text{bulk}}\, |k\rangle = \sum_{\alpha,\beta \in \{A,B\}} \langle k,\alpha|\, H_{\text{bulk}}\, |k,\beta\rangle \cdot |\alpha\rangle\langle\beta|$$

Bulk Hamiltonian

Periodicity in wavenumber:

- Fourier transform above acts only on the external degree of freedom →periodicity in the Brillouin zone

$$\hat{H}(k+2\pi)=\hat{H}(k) \qquad |u_n(k+2\pi)\rangle = |u_n(k)\rangle$$

- For a system consisting of N=4 unit cells with the bulk Hamiltonian and the Bloch eigenstates the matrix eigenvalue equation reads:

$$\begin{pmatrix} 0 & v & 0 & 0 & 0 & 0 & 0 & w \\ v & 0 & w & 0 & 0 & 0 & 0 & 0 \\ 0 & w & 0 & v & 0 & 0 & 0 & 0 \\ 0 & 0 & v & 0 & w & 0 & 0 & 0 \\ 0 & 0 & 0 & w & 0 & v & 0 & 0 \\ 0 & 0 & 0 & 0 & v & 0 & w & 0 \\ 0 & 0 & 0 & 0 & 0 & w & 0 & v \\ w & 0 & 0 & 0 & 0 & 0 & v & 0 \end{pmatrix} \begin{pmatrix} a(k)e^{ik} \\ b(k)e^{ik} \\ a(k)e^{2ik} \\ b(k)e^{2ik} \\ a(k)e^{3ik} \\ b(k)e^{3ik} \\ a(k)e^{Nik} \\ b(k)e^{Nik} \end{pmatrix} = E(k) \begin{pmatrix} a(k)e^{ik} \\ b(k)e^{ik} \\ a(k)e^{2ik} \\ b(k)e^{2ik} \\ a(k)e^{3ik} \\ b(k)e^{3ik} \\ a(k)e^{Nik} \\ b(k)e^{Nik} \end{pmatrix}$$

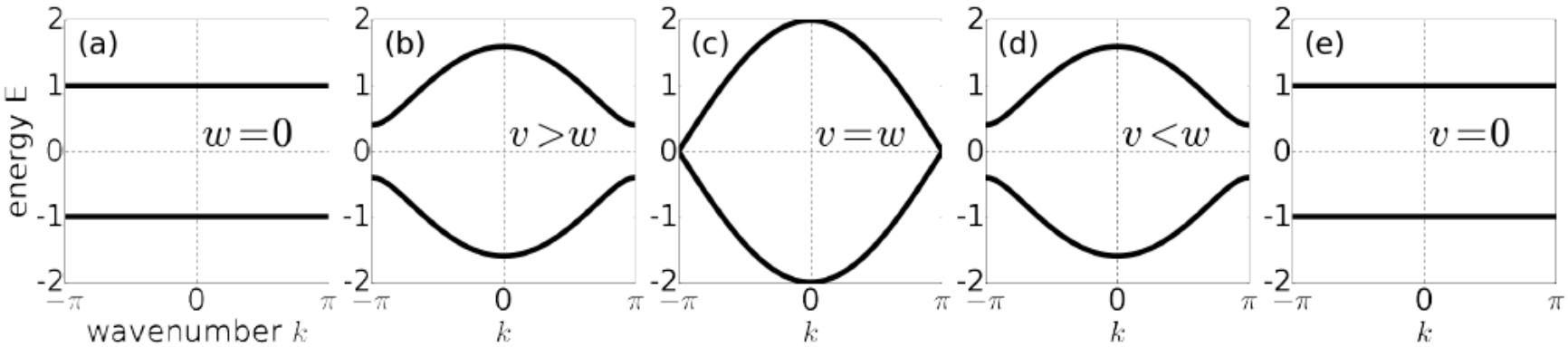
Bulk Hamiltonian

- For the bulk momentum-space Hamiltonian one can find:

$$H(k) = \begin{pmatrix} 0 & v + we^{-ik} \\ v + we^{ik} & 0 \end{pmatrix} \quad H(k) \begin{pmatrix} a(k) \\ b(k) \end{pmatrix} = E(k) \begin{pmatrix} a(k) \\ b(k) \end{pmatrix}$$

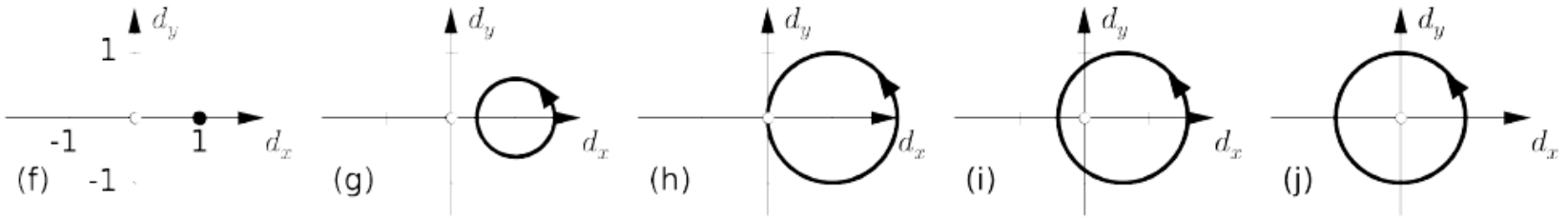
- With this equation one can find the dispersion relation

$$E(k) = \left| v + e^{-ik} w \right| = \sqrt{v^2 + w^2 + 2vw\cos k}$$



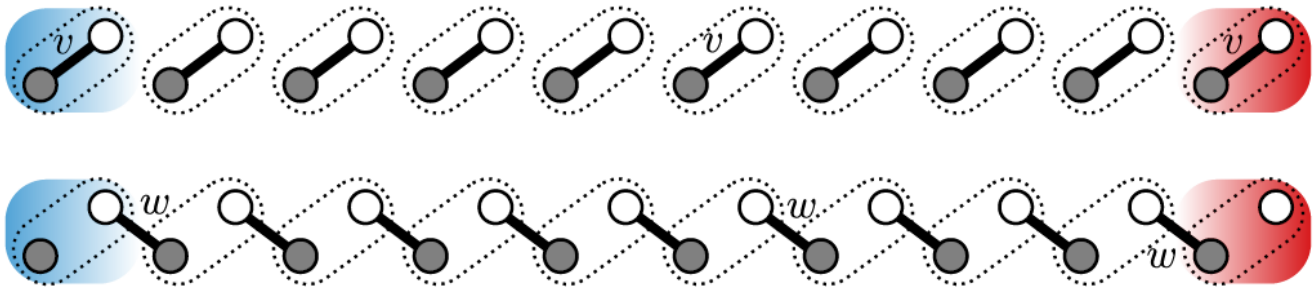
Bulk Hamiltonian

- For staggered hopping amplitudes a gap of 2Δ seperates the lower filled band from the upper empty band
- If not staggered → conductor $\Delta = \min_k E(k) = |v - w|$
- Staggering is energetically favourable
- Internal structure of stationary states given by conponents of H(k): $d_x(k) = v + w\cos k; \quad d_y(k) = w\sin k; \quad d_z(k) = 0$
- Endpoint of vector for k=0→2π : closed loop, here circle, avoids origin for insulators. Topology of loop characterised by bulk winding number, number of times the loop winds around the origin of the xy-plane



Edge states

- Distinguish edge and bulk states by their localised/delocalised behaviour in the thermodynamic limit
- Fully dimerised limits: Intercell hopping vanishes, intracell hopping set to 1 or vice versa



- The bulk has flat bands here, A set of energy eigenstates restricted to one dimer each.
- Consist of even and odd superpositions of the two sites forming a dimer

Edge States

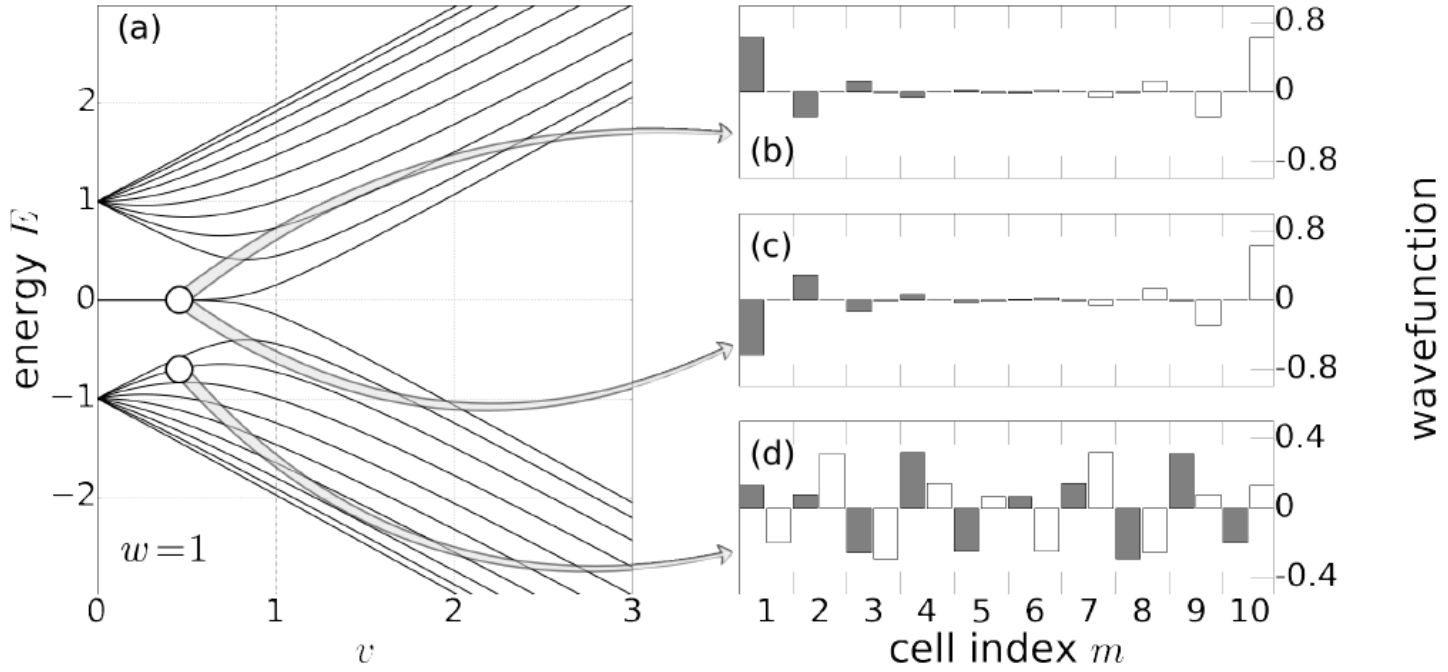
- „Trivial“ Case: v=1, w=0: $\hat{H}(|m,A\rangle \pm |m,B\rangle) = \pm(|m,A\rangle \pm |m,B\rangle)$
  → $\hat{H}(k) = \hat{\sigma}_x$ independent of wavefunction k
- „Topological“ Case: v=0, w=1:
  $\hat{H}(|m,B\rangle \pm |m+1,A\rangle) = \pm(|m,B\rangle \pm |m+1,A\rangle)$
  → $\hat{H}(k) = \hat{\sigma}_x \cos k + \hat{\sigma}_y \sin k$
- Energy eigenvalues independent of wavenumber k $E(k) = 1$
- Group velocity zero
- Edges can host zero energy states in this limit: In the topological case each end hosts an eigenstate at energy zero

$$\hat{H}\,|1,A\rangle = \hat{H}\,|N,B\rangle = 0$$

- Support on one side only, E=0 because no onsite pot. allowed

Edge States

- Move away from fully dimerised limit by turning on v continuously



Chiral symmetry

- Definition: $\hat{\Gamma}\hat{H}\hat{\Gamma}^{\dagger} = -\hat{H}$ where $\hat{\Gamma}$ it unitary and Hermitian

  further requirements:
  - Local: for $m \neq m'$ is $\langle m, \alpha | \hat{\Gamma} | m', \alpha' \rangle = 0$

    → consists of $\hat{\Gamma} = \hat{\gamma} \oplus \hat{\gamma} \oplus \ldots \oplus \hat{\gamma} = \bigoplus_{m=1}^{N} \hat{\gamma}$
  - Robust: Independent of variation of local parameters
- Consequences:
  - Sublattice symmetry: By defining $\hat{P}_A = \frac{1}{2}\left(\mathbb{I} + \hat{\Gamma}\right)$, $\hat{P}_B = \frac{1}{2}\left(\mathbb{I} - \hat{\Gamma}\right)$ and requiring no transitions from site to site on the same sublattice are induced by H: $\hat{P}_A \hat{H} \hat{P}_A = P_B \hat{H} \hat{P}_B = 0$

    → $\hat{H} = \hat{P}_A \hat{H} \hat{P}_B + \hat{P}_B \hat{H} \hat{P}_A$

Chiral Symmetry

- Consequences:
  - Symmetric spectrum:

    $$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle \quad \Longrightarrow \quad \hat{H}\hat{\Gamma}|\psi_n\rangle = -\hat{\Gamma}\hat{H}|\psi_n\rangle = -\hat{\Gamma}E_n|\psi_n\rangle = -E_n\hat{\Gamma}|\psi_n\rangle$$

  - If $E_n \neq 0$ then $0 = \langle\psi_n|\hat{\Gamma}|\psi_n\rangle = \langle\psi_n|P_A|\psi_n\rangle - \langle\psi_n|P_B|\psi_n\rangle$

    If $E_n = 0$ zero energy eigenstates can be chosen to have support only on one sublattice.

Chiral Symmetry

- Bulk winding number
  - Recall vector **d**(k), restricted to xy-plane due to chiral symmetry $\sigma_z \hat{H}(k)\sigma_z = 0 \rightarrow d_z = 0$
  - Endpoint curve direct closed loop on plane, well defined integer winding number, has to avoid origin (insulator)
  - Integral definition of winding number:

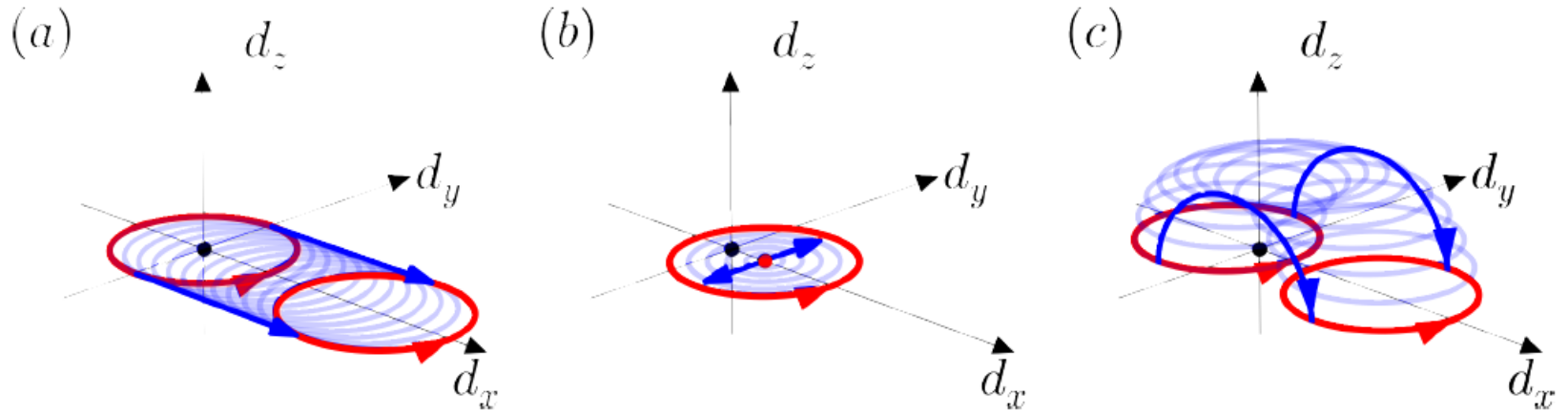
$$\tilde{\mathbf{d}} = \frac{\mathbf{d}}{|\mathbf{d}|} \qquad \nu = \frac{1}{2\pi}\int \left(\tilde{\mathbf{d}}(k) \times \frac{d}{dk}\tilde{\mathbf{d}}(k)\right)_z dk \qquad H(k) = \begin{pmatrix} 0 & h(k) \\ h^*(k) & 0 \end{pmatrix}$$

$$h(k) = d_x(k) - i d_y(k)$$

$$\nu = \frac{1}{2\pi i}\int_{-\pi}^{\pi} dk \frac{d}{dk}\log h(k)$$

Winding Number of SSH model

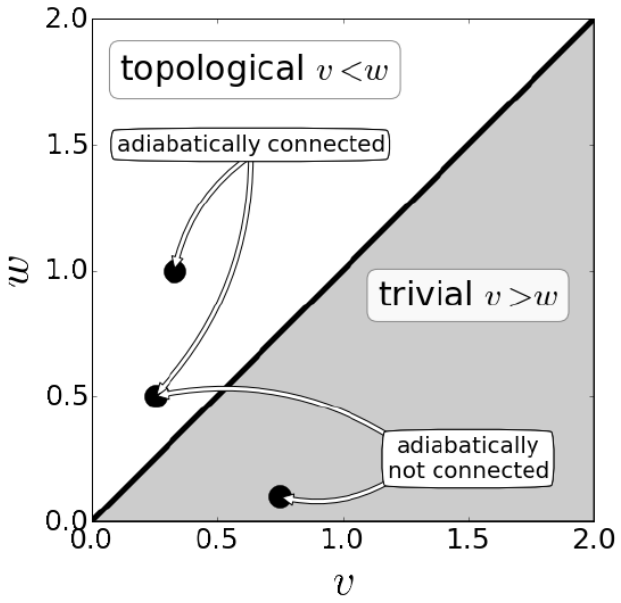
- Trivial case with dominant intracell hopping winding number 0
- Topological case: winding number 1
- To change the winding number of the SSH model eiter close



bulk gap or break chiral symmetry.

Number of edge states as topological invariant

- Definition of adiabatic deformation of insulating Hamiltonian
  - Continous change of parameters
  - Maintaining important symmetries
  - Keeping the gap around zero energy open
- Definition of adiabatic equivalence of Hamiltonians
  - Two insulating Hamiltonians are adiabatically connected if they are connected by adiabatic transformation
  - Path can be drawn that does not cross gapless phase boundary w=v



Number of edge states as topological invariant

- Topological invariant
  - Integer number characterising insulating Hamiltonian if it cannot change under adiabatic deformations
  - Only well defined in thermodynamic limit,
  - Depends on Symmetries that need to be respected
  - Winding Number of SSH model is topological invariant
- Number of edge states as topological invariant
  - Gapped chiral symmetric one-dimensional Hamiltonian
  - Energy window $-\varepsilon < E < \varepsilon$ where ε is the bulk gap
  - Zero and nonzero edge states possible
  - Nonzero energy state has chiral symmetric parnter occupying same unit cell

Number of edge states as topological invariant

- Finite number of zero energy states (bulk gap)
- Restriction to single sublattice: N_A states on sublattice A and N_B states on sublattice B
- Consider effect of adiabatic deformation with continuous parameter d: 0 → 1 on $N_A - N_B$
  - Nonzero energy edge state can be brought to zero energy for $d \geq d'$
  - Chiral symmetric partner moves simultaneously to zero energy

$$|\Psi_0(d=0)\rangle \qquad \Gamma\,|\Psi_0(d)\rangle \qquad E_0(d)=0$$

$$\hat{P}_A\,|\Psi_0(d')\rangle \qquad \hat{P}_B\,|\Psi_0(d')\rangle$$

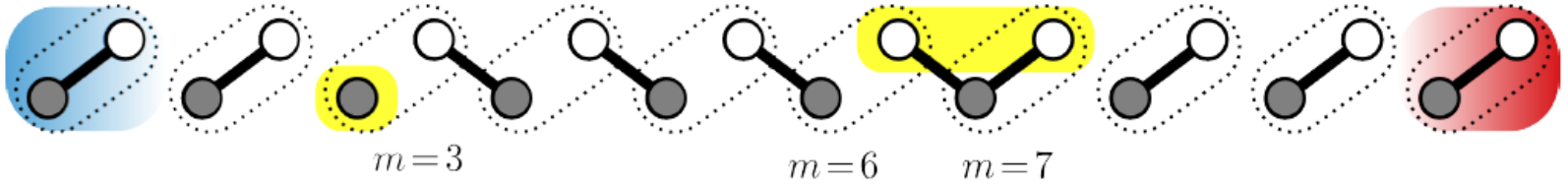
  - $N_A - N_B$ unchanged

Number of edge states as topological invariant

- Timereverse process also possible, bring zero energy state to nonzero energy at time d=d‘
  - Both sublattice numbers decrease by one so difference unchanged
- Bringing nonzero energy states out of the energy range of above does not change difference
- Zero energy eigenstate can change, extending deeper into the bulk; due to gap condition exponential decay of wavefunction
  - Cannot move states away from the edge, thus no change of the numbers
- $N_A - N_B$ is net number of edge states on sublattice A at the left edge
  - This is a topological invariant.
- Winding number (bulk) allows predictions about low energy physics at the edge: trivial case both zero, topological case both one
  - Example for bulk-boundary correspondence

Number of edge states as topological invariant

- Consider interfaces between different insulating domains



- $\hat{H}(|6,B\rangle - |7,B\rangle) = 0$ zero energy eigenstate
- Consider SSH system that is not in the fully dimerized limit
  - Edge state wave functions at domain walls penetrate into the bulk
  - Hybridization of two edge states at domainwalls with distance M forming bonding and anti-bonding states
  - Only negative energy eigenstate will be occupied at half filling
  - Each domain wall carries half an electronic charge: fractionalisation

Number of edge states as topological invariant

- Zero energy edge states can be calculated without translational invariance

$$\hat{H} = \sum_{m=1}^{N} \left(v_m \left| m,B \right\rangle \left\langle m,A \right| + h.c. \right) + \sum_{m=1}^{N-1} \left(w_m \left| m+1,A \right\rangle \left\langle m,B \right| + h.c. \right)$$

$$\hat{H} \sum_{m-1}^{N} \left(a_m \left| m,A \right\rangle + b_m \left| m,B \right\rangle \right) = 0$$

$$m = 1,\ldots,N-1: \qquad v_m a_m + w_m a_{m+1} = 0; \qquad w_m b_m + v_{m+1} b_{m+1} = 0$$

$$\text{boundaries}: \qquad v_N a_N = 0; \qquad v_1 b_1 = 0$$

$$m = 2,\ldots,N: \qquad a_m = \prod_{j=1}^{m-1} \frac{-v_j}{w_j} a_1;$$

$$m = 1,\ldots,N-1: \qquad b_m = \frac{-v_N}{w_m} \prod_{j=m+1}^{N-1} \frac{-v_j}{w_j} b_N$$

Number of edge states as topological invariant

- In general no zero energy state but approximately in the thermodynamic limit for strong intercell hopping

$$\overline{\log|v|} = \frac{1}{N-1}\sum_{m=1}^{N-1}\log|v_m|; \qquad \overline{\log|w|} = \frac{1}{N-1}\sum_{m=1}^{N-1}\log|w_m|$$

$$|a_N| = |a_1|\,e^{-(N-1)/\xi}; \qquad |b_1| = |b_N|\,e^{-(N-1)/\xi}\,\frac{|v_N|}{|v_1|}$$

  - Localisation length $\xi = \dfrac{1}{\overline{\log|w|} - \overline{\log|v|}}$
  - for $\xi > 0$ solutions

$$|L\rangle = \sum_{m=1}^{N} a_m\,|m,A\rangle; \qquad |R\rangle = \sum_{m=1}^{N} b_m\,|m,B\rangle$$

Number of edge states as topological invariant

- Exponentially small hybridisation of states above under H
- Overlap central quantity $\langle R|\hat{H}|L\rangle = \left|a_1 e^{-(N-1)/\xi} v_N b_N\right| e^{i\phi}$

- This leads to approximated energy eigenstates and energies

$$|0+\rangle = \frac{e^{-i\phi/2}|L\rangle + e^{i\phi/2}|R\rangle}{\sqrt{2}}; \qquad E_+ = \left|a_1 e^{-(N-1)/\xi} v_N b_N\right|;$$

$$|0-\rangle = \frac{e^{-i\phi/2}|L\rangle - e^{i\phi/2}|R\rangle}{\sqrt{2}}; \qquad E_- = -\left|a_1 e^{-(N-1)/\xi} v_N b_N\right|$$

- Energy exponentially small in the system size (N)

This is the end!

Thank you for your attention!