Topological insulators and superconductors

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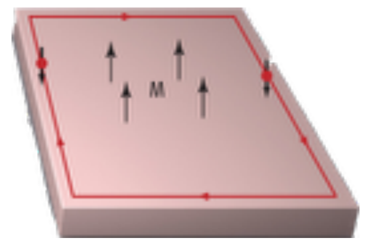
Zoo of topological materials

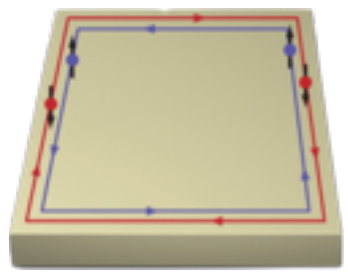
Chern insulator

Cr-doped $(Bi,Sb)_2Te_3$



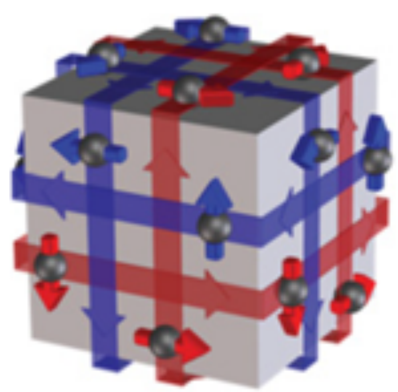
Quantum spin Hall state

HgTe/CdTe quantum wells



3D topological insulator

Bi_2Se_3



[pictures courtesy Lanzara and S. Zhang et al.]

Over the last years, the number of known topological materials has exploded

? Can we bring some order in this zoo of topological materials?

Zoo of topological materials

Chern insulator

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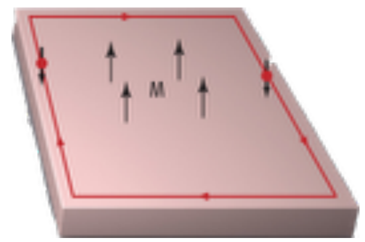
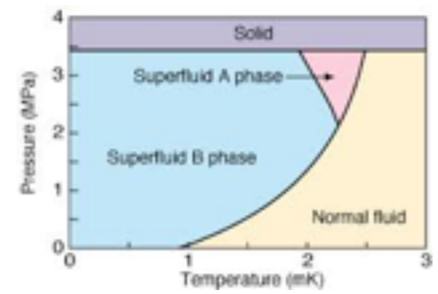


the B phase of ^3He



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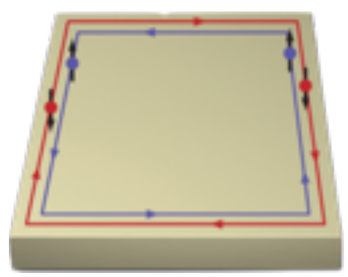
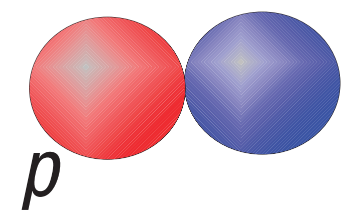
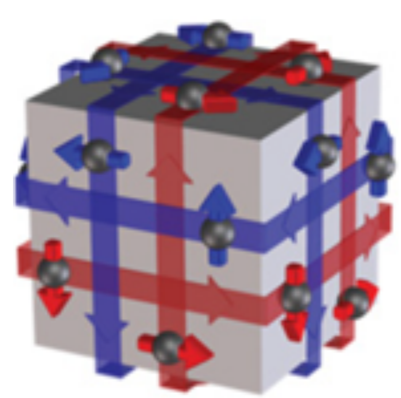


chiral p-wave superconductor



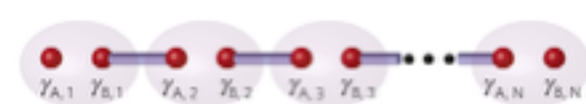
Sr_2RuO_4

3D topological insulator

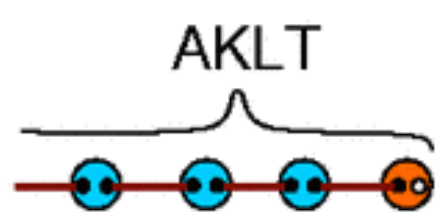


Bi_2Se_3

1D p-wave superconductor



InSb-nanowire heterostructures



Haldane AFM spin-1 chain

Over the last years, the number of known topological materials has exploded

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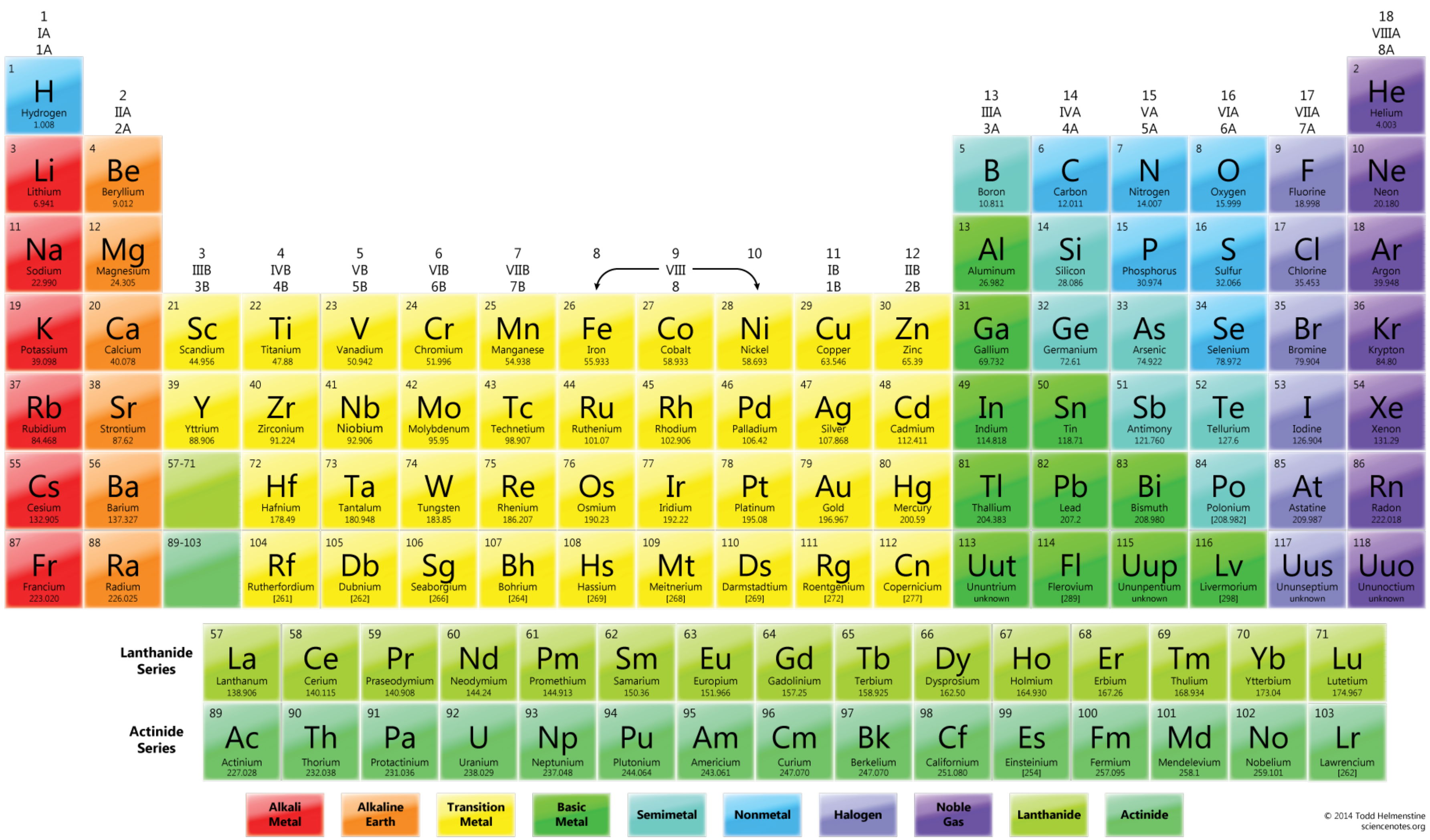
[pictures courtesy Lanzara and S. Zhang et al.]

Classification of chemical elements

Periodic table of the elements

Organize elements according to symmetries of electronic configurations

1860s Dimitri Mendeleev



⟹ prediction of new elements: Ge, Sc, Tc, Ga

? **Can topological materials be classified in a similar fashion?**

Topological insulators and superconductors

1. Topological band theory
    - What is topology?
    - SSH model (polyacetylene)

2. Chern insulators and IQHE
    - Integer quantum Hall effect
    - Chern insulator on square lattice

3. Topological insulators w/ time-reversal symmetry
    - Quantum spin Hall state
    - Z_2 invariants in 2D & 3D

4. Topological superconductors
    - Topological superconductors in 1D & 2D
    - Topological superconductors w/ TRS

5. Classification scheme and topological semi-metals
    - Tenfold classification of TIs and SCs
    - Topological semi-metals and nodal superconductors

Books and review articles

Review articles:

- M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. **82**, 3045 (2010)
- X.L. Qi and S.C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011)
- S. Ryu, A. P. Schnyder, A. Furusaki, A. Ludwig, New J. Phys. **12**, 065010 (2010)
- C.-K. Chiu, J. C. Y. Teo, A. P. Schnyder, S. Ryu, arXiv:1505.03535
- C. Beenakker, Annual Review of Cond. Mat. Phys. **4**, 113 (2013)
- J. Alicea, Rep. Prog. Phys. **75**, 076501 (2012)
- Y. Ando, J. Phys. Soc. Jpn. **82**, 102001 (2013)
- Y. Ando and L. Fu, arXiv:1501.00531
- A. P. Schnyder, P. M. R. Brydon, arXiv:1502.03746

Books:

- Shun-Qing Shen, “Topological insulators”, Springer Series in Solid-State Sciences, Volume **174** (2012)
- B. Andrei Bernevig, "Topological Insulators and Topological Superconductors”, Princeton University Press (2013)
- Mikio Nakahara, "Geometry, Topology and Physics", Taylor & Francis (2003)
- A. Bohm, A. Mostafazadeh, H. Koizumi, Q. Niu, J. Zwanziger, “The geometric phase in quantum systems”, Springer (2003)
- M. Franz and L. Molenkamp, “Topological Insulators”, Contemporary Concepts of Condensed Matter Science, Elsevier (2013)

1st lecture: Topological band theory

1. Introduction
   - What is topology?
   - Bloch theorem
   - Topological band theory

2. Topological insulators in 1D
   - Berry phase
   - Simple example: Two-level system
   - Polyacetylene (Su-Schrieffer-Heeger model)
   - Domain wall states

What is topology?

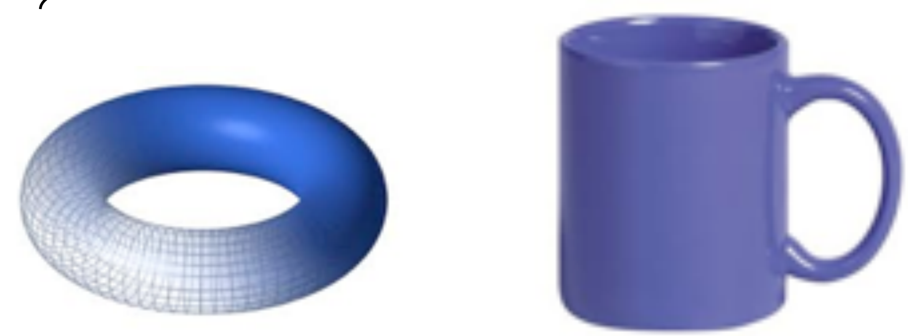
The study of geometric properties that are insensitive to smooth deformations

For example, consider two-dimensional surfaces in three-dimensional space

Closed surfaces are characterized by their genus g = # holes

$g = 0$

$g = 1$



▶ **Topological equivalence:**

> Two surfaces are equivalent if they can be continuously deformed into one another without cutting a hole.

▶ topological equivalence classes distinguished by genus g (topological invariant)

Gauss-Bonnet Theorem

Genus can be expressed in terms of an integral of the Gauss curvature over the surface

$$\int_S \kappa \, dA = 4\pi(1 - g)$$

topological invariant

Band theory of solids and topology

Bloch's theorem: consider electron wavefunction in periodic crystal potential

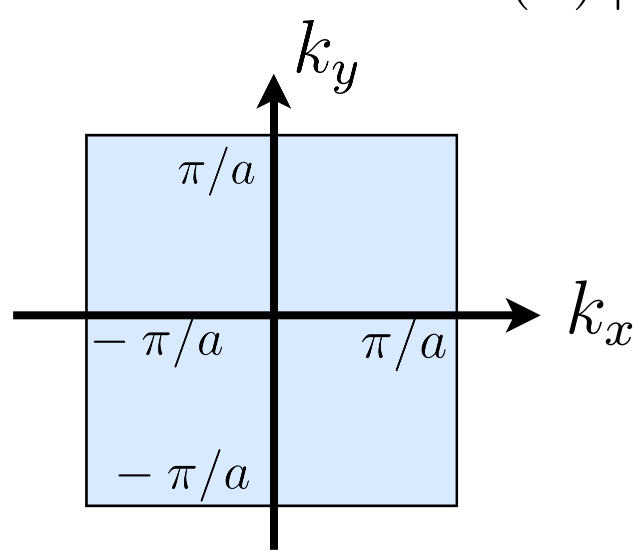
Electron wavefunction in crystal $|\psi_n\rangle = e^{i\boldsymbol{k}\boldsymbol{r}}\,|u_n(\boldsymbol{k})\rangle$

crystal momentum

Bloch wavefunction
has periodicity of potential

Bloch Hamiltonian $H(\boldsymbol{k}) = e^{-i\boldsymbol{k}\boldsymbol{r}} H e^{+i\boldsymbol{k}\boldsymbol{r}}$ $\quad H(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle$

$\boldsymbol{k} \in \text{Brillouin Zone}$



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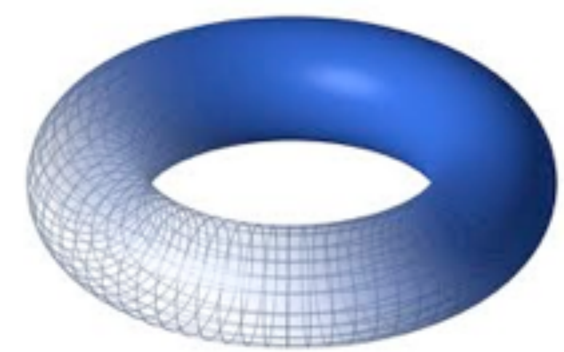
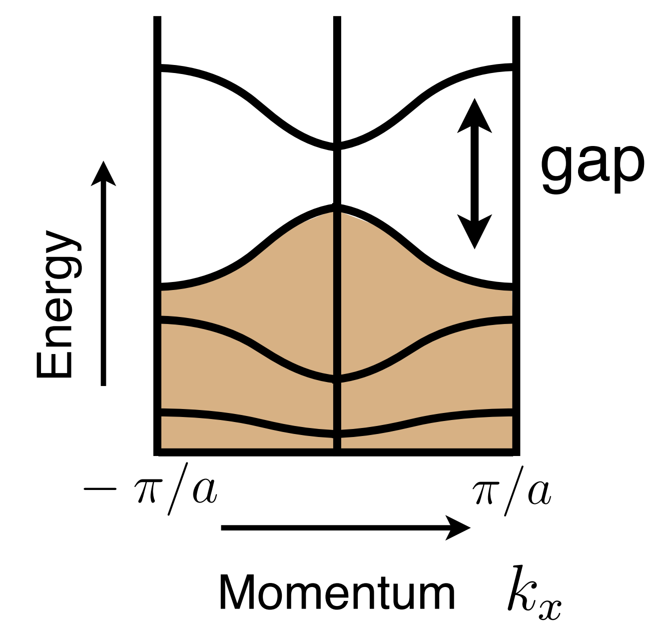


Band structure defines a mapping:

Brillouin zone $\longmapsto$ $H(\boldsymbol{k})$ Hamiltonians with energy gap



Topological equivalence:

Band structures are equivalent if they can be continuously deformed into one another without closing the energy gap

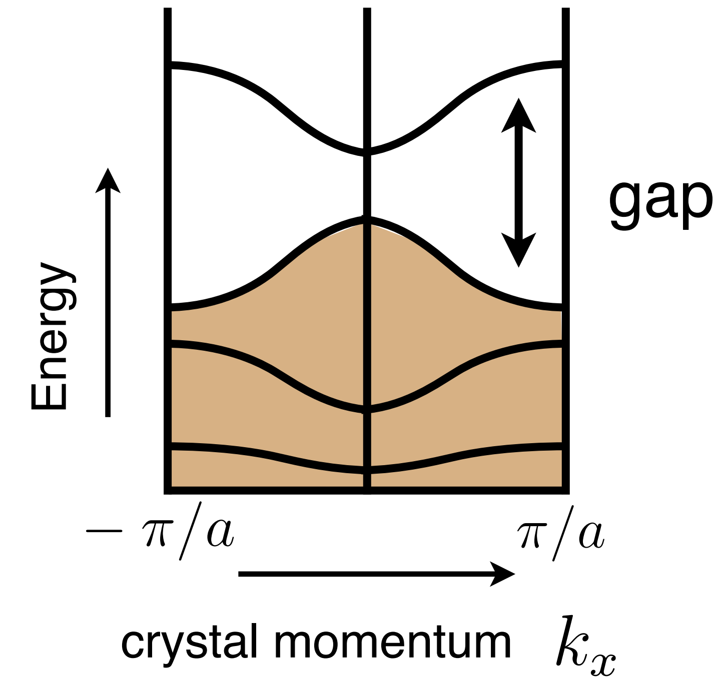
Topological band theory

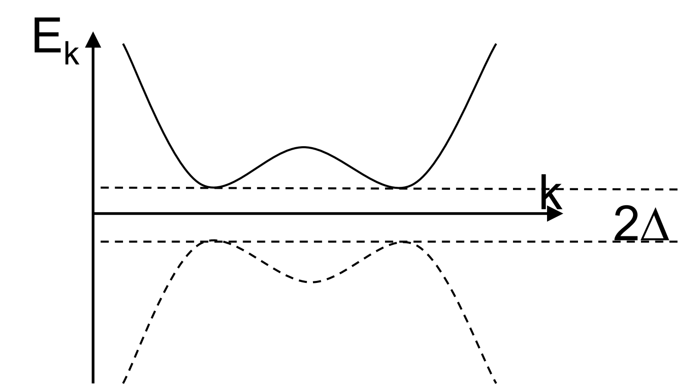
- Consider band structure with a gap:

$$H(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle$$

— *band insulator:* E_F between conduction and valence bands

— *superconductor:* band structure of Bogoliubov quasiparticles





- **Topological equivalence:**

> Two band structures are equivalent if they can be continuously deformed into one another without closing the energy gap and without breaking the **symmetries** of the band structure.

▷ symmetries to consider:

— particle-hole symmetry, time-reversal symmetry

— reflection symmetry, rotation symmetry, etc.

▷ top. equivalence classes distinguished by:

Berry curvature

topological invariant (e.g. Chern no): $n_{\mathbb{Z}} = \frac{i}{2\pi} \int_{\text{filled states}} \mathcal{F}\, d\mathbf{k} \in \mathbb{Z}$

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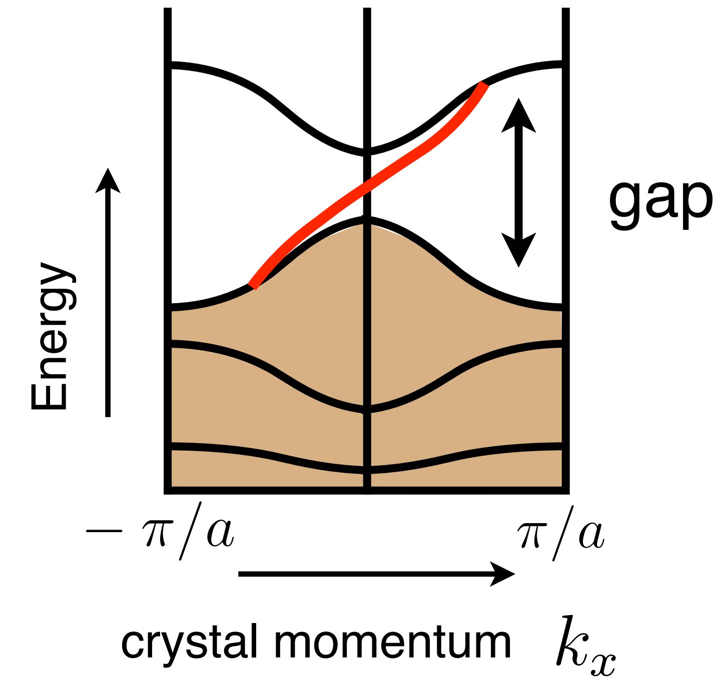

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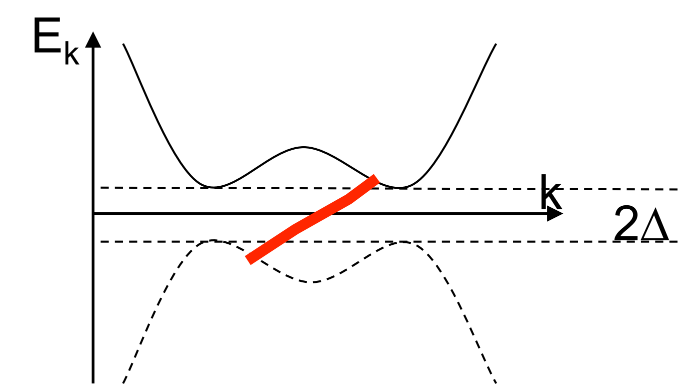

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- **Bulk-boundary correspondence:**

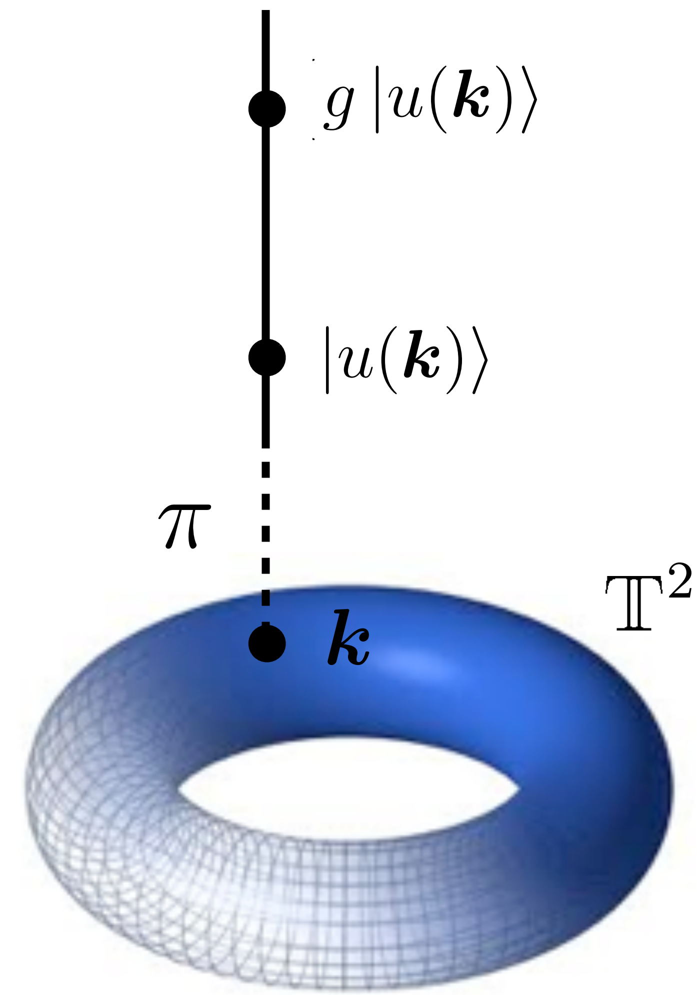
$$|n_{\mathbb{Z}}| = \#\,\text{gapless edge states (or surface states)}$$

Band theory and topology

Berry phase:

Phase ambiguity of wavefucntion $|u(\boldsymbol{k})\rangle \rightarrow e^{i\phi_{\boldsymbol{k}}}|u(\boldsymbol{k})\rangle$

U(1) fiber bundle: to each $\boldsymbol{k}$ attach fiber $\{g\,|u(\boldsymbol{k})\rangle \mid g \in U(1)\}$



define Berry connection: (like EM vector potential)

$$\mathcal{A} = \langle u_{\boldsymbol{k}}| - i\nabla_k |u_{\boldsymbol{k}}\rangle$$

under gauge transformation:

$$|u(\boldsymbol{k})\rangle \rightarrow e^{i\phi_{\boldsymbol{k}}}|u(\boldsymbol{k})\rangle \quad \Longrightarrow \quad \mathcal{A} \rightarrow \mathcal{A} + \nabla_{\boldsymbol{k}}\phi_{\boldsymbol{k}}$$

Berry phase: (gauge invariant quantity)

change in phase on a closed loop $\gamma_C = \oint_C \mathcal{A} \cdot d\boldsymbol{k}$

Berry curvature tensor: (gauge independent) $\mathcal{F}_{\mu\nu}(\mathbf{k}) = \frac{\partial}{\partial k_\mu}\mathcal{A}_\nu(\boldsymbol{k}) - \frac{\partial}{\partial k_\nu}\mathcal{A}_\mu(\boldsymbol{k})$

For 3D: $\boldsymbol{\mathcal{F}} = \nabla_{\boldsymbol{k}} \times \mathcal{A}$ $\quad \mathcal{F}_{\mu\nu} = \epsilon_{\mu\nu\xi}\boldsymbol{\mathcal{F}}_\xi$ $\quad$ Stokes: $\gamma_C = \int_S \boldsymbol{\mathcal{F}} \cdot d\boldsymbol{k}$

Topological invariants of band structures:

Topological property of insulating material
given by Chern number (or winding number):

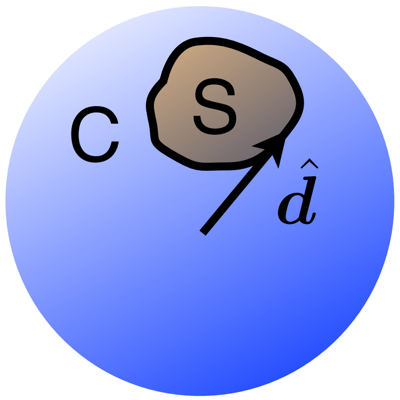
$$n = \frac{i}{2\pi}\sum_{\substack{\text{filled}\\\text{states}}}\int \mathcal{F} d^2k$$

Berry phase for two-band model

Two-level Hamiltonian: $$H(\boldsymbol{k}) = \boldsymbol{d}(\boldsymbol{k}) \cdot \boldsymbol{\sigma} = \begin{pmatrix} d_z & d_x - i d_y \\ d_x + i d_y & -d_z \end{pmatrix}$$

param. by spherical coord.: $\boldsymbol{d}(\boldsymbol{k}) = |\boldsymbol{d}|(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$

two eigenvectors with energies $E_\pm = \pm|\boldsymbol{d}|$ (north pole gauge)



$$|u_{\boldsymbol{k}}^-\rangle = \begin{pmatrix} \sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2) \end{pmatrix} \qquad |u_{\boldsymbol{k}}^+\rangle = \begin{pmatrix} \cos(\theta/2)e^{-i\phi} \\ \sin(\theta/2) \end{pmatrix}$$

$$2\gamma_C = \begin{matrix}\text{solid angle} \\ \text{swept out by } \hat{\boldsymbol{d}}(\boldsymbol{k})\end{matrix}$$

Berry vector potential: (gauge dependent)

$$A_\theta = i\left\langle u_{\boldsymbol{k}}^-\right| \partial_\theta \left|u_{\boldsymbol{k}}^-\right\rangle = 0 \qquad A_\phi = i\left\langle u_{\boldsymbol{k}}^-\right| \partial_\phi \left|u_{\boldsymbol{k}}^-\right\rangle = \sin^2(\theta/2)$$

Berry curvature: (gauge independent) $$\mathcal{F}_{\theta\phi} = \partial_\theta A_\phi - \partial_\phi A_\theta = \frac{\sin\theta}{2}$$

If $\boldsymbol{d}(\boldsymbol{k})$ depends on parameters $\boldsymbol{k}$: $$\mathcal{F}_{k_i,k_j} = \frac{\sin\theta}{2}\frac{\partial(\theta,\phi)}{\partial(k_i,k_j)}$$ ← Jacobian matrix

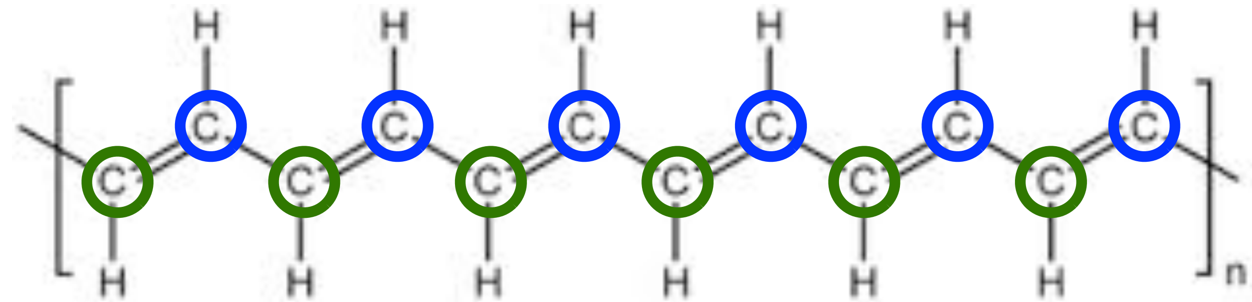
Simple example: $\boldsymbol{d}(\boldsymbol{k}) = \boldsymbol{k}$

$$\boldsymbol{\mathcal{F}} = \frac{1}{2}\frac{\hat{\boldsymbol{k}}}{k^2}$$ (monopole field)

$$\gamma_C = \int_S \mathcal{F}_{\theta\phi}\, d\theta d\phi = \frac{1}{2}\left(\begin{matrix}\text{solid angle} \\ \text{swept out by } \hat{\boldsymbol{d}}(\boldsymbol{k})\end{matrix}\right)$$

Polyacetylene (Su-Schrieffer-Heeger model)

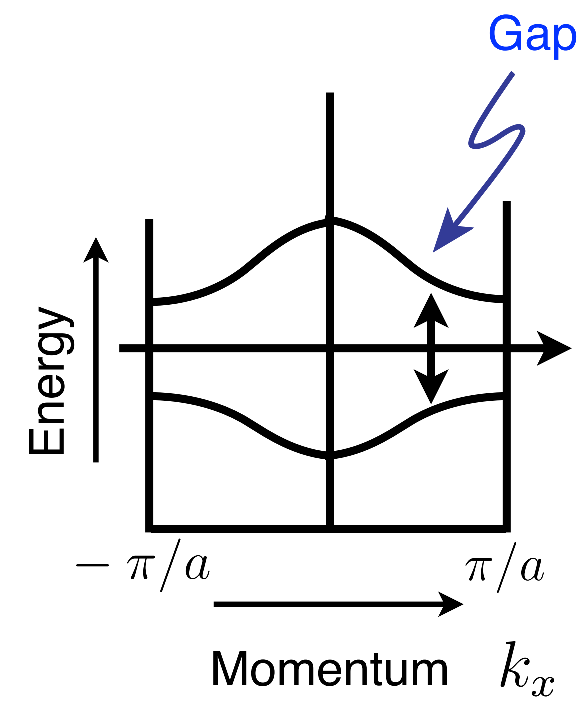
[Su, Schreiffer, Heeger 79]



Su-Schrieffer-Heeger model
describes polyacetylene $[\mathrm{C_2H_2}]_n$

Hamiltonian:

$$\mathcal{H} = \sum_i \left[(t+\delta t) c^\dagger_{Ai} c_{Bi} + (t-\delta t) c^\dagger_{Ai+1} c_{Bi} + \text{h.c.} \right]$$

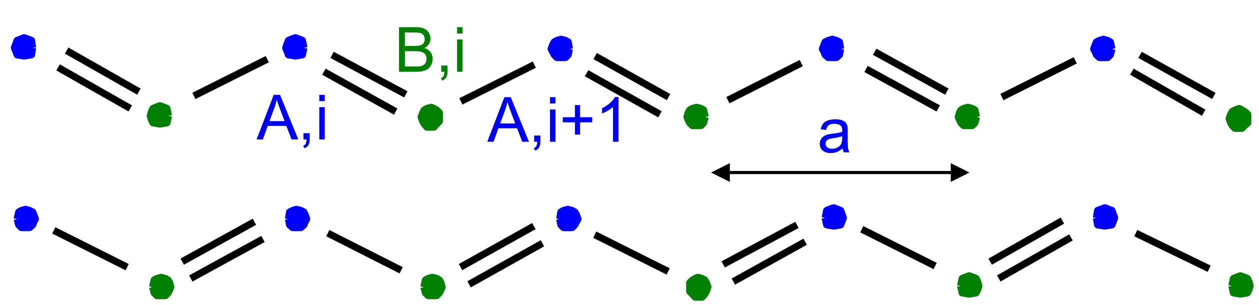


phonons lead to Peierls instability $\longrightarrow$ finite δt

two degenerate ground states:

$\delta t > 0$

$\delta t < 0$



in momentum space: $\mathcal{H}(k) = \boldsymbol{d}(k) \cdot \boldsymbol{\sigma} = \begin{pmatrix} 0 & h(k) \\ h^\dagger(k) & 0 \end{pmatrix}$

$d_x(k) = (t+\delta t) + (t-\delta t)\cos k$ $\qquad d_y(k) = (t-\delta t)\sin k$ $\qquad d_z(k) = 0$

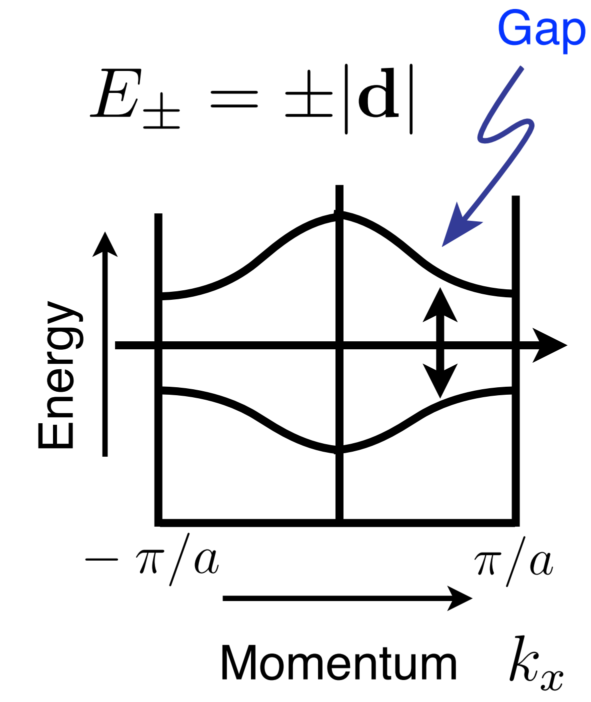
Sublattice symmetry: $\sigma_z \mathcal{H}(k) + \mathcal{H}(k)\sigma_z = 0 \longrightarrow d_z = 0$ (energy spectrum is symmetric)

Energy spectrum: $E_\pm = \pm|\mathbf{d}| = \pm\sqrt{2}\sqrt{t^2 + (\delta t)^2 + [t^2 - (\delta t)^2]\cos k}$

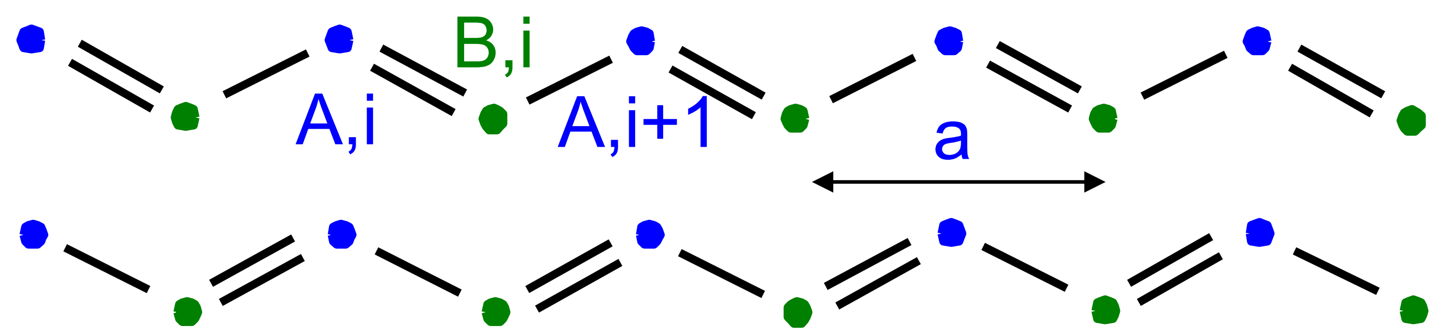
Polyacetylene (Su-Schrieffer-Heeger model)

Su-Schrieffer-Heeger model describes polyacetylene $[\mathrm{C_2H_2}]_n$

$$E_\pm = \pm|\mathbf{d}|$$



$\delta t > 0$

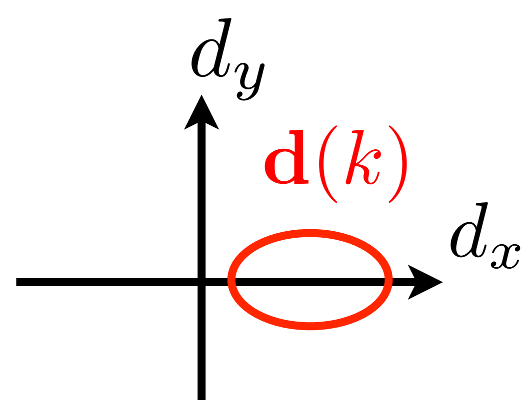


$\delta t < 0$

$$\mathcal{H}(k) = \boldsymbol{d}(k)\cdot\boldsymbol{\sigma} = \begin{pmatrix} 0 & h(k) \\ h^\dagger(k) & 0 \end{pmatrix}$$

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

$$d_y(k) = (t-\delta t)\sin k \qquad d_z(k) = 0$$



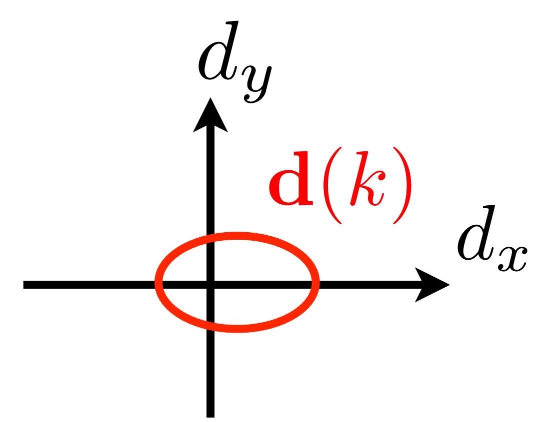
$\delta t > 0:$

Berry phase 0

$\nu_1 = 0$

Winding no: $\nu_1 = \dfrac{i}{2\pi}\displaystyle\int dk\,\mathrm{Tr}\left[q^{-1}\partial_k q\right]$

$$q(k) = \frac{h(k)}{|\mathbf{d}(k)|} \qquad q(k): S^1 \longrightarrow S^1 \qquad \pi_1(S^1) = \mathbb{Z}$$



$\delta t < 0:$

Berry phase π

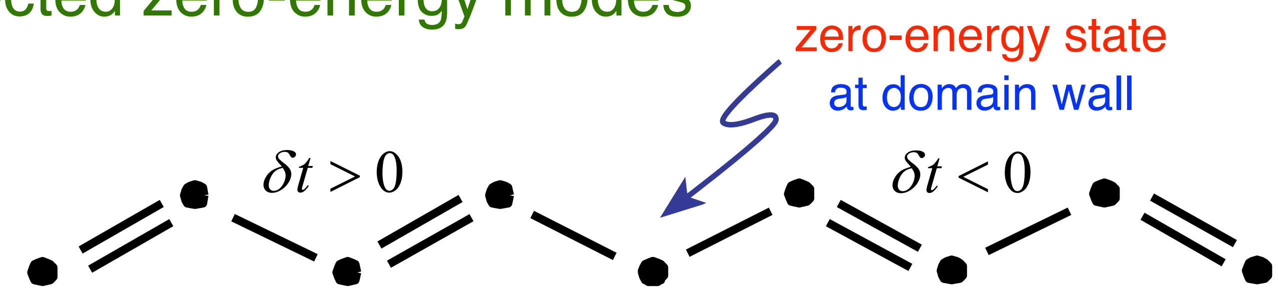
$\nu_1 = 1$

Provided $d_z = 0$ (required by sublattice symmetry) states with $\delta t > 0$ and $\delta t < 0$ are topologically distinct

Domain Wall States in Polyacetylene

[Su, Schreiffer, Heeger 79]
[Jackiw, Rebbi]

Domain wall between different topological states has topologically protected zero-energy modes



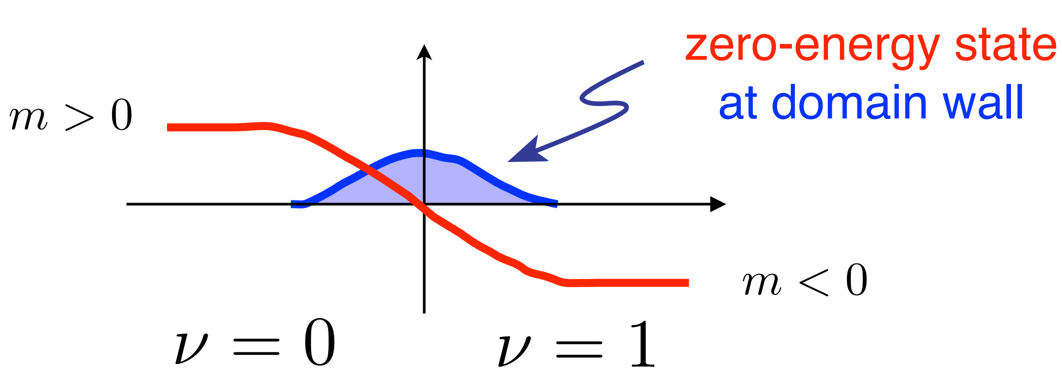
Effective low-energy continuum theory: (expand around $k_0 = \pi$) $\quad k \to -i\partial_x$

$$H(x) = -i\sigma_y \partial_x + m(x)\sigma_x \qquad m(x) = 2\delta t$$

Dirac Hamiltonian with a mass: $E(q) = \pm\sqrt{q^2 + m^2}$

Sublattice symmetry (“chiral symmetry”): $\{\sigma_z, H\} = 0 \quad \longrightarrow \quad \sigma_z \left|\psi_E\right\rangle = \left|\psi_{-E}\right\rangle$

Consider domain wall:



Ansatz for boundstate: $\psi_0 = \chi e^{-\int_0^x m(x')dx'}$

$$H\psi_0 = 0 \Rightarrow \chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Bulk-boundary correspondence: $\Delta\nu = |\nu_\mathrm{R} - \nu_\mathrm{L}| = \#\,\mathrm{zero\ modes}$ (topological invariant characterizing domain wall)