Topology and Symmetry in Carbon Nanoribbons

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Topology and Symmetry

Introduction

(Non-rigorous) Definition

Topology is the study of *continuity*

Topological Condensed Matter

Umbrella term of various problems in condensed matter that can be explained with the aid of topology

Topology and Symmetry

Example: Bloch's Theorem

Definition

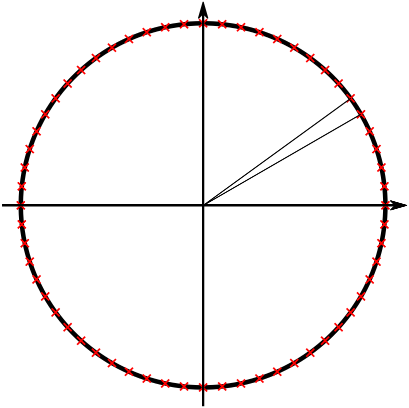
Translationally invariant Hamiltonian has eigenstates of the form

$$\psi_n(x) = e^{ikx} u_{nk}(x)$$

- Idealized lattice - $\mathbb{Z}$
- Real lattice of size L
  - Born-von Karman PBC is assumed
  - Symmetry breaks to $\mathbb{Z} \to \mathbb{Z}_L = \langle g | g^L = e \rangle$
- $\psi \mapsto D(g)\psi$

Topology and Symmetry

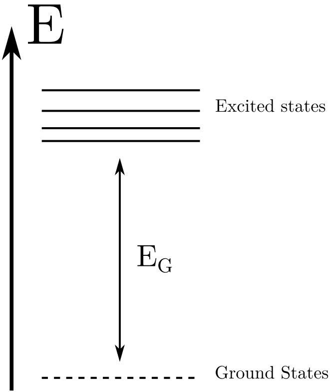
Bloch's Theorem cont'd



- Irreps of $\mathbb{Z}_N$ are characterized by integer m: $D^m(g^n) = e^{i\frac{2\pi m}{L}n} \equiv e^{ik_m n}$
- Translational invariance $\implies$ quantum number k_m
- Representation of $\mathbb{Z}$ is $U(1)$
- Same technique used in
  - Dispersion of crystals [1]
  - Dispersion of CNRs [6]

Topology and Symmetry

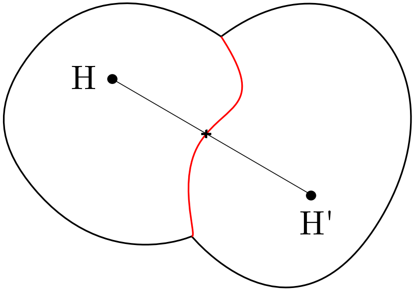
Example: Gapped Systems



- E_G - Energy gap between ground and excited states
- Finite in thermodynamic limit $\implies$ System is gapped

Topology and Symmetry

Example: Gapped Systems cont'd



- Gapped Hamiltonians H, H'
- Adiabatic transport $H \to H'$
  - Timescale defined by E_G^{-1}
  - System stays in GS
  - Nonequivalent phases
    $\implies$ Gap closing

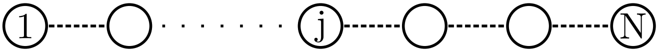
Kitaev Model

Hamiltonian

Model Hamiltonian

$$\frac{H}{t} = -\sum_{j=1}^{L-1}(c_j^\dagger c_{j+1} + h.c.) + \frac{\Delta}{t}\sum_{j=1}^{L-1}(c_j c_{j+1} + h.c.) - \frac{\mu}{t}\sum_{j=1}^{L} c_j^\dagger c_j$$

- t - Hopping strength
- Δ - SC pairing strength
- μ - Chemical potential



Kitaev Model

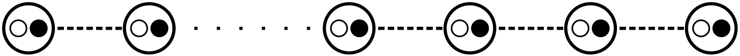
Majorana Fermions

Definition

$$c_j = \frac{\gamma_{ja} + i\gamma_{jb}}{2} \qquad c_j^\dagger = \frac{\gamma_{ja} - i\gamma_{jb}}{2}$$

with properties

$$\{\gamma_{j\lambda}, \gamma_{k\lambda'}\} = \delta_{jk}\delta_{\lambda\lambda'} \qquad \gamma_{j\lambda}^\dagger = \gamma_{j\lambda}$$



Kitaev Model

Phases

Hamiltonian at Symmetric Lines ($\Delta = t$)

$$H = -t \sum_{j=1}^{L-1} i\gamma_{jb}\gamma_{j+1a} - \frac{\mu}{2} \sum_{j=1}^{L} (1 + i\gamma_{ja}\gamma_{jb})$$

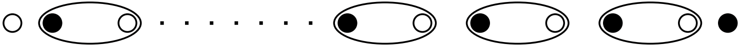
- $\mu \gg t$
  - Trivial
  - Unique GS
  - No MZM

Kitaev Model

Phases cont'd

Hamiltonian at Symmetric Lines ($\Delta = t$)

$$H = -t \sum_{j=1}^{L-1} i\gamma_{jb}\gamma_{j+1a} - \frac{\mu}{2}\sum_{j=1}^{L}(1+\gamma_{ja}\gamma_{jb})$$



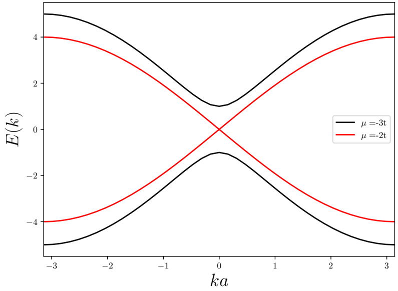
- $\mu \ll t$
  - Topological
  - GSD due to *parity* - $\mathcal{P} = \prod_{j=1}^{L}(-i\gamma_{ja}\gamma_{jb})$
  - MZM - Edge states $\sim \gamma_{1a} \pm i\gamma_{Lb}$

Kitaev Model

Gap Closing

Dispersion Relation ($\Delta = t$)

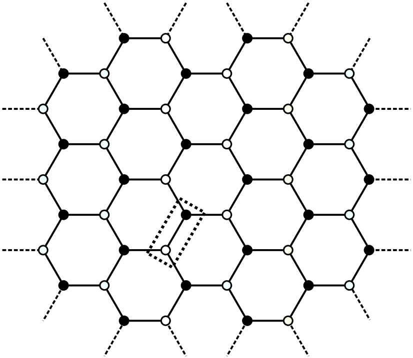
$$E(k) = \pm\sqrt{\mu^2 + 4t^2 + 4\mu t\cos(ka)}$$



- $H_{\text{eff}} = -(\mu + 2t)\sigma_z + 2tk\sigma_y$
- Gap closing at $\mu = -2t$
  - Dirac for massless particle
  - Chiral states
  - $v = 2t$

Carbon Nanoribbon

Graphene



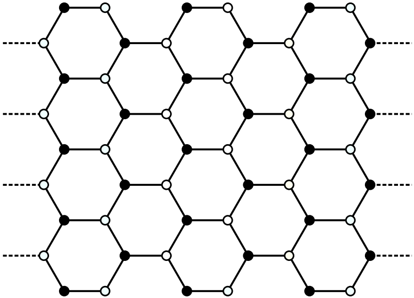
Hamiltonian in Momentum Space

$$H(k) = t\sum_i \sigma_x \cos(\mathbf{k}\cdot\mathbf{a}_i) - \sigma_y \sin(\mathbf{k}\cdot\mathbf{a}_i)$$

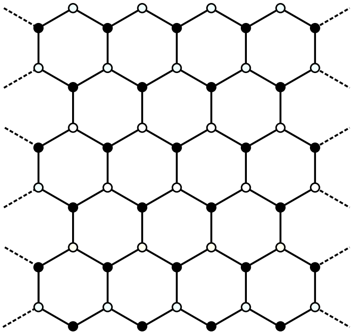
- Sublattice - σ_z
- Spinless time reversal - K

Carbon Nanoribbon

Edge Geometry



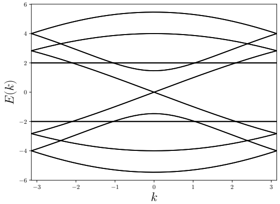
Armchair nanoribbon (ANR)



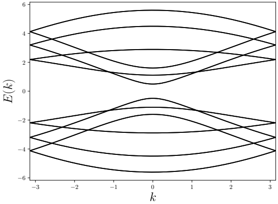
Zigzag nanoribbon (ZNR)

Carbon Nanoribbon

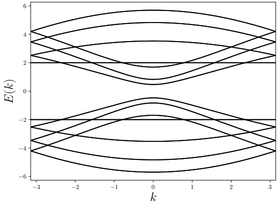
Dispersion Relations: Armchair



$W = 5$



$W = 6$

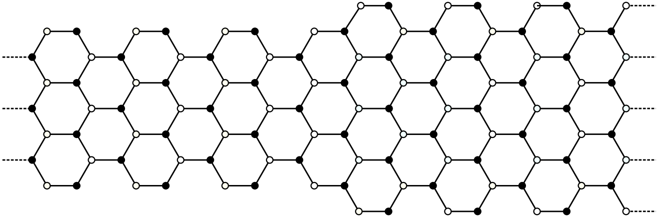


$W = 7$

- Energy depends on widths
- Zero crossing for $3m - 1$

Carbon Nanoribbon

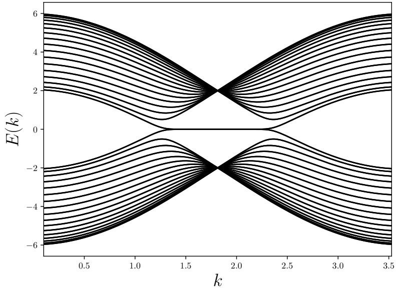
Dispersion Relations: Armchair cont'd



- Different ANRs can be stacked [2] [5]
- Topological states at junctions
- Other geometries possible

Carbon Nanoribbon

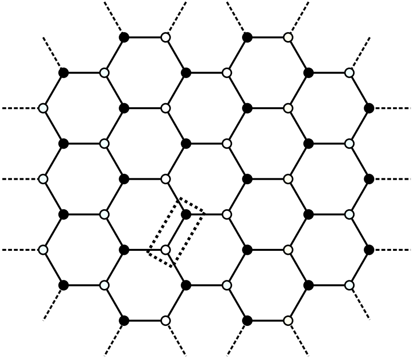
Dispersion Relations: Zigzag



- No width dependence
- Flatband around $\frac{2\pi}{3} \leq |k| \leq \pi$
- Edge states

BCS-Hubbard

Bipartite Lattice



BCS-Hubbard [3]

$$H_0 = -\sum_{\langle i,j\rangle\sigma} t c^\dagger_{i\sigma} c_{j\sigma} + \Delta c_{i\sigma} c_{j\sigma} + h.c.$$

$$H_{\text{int}} = -U \sum_l \left(n_{l\uparrow} - \frac{1}{2}\right)\left(n_{l\downarrow} - \frac{1}{2}\right)$$

- $\langle i,j\rangle$ - Nearest neighbors
- n - Number operator
- σ - Spin

BCS-Hubbard

Composite Fermions

Definition

$$d_{l1} = d_{l2} = \frac{1}{i\sqrt{2}}(c_{l\leftarrow} - c^{\dagger}_{l\rightarrow}) \equiv d_{l\leftarrow} \qquad l \in A$$

$$d_{l2} = d_{l1} = \frac{1}{\sqrt{2}}(c_{l\rightarrow} + c^{\dagger}_{l\leftarrow}) \equiv d_{l\rightarrow} \qquad l \in B$$

Conserved Quantities

$$\xi_l D_l = (2d^{\dagger}_{l2} d_{l2} - 1) \in \{-1, 1\}$$

BCS-Hubbard

Diagonal Hamiltonian

Hamiltonian

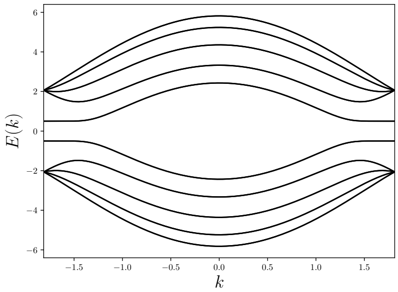
$$H = -4it \sum_{\langle i,j \rangle} d_{i1} d_{j1} + d_{i1}^{\dagger} d_{j1}^{\dagger} + U \sum_{l} \xi_l D_l \left(n_{l1} - \frac{1}{2} \right)$$

Hilbert Space

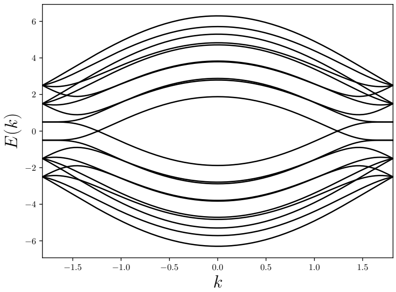
- Split into non-interacting 2^N sectors
- Sectors Labeled by the set $\{\xi_l D_l\}$
- For each sector Hamiltonian is solvable [7] [4]

BCS-Hubbard

Nanoribbon: Zigzag



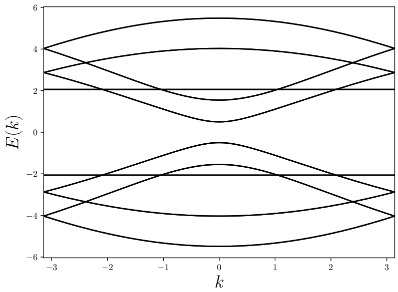
Anti-Ferromagnetic



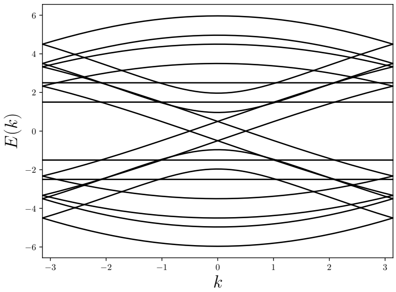
Ferromagnetic

BCS-Hubbard

Nanoribbon: Armchair



Anti-Ferromagnetic



Ferromagnetic

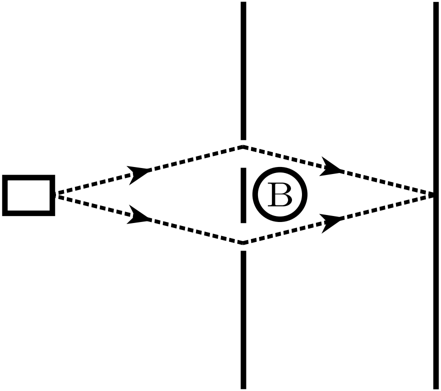
Conclusion

- Topological matter is in between abstract mathematics and physics of materials
- Allows us to extend and formalize the classification of states of matter
  - Fractional quantities
  - Edge states
  - Anyions

Thank You!

Topology and Symmetry

Example: Ahronov-Bohm Effect



- $|e^{iS_1} + e^{iS_2}| \sim e^{i\Delta S}$
- $\Delta S \propto \oint \vec{A} \cdot \mathrm{d}\vec{l} = \Phi_B$
- Due to solenoid the space is $M = \mathbb{R}^3 \backslash \mathbb{R} \simeq S^1$
- $\pi_1(S^1) = \mathbb{Z} \implies$ paths characterized by *winding number*

References I

[1] H. Bethe. Termaufspaltung in kristallen. *Annalen der Physik*, 395(2):133–208, 1 1929.

[2] Cao et al. Topological phases in graphene nanoribbons: Junction states, spin centers, and quantum spin chains. *Phys. Rev. Lett.*, 119:076401, Aug 2017.

[3] Chen et al. Exactly solvable bcs-hubbard model in arbitrary dimensions. *Phys. Rev. Lett.*, 120:046401, Jan 2018.

[4] Miao et al. Exact solution to the haldane-bcs-hubbard model along the symmetric lines: Interaction-induced topological phase transition. *Phys. Rev. B*, 99:245154, Jun 2019.

[5] Rizzo et al. Topological band engineering of graphene nanoribbons. *Nature*, 560:204–208, 2018.

[6] Saito et al. Electronic structure of graphene tubules based on c_{60}. *Phys. Rev. B*, 46:1804–1811, Jul 1992.

References II

[7] Motohiko Ezawa. Exact solutions for two-dimensional topological superconductors: Hubbard interaction induced spontaneous symmetry breaking. *Phys. Rev. B*, 97:241113, Jun 2018.