# Topological Superconductivity

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### UPPSALA UNIVERSITET

Quantum Matter Theory

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Ångström laboratory

Open postdoc positions this fall



- Introduction to superconductivity
  - BCS, BdG, group theory

- Topological superconductivity
  - Chiral superconductors
  - "Spinless" superconductors  $\rightarrow$  Majorana fermions



# Introduction to Superconductivity

What is it?

How do we describe it?



### What is Superconductivity? UNIVERSITET

- Electric transport without resistance

– Meissner effect











- But how do electrons move without resistance?
  - All electrons in coherent quantum state with fixed phase (condensate)

$$\Psi = \Delta_0 e^{i \varphi}$$

- Bardeen-Cooper-Schrieffer (BCS) theory
  - Condensation of electron (Cooper) pairs (with fermionic wave function)
  - Many-body state, but possible to describe within mean-field theory



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## BCS Hamiltonian

### Pairing Hamiltonian:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}$$
  
Electron pairing  
Kinetic (band) energy  
$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -g_0/V, & (|\epsilon_{\mathbf{k}}| < \omega_D) \\ 0 & (\text{otherwise}) \end{cases}$$

Mean-field theory with  $F_{\bf k}=\langle c_{-{\bf k}\downarrow}c_{{\bf k}\uparrow}\rangle$  (pair amplitude at  ${\bf k}$ )

Set order parameter 
$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} F_{\mathbf{k}'} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle$$
  
 $\rightarrow H_{\mathrm{MF}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\downarrow} c^{\dagger}_{\mathbf{k}\uparrow} + \mathrm{H.c.} + \sum_{\mathbf{k}} \frac{V}{g_0} \Delta^{\dagger}_{\mathbf{k}} \Delta_{\mathbf{k}}$ 

See e.g. Tinkham: Introduction to superconductivity



Define the Nambu spinor 
$$\psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} \quad \psi^{\dagger}_{\mathbf{k}} = \begin{pmatrix} c^{\dagger}_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow} \end{pmatrix}$$

$$\rightarrow \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} (c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} - c_{-\mathbf{k}\downarrow} c^{\dagger}_{-\mathbf{k}\downarrow} + 1) = (c^{\dagger}_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}) \begin{bmatrix} \epsilon_{\mathbf{k}} & 0\\ 0 & -\epsilon_{\mathbf{k}} \end{bmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow}\\ \bar{c}^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}$$

$$\text{TRS: } \varepsilon_{\mathbf{k}} = \varepsilon_{-\mathbf{k}}$$

$$\rightarrow \epsilon_{\mathbf{k}} \sum_{\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \left[ \bar{\Delta} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \Delta \right] = \left( c^{\dagger}_{\mathbf{k}\uparrow}, \ c_{-\mathbf{k}\downarrow} \right) \begin{bmatrix} \epsilon_{\mathbf{k}} & \Delta \\ \bar{\Delta} & -\epsilon_{\mathbf{k}} \end{bmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ \bar{\Delta} & -\epsilon_{\mathbf{k}} \end{bmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix}$$

### Bogliubov-de Gennes (BdG) formulation

2x2 matrix problem → Solve by finding eigenvalues and vectors



## Eigenstates = Quasiparticles

QP energies (eigenvalues):  $E_{\mathbf{k}} = \pm \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$ 

QP operators (eigenvectors):  $\begin{cases} a^{\dagger}_{\mathbf{k}\uparrow} = \psi^{\dagger}_{\mathbf{k}} \cdot \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = c^{\dagger}_{\mathbf{k}\uparrow} u_{\mathbf{k}} + c_{-\mathbf{k}} \\ a_{-\mathbf{k}\downarrow} = \psi^{\dagger}_{\mathbf{k}} \cdot \begin{pmatrix} -v_{\mathbf{k}}^{*} \\ u_{\mathbf{k}}^{*} \end{pmatrix} = c_{-\mathbf{k}\downarrow} u_{\mathbf{k}}^{*} - c^{\dagger}_{\mathbf{k}\downarrow} \end{cases}$ 

$$k \downarrow V_k$$
 Bogoliubov  
tranformation

$$u_{\mathbf{k}} = \sqrt{\frac{1}{2} \left[ 1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \right]} \quad v_{\mathbf{k}} = \sqrt{\frac{1}{2} \left[ 1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \right]}$$

Band structure







Superconducting Order

Self-consistent order parameter:

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle = \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'}^* \langle a_{\mathbf{k}'\uparrow}^{\dagger} a_{\mathbf{k}'\uparrow} + a_{-\mathbf{k}'\downarrow}^{\dagger} a_{\mathbf{k}'\downarrow} - 1 \rangle$$

$$\langle a_{\mathbf{k}'\sigma}^{\dagger} a_{\mathbf{k}'\sigma} \rangle = (1 + e^{E_{\mathbf{k}'}/k_BT})^{-1}$$
Fermi-Dirac distribution

Generalized order: fermionic, odd under particle exchange:

$$\Delta_{\alpha\beta}(\mathbf{k}) = -\Psi_{\beta\alpha}(-\mathbf{k})$$
$$\Delta_{\alpha\beta}(\mathbf{k}) = \Delta e^{i\varphi} \eta(\mathbf{k}) \chi_{\alpha\beta}$$
$$\uparrow_{\text{orbital spin}}$$

$$\chi_{\alpha\beta} \rightarrow \begin{cases} \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) & (S=0) & \rightarrow \eta \text{ even function in } \mathbf{k} \\ |\uparrow\uparrow\rangle & (S=1, S_z=1) \\ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) & (S=1, S_z=0) \\ |\downarrow\downarrow\rangle & (S=1, S_z=-1) \end{cases} \rightarrow \eta \text{ odd function in } \mathbf{k} \end{cases}$$



# Spatial Symmetries

- Conventional superconductors:
  - Spin-singlet, s-wave ( $\eta$  k-independent)
- Cuprate (high-Tc) superconductors:
  - Spin-singlet, *d*-wave  $(\eta = k_x^2 k_y^2)$

### UNCONVENTIONAL

 $k_x + ik_y$ 

- *p*-wave superconductors:
  - Spin-triplet, *p*-wave ( ${}^{3}$ He, Sr<sub>2</sub>RuO<sub>4</sub>?)
  - Topological "spinless" superconductors with Majorana fermions



# <sup>T</sup> Superconducting Pairing

 $\mathrm{V}_{k,k'}$  (and the band structure) determine the pairing symmetry, but often very hard to determine

- Lattice fluctations (phonon): spin-singlet *s*-wave **CONVENTIONAL**
- Antiferromagnetic spin fluctuations: spin-singlet *d*-wave (extended *s*-wave)
- Ferromagnetic spin fluctuations: spin-triplet *p*-wave
- Strong on-site repulsion (Heisenberg interaction): spin-singlet *d*-wave

• .

Can we determine the possible pairing symmetries in a material without knowing V<sub>k,k'</sub>?

Yes, by a general group theory analysis

See e.g. Sigrist and Ueda, RMP **63**, 239 (1991)



General Hamiltonian

General Hamiltonian:  $\mathcal{H} = \sum_{\mathbf{k},s} \varepsilon(\mathbf{k}) a_{\mathbf{k}s}^{\dagger} a_{\mathbf{k}s}$ 

$$+ \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',s_1,s_2,s_3,s_4} V_{s_1s_2s_3s_4}(\mathbf{k},\mathbf{k}') a_{-\mathbf{k}s_1}^{\dagger} a_{\mathbf{k}s_2}^{\dagger} a_{\mathbf{k}'s_3} a_{-\mathbf{k}'s_4}$$

Mean-field order: 
$$\Delta_{ss'}(\mathbf{k}) = -\sum_{\mathbf{k}', s_3, s_4} V_{s'ss_3s_4}(\mathbf{k}, \mathbf{k'}) \langle a_{\mathbf{k}'s_3} a_{-\mathbf{k}'s_4} \rangle$$

$$\rightarrow \tilde{\mathcal{H}} = \sum_{\mathbf{k},s} \varepsilon(\mathbf{k}) a_{\mathbf{k}s}^{\dagger} a_{\mathbf{k}s} + \frac{1}{2} \sum_{\mathbf{k},s_1,s_2} \left[ \Delta_{s_1 s_2}(\mathbf{k}) a_{\mathbf{k}s_1}^{\dagger} a_{-\mathbf{k}s_2}^{\dagger} - \Delta_{s_1 s_2}^{\ast}(-\mathbf{k}) a_{-\mathbf{k}s_1} a_{\mathbf{k}s_2} \right]$$



### Matrix Formulation LINIVERSITET

4-component notation (Nambu):  $\mathbf{a}_{\mathbf{k}} = (a_{\mathbf{k}\uparrow}, a_{\mathbf{k}\downarrow}, a_{-\mathbf{k}\uparrow}^{\dagger}, a_{-\mathbf{k}\downarrow}^{\dagger})^{\dagger}$ 

$$\rightarrow \tilde{\mathcal{H}} = \mathbf{a}_{\mathbf{k}}^{\dagger} \begin{pmatrix} \varepsilon(\mathbf{k})\sigma_{0} & \hat{\Delta}(\mathbf{k}) \\ \hat{\Delta}^{\dagger}(\mathbf{k}) & -\varepsilon(\mathbf{k})\sigma_{0} \end{pmatrix} \mathbf{a}_{\mathbf{k}}$$
Spin-singlet pairing:  $\hat{\Delta}(\mathbf{k}) = i\hat{\sigma}_{y}\psi(\mathbf{k}) = \begin{bmatrix} 0 & \psi(\mathbf{k}) \\ -\psi(\mathbf{k}) & 0 \end{bmatrix}$   $\psi$  even function of  $\mathbf{k}$ 

$$\begin{bmatrix} \psi(\mathbf{k})[c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger} - c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}] \end{bmatrix}$$

Spin-triplet pairing:  $\hat{\Delta}(\mathbf{k}) = i(\mathbf{d}(\mathbf{k}) \cdot \hat{\boldsymbol{\sigma}}) \hat{\boldsymbol{\sigma}}_{y}$ 

 $= \begin{bmatrix} -d_x(\mathbf{k}) + id_y(\mathbf{k}) & d_z(\mathbf{k}) \\ d_z(\mathbf{k}) & d_x(\mathbf{k}) + id_y(\mathbf{k}) \end{bmatrix}$ 

**d** vector odd function of **k** 

 $\begin{pmatrix} \mathbf{m}_{z} = 0: & d_{z}(\mathbf{k})[c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger} + c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}] \\ \mathbf{m}_{z} = 1: & [-d_{x}(\mathbf{k}) + id_{y}(\mathbf{k})]c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\uparrow}^{\dagger} \end{pmatrix}$ 



# General Solution

QP energy (eigenvalue): 
$$E_{\mathbf{k}} = \sqrt{\varepsilon(\mathbf{k})^2 + |\psi(\mathbf{k})|^2}$$
  
 $E_{\mathbf{k}} = \sqrt{\varepsilon(\mathbf{k})^2 + |\mathbf{d}(\mathbf{k})|^2 \pm \mathbf{q}(\mathbf{k})|}$ 

$$\begin{pmatrix} \widehat{\Delta}\widehat{\Delta}^{\dagger} = |\mathbf{d}|^2 \widehat{\sigma}_0 + \mathbf{q} \cdot \widehat{\sigma} \\ \mathbf{q} = i(\mathbf{d} \times \mathbf{d}^*) \\ \text{Finite } \mathbf{q} = \text{non-unitary} \end{cases}$$

Self-consistency equation, linear close to T<sub>c</sub>:

$$v\Delta_{s_1s_2}(\mathbf{k}) = -\sum_{s_3s_4} \langle V_{s_2s_1s_3s_4}(\mathbf{k},\mathbf{k}')\Delta_{s_3s_4}(\mathbf{k}')\rangle_{\mathbf{k}}$$
$$\frac{1}{v} = N(0)\int_0^{\varepsilon_c} d\varepsilon \frac{\tanh\left[\frac{\beta_c\varepsilon(k)}{2}\right]}{\varepsilon(\mathbf{k})} = \ln(1.14\beta_c\varepsilon_c)$$

- Largest eigenvalue gives T<sub>c</sub>
- Eigenfunction (Δ) belongs to irreducible representation (irrep) of symmetry group

 $\rightarrow$  Possible SC symmetries belong to irreps of symmetry group of H

 $\rightarrow$  SC state always breaks U(1), can also break

- Crystal lattice, spin-rotation, time-reversal, ... symmetries



### Basis Gap Functions: D<sub>4h</sub> UNIVERSITET

•  $D_{4h}$  = tetragonal symmetry (cuprates with  $k_z = 0$ )

Irreducible representation $\Gamma$	Basis function
$     \Gamma_{1}^{+} \\     \Gamma_{2}^{+} \\     \Gamma_{3}^{+} \\     \Gamma_{4}^{+} \\     \Gamma_{5}^{+}   $	(a) Spin-singlet $\psi(\Gamma_1^+;\mathbf{k}) = 1, \ k_x^2 + k_y^2, \ k_z^2  s\text{-wave, extended } s\text{-wave}$ $\psi(\Gamma_2^+;\mathbf{k}) = k_x k_y (k_x^2 - k_y^2)$ $\psi(\Gamma_3^+;\mathbf{k}) = k_x^2 - k_y^2  d(x^2 - y^2) \text{-wave}$ $\psi(\Gamma_4^+;\mathbf{k}) = k_x k_y  d(xy) \text{-wave}$ $\psi(\Gamma_5^+, 1;\mathbf{k}) = k_x k_z$ $\psi(\Gamma_5^+, 2;\mathbf{k}) = k_y k_z$
$\Gamma_{1}^{-}$ $\Gamma_{2}^{-}$ $\Gamma_{3}^{-}$ $\Gamma_{4}^{-}$ $\Gamma_{5}^{-}$	(b) Spin-triplet $d(\Gamma_{1}^{-};\mathbf{k}) = \hat{\mathbf{x}}k_{x} + \hat{\mathbf{y}}k_{y}, \hat{\mathbf{z}}k_{z}$ $d(\Gamma_{2}^{-};\mathbf{k}) = \hat{\mathbf{x}}k_{y} - \hat{\mathbf{y}}k_{x}$ $d(\Gamma_{3}^{-};\mathbf{k}) = \hat{\mathbf{x}}k_{x} - \hat{\mathbf{y}}k_{x}$ $d(\Gamma_{4}^{-};\mathbf{k}) = \hat{\mathbf{x}}k_{y} + \hat{\mathbf{y}}k_{x}$ $d(\Gamma_{5}^{-},1;\mathbf{k}) = \hat{\mathbf{x}}k_{z}, \hat{\mathbf{z}}k_{x}$ $d(\Gamma_{5}^{-},2;\mathbf{k}) = \hat{\mathbf{y}}k_{z}, \hat{\mathbf{z}}k_{y}$ $p(\mathbf{x}) - \text{ and } p(\mathbf{y}) - \text{ wave degenerated}$

Sigrist and Ueda, RMP **63**, 239 (1991)



Basis Gap Functions: D<sub>6h</sub>

•  $D_{6h}$  = hexagonal symmetry (graphene, Bi<sub>2</sub>Se<sub>3</sub> TIs with  $k_z = 0$ ,)

Irreducible representation $\Gamma$	Basis functions
$\Gamma_1^+$ $\Gamma_2^+$ $\Gamma_3^+$ $\Gamma_4^+$	(a) Spin-singlet $\psi(\Gamma_1^+;\mathbf{k})=1, k_x^2+k_y^2, k_z^2 \qquad s\text{-wave, extended } s\text{-wave}$ $\psi(\Gamma_2^+;\mathbf{k})=k_x k_y (k_x^2-3k_y^2)(k_y^2-3k_x^2)$ $\psi(\Gamma_3^+;\mathbf{k})=k_z k_x (k_x^2-3k_y^2)$ $\psi(\Gamma_4^+;\mathbf{k})=k_z k_y (k_y^2-3k_x^2)$
$\Gamma_5^+$	$\psi(\Gamma_5^+, 1; \mathbf{k}) = k_x k_z$ $\psi(\Gamma_5^+, 2; \mathbf{k}) = k_y k_z$
$\Gamma_6^+$	$\psi(\Gamma_{6}^{+},1;\mathbf{k}) = k_{x}^{2} - k_{y}^{2}$ $\psi(\Gamma_{6}^{+},2;\mathbf{k}) = 2k_{x}k_{y}$ (b) Spin-triplet
$\Gamma_1^-$ $\Gamma_2^-$ $\Gamma_3^-$	$\mathbf{d}(\Gamma_1^-;\mathbf{k}) = \mathbf{\hat{x}}k_x + \mathbf{\hat{y}}k_y, \mathbf{\hat{z}}k_z$ $\mathbf{d}(\Gamma_2^-;\mathbf{k}) = \mathbf{\hat{x}}k_y - \mathbf{\hat{y}}k_x$ $\mathbf{d}(\Gamma_3^-;\mathbf{k}) = \mathbf{\hat{z}}k_x(k_x^2 - 3k_y^2),$ $k_z[(k_x^2 - k_y^2)\mathbf{\hat{x}} - 2k_xk_y\mathbf{\hat{y}}]$
$\Gamma_4^-$	$\mathbf{d}(\Gamma_4^-;\mathbf{k}) = \hat{\mathbf{z}}k_y(k_y^2 - 3k_x^2), \\ k_z[(k_y^2 - k_x^2)\hat{\mathbf{y}} - 2k_xk_y\hat{\mathbf{x}}]$
$\Gamma_5^-$	$\mathbf{d}(\Gamma_5^-, 1; \mathbf{k}) = \mathbf{\hat{x}} k_z, \mathbf{\hat{z}} k_x$ $\mathbf{d}(\Gamma_5^-, 2; \mathbf{k}) = \mathbf{\hat{y}} k_z, \mathbf{\hat{z}} k_y$
Γ <sub>6</sub>	

Sigrist and Ueda, RMP **63**, 239 (1991)



### UPPSALA NIVERSITET Multiple Order Parameters

Superconducting state highly unconventional if multiple components at  $\rm T_{\rm c}$ 

- Two-dimensional irreps often gives  $\Delta_1 + i\Delta_2$  at  $T < T_c$ 
  - Only combination with fully gap  $\rightarrow$  Highest energy gain
  - Singlet  $d(x^2-y^2)+id(xy)$ -wave for hexagonal lattices (graphene?)
  - Triplet (m<sub>z</sub> = 0) p(x)+ip(y)-wave for square lattices

## **Topological (chiral) superconductors**

Break time-reversal symmetry (TRS) Fully gapped bulk energy spectrum



# Introduction to Superconductivity

What is it?

A charged superfluid of Cooper pairs (2 electrons) with fermionic character

Cooper pairs formed by effective attractive interaction

How do we describe it?

BCS theory (mean-field theory of condensation)

BdG matrix formalism

Symmetry of order parameter (group theory)



# **Topological Superconductivity**

Chiral superconductors Spin-singlet *d*+i*d*'-wave (spin-triplet *p*+i*p*'-wave) superconductors

Spinless superconductors Majorana fermions Engineered systems



# UPPSALA Topology



Topologically speaking: coffee  $\sup_{1 \text{ hole}} = \operatorname{donut} \neq \lim_{0 \text{ hole}} \sup_{1 \text{ hole}} = \operatorname{donut} \neq \operatorname{bun}_{0 \text{ hole}}$ 



## Classification

- All forms of matter can be classified according to the symmetry they break (translation, spin, gauge, time-reversal, ...)
- Except topological matter

Topological insulators: 2005 (quantum Hall effect: 1980)

- Ordered but no symmetry breaking
- Topology of the wave function





Trivial

Non-trivial







### **Topological Band Theory** UNIVERSITET

Anything else than metals and insulators? + spin-orbit coupling  $\rightarrow$  Band inversion





### UPPSALA UNIVERSITET HgTe & CdTe Semiconductors



Bernevig et al., Science 314, 1757 (2006)





UPPSALA UNIVERSITET TOpological Matter

Topological states of matter have

- Bulk topological invariant
  - Number classifying the topological class
  - Only changes with bulk gap closing
- Protected boundary states
  - At any boundary to other topological region (vacuum, normal metal, s-wave SC = trivial topological order)

## **Bulk-boundary correspondence**

# of boundary states = change in topological invariant at boundary



### **Topological Superconductors** UPPSALA UNIVERSITET

Same band theory in insulators and superconductors



Same low-energy excitation spectrum





# Topological Classification

Non-interacting (single-particle) insulators and superconductors: 10-fold way

		time-reversa	l subl	ittice (ch	iral) Top	ological in	variants
·		TRS	particle-hole	SLS	d=1	d=2	d=3
Standard	A (unitary)	0	0	0	-	Z	-
(Wigner-Dyson)	AI (orthogonal)	+1	0	0	-	-	-
	AII (symplectic)	-1	0	0	-	$\mathbb{Z}_2$	$\mathbb{Z}_2$
Chiral	AIII (chiral unitary)	0	0	1	Z	-	Z
(sublattice)	BDI (chiral orthogonal)	+1	+1	1	Z	-	_
	CII (chiral symplectic)	-1	-1	1	Z	-	$\mathbb{Z}_2$
BdG	D	0	+1	0	$\mathbb{Z}_2$	Z	-
	С	0	-1	0	-	Z	-
	DIII	-1	+1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	Z
	CI	+1	-1	1	-	-	Z



# Superconductors

AZ class	SU(2)	TRS	Examples in two dimensions						
D	×	×	Spinless chiral $(p \pm ip)$ wave						
DIII	×	0	Superposition of $(p+ip)$ and $(p-ip)$ waves						
Α	$\triangle$	×	Spinful chiral $(p \pm ip)$ wave						
AIII	$\triangle$	0	Spinful $p_x$ or $p_y$ wave						
С	0	×	$(d \pm id)$ wave						
CI	0	0						0	$d_{x^2-y^2}$ or $d_{xy}$ wave
			TRS	PHS	SLS	<i>d</i> =1	<i>d</i> =2	<i>d</i> =3	
Standard		A (unitary)	0	0	0	-	Z	-	
(Wigner-Dyson	Wigner-Dyson) AI (orthogonal)		+1	0	0	-	-	-	
AII (symplectic) Chiral AIII (chiral unitary)		-1	0	0	-	$\mathbb{Z}_2$	$\mathbb{Z}_2$		
		0	0	1	Z	-	Z	Spinless $p+ip'$ -wave in 1D $\rightarrow$ BC	
(sublattice)	BDI (	chiral orthogonal)	+1	+1	1	Z	-	-	because effective TRS
	CII (c	chiral symplectic)	-1	-1	1	Z	-	$\mathbb{Z}_2$	because effective TRS
BdG		D	0	+1	0	$\mathbb{Z}_2$	Z	-	
		С	0	-1	0	-	Z	-	
		DIII	-1	+1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	Z	
		CI	+1	-1	1	-	-	Z	

Schnyder et al., PRB 78, 195125 (2008)



# **Topological Superconductivity**

Chiral superconductors Spin-singlet *d*+i*d*-wave (spin-triplet *p*+i*p*-wave) superconductors

Spinless superconductors Topology and Majorana fermions



### d-wave SC from Strong Repulsion LINIVERSITET

Strong Coulomb repulsion, antiferromagnetic correlations (e.g. Hubbard model near half-filling)

 $\rightarrow$  Spin-singlet pairing

- $\rightarrow$  Double electron occupation unfavorable
  - $\rightarrow$  No *s*-wave pairing
- $\rightarrow$  Spin-singlet *d*-wave pairing (best state = least number of nodes)

2D hexagonal lattice  $\rightarrow$ 

Spin-singlet  $d(x^2-y^2)+id(xy)$  pairing (Only combination with energy gap)

and a second		
Irreducible		
epresentation $\Gamma$	Basis functions	
	(a)	
$\Gamma_1^+$	$\psi(\Gamma_1^+;\mathbf{k})=1, k_x^2+k_y^2, k_z^2$	
$\Gamma_2^+$	$\psi(\Gamma_{2}^{+};\mathbf{k}) = k_{x}k_{y}(k_{x}^{2} - 3k_{y}^{2})(k_{y}^{2} - 3k_{x}^{2})$	
$\Gamma_3$	$\psi(\Gamma_{3};\mathbf{k}) = k_{z}k_{x}(k_{x}^{z} - 3k_{y}^{z})$	
14	$\psi(1_4,\mathbf{K}) - \kappa_z \kappa_y (\kappa_y - 3\kappa_x)$	
$\Gamma_5^+$	$\psi(\Gamma_5^+, 1; \mathbf{k}) = k_x k_z$ $\psi(\Gamma_5^+, 2; \mathbf{k}) = k_y k_z$	
$\Gamma_6^+$	$\psi(\Gamma_{6}^{+},1;\mathbf{k}) = k_{x}^{2} - k_{y}^{2} d(X^{2} - Y^{2})$ $\psi(\Gamma_{6}^{+},2;\mathbf{k}) = 2k_{x}k_{y} d(X^{2} - Y^{2})$	+id(xy)
	(b)	
$\Gamma_1^-$	$\mathbf{d}(\boldsymbol{\Gamma}_1^-;\mathbf{k}) = \mathbf{\hat{x}}k_x + \mathbf{\hat{y}}k_y, \mathbf{\hat{z}}k_z$	
$\Gamma_2^-$	$\mathbf{d}(\Gamma_2^-;\mathbf{k}) = \mathbf{\hat{x}} k_y - \mathbf{\hat{y}} k_x$	
Ι <sub>3</sub>	$\mathbf{d}(1_{3};\mathbf{k}) = \mathbf{z}k_{x}(k_{x}^{2} - 3k_{y}^{2}),$ $k_{z}[(k_{x}^{2} - k_{y}^{2})\mathbf{\hat{x}} - 2k_{x}k_{y}\mathbf{\hat{y}}]$	
$\Gamma_4^-$	$\mathbf{d}(\boldsymbol{\Gamma}_{4}^{-};\mathbf{k}) = \widehat{\mathbf{z}}k_{y}(k_{y}^{2}-3k_{x}^{2}), \\ k_{z}[(k_{y}^{2}-k_{x}^{2})\widehat{\mathbf{y}}-2k_{x}k_{y}\widehat{\mathbf{x}}]$	
$\Gamma_5^-$	$\mathbf{d}(\Gamma_5^-, 1; \mathbf{k}) = \mathbf{\hat{x}} k_z, \mathbf{\hat{z}} k_x$ $\mathbf{d}(\Gamma_5^-, 2; \mathbf{k}) = \mathbf{\hat{y}} k_z, \mathbf{\hat{z}} k_y$	
$\Gamma_6^-$	$\mathbf{d}(\Gamma_6^-, 1; \mathbf{k}) = \mathbf{\hat{x}} k_x - \mathbf{\hat{y}} k_y$ $\mathbf{d}(\Gamma_6^-, 2; \mathbf{k}) = \mathbf{\hat{x}} k_y - \mathbf{\hat{y}} k_x$	



### UPPSALA UNIVERSITET Bulk and Edge Properties

• Fully gapped bulk  $E_{QP}(\mathbf{k}) = \sqrt{\varepsilon(\mathbf{k})^2 + |\Delta(\mathbf{k})|^2}$ 



• Two chiral (co-propagating) edge states per edge



ABS, PRL 109, 197001 (2012)


#### UPPSALA UNIVERSITET TOpological Invariant

d+id'-wave SC breaks TRS  $\rightarrow$  Chern number invariant

$$\mathcal{N} = \frac{1}{4\pi} \int_{\mathrm{BZ}} \mathrm{d}^2 k \, \hat{\mathbf{m}} \cdot \left( \frac{\partial \hat{\mathbf{m}}}{\partial k_x} \times \frac{\partial \hat{\mathbf{m}}}{\partial k_y} \right)$$

Skyrmion number 
$$\hat{\mathbf{m}} = \frac{1}{\sqrt{\varepsilon(\mathbf{k})^2 + |\Delta(\mathbf{k})|^2}} \begin{pmatrix} \operatorname{Re} \Delta(\mathbf{k}) \\ \operatorname{Im} \Delta(\mathbf{k}) \\ \varepsilon(\mathbf{k}) \end{pmatrix}$$

Counts unit sphere area spanned by **m** as **k** covers the BZ

Bottom of band: m ~ -z Top of band: m ~ z → Non-zero N iff Δ has finite winding along lines of constant ε

d+id'-wave winds twice around  $\Gamma \rightarrow |\mathcal{N}| = 2$  $\rightarrow 2$  chiral edge states



ABS and Honerkamp JPCM **26**, 423201 (2014)



#### UPPSALA NIVERSITET Chiral p+ip SC Properties

Spin-triplet p(x)+ip(y)-wave spin-triplet,  $\mathbf{d} = (0, 0, k_x+ik_y)$ 

• Fully gapped in the bulk  $E_{\rm QP}(\mathbf{k}) = \sqrt{\varepsilon(\mathbf{k})^2 + |\Delta(\mathbf{k})|^2}$ 



• Break TRS  $\rightarrow$  finite Chern number/Skyrmion winding

$$\mathcal{N} = \frac{1}{4\pi} \int_{\mathrm{BZ}} \mathrm{d}^2 k \, \hat{\mathbf{m}} \cdot \left( \frac{\partial \hat{\mathbf{m}}}{\partial k_x} \times \frac{\partial \hat{\mathbf{m}}}{\partial k_y} \right)$$
$$\hat{\mathbf{m}} = \frac{1}{\sqrt{\varepsilon(\mathbf{k})^2 + |\Delta(\mathbf{k})|^2}} \begin{pmatrix} \operatorname{Re} \Delta(\mathbf{k}) \\ \operatorname{Im} \Delta(\mathbf{k}) \\ \varepsilon(\mathbf{k}) \end{pmatrix}$$

- p+ip'-wave winds once around  $\Gamma \rightarrow |\mathcal{N}| = 1$ 
  - $\rightarrow$  One chiral edge state per edge



# Doped Graphene, d+id'SC?

Honeycomb lattice



Band structure with van Hove singularities



# Pairing from repulsive interactions

- Strong interactions [1]
- Perturbative RG [2]
- Functional RG [3]



[1]: ABS and Doniach, PRB 75, 134512 (2007), [2]: Nandkishore et al., Nat. Phys. 8, 158 (2012), [3]: Kiesel et al., PRB 86, 020507 (2012)



## UPPSALA Other Chiral d+id'SCs?

- SrPtAs
- $Na_xCoO_2 \bullet yH_2O$
- $\beta$ -MNCl
- $\kappa$ -(BEDT-TTF)<sub>2</sub>X
- (111) bilayer SrIrO<sub>3</sub>
- $In_3Cu_2VO_9$
- Twisted (~45°) cuprate bilayers

See e.g. review: ABS and Honerkamp JPCM 26, 423201 (2014)



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#### Twisted Bilayer Graphene UNIVERSITET





#### UPPSALA NIVERSITET Why are Flat Bands Interesting?

### Locally or regionally flat bands $\rightarrow$ divergent DOS

### Electronic ordering, even with weak interactions

Magnetism (Stoner criterion):  $DOS(E_F)U > 1$ 

Superconductivity (BCS):  $T_c \propto e^{-\frac{1}{DOS(E_F)V}}$ 



1.06°

1.16 1.14°

1.10

Insulator

- 1.27° (1.33 GPa)

3





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 $T_c$  at magic angle with doping at DOS peak



- Two-fold solution:  $\hat{\Delta}_x, \hat{\Delta}_y$ Top  $|\vec{\Delta}(\vec{x})|/Max |\vec{\Delta}(\vec{x})|$ 0.2 0.4 0.6 0.8 1.0 0
- Highest T<sub>c</sub> for two-fold degenerate solution
- Very low J for realistic  $T_c$  at magic angle
- Peaks in AA regions •
- Moiré-scale nematicity (breaks  $C_3$  rotation)

Löthman, Schmidt, Parhizgar, ABS, Commun. Phys. 5, 92 (2022)



Moiré-scale Nematicity

#### At T<sub>c</sub> all linear combinations are solutions: $\hat{\Delta}(\Theta, \varphi) = \|\hat{\Delta}\| \left(\cos \Theta \hat{\Delta}_x + e^{i\varphi} \sin \Theta \hat{\Delta}_y\right)$







- 3-fold degenerate nematic ground state
- Real valued
- Chiral solution worst!



Cp. gapped chiral *d*-wave in graphene & nodal *d*-wave in cuprates

Löthman, Schmidt, Parhizgar, ABS, Commun. Phys. 5, 92 (2022)



## Atomic-scale *d*-wave Nematicity

Decompose order on bonds:  $\Delta(\vec{x}_i) = |\Delta(\vec{x}_i)| \left( \cos \tau(\vec{x}_i) f_{d_{x^2-y^2}} + \sin \tau(\vec{x}_i) f_{d_{xy}} \right)$ Vector field for *d*-wave order:  $\vec{\chi}(\vec{x}_i) = \cos \tau(\vec{x}_i) \hat{x} + \sin \tau(\vec{x}_i) \hat{y}$ *d*-wave form factors



- Atomic-scale *d*-wave nematicity
- Aligned with moiré-scale nematicity in AA regions
- Vortex structure outside AA regions

Cuprate  $\rightarrow$  Nodal *d*-wave

Graphene  $\rightarrow$  Gapped chiral *d*+i*d*-wave

Twisted bilayer graphene  $\rightarrow$ Gapped inhomogeneous (nematic) *d*-wave



# **Topological Superconductivity**

Chiral superconductors

Spin-singlet d+id'-wave (spin-triplet p+ip'-wave) superconductors

Appears often for 2D irreps Fully gapped bulk Finite Chern number  $\mathcal{N}$ , set by phase winding of  $\Delta$ Chiral edge states crossing bulk gap,  $\# = \mathcal{N}$ Breaks TRS, preserves at least  $S_z$  symmetry



# **Topological Superconductivity**

Chiral superconductors Spin-singlet *d*+i*d*'-wave (spin-triplet *p*+i*p*'-wave) superconductors

Spinless superconductors Majorana fermions Engineered systems



#### UPPSALA NIVERSITET "Spinless" p+ip'Superconductor

- Spinless superconductor  $\rightarrow p$ -wave pairing
- No known intrinsic "spinless" SC
- Multiple proposals for engineered "spinless" *p*+i*p*' superconductors last ~ 10 years
  - 1D spinless  $\Delta \sim k$  (class BDI)
  - 2D spinless  $\Delta \sim k_x + ik_y$  (class D)

#### Can be topological superconductors

Topological boundary states are Majorana Fermions (MFs)

1D: Localized zero-energy end states

2D: dispersive edge modes or localized

zero-energy vortex states





# Majorana Fermions

#### New particle $\sim 1/2$ electron

- Emergent particle
- Appears in pairs





### Non-Abelian statistics in 2D

→ Robust quantum computation by braiding



Quantum gate operation = particle braiding



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# Excitations in Superconductors

Quasiparticles in a superconductor:

- Part electron and part hole
- Mixed spin-up and spin-down

$$\begin{cases} a = uc_{\uparrow}^{\dagger} + vc_{\downarrow} \\ a^{\dagger} = u^{*}c_{\uparrow} + v^{*}c_{\downarrow}^{\dagger} \\ |v_{\mathbf{k}}|^{2} = 1 - |u_{\mathbf{k}}|^{2} = \frac{1}{2} \left(1 - \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \end{cases}$$

**h** +1 + -2 =

 $\rightarrow$  E = 0 states are Majorana fermions:  $\gamma^{\dagger} = \gamma$  (if we ignore spin)

But ...

• Superconductors often have an energy gap

- Topological SCs have E = 0 boundary states

• E = 0 states are often spin-degenerate (2 Majorana  $\rightarrow$  1 electron)

#### $\rightarrow$ "Spinless" topological superconductor



Kitaev, arXiv:cond-mat/0010440 (2001)



UPPSALA UNIVERSITET Majorana Basis

$$H = -\mu \sum_{i} c_{i}^{\dagger} c_{i} - \frac{1}{2} \sum_{i} t c_{i}^{\dagger} c_{i+1} + \Delta c_{i} c_{i+1} + \text{H.c.}$$

$$c_{i} = \frac{1}{2} (\gamma_{i}^{B} + i \gamma_{i}^{A}) \longrightarrow \begin{array}{c} (\gamma_{i}^{\alpha})^{\dagger} = \gamma_{i}^{\alpha} \\ \{\gamma_{i}^{\alpha}, \gamma_{j}^{\beta}\} = 2\delta_{ij}\delta_{\alpha\beta} \\ \text{Majorana fermions} \end{array}$$

$$H = -\frac{\mu}{2} \sum_{i}^{N} (1 + i \gamma_{i}^{B} \gamma_{i}^{A}) - \frac{i}{4} \sum_{i}^{N-1} \left[ (\Delta + t) \gamma_{i}^{B} \gamma_{i+1}^{A} + (\Delta - t) \gamma_{i}^{B} \gamma_{i+1}^{A} \right]$$

$$H = -\frac{\mu}{2} \sum_{i=1}^{n} (1 + i\gamma_i^B \gamma_i^A) - \frac{i}{4} \sum_{i=1}^{n} \left[ (\Delta + t)\gamma_i^B \gamma_{i+1}^A + (\Delta - t)\gamma_i^A \gamma_{i+1}^B \right]$$
  
A:
  
B:
  
 $i = 1$ 
  
 $i = 1$ 
  
 $j = 1$ 
  



### Trivial Phase

$$H = -\frac{\mu}{2} \sum_{i=1}^{N} (1 + i\gamma_{i}^{B}\gamma_{i}^{A}) - \frac{i}{4} \sum_{i=1}^{N-1} \left[ (\Delta + t)\gamma_{i}^{B}\gamma_{i+1}^{A} + (\Delta - t)\gamma_{i}^{A}\gamma_{i+1}^{B} \right]$$

Topological trivial phase:  $\Delta = t = 0, \mu < 0$ 



#### Unique ground state

- Vacuum state for electrons
- Bulk gap ( $|\mu|$  lowest excitation energy)



## Non-Trivial Phase

$$H = -\frac{\mu}{2} \sum_{i=1}^{N} (1 + i\gamma_{i}^{B}\gamma_{i}^{A}) - \frac{i}{4} \sum_{i=1}^{N-1} \left[ (\Delta + t)\gamma_{i}^{B}\gamma_{i+1}^{A} + (\Delta - t)\gamma_{i}^{A}\gamma_{i+1}^{B} \right]$$





#### UPPSALA NIVERSITET Majorana Fermions in BdG

How can we get "1/2 electron" in the BdG formalism?

Never if 
$$\epsilon_{\mathbf{k}} \sum_{\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \left[ \bar{\Delta} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \Delta \right] = \left( c^{\dagger}_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow} \right) \begin{bmatrix} \epsilon_{\mathbf{k}} & \Delta \\ \bar{\Delta} & -\epsilon_{\mathbf{k}} \end{bmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix}$$

→ Not in spindegenerate (e.g. chiral p+ip' or d+id') superconductors

But if 
$$\tilde{\mathcal{H}} = \mathbf{a}_{\mathbf{k}}^{\dagger} \begin{pmatrix} \varepsilon(\mathbf{k})\sigma_{0} & \hat{\Delta}(\mathbf{k}) \\ \hat{\Delta}^{\dagger}(\mathbf{k}) & -\varepsilon(\mathbf{k})\sigma_{0} \end{pmatrix} \mathbf{a}_{\mathbf{k}} \quad \left[ \mathbf{a}_{\mathbf{k}} = (a_{\mathbf{k}\uparrow}, a_{\mathbf{k}\downarrow}, a_{-\mathbf{k}\uparrow}^{\dagger}, a_{-\mathbf{k}\downarrow}^{\dagger}) \right]$$

1 electron represented by 2 vector components

 $\rightarrow$  MF if E=0 eigenstate has no spatial overlap with other states



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Spin-orbit coupled (SOC) semiconductor + magnetic field



4x4 BdG description needed due to SOC + Zeeman field Spinless p+ip' superconductor with MFs if  $|V_z| > |\Delta|$ 

2D: Sau et al. PRL 104, 040502 (2010). 1D: Lutchyn et al. PRL 105, 077001 (2010), Oreg et al. PRL 104, 077002 (2010)



MFs?

## Experimental Hunt in Nanowires

1D InSb nanowire (Semiconductor with strong SOC)

+ *s*-wave superconductor

s-wave superconductor

+ Magnetic field









Nadj-Perge et al., Science 346, 602 (2014), Jeon et al., Science 358, 772 (2017)



Nadj-Perge et al., Science 346, 6209 (2014), Li et al., Nat. Commun. 7, 12297 (2016)



Flexible Setup

### Self-consistent solution for the superconducting order parameter $\begin{bmatrix} \Delta_{\mathbf{i}} = -V_{sc} \langle c_{\mathbf{i}\downarrow} c_{\mathbf{i}\uparrow} \rangle \end{bmatrix}$ Single magnetic impurity





# Magnetic Impurity Wire Networks

Are there simple, but unique, signals of MFs?





### UPPSALA Ferromagnetic Atom Wire Networks

#### Wire network of ferromagnetic atoms on SOC superconductor





# UPPSALA Odd- and Even-Wire Junctions



Björnson and ABS, PRB 94, 100501(R) (2016)



# Parameter Dependencies

B

#### SOC: increased gap



#### SC order parameter: increased gap



#### Magnetic moment: TPT



Large LDOS difference between even- and odd-wire junctions for all parameters

Björnson and ABS, PRB 94, 100501(R) (2016)



### **Majorana Oscillations and Localization**

#### How are MFs interacting with other states?





UPPSALA UNIVERSITET VSR Subgap States

Magnetic impurity (classical spin  $S = V_z$ ) in *s*-wave SC

• Yu-Shiba-Rusinov (YSR) subgap states

$$E_{\rm YSR}^{\pm} = \pm \Delta \left[ 1 - \left(\frac{\pi \rho S}{2}\right)^2 \right] \middle/ \left[ 1 + \left(\frac{\pi \rho S}{2}\right)^2 \right]$$



Quantum phase transition (QPT)

$$|\Psi_0\rangle$$
  $(\Psi_1\rangle$   $(\Psi_1$ 









Self-consistency:  $(\Delta_{\mathbf{i}} = -V_{sc} \langle c_{\mathbf{i}\downarrow} c_{\mathbf{i}\uparrow} \rangle)$ 

MFs?

- $\Delta$  suppressed on chain sites
- Phase transition at lower  $V_z$
- Energy oscillations
- YSR states lower energies






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#### Higher Energy State at High V<sub>z</sub> UNIVERSITET



Oscillations from MF or YSR?



# Clean MF and YSR States at TPT

### At TPT, well-behaved states $\rightarrow$ Basis states





# Basis Decomposition

#### Using states at TPT as a basis:











Topological boundary mode =  $MF \sim first$  peak in lowest state

Localization increases with  $V_z$  (opposite to SC coherence length)



Lowest energy state = MF (topo. boundary mode) + YSRs

- Energy and amplitude oscillations due to YSR contributions
- MF ~ first peak in lowest state
- Enhanced effects by self-consistent treatment of superconductivity





# **Nanowire SNS Junctions**

### When do false MFs appear and how to detect them?





# UPPSALA Are zero-Energy states MFs?

Interfaces/edges/impurities often host trivial zero-energy Andreev bound states (ABS)

## How to distinguish MFs?

- Stable zero-energy peak
- Quantized conductance
- Bulk gap closing



B (T)

Zhang et al., arXiv:2101.11456, see also Prada et al., Nat. Rev. Phys. 2, 575 (2020)





Awoga, Cayao, and ABS, PRL 123, 117001 (2019), see also Reeg et al. PRB 97, 165425 (2018)









# Phase Dependent Spectrum





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#### $\pi$ -Shifted Supercurrent UNIVERSITET



### False MFs $\leftarrow \rightarrow \pi$ -shifted supercurrent



# Nanowire SNS junctions



- False MFs common in short junctions
  - Due to spontaneous QD formation
  - Distinguishable by  $\pi$ -shifted supercurrent





# **Topological Superconductivity**

Spinless superconductors

- Majorana fermions
- Engineered systems

Prototype: Kitaev model for 1D spinless SC Materials: SOC + magnetism + *s*-wave SC Majorana fermion:

- Non-local, "<sup>1</sup>/<sub>2</sub> electron"
- Topological boundary state in spinless SCs
- Topological quantum computation



- Introduction to superconductivity
  - BCS, BdG, group theory
- Topological superconductivity
  - Chiral superconductors: p+ip' and d+id' superconductors
    - Appears often in 2D irreps
    - Topology set by Chern/winding number of order parameter
    - Chiral edge states
  - "Spinless" superconductors  $\rightarrow$  Majorana fermions
    - SOC + magnetism + *s*-wave superconductivity
    - Topological edge state = Majorana fermion ~ non-local "1/2 electron"



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