

# Symmetry and topology of noncentrosymmetric superconductors

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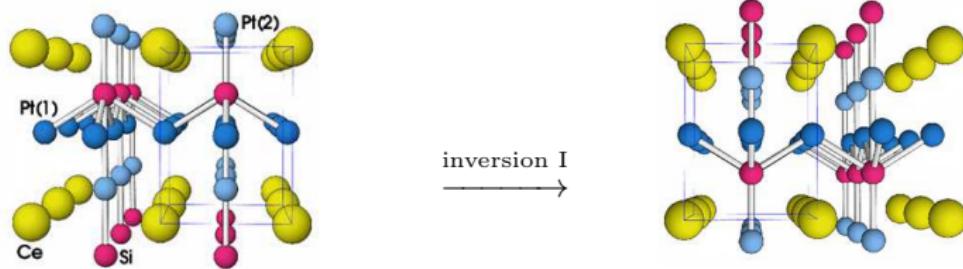
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- ▶ Electron-lattice spin-orbit coupling
- ▶ Topology in normal state
- ▶ Cooper pairing in nondegenerate bands
- ▶ Unusual nonuniform states (helical states, phase solitons, etc)
- ▶ Topology in superconducting state and Andreev boundary modes

# 3D noncentrosymmetric superconductors

<b>O</b>	Li <sub>2</sub> Pt <sub>3</sub> B (2K), Li <sub>2</sub> Pd <sub>3</sub> B (8K), Mo <sub>3</sub> Al <sub>2</sub> C (10K)
<b>T<sub>d</sub></b>	Ti <sub>5</sub> Re <sub>24</sub> (6.6K), Y <sub>2</sub> C <sub>3</sub> (17K), TLa <sub>3</sub> S <sub>4</sub> (8K)
<b>T</b>	LaRhSi (4K), LaIrSi (2K)
<b>C<sub>4v</sub></b>	<b>CePt<sub>3</sub>Si (0.5K)</b> , CeRhSi <sub>3</sub> (1K), CeIrSi <sub>3</sub> (1.5K)
<b>C<sub>4</sub></b>	La <sub>5</sub> B <sub>2</sub> C <sub>6</sub> (7K)
<b>C<sub>6v</sub></b>	MoN (15K), GaN (6K)
<b>D<sub>3h</sub></b>	MoC (9K), NbSe (6K), ZrPuP (13K)
<b>C<sub>3v</sub></b>	MoS <sub>2</sub> (1K)
<b>C<sub>2</sub></b>	Ui <sub>r</sub> (0.1K)



(from E. Bauer *et al*, PRL 92, 027003 (2004))

# 2D noncentrosymmetric superconductors

Insulator/insulator interface:

$\text{LaAlO}_3/\text{SrTiO}_3$  (LAO/STO)

$\text{LaTiO}_3/\text{SrTiO}_3$  (LTO/STO)

Metal/insulator interface:

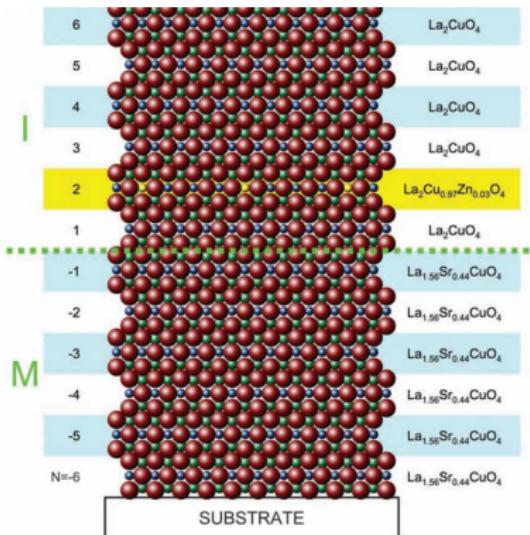
LSCO/LCO

Doped insulator surface:

$\text{STO}$ ,  $\text{WO}_3$

Typically:  $T_c < 1\text{K}$

FeSe single layers on doped STO substrate:  $T_c=109\text{K}$



(from J. Pereiro *et al*, Phys. Express **1**, 208 (2011))

# Electron bands

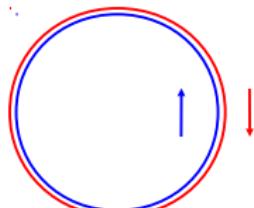
No inversion + SO coupling → nondegenerate, topologically nontrivial bands

Time-reversal  $K$  ( $K = i\hat{\sigma}_2 K_0$ )

and inversion  $I$ :

$|\mathbf{k}\rangle, KI|\mathbf{k}\rangle$  belong to  $\mathbf{k}$

$K|\mathbf{k}\rangle, I|\mathbf{k}\rangle$  belong to  $-\mathbf{k}$

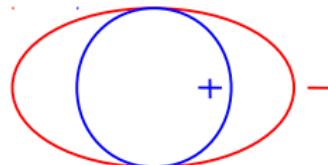


bands twofold degenerate at all  $\mathbf{k}$

Time-reversal  $K$ , no inversion:

$|\mathbf{k}\rangle$  belongs to  $\mathbf{k}$

$K|\mathbf{k}\rangle$  belongs to  $-\mathbf{k}$



bands nondegenerate at (almost) all  $\mathbf{k}$

# Spin-orbit coupling

Electron-lattice SO coupling:  $H_0 = \frac{\hat{\mathbf{p}}^2}{2m} + U(\mathbf{r}) + \frac{\hbar}{4m^2c^2} \hat{\boldsymbol{\sigma}} [\nabla U(\mathbf{r}) \times \hat{\mathbf{p}}]$

Noninteracting electrons:

$$\hat{H}_0 = \sum_{\mathbf{k}, \mu\nu} \sum_{\alpha, \beta = \uparrow, \downarrow} [\underbrace{\epsilon_\mu(\mathbf{k}) \delta_{\mu\nu} \delta_{\alpha\beta}}_{I-\text{symmetric}} + \underbrace{i A_{\mu\nu}(\mathbf{k}) \delta_{\alpha\beta} + \mathbf{B}_{\mu\nu}(\mathbf{k}) \boldsymbol{\sigma}_{\alpha\beta}}_{I-\text{asymmetric}}] \hat{a}_{\mathbf{k}\mu\alpha}^\dagger \hat{a}_{\mathbf{k}\nu\beta}$$

pseudospin 

$$A_{\mu\nu}(\mathbf{k}) = -A_{\nu\mu}(\mathbf{k}) = -A_{\mu\nu}(-\mathbf{k})$$

$$\mathbf{B}_{\mu\nu}(-\mathbf{k}) = \mathbf{B}_{\nu\mu}(\mathbf{k}) = -\mathbf{B}_{\mu\nu}(\mathbf{k})$$

+ additional constraints due to point-group symmetry

If  $\mathbf{B}_{\mu\nu}(\mathbf{k}) \neq 0 \Rightarrow$  nondegenerate Bloch bands  $\xi_n(\mathbf{k}) = \xi_n(-\mathbf{k})$

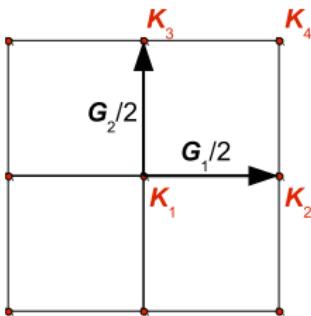
# Spin-orbit coupling

TR invariant points:  $-\mathbf{K} = \mathbf{K} + \mathbf{G}$

2D square lattice (spacing =  $d$ )

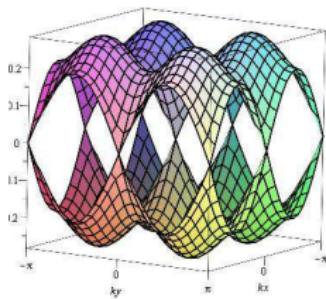
$$\{\mathbf{K}_i\} = \left\{ \mathbf{0}, \frac{\mathbf{G}_1}{2}, \frac{\mathbf{G}_2}{2}, \frac{\mathbf{G}_1 + \mathbf{G}_2}{2} \right\}$$

$$\mathbf{G}_1 = \frac{2\pi}{d} \hat{x}, \quad \mathbf{G}_2 = \frac{2\pi}{d} \hat{y}$$



$$\mathbf{B}_{\mu\nu}(\mathbf{K}) = -\mathbf{B}_{\mu\nu}(-\mathbf{K}) = -\mathbf{B}_{\mu\nu}(\mathbf{K} + \mathbf{G}) = -\mathbf{B}_{\mu\nu}(\mathbf{K}) = 0, \quad \mathbf{A}_{\mu\nu}(\mathbf{K}) = 0$$

Bloch bands  $\xi_n(\mathbf{k})$  remain pairwise degenerate at the TRI points



# Minimal model of SO coupling

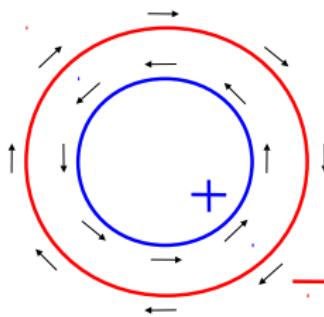
Generalized Rashba model:  $\hat{H}_0 = \sum_{\mathbf{k}, \alpha\beta=\uparrow,\downarrow} [\epsilon_0(\mathbf{k})\delta_{\alpha\beta} + \gamma(\mathbf{k})\sigma_{\alpha\beta}] \hat{a}_{\mathbf{k}\alpha}^\dagger \hat{a}_{\mathbf{k}\beta}$

antisymmetric SO coupling,  $B_{00}(\mathbf{k}) \equiv \gamma(\mathbf{k}) = -\gamma(-\mathbf{k})$

Two Bloch bands:  $\xi_\lambda(\mathbf{k}) = \epsilon(\mathbf{k}) + \lambda|\gamma(\mathbf{k})|$  (band index  $\lambda = \pm$  – helicity)

The original Rashba model:

$$\gamma(\mathbf{k}) = a(k_y \hat{x} - k_x \hat{y})$$
$$\xi_\lambda(\mathbf{k}) = \epsilon(\mathbf{k}) + |a| \sqrt{k_x^2 + k_y^2}$$



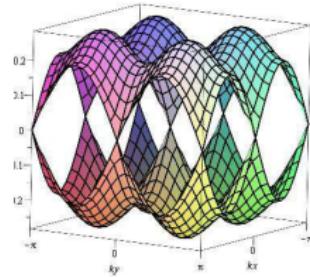
# Minimal model of SO coupling

At TRI points:  $\gamma(\mathbf{K}) = 0$

Isolated band degeneracies = Weyl points = Berry “monopoles”

Example: 2D square lattice with  $\gamma(\mathbf{k}) = \gamma_0(\hat{x} \sin k_y d - \hat{y} \sin k_x d)$

$$\{\mathbf{K}_i\} = \left\{ \mathbf{0}, \frac{\mathbf{G}_1}{2}, \frac{\mathbf{G}_2}{2}, \frac{\mathbf{G}_1 + \mathbf{G}_2}{2} \right\}$$
$$\mathbf{G}_1 = \frac{2\pi}{d}\hat{x}, \mathbf{G}_2 = \frac{2\pi}{d}\hat{y}$$



# Symmetry of the SO coupling

Point-group symmetry:  $g\gamma(g^{-1}\mathbf{k}) = \gamma(\mathbf{k})$  ( $g$  - lattice rotation or reflection)

## 21 point groups in 3D

**O**

$$\underline{\gamma_{3D}(\mathbf{k})}$$

$$a(k_x\hat{x} + k_y\hat{y} + k_z\hat{z})$$

**C<sub>4v</sub>**

$$\textcolor{red}{a_1(k_y\hat{x} - k_x\hat{y})} + ia_2(k_+^4 - k_-^4)k_z\hat{z}$$

**T<sub>d</sub>**

$$a[k_x(k_y^2 - k_z^2)\hat{x} + k_y(k_z^2 - k_x^2)\hat{y} + k_z(k_x^2 - k_y^2)\hat{z}]$$

...

...

## 10 point groups in 2D

**C<sub>1</sub>**

$$\underline{\gamma_{2D}(\mathbf{k})}$$

$$(a_1k_x + a_2k_y)\hat{x} + (a_3k_x + a_4k_y)\hat{y} + (a_5k_x + a_6k_y)\hat{z}$$

**C<sub>2</sub>**

$$(a_1k_x + a_2k_y)\hat{x} + (a_3k_x + a_4k_y)\hat{y}$$

**C<sub>3</sub>**

$$(a_1k_x + a_2k_y)\hat{x} + (-a_2k_x + a_1k_y)\hat{y} + (bk_+^3 + b^*k_-^3)\hat{z}$$

**C<sub>4</sub>**

$$(a_1k_x + a_2k_y)\hat{x} + (-a_2k_x + a_1k_y)\hat{y}$$

**C<sub>6</sub>**

$$(a_1k_x + a_2k_y)\hat{x} + (-a_2k_x + a_1k_y)\hat{y}$$

**D<sub>1</sub>**

$$a_1k_y\hat{x} + a_2k_x\hat{y} + a_3k_x\hat{z}$$

**D<sub>2</sub>**

$$a_1k_y\hat{x} + a_2k_x\hat{y}$$

**D<sub>3</sub>**

$$a_1(k_y\hat{x} - k_x\hat{y}) + a_2(k_+^3 + k_-^3)\hat{z}$$

**D<sub>4</sub>**

$$\textcolor{red}{a(k_y\hat{x} - k_x\hat{y})}$$

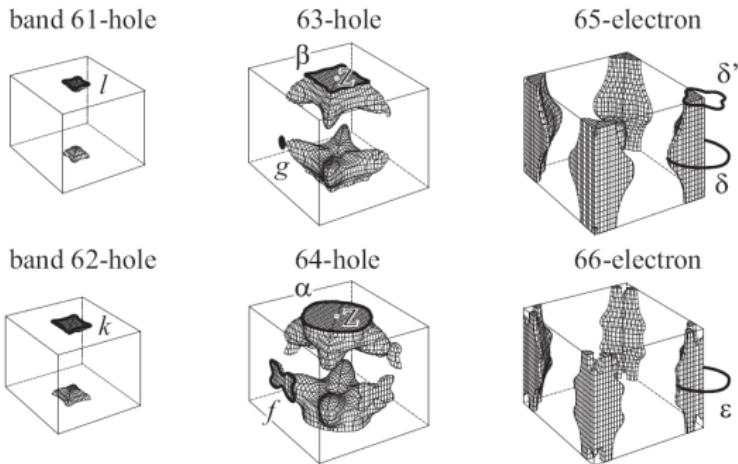
**D<sub>6</sub>**

$$a(k_y\hat{x} - k_x\hat{y})$$

← oxide interface SC

# Electron band structure

Band structure of  
 $\text{CePt}_3\text{Si}$ :



SO band splitting:

- $\text{CePt}_3\text{Si}: E_{\text{SO}} \simeq 200 \text{ meV}$   
 $\text{Li}_2\text{Pd}_3\text{B}: E_{\text{SO}} \simeq 30 \text{ meV}$   
 $\text{Li}_2\text{Pt}_3\text{B}: E_{\text{SO}} \simeq 200 \text{ meV}$   
 $\text{LAO/STO}: E_{\text{SO}} \simeq 1..10 \text{ meV}$

$E_{\text{SO}} \gg \text{SC energy scales}$

# Bloch band topology in 3D

Berry curvature of the Bloch wave functions:

$$\mathcal{F}_{n,ij}(\mathbf{k}) = i \left( \frac{\partial \langle \mathbf{k}, n |}{\partial k_i} \frac{\partial |\mathbf{k}, n \rangle}{\partial k_j} - \frac{\partial \langle \mathbf{k}, n |}{\partial k_j} \frac{\partial |\mathbf{k}, n \rangle}{\partial k_i} \right) = e_{ijk} \underbrace{\mathcal{B}_{n,k}(\mathbf{k})}_{\text{Berry field}}$$

First Chern number of the FS:  $\text{Ch}_n = \frac{1}{2\pi} \int_{FS_n} \mathcal{B}_n(\mathbf{k}) \cdot d\mathbf{S} = \text{Berry flux}$

Example: in the two-band model  $\mathcal{B}_{\lambda,k} = -\frac{\lambda}{4} e_{ijk} \hat{\gamma} \left( \frac{\partial \hat{\gamma}}{\partial k_i} \times \frac{\partial \hat{\gamma}}{\partial k_j} \right)$

Isolated TRI point  $\mathbf{K}_i$  = Berry monopole:  $\nabla_{\mathbf{k}} \mathcal{B}_{\lambda} = 4\pi q_{\lambda} \delta^3(\mathbf{k} - \mathbf{K}_i)$

$$q_{\lambda} = -\frac{1}{2} \int_{\sigma} e_{ijk} \hat{\gamma} \left( \frac{\partial \hat{\gamma}}{\partial k_i} \times \frac{\partial \hat{\gamma}}{\partial k_j} \right) \frac{dS_k}{8\pi} = -\frac{1}{2} \operatorname{sgn} \det \left| \left| \frac{\partial \gamma_l}{\partial k_m} \right| \right|_{\mathbf{k}=\mathbf{K}_i}$$

Fermi-surface Chern number =  $2 \times (\text{total monopole charge inside the FS})$

# Bloch band topology in 3D. Semiclassical electron dynamics

Modified Poisson brackets  
(quantum corrections  $\mathcal{O}(\hbar)$ )

$$\begin{aligned}\{r_i, r_j\} &= \hbar \mathcal{F}_{\lambda,ij} \\ \{r_i, P_j\} &= \delta_{ij} + \frac{\hbar e}{c} \sum_k \mathcal{F}_{\lambda,ik} F_{kj} \\ \{P_i, P_j\} &= -\frac{e}{c} F_{ij} - \hbar \left(\frac{e}{c}\right)^2 \sum_{kl} F_{ik} \mathcal{F}_{\lambda,kl} F_{lj}\end{aligned}$$

Classical band Hamiltonian:

$$\mathcal{H}_\lambda(\mathbf{r}, \mathbf{P}) = \varepsilon(\mathbf{P}) + \lambda |\mathbf{g}(\mathbf{P})| - e\phi(\mathbf{r}) - \mathbf{m}_\lambda(\mathbf{P}) \cdot \mathbf{B}$$

Magnetic moment:  $\mathbf{m}_\lambda(\mathbf{P}) = -\lambda \mu_m \hat{\mathbf{g}}(\mathbf{P}) + \lambda \underbrace{\frac{\hbar e}{c} |\mathbf{g}(\mathbf{P})| \mathcal{B}_\lambda(\mathbf{P})}_{\mathcal{O}(E_{SO}/\epsilon_F)}$

Semiclassical equations of motion:

$$\frac{d\mathbf{r}}{dt} = \frac{\partial \mathcal{H}_\lambda}{\partial \mathbf{P}} - \underbrace{\hbar \frac{d\mathbf{P}}{dt} \times \mathcal{B}_\lambda(\mathbf{P})}_{\text{anomalous velocity}}, \quad \frac{d\mathbf{P}}{dt} = -e\mathbf{E}(\mathbf{r}) - \frac{e}{c} \frac{d\mathbf{r}}{dt} \times \mathbf{B}(\mathbf{r})$$

Semiclassical orbit  $\Gamma_\lambda(\epsilon, P_B)$ :

intersection of  $\varepsilon(\mathbf{P}) + \lambda|\mathbf{g}(\mathbf{P})| = \epsilon$  with  $\frac{\mathbf{P} \cdot \mathbf{B}}{B} = P_B$

Lifshitz-Onsager quantization condition:

area of the orbit  $S_\lambda(\epsilon, P_B) = \frac{2\pi e H}{\hbar c} \left( n + \frac{1}{2} - \frac{\Phi_\lambda^m + \Phi_\lambda^B}{2\pi} \right)$

corrections due to  
the “Zeeman” deformation of  $\Gamma_\lambda$   
and the Berry phase around  $\Gamma_\lambda$

dHvA frequencies  $F_\lambda = \frac{\hbar c}{2\pi e} S_\lambda^{ext}$  are changed by the quantum corrections

# Bloch band topology in 2D: $Z_2$ invariant

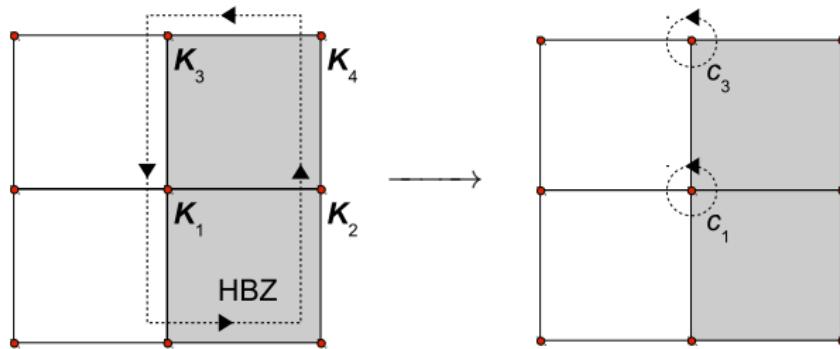
Time-reversed Bloch states:

$$K|\mathbf{k}, n\rangle = t_n(\mathbf{k})|-\mathbf{k}, n\rangle$$
$$|t_n(\mathbf{k})| = 1, \quad t_n(\mathbf{k}) = -t_n(-\mathbf{k})$$

Maps  $\mathbf{k} \rightarrow t_n(\mathbf{k})$  are classified by the topological invariant

$$D_n = -\frac{1}{2\pi} \left[ \oint_{\partial(\text{HBZ})} \alpha_n \right] \text{ mod } 2, \quad \alpha_n = -id \ln t_n$$

invariant under  $|\mathbf{k}, n\rangle \rightarrow e^{i\theta_n(\mathbf{k})} |\mathbf{k}, n\rangle$ ,  $\alpha_n(\mathbf{k}) \rightarrow \alpha_n(\mathbf{k}) - d[\theta_n(\mathbf{k}) + \theta_n(-\mathbf{k})]$



## Bloch band topology in 2D: $Z_2$ invariant

Focus on the TRI points:  $D_n = -\frac{1}{2\pi} \left( \sum_{i=1}^{N_{\text{TRI}}/2} \oint_{c_i} \alpha_n \right) \bmod 2$

The band structure near  $\mathbf{K}_i$  is described by the generalized Rashba model:  
 $\hat{\gamma} = \gamma/|\gamma| = (\sin \alpha \cos \beta, \sin \alpha \sin \beta, \cos \alpha) \Rightarrow t_\lambda(\mathbf{k}) = \lambda e^{-i\beta(\mathbf{k})}$

$$D_n = \left[ \sum_{i=1}^{N_{\text{TRI}}/2} N_\beta(\mathbf{K}_i) \right] \bmod 2$$

Winding number:  $N_\beta(\mathbf{K}_i) = \frac{1}{2\pi} \oint_{c_i} d\beta = \pm 1$

even  $N_{\text{TRI}}/2 \Rightarrow D_n = 0$  (square lattice, point group  $\mathbf{D}_4$ )

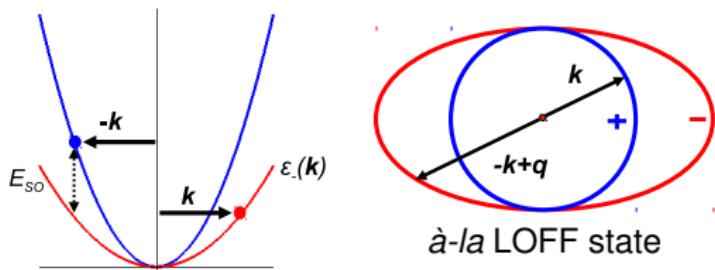
odd  $N_{\text{TRI}}/2 \Rightarrow D_n = 1$  (hexagonal lattice, point group  $\mathbf{D}_6$ )

# Superconducting pairing in nondegenerate bands

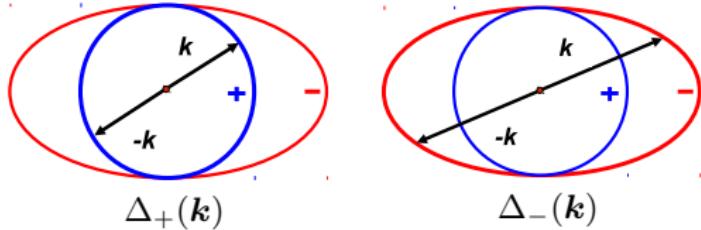
In real noncentrosymmetric SCs:

$$T_c \ll \varepsilon_c \ll E_{SO}, \epsilon_F$$

interband pairing  
is suppressed



only intraband  
pairing survives



# Superconducting pairing in nondegenerate bands

Cooper pairing of the time-reversed states in the same band:

$$\hat{H}_{int} = \frac{1}{2\mathcal{V}} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \sum_{nn'} V_{nn'}(\mathbf{k}, \mathbf{k}') \hat{c}_{\mathbf{k}+\mathbf{q}, n}^\dagger \hat{c}_{\mathbf{k}, n}^\dagger \hat{c}_{\mathbf{k}', n'} \hat{c}_{\mathbf{k}'+\mathbf{q}, n'}$$

$$\hat{c}_{\mathbf{k}, n}^\dagger = K \hat{c}_{\mathbf{k}, n}^\dagger K^{-1} = t_n(\mathbf{k}) \hat{c}_{-\mathbf{k}, n}^\dagger, \quad t_n(\mathbf{k}) = -t_n(-\mathbf{k})$$

Mean field ( $M$  = # of nondegenerate bands crossing the Fermi level):

$$\hat{H}_{MF} = \sum_{\mathbf{k} \in \text{HBZ}} \sum_{n=1}^M \left[ \Delta_n(\mathbf{k}) \hat{c}_{\mathbf{k}, n}^\dagger \hat{c}_{\mathbf{k}, n} + \Delta_n^*(\mathbf{k}) \hat{c}_{\mathbf{k}, n} \hat{c}_{\mathbf{k}, n}^\dagger \right]$$

Gap functions are even:  $\Delta_n(\mathbf{k}) = \Delta_n(-\mathbf{k})$

# Superconducting pairing in nondegenerate bands

Symmetry properties:  $K : \Delta_n(\mathbf{k}) \rightarrow \Delta_n^*(\mathbf{k})$

$g \in \mathbb{G} : \Delta_n(\mathbf{k}) \rightarrow \Delta_n(g^{-1}\mathbf{k})$

Basis-function expansion:  $\Delta_n(\mathbf{k}) = \sum_{a=1}^{d_\Gamma} \eta_{n,a} \phi_a(\mathbf{k}), \quad \phi_a(\mathbf{k}) = \phi_a(-\mathbf{k})$

*Md<sub>Γ</sub> order parameter components*

Example:  $\mathbb{G}_{2D} = \mathbf{D}_4$  (e.g. oxide interfaces)

$\Gamma$	$d_\Gamma$	$\phi_\Gamma(\mathbf{k}) = \phi_\Gamma(-\mathbf{k})$
$A_1$	1	1
$A_2$	1	$k_x k_y (k_x^2 - k_y^2)$
$B_1$	1	$k_x^2 - k_y^2$
$B_2$	1	$k_x k_y$
$E$	2	—

# Superconducting pairing in two-band model

Band representation:  $\Delta_+(\mathbf{k}) = \Delta_+(-\mathbf{k}), \quad \Delta_- (\mathbf{k}) = \Delta_- (-\mathbf{k})$

Spin representation:

$$\hat{\Delta}_{\alpha\beta} = \Delta_s(\mathbf{k})(i\hat{\sigma}_2)_{\alpha\beta} + \underbrace{\Delta_t(\mathbf{k})\hat{\gamma}(\mathbf{k})}_{d(\mathbf{k})=-d(-\mathbf{k})}(i\hat{\sigma}\hat{\sigma}_2)_{\alpha\beta} \quad \text{singlet-triplet mixing}$$

$$\Delta_s(\mathbf{k}) = \frac{\Delta_+(\mathbf{k}) + \Delta_-(\mathbf{k})}{2}, \quad \Delta_t(\mathbf{k}) = \frac{\Delta_+(\mathbf{k}) - \Delta_-(\mathbf{k})}{2}$$

Spin representation:

- ▶ does not fit into the conceptual frameworks of the Fermi-liquid and BCS theories
- ▶ more complicated technically (awkward phase factors in the gap functions, etc)

# Novel features in superconducting state

This talk:

- ▶ Unusual nonuniform states: helical, phase solitons, zero-field instabilities
- ▶ Topological invariants and boundary modes

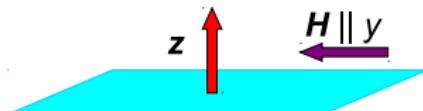
Not today:

- ▶ Magnetoelectric effect
- ▶ Unusual impurity effects on  $T_c$  and spin susceptibility
- ▶ Non-Helfand-Werthamer behaviour of  $H_{c2}$
- ▶ ...

# Ginzburg-Landau free energy

Simplest case: 1D IREP, two bands:  $n = \lambda = \pm \Rightarrow$  two OPs  $\eta_+(\mathbf{r}), \eta_-(\mathbf{r})$

2D SC  
in a parallel field



GL free energy density:  $F = F_+ + F_- + F_m$

Intraband:

$$F_\lambda = \alpha_\lambda |\eta_\lambda|^2 + \beta_\lambda |\eta_\lambda|^4 + K_\lambda |\nabla \eta_\lambda|^2 + \underbrace{\tilde{K}_\lambda \operatorname{Im} [\eta_\lambda^* (\mathbf{H} \times \nabla)_z \eta_\lambda]}_{\text{Lifshitz invariant}} + L_\lambda H^2 |\eta_\lambda|^2$$

$$K_\lambda \sim \frac{N_{F,\lambda}}{T_{c0}^2} v_{F,\lambda}^2, \quad \tilde{K}_\lambda \sim \frac{N_{F,\lambda}}{T_{c0}^2} \mu_B v_{F,\lambda}, \quad L_\lambda \sim \frac{N_{F,\lambda}}{T_{c0}^2} \mu_B^2$$

Interband (“Josephson”) pair tunneling:  $F_m = \gamma_m (\eta_+^* \eta_- + \eta_-^* \eta_+)$

Lifshitz invariants  $\Rightarrow$  unusual nonuniform SC states

## Low fields: helical state

Helical state = weak-field counterpart of the FF state

$$\eta_\lambda(\mathbf{r}) = \eta_\lambda e^{iqx}$$

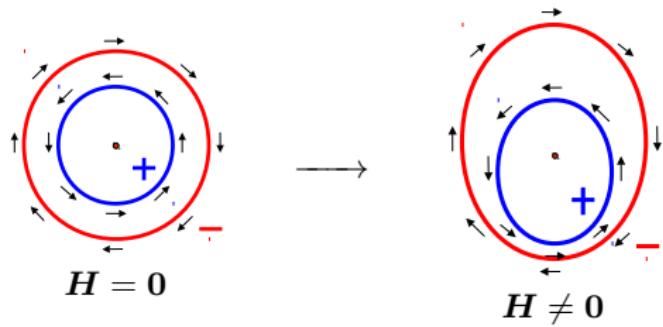
$$q = C_1 H, \quad T_c(H) = T_{c0} - C_2 H^2$$

$$C_{1,2} = C_{1,2}(\alpha_\pm, K_\pm, \tilde{K}_\pm, L_\pm)$$

No supercurrent in the helical state:  $j_x = -\frac{c}{\mathcal{V}} \frac{\partial \mathcal{F}}{\partial A_x} = \frac{2e}{\mathcal{V}} \frac{\partial \mathcal{F}}{\partial q} = 0$

Origin of the helical instability: FS displacement and deformation by  $\mathbf{H}$

$$\xi_\lambda(\mathbf{k}) \rightarrow \Xi_\lambda(\mathbf{k}) = \xi_\lambda(\mathbf{k}) - \lambda \mu_B \hat{\gamma}(\mathbf{k}) \mathbf{H}, \quad \Xi_\lambda(\mathbf{k}) \neq \Xi_\lambda(-\mathbf{k})$$



## Low fields: helical state

How to probe the helical state  $\eta_\lambda(\mathbf{r}) = \eta_\lambda e^{i\mathbf{q}\cdot\mathbf{r}}$  by tunneling:

BdG Hamiltonian can be made  $\mathbf{k}$ -diagonal by a unitary transformation

$$H_\lambda(\mathbf{k}, \mathbf{k}') = \delta_{\mathbf{k}, \mathbf{k}'} \begin{pmatrix} \xi_\lambda(\mathbf{k}) + \Omega_\lambda(\mathbf{k}) & \eta_\lambda \\ \eta_\lambda^* & -\xi_\lambda(\mathbf{k}) + \Omega_\lambda(\mathbf{k}) \end{pmatrix}$$
$$\Omega_\lambda(\mathbf{k}) = \underbrace{\frac{1}{2} \mathbf{v}_\lambda(\mathbf{k}) \mathbf{q}}_{\text{helical}} - \underbrace{\lambda \mu_B \hat{\boldsymbol{\gamma}}(\mathbf{k}) \mathbf{H}}_{\text{Zeeman}}$$

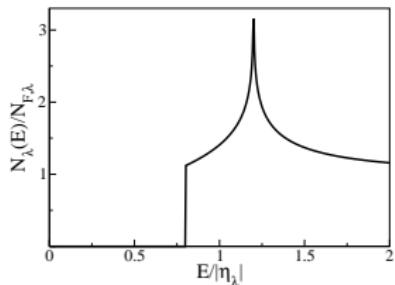
Quasiparticle DoS:

$$N_\lambda(E) = N_{F,\lambda} \left\langle \frac{|E - \Omega_\lambda(\mathbf{k})|}{\sqrt{[E - \Omega_\lambda(\mathbf{k})]^2 - |\eta_\lambda|^2}} \right\rangle_{FS_\lambda}$$

## Low fields: helical state

For a circular Fermi surface & Rashba SO coupling  $\gamma(\mathbf{k}) = \gamma_0(k_y, -k_x)$ :

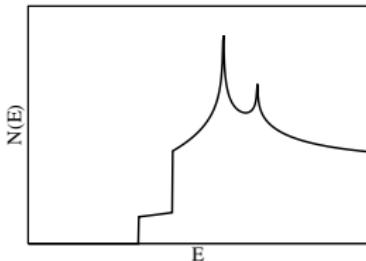
$$N_\lambda(E) = N_{F,\lambda} I\left(\frac{E}{|\eta_\lambda|}, \frac{\mu_\lambda H}{|\eta_\lambda|}\right)$$
$$I(x, y) = \int_0^{2\pi} \frac{d\phi}{2\pi} \frac{|x - y \cos \phi|}{\sqrt{(x - y \cos \phi)^2 - 1}}$$



Field-dependent gap edge:  $\Delta_\lambda(H) = |\eta_\lambda| - \mu_\lambda H$

DoS singularity:

$$\frac{N_\lambda(E)}{N_{F,\lambda}} = \frac{1}{2\pi} \sqrt{\frac{|\eta_\lambda|}{\mu_\lambda H}} \ln \frac{\mu_\lambda H}{|E - (|\eta_\lambda| + \mu_\lambda H)|}$$



Total DoS

$$N(E) = N_+(E) + N_-(E)$$

## High fields: phase soliton lattice

London approximation:  $\eta_\lambda(\mathbf{r}) = |\eta_\lambda| e^{i\varphi_\lambda(x)}$

Supercurrent:  $j_x = -4e \sum_\lambda K_\lambda |\eta_\lambda|^2 \nabla_x \varphi_\lambda + 2eH \sum_\lambda \tilde{K}_\lambda |\eta_\lambda|^2 = 0$

current conservation + boundary conditions

$$\nabla_x \varphi_+ = \frac{1}{1+\rho} \nabla_x \theta + q, \quad \nabla_x \varphi_- = -\frac{\rho}{1+\rho} \nabla_x \theta + q$$

$$\theta = \varphi_+ - \varphi_- \quad - \text{ relative phase,} \quad \rho = \frac{K_+ |\eta_+|^2}{K_- |\eta_-|^2}, \quad q = \frac{H}{2} \frac{\sum_\lambda \tilde{K}_\lambda |\eta_\lambda|^2}{\sum_\lambda K_\lambda |\eta_\lambda|^2}$$

$\varphi_+$  and  $\varphi_-$  are locked ( $\theta = 0$  or  $\pi$ )  $\Rightarrow$  **helical state**

$\nabla_x \theta \neq 0 \Rightarrow$  **phase soliton state**

# High fields: phase soliton lattice

London free energy density:  $f = (\dots) + \frac{1}{2}(\nabla_x \theta)^2 + V_0(1 - \cos \theta) - \underbrace{h(\nabla_x \theta)}_{\text{bias}}$

$$h = \frac{H}{2} \left( \frac{\tilde{K}_+}{K_+} - \frac{\tilde{K}_-}{K_-} \right), \quad V_0 \propto |\gamma_m|$$

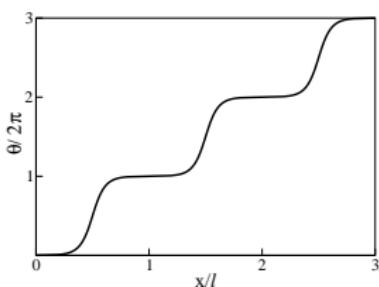
Sine-Gordon equation

$$\nabla_x^2 \theta - V_0 \sin \theta = 0$$

single soliton ( $\gamma_m < 0$ ):  
 $\theta(x) = \pi + 2 \arcsin \tanh(x/\xi_s)$   
 $\xi_s = 1/\sqrt{V_0}$ , energy =  $\epsilon_1$

At low soliton density  $n_s$ :  $F_{\text{solitons}} - F_{\text{no solitons}} = (\epsilon_1 - 2\pi h)n_s + \dots$

**Soliton lattice**  
at  $h > h_s = \epsilon_1/2\pi$   
lattice spacing  
 $\simeq 2\xi_s \ln H_s / (H - H_s)$



# Zero-field nonuniform superconducting states

Lifshitz gradient terms are possible even at  $\mathbf{H} = \mathbf{0}$ !

GL energy for a tetragonal SC, two bands (Rashba), point group  $\mathbf{C}_{4v}$ :  
 $F = F_+ + F_- + F_m + \textcolor{red}{F_L}$

Additional Lifshitz invariant:  $F_L = K_L \operatorname{Re}(\eta_+^* \nabla_z \eta_- - \eta_-^* \nabla_z \eta_+)$

Nonuniform instability:  $\eta_\lambda = \eta_{\lambda,0} e^{iqz}$  if  $K_L > K_{L,c}$

Semi-microscopic derivation:

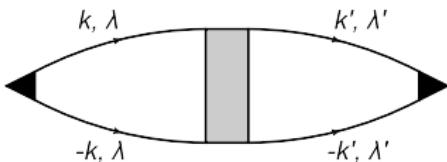
$$\hat{H}_{int} = \frac{1}{2\mathcal{V}} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \sum_{nn'} V_{nn'}(\mathbf{k}, \mathbf{k}'; \mathbf{q}) \hat{c}_{\mathbf{k}+\mathbf{q}, n}^\dagger \hat{\tilde{c}}_{\mathbf{k}, n}^\dagger \hat{\tilde{c}}_{\mathbf{k}', n'} \hat{c}_{\mathbf{k}'+\mathbf{q}, n'}$$

Expand in powers of  $\mathbf{q}$ :  $V_{\lambda\lambda'}(\mathbf{k}, \mathbf{k}'; \mathbf{q}) = v_{\lambda\lambda'}(\mathbf{k}, \mathbf{k}') + \textcolor{red}{i\mathbf{b}_{\lambda\lambda'}(\mathbf{k}, \mathbf{k}')\mathbf{q}} + \mathcal{O}(q^2)$

↑  
treat as a perturbation

# Zero-field nonuniform superconducting states

Correction to the free energy =



Magnitude of the Lifshitz term:  $K_L = \frac{1}{2} N_+ N_- \ln^2 \left( \frac{2e^{\mathbb{C}} \epsilon_c}{\pi T_c} \right) |\beta|$

$\beta = \langle b_{+-}(\hat{k}, \hat{k}') \rangle_{\hat{k}, \hat{k}'}$  – invariant polar vector (for  $C_{4v}$ :  $\beta \parallel \hat{z}$ )

$\beta \neq 0$  in **pyroelectric crystals**:

for  $G = C_1, C_s, C_2, C_{2v}, C_4, C_{4v}, C_3, C_{3v}, C_6, C_{6v}$

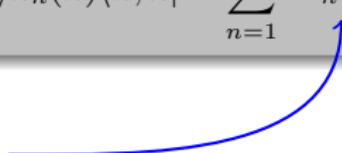
# Bogoliubov-de Gennes Hamiltonian

Spectrum of fermionic excitations = eigenvalues of the BdG Hamiltonian:

$$\mathcal{H}_{BdG}(\mathbf{k}) = \sum_{n=1}^M |\mathbf{k}, n\rangle \hat{h}_n(\mathbf{k}) \langle \mathbf{k}, n| = \sum_{n=1}^M \hat{\Pi}_n(\mathbf{k}) \otimes \hat{h}_n(\mathbf{k})$$

Bloch band projector

$$\hat{\Pi}_n(\mathbf{k}) = |\mathbf{k}, n\rangle \langle \mathbf{k}, n|$$



$$\hat{h}_n(\mathbf{k}) = \begin{pmatrix} \xi_n(\mathbf{k}) & \Delta_n(\mathbf{k}) \\ \Delta_n^*(\mathbf{k}) & -\xi_n(\mathbf{k}) \end{pmatrix} = \boldsymbol{\nu}_n(\mathbf{k}) \hat{\tau}, \quad \boldsymbol{\nu}_n(\mathbf{k}) = \begin{pmatrix} \text{Re}\Delta_n(\mathbf{k}) \\ -\text{Im}\Delta_n(\mathbf{k}) \\ \xi_n(\mathbf{k}) \end{pmatrix}$$

Electron-hole symmetry:  $\hat{\tau}_2 \hat{h}_n(\mathbf{k}) \hat{\tau}_2 = -\hat{h}_n^*(\mathbf{k}) \Rightarrow$  eigenvalues  $= \pm E_n(\mathbf{k})$

Bogoliubov excitation energy:  $E_n(\mathbf{k}) = \sqrt{\xi_n^2(\mathbf{k}) + |\Delta_n(\mathbf{k})|^2} \geq 0$

# Topology in 3D. TR breaking states

How to characterize topological classes of bulk SC states?

Consider the map of 3D BZ:  $\mathbf{k} \rightarrow \mathcal{H}_{BdG}(\mathbf{k}) = \sum_{n=1}^M \hat{\Pi}_n(\mathbf{k}) \otimes \boldsymbol{\nu}_n(\mathbf{k}) \hat{\tau}$

Maurer-Cartan 1-form:  $\omega = \mathcal{H}_{BdG}^{-1} d\mathcal{H}_{BdG}$  –  $2M \times 2M$  matrix

Topological invariant:  $\mathcal{N}_3 = \frac{1}{24\pi^2} \int_{BZ} \text{Tr } \omega^3$

$$\text{Tr } \omega^3 = d \left\{ 3 \sum_{m \neq n} \left[ \left( \frac{E_m}{E_n} - \frac{E_n}{E_m} \right) (\hat{\boldsymbol{\nu}}_m \hat{\boldsymbol{\nu}}_n) - 2 \ln \frac{E_m}{E_n} \right] \mathcal{A}_{mn} \mathcal{A}_{nm} \right\}$$

$\mathcal{A}_{mn}(\mathbf{k}) = i \langle \mathbf{k}, m | d | \mathbf{k}, n \rangle$  – Berry potential

$$\mathcal{N}_3 = 0$$

# Topology in 3D. TR invariant states

TR invariant superconducting state = real  $\Delta_n$

$$U\mathcal{H}_{BdG}U^\dagger = \sum_{n=1}^M E_n \hat{\Pi}_n^B \otimes \begin{pmatrix} 0 & e^{i\theta_n} \\ e^{-i\theta_n} & 0 \end{pmatrix}$$
$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}, \quad e^{i\theta_n} = \frac{\xi_n + i\Delta_n}{\sqrt{\xi_n^2 + \Delta_n^2}}$$

Consider the map of 3D BZ:  $\mathbf{k} \rightarrow \hat{q}(\mathbf{k}) = \sum_n E_n(\mathbf{k}) e^{i\theta_n(\mathbf{k})} \hat{\Pi}_n^B(\mathbf{k})$

Topological invariant:

$$\mathcal{N}_3^{\text{TRI}} = \frac{1}{24\pi^2} \int_{\text{BZ}} \text{tr} (\hat{q}^{-1} d\hat{q})^3 = -\frac{1}{4\pi^2} \sum_n \int_{\text{BZ}} \underbrace{(\mathbf{B}_n \cdot \nabla_{\mathbf{k}} \theta_n)}_{\neq 0 \text{ near FS}} d^3 \mathbf{k}$$

$B_n = d\mathcal{A}_{nn}$  – Berry field in the  $n$ th Bloch band

# Topology in 3D. TR invariant states

$$\mathcal{N}_3^{\text{TRI}} = \frac{1}{2} \sum_{n=1}^M \text{Ch}_n \operatorname{sgn} \Delta_n$$

depends on the Bloch band topology  
and SC properties

First Chern number = Berry flux through the Fermi surface

$$\text{Ch}_n = \frac{1}{2\pi} \int_{\text{FS}_n} \mathbf{B}_n(\mathbf{k}) \cdot d\mathbf{S}$$

Rashba SC, isolated band degeneracy (“Berry monopole”) at  $\mathbf{k} = \mathbf{K}$ :

$$\text{Ch}_\lambda = -\lambda \operatorname{sgn} \det \left| \left| \frac{\partial \gamma_i}{\partial k_j} \right| \right|_{\mathbf{k}=\mathbf{K}} = \pm 1$$

$$|\mathcal{N}_3^{\text{TRI}}| = \frac{1}{2} |\operatorname{sgn} \Delta_+ - \operatorname{sgn} \Delta_-|$$

Topologically trivial:  $\operatorname{sgn} \Delta_+ \operatorname{sgn} \Delta_- = 1$  (singlet channel dominates)

Topologically nontrivial:  $\operatorname{sgn} \Delta_+ \operatorname{sgn} \Delta_- = -1$  (triplet channel dominates)

# Topology in 2D. Winding numbers

Add one **extra dimension**:  $k_0$  – real “frequency”

Use the BdG Green's function:  $\mathcal{G}(\mathbf{k}, k_0) = [ik_0 - \mathcal{H}_{BdG}(\mathbf{k})]^{-1}$  to define

topological invariant:  $\mathcal{N}_{2+1} = \frac{1}{24\pi^2} \int_{BZ \times S^1} \text{Tr} (\mathcal{G} d\mathcal{G}^{-1})^3$

$$\mathcal{N}_{2+1} = -\frac{1}{8\pi} \sum_{n=1}^M \int_{BZ} \hat{\nu}_n (d\hat{\nu}_n \times d\hat{\nu}_n) \quad \leftarrow \text{only SC properties}$$

For a fully gapped superconducting state  $\Delta_n(\mathbf{k}) = \Delta_n(-\mathbf{k}) = |\Delta_n(\mathbf{k})| e^{i\varphi_n(\mathbf{k})}$

$$\mathcal{N}_{2+1} = -\sum_{n=1}^M N_n$$

$N_n = \frac{1}{2\pi} \oint_{FS_n} d\varphi_n$  – phase winding number  
 $N_n$  is **even!**

# Topology in 2D. Wilson loops

BdG eigenfunctions at given  $\mathbf{k}$ :

$$\mathcal{H}_{BdG}(\mathbf{k}) (|\mathbf{k}, n\rangle \otimes |\mathbf{k}, n; s\rangle) = s E_n(\mathbf{k}) (|\mathbf{k}, n\rangle \otimes |\mathbf{k}, n; s\rangle)$$

Bloch Berry potential:  $A_n(\mathbf{k}) = i\langle \mathbf{k}, n | d | \mathbf{k}, n \rangle = \mathcal{A}_{nn}(\mathbf{k})$

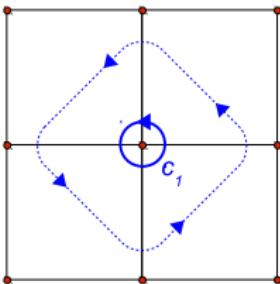
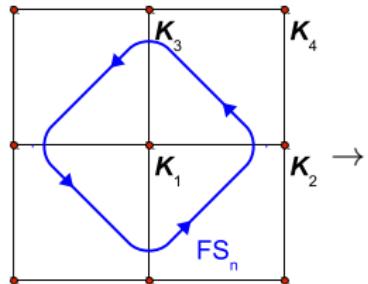
Nambu Berry potential:  $a_{n,s}(\mathbf{k}) = i\langle \mathbf{k}, n; s | d | \mathbf{k}, n; s \rangle$

Bloch Wilson loop:  $w_n^B = e^{i \oint_{FS_n} A_n}$

For the point groups containing “2D inversion”  $C_{2z}$  ( $\mathbb{G} = \mathbf{C}_{2,4,6}, \mathbf{D}_{2,4,6}$ ):

$\mathcal{B}_n(-\mathbf{k}) = -\mathcal{B}_n(\mathbf{k})$  (TR) and  $\mathcal{B}_n(-\mathbf{k}) = \mathcal{B}_n(\mathbf{k})$  ( $C_{2z}$ )  $\Rightarrow$

Berry field  $\mathcal{B}_n(\mathbf{k}) = 0$  everywhere, except the TRI points  $\mathbf{K}_i$



$$\oint_{FS_n} A_n = \sum'_{\mathbf{K}_i} \oint_{c_i} A_n$$

# Topology in 2D. Wilson loops

Near  $\mathbf{K}_i$  – use two-band model with  $\gamma = |\gamma|(\sin \alpha \cos \beta, \sin \alpha \sin \beta, \cos \alpha)$

$$A_\lambda = -\frac{1}{2}(1 - \lambda \cos \alpha)d\beta \quad \Rightarrow \quad \oint_{c_i} A_\lambda = -\pi N_\beta(\mathbf{K}_i)$$

$N_\beta(\mathbf{K}_i)$  = the index of the critical point  $\mathbf{K}_i$  of the vector field  $\gamma_{||} = (\gamma_x, \gamma_y, 0)$

$$N_\beta(\mathbf{K}_i) = \operatorname{sgn} \det \left\| \frac{\partial \gamma_{||,l}}{\partial k_m} \right\|_{\mathbf{k}=\mathbf{K}_i} = \pm 1$$

$$w_\lambda^B = (-1)^{\sum_i' N_\beta(\mathbf{K}_i)} = (-1)^{M_n} \quad Z_2 \text{ invariant}$$

$M_n$  = number of the TRI points enclosed by  $\text{FS}_n$

# Topology in 2D. Wilson loops

Nambu Wilson loop:  $w_{n,s}^N = e^{i \oint_{FS_n} a_{n,s}}$

$$\hat{h}_n(\mathbf{k}) = \boldsymbol{\nu}_n(\mathbf{k})\hat{\tau}, \quad \boldsymbol{\nu}_n(\mathbf{k}) = \begin{pmatrix} \text{Re}\Delta_n(\mathbf{k}) \\ -\text{Im}\Delta_n(\mathbf{k}) \\ \xi_n(\mathbf{k}) \end{pmatrix} = E_n(\mathbf{k}) \begin{pmatrix} \sin \tilde{\alpha}_n \cos \tilde{\beta}_n \\ \sin \tilde{\alpha}_n \sin \tilde{\beta}_n \\ \cos \tilde{\alpha}_n \end{pmatrix}$$

Nambu Berry connection:

$$a_{n,s} = -\frac{1}{2}(1 - s \cos \tilde{\alpha}_n)d\tilde{\beta}_n, \quad \oint_{FS_n} a_{n,s} = \underbrace{-\pi N_{\tilde{\beta}_n}}_{\text{for } \Delta_n = |\Delta_n|e^{i\varphi_n}} = \pi N_n$$

$w_{n,s}^N = (-1)^{N_n} = 1$

$Z_2$  invariant =  
parity of the phase winding number  $N_n$

# Bulk topology and boundary modes

Manifestation of nontrivial topology – **subgap fermionic boundary modes**

Andreev equations:  $\begin{pmatrix} -iv_{F,x}\nabla_x & \Delta(\mathbf{k}_F) \\ \Delta^*(\mathbf{k}_F) & iv_{F,x}\nabla_x \end{pmatrix} \psi_{\mathbf{k}_F} = E\psi_{\mathbf{k}_F}$

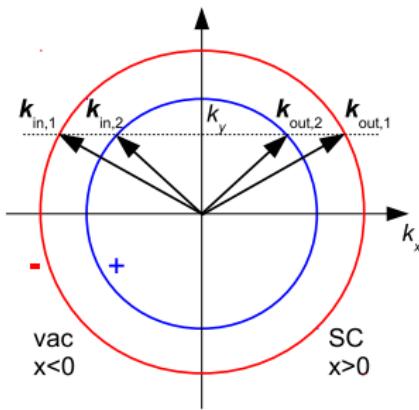
Surface bound state (ABS):

$$\psi_{\mathbf{k}_F}(x) = C(\mathbf{k}_F) \underbrace{\begin{pmatrix} \Delta(\mathbf{k}_F) \\ \frac{E - i\Omega \operatorname{sgn} v_{F,x}}{1} \end{pmatrix}}_{\phi(\mathbf{k}_F) \equiv \psi_{\mathbf{k}_F}(x=0)} e^{-\frac{\Omega x}{|v_{F,x}|}}, \quad \Omega = \sqrt{|\Delta|^2 - E^2}$$

Specular surface reflection  $\Rightarrow k_y = \text{const}$

$\mathcal{N}$  incident waves

$\mathcal{N}$  reflected waves



# Andreev boundary states in 2D

Boundary conditions  
for  $\phi(\mathbf{k}_F) \equiv \psi_{\mathbf{k}_F}(x = 0)$ :

$$\phi(\mathbf{k}_{\text{out},i}) = \sum_{j=1}^{\mathcal{N}} S_{ij} \phi(\mathbf{k}_{\text{in},j})$$

surface scattering matrix

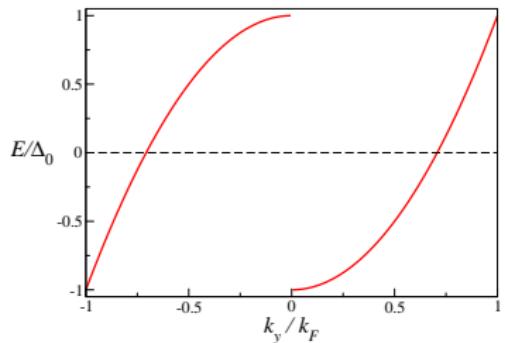
$S$ -matrix: normal-state property (electron-hole scalar),  
 $\hat{S}^\dagger \hat{S} = 1$  + additional symmetries (e.g. TR)

$2\mathcal{N}$  equations for  $\{C(\mathbf{k}_{\text{in},i})\}$ ,  $\{C(\mathbf{k}_{\text{out},i})\}$   $\rightarrow$  equation for  $E(k_y)$

# Andreev boundary states in 2D

Example: single band,  $\Delta(\mathbf{k}) = \Delta_0 e^{iN\theta}$  ( $N$  – phase winding number)

$$E_{ABS}(\theta) = -\Delta_0 \cos(N\theta) \operatorname{sgn} [\sin(N\theta)], \quad k_y = k_F \sin \theta$$



e.g. chiral *d*-wave state ( $N = 2$ ):  
 $\Delta(\mathbf{k}) = \Delta_0 (\hat{k}_x^2 - \hat{k}_y^2 + 2i\hat{k}_x\hat{k}_y)$

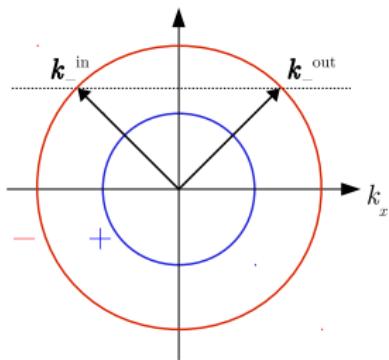
# of zero modes = phase winding number

$$\theta_m = \pm \frac{\pi}{2|N|} (2m + 1), \quad m = 0, \dots, \frac{|N|}{2} - 1$$

# Andreev boundary states in a 2D Rashba SC

Isotropic Rashba model:  $\hat{H}_0(\mathbf{k}) = \left( \frac{\mathbf{k}^2}{2m^*} - \epsilon_F \right) \hat{\sigma}_0 + \gamma_0 (k_y \hat{\sigma}_x - k_x \hat{\sigma}_y)$

Fermi surfaces are circular:  $k_{F,\lambda} = \sqrt{k_F^2 + (m^* \gamma_0)^2} - \lambda m^* \gamma_0$   
 $(k_{F,-} > k_{F,+})$



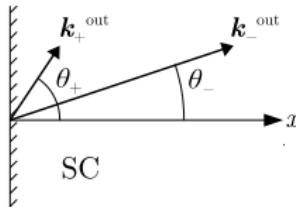
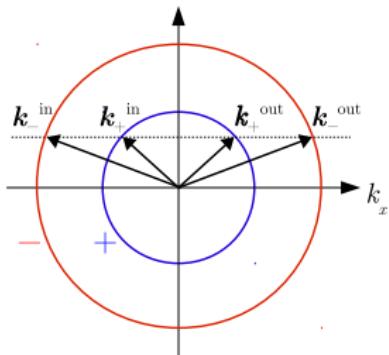
ABS energy equation at given  $k_y$ :

$$\frac{E + i\sqrt{|\Delta(\mathbf{k}_-^{\text{in}})|^2 - E^2}}{E - i\sqrt{|\Delta(\mathbf{k}_-^{\text{out}})|^2 - E^2}} = \frac{\Delta(\mathbf{k}_-^{\text{in}})}{\Delta(\mathbf{k}_-^{\text{out}})}$$

does not depend on surface scattering!

$$\mathcal{N} = 1$$

# Andreev boundary states in a 2D Rashba SC



angles of reflection  $|\theta_{\pm}| < \pi/2$

$$\mathcal{N} = 2$$

ABS energy equation  
at given  $k_y$ :

$$\frac{(\alpha_-^{\text{in}} - \alpha_-^{\text{out}})(\alpha_+^{\text{in}} - \alpha_+^{\text{out}})}{(\alpha_-^{\text{in}} - \alpha_+^{\text{out}})(\alpha_+^{\text{in}} - \alpha_-^{\text{out}})} = \frac{S_{-+}S_{+-}}{S_{--}S_{++}}$$

$$\alpha_{\lambda}^{\text{in}} = \frac{\Delta(\mathbf{k}_{\lambda}^{\text{in}})}{E + i\sqrt{|\Delta(\mathbf{k}_{\lambda}^{\text{in}})|^2 - E^2}}, \quad \alpha_{\lambda}^{\text{out}} = \frac{\Delta(\mathbf{k}_{\lambda}^{\text{out}})}{E - i\sqrt{|\Delta(\mathbf{k}_{\lambda}^{\text{out}})|^2 - E^2}}$$

# Andreev boundary states in a 2D Rashba SC

$S$ -matrix in the Rashba model (surface potential =  $\infty$ , no TRS breaking):

$$\hat{S} = -\frac{1}{e^{i\theta_-} + e^{i\theta_+}} \begin{pmatrix} e^{i\theta_+} - e^{-i\theta_-} & 2\sqrt{\cos\theta_- \cos\theta_+} \\ 2\sqrt{\cos\theta_- \cos\theta_+} & e^{i\theta_-} - e^{-i\theta_+} \end{pmatrix}$$

- ▶ unitarity:  $\hat{S}^\dagger(k_y)\hat{S}(k_y) = 1$
- ▶ TR invariance:  $S_{\lambda\lambda'}(-k_y) = -\lambda\lambda' e^{i(\theta_\lambda + \theta_{\lambda'})} S_{\lambda'\lambda}(k_y)$
- ▶ for normal incidence:  $\hat{S}(k_y = 0) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$  – no intraband scattering

# Andreev boundary states: $s$ -wave SC

Isotropic  $s$ -wave state  
 $(\Delta_{\pm} > 0)$

$$\Delta_{-}(\mathbf{k}) = \Delta_{-}, \quad \Delta_{+}(\mathbf{k}) = \Delta_{+} e^{i\chi}$$

$0 \leq \chi \leq \pi$  – phenomenologically possible in two-band GL free energy

TR invariant states:

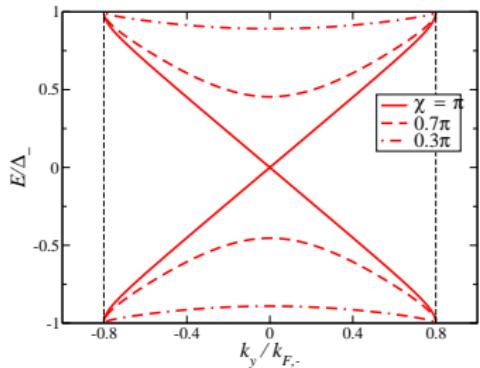
$\chi = 0$ :  $\Delta_{-}(\mathbf{k}) = \Delta_{-}, \Delta_{+}(\mathbf{k}) = \Delta_{+} \Rightarrow |\Delta_s| > |\Delta_t|$  –  $Z_2$  trivial

$\chi = \pi$ :  $\Delta_{-}(\mathbf{k}) = \Delta_{-}, \Delta_{+}(\mathbf{k}) = -\Delta_{+} \Rightarrow |\Delta_t| > |\Delta_s|$  –  $Z_2$  nontrivial

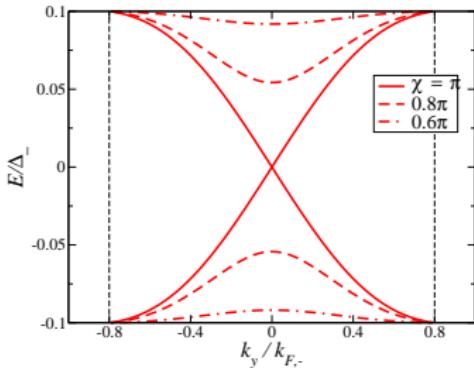
$Z_2$  topological invariant = # of Kramers pairs of zero-energy ABSs

How do the ABS evolve under intrinsic TR symmetry breaking?

# Andreev boundary states: $s$ -wave SC



$$\Delta_+ = \Delta_-, \quad k_{F,+} = 0.8k_{F,-}$$



$$\Delta_+ = 0.1\Delta_-, \quad k_{F,+} = 0.8k_{F,-}$$

ABS exists only at  $\chi_c < \chi \leq \pi$ ,  $\chi_c = \arccos \left[ \min \left( \frac{\Delta_-}{\Delta_+}, \frac{\Delta_+}{\Delta_-} \right) \right]$

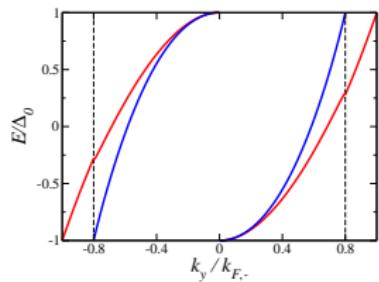
TR symmetry breaking  $\rightarrow$  **gap in the ABS spectrum**

# Andreev boundary states: chiral $d$ -wave SC

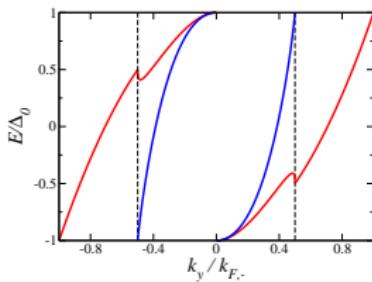
Chiral  $d$ -wave state  
( $d + id$  state)

$$\Delta_-(\mathbf{k}) = \Delta_+(\mathbf{k}) = \Delta_0(\hat{k}_x^2 - \hat{k}_y^2 + 2i\hat{k}_x\hat{k}_y)$$

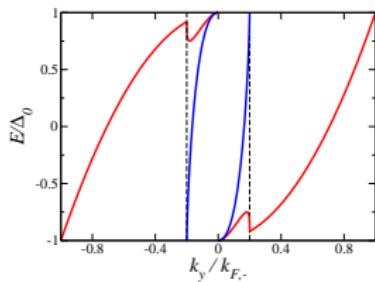
Phase winding numbers:  $N_- = N_+ = 2$



$$k_{F,+} = 0.8k_{F,-}$$



$$k_{F,+} = 0.5k_{F,-}$$



$$k_{F,+} = 0.2k_{F,-}$$

# of the ABS zero modes = total phase winding number  $N_- + N_+ = 4$

# Andreev boundary states: $d_{xy}$ -wave SC

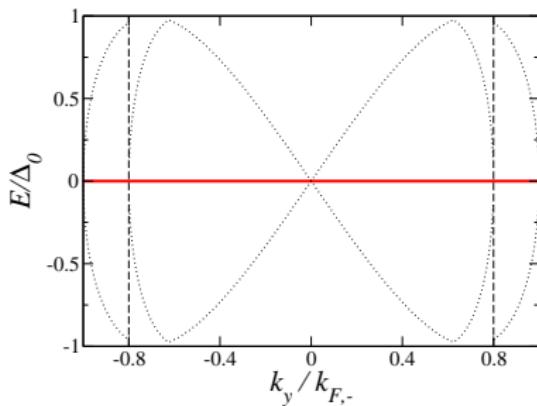
$d_{xy}$ -wave state  
(TR invariant)

$$\Delta_-(\mathbf{k}) = \Delta_+(\mathbf{k}) = 2\Delta_0 \hat{k}_x \hat{k}_y$$

$\Delta_\pm(-k_x, k_y) = -\Delta_\pm(k_x, k_y)$  – **sign change** upon surface reflection, at all  $k_y$

$$E_{ABS}(k_y) = 0$$

dotted line = bulk gap edge  
 $\min(|\Delta_-(k_y)|, |\Delta_+(k_y)|)$



$$k_{F,+} = 0.8k_{F,-}$$

## Andreev boundary states: $d_{x^2-y^2}$ -wave SC

$d_{x^2-y^2}$ -wave state  
(TR invariant)

$$\Delta_-(\mathbf{k}) = \Delta_+(\mathbf{k}) = \Delta_0(\hat{k}_x^2 - \hat{k}_y^2)$$

$\Delta_\pm(-k_x, k_y) = \Delta_\pm(k_x, k_y)$  – no sign change upon surface reflection into the same helicity band

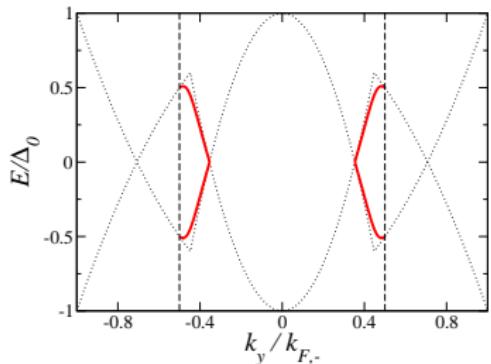
If  $\Delta_-(k_y)\Delta_+(k_y) = \Delta_0^2 \cos(2\theta_-) \cos(2\theta_+) < 0$



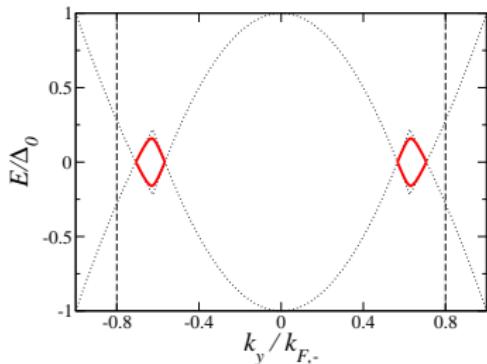
gap function changes sign upon interband reflection  
(probability =  $|S_{+-}|^2 = |S_{-+}|^2 < 1$ )

# Andreev boundary states: $d_{x^2-y^2}$ -wave SC

$$\Delta_-(\mathbf{k}) = \Delta_+(\mathbf{k}) = \Delta_0(\hat{k}_x^2 - \hat{k}_y^2)$$



$$k_{F,+} = 0.5k_{F,-}$$



$$k_{F,+} = 0.8k_{F,-}$$

dotted line: bulk gap edge =  $\min(|\Delta_-(k_y)|, |\Delta_+(k_y)|)$

# Topology of TR invariant $d$ -wave states

BdG Hamiltonian:  $\mathcal{H}_{BdG}(\mathbf{k}) = \sum_{\lambda=\pm} \hat{\Pi}_\lambda(\mathbf{k}) \otimes \hat{h}_\lambda(\mathbf{k})$

Electron-hole symmetry  $\hat{\tau}_2 \hat{h}_\lambda(\mathbf{k}) \hat{\tau}_2 = -\hat{h}_\lambda^*(\mathbf{k})$  + TR symmetry  $\hat{h}_\lambda^*(\mathbf{k}) = \hat{h}_\lambda(\mathbf{k})$



Chiral symmetry:  $\{\mathcal{C}, \mathcal{H}_{BdG}(\mathbf{k})\} = 0, \quad \mathcal{C} = \sum_\lambda \hat{\Pi}_\lambda(\mathbf{k}) \otimes \hat{\tau}_2$

Symmetry-protected Maurer-Cartan topological invariant:

$$N_1 = \frac{1}{4\pi i} \oint_{k_y=\text{const}} \text{Tr} (\mathcal{C}\omega), \quad \omega = \mathcal{H}_{BdG}^{-1} d\mathcal{H}_{BdG}$$

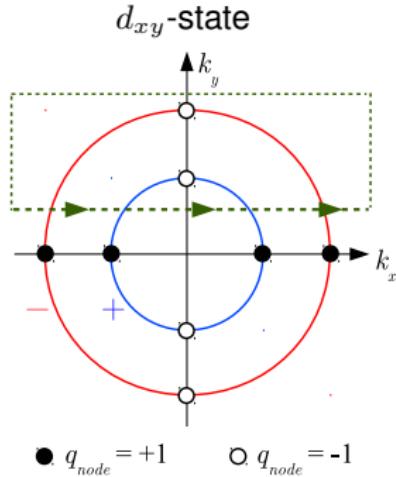
# of the zero-energy Andreev surface modes =  $|N_1(k_y)|$

$$N_1 = \frac{1}{2\pi} \sum_\lambda \oint d\tilde{\Phi}_\lambda, \quad e^{i\tilde{\Phi}_\lambda(\mathbf{k})} = \frac{\xi_\lambda(\mathbf{k}) + i\Delta_\lambda(\mathbf{k})}{\sqrt{\xi_\lambda^2(\mathbf{k}) + \Delta_\lambda^2(\mathbf{k})}}$$

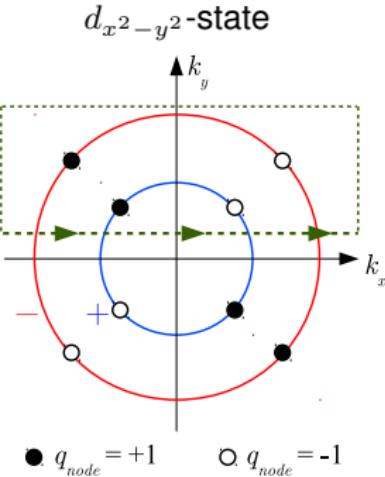
not defined at gap nodes

# Topology of TR invariant $d$ -wave states

$$N_1 = \sum_{\lambda,i} q_{\lambda,i}, \quad q_{\lambda,i} = \frac{1}{2\pi} \oint_{c_{\lambda,i}} d\tilde{\Phi}_{\lambda} - \text{"topological charge" of the node}$$



$$|N_1| = 2 \text{ or } 1$$



$$|N_1| = 0$$

# Conclusions

- ▶ Absence of inversion symmetry + strong SOC result in nondegenerate electron bands with nontrivial topological properties
- ▶ Symmetry classification of the SC states in noncentrosymmetric crystals differs from the centrosymmetric case (gap functions are even in  $k$ )
- ▶ Linear gradient terms in the GL energy (Lifshitz invariants) are responsible for a variety of novel nonuniform SC states, even at  $H = 0$
- ▶ SC states in the bulk can have nontrivial topology, which manifests itself in the Andreev surface modes

Thanks to

