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Surface properties of chiral *d*-wave superconductor with hexagonal symmetry

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@YITP

In collaboration with...

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Manfred Sigrist (ETH Zurich)

symmetry breaking
& ***topology*** } ***exotic phenomena***

Pnictide superconductor SrPtAs

Y.Nishikubo, K.Kudo, M.Nohara, JPSJ **80**, 055002 (2011)

Contents:

- SrPtAs normal state

  local lack of inversion symmetry
  ⇒ spin-orbit coupling of Kane-Mele type "KM metal"

- Superconductivity and its pairing symmetry

  topological chiral *d*-wave with
  time-reversal-symmetry breaking is highly expected

- Surface properties

  Spontaneous ***charge*** & ***spin currents***, and ***spin polarization***

  Goryo,Imai,Rui,Sigrist, and Schnyder, PRB (2017)

Symmetry breaking
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  Topological chiral d-wave with
  Time Rev. Sym. Breaking (?)

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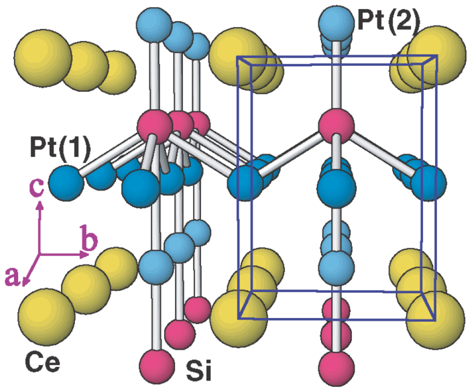
Inversion-symmetry breaking

Inversion transformation: $\boldsymbol{r} \rightarrow -\boldsymbol{r}$

ex) $CePt_3Si$



Inversion symmetry breaking along c-axis (C_{4v})

$$\alpha \sum_{\boldsymbol{k}ss'} \boldsymbol{\lambda}_{\boldsymbol{k}} \cdot \boldsymbol{\sigma}_{ss'} c^{\dagger}_{\boldsymbol{k}s} c_{\boldsymbol{k}s'}$$

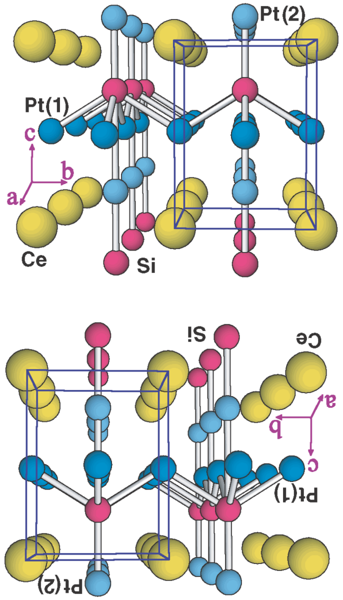
$$\boldsymbol{\lambda}_{\boldsymbol{k}} = \hat{\boldsymbol{z}} \times \boldsymbol{k} = -\boldsymbol{\lambda}_{-\boldsymbol{k}}$$

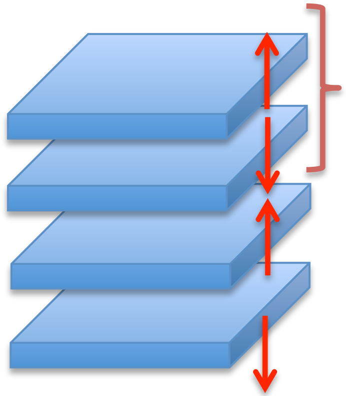
Rashba anti-symmetric spin-orbit coupling

local lack of inversion symmetry

Artificial layered system of $CePt_3Si$:

Maruyama, Sigrist, Yanase, JPSJ (2011)





- bilayer system
- inversion center exists in between (does not in) two sublayers

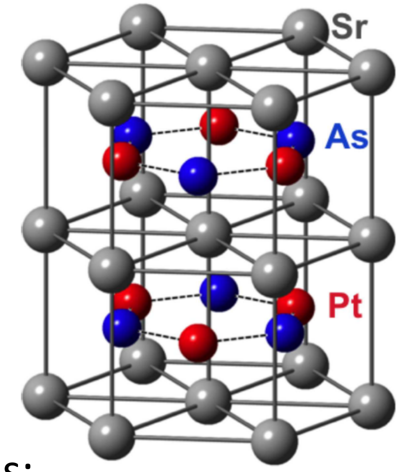
"local lack of inversion-symmetry"

Staggered Rashba SOC

$$(-1)^l \times \alpha \sum_{kss'} \boldsymbol{\lambda}_{\boldsymbol{k}} \cdot \boldsymbol{\sigma}_{ss'} c^{\dagger}_{\boldsymbol{k}s} c_{\boldsymbol{k}s'}$$

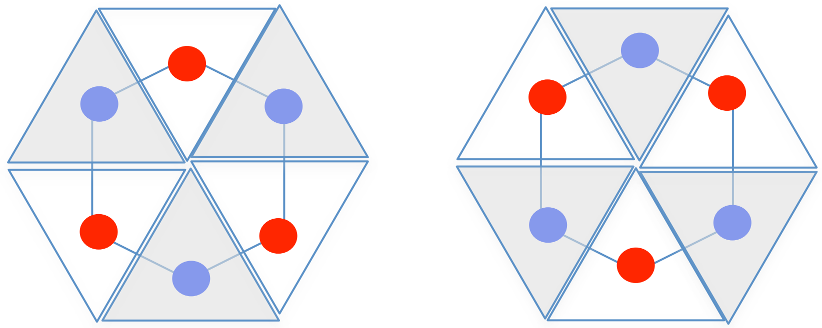
$$\boldsymbol{\lambda}_{\boldsymbol{k}} = \hat{\boldsymbol{z}} \times \boldsymbol{k} = -\boldsymbol{\lambda}_{-\boldsymbol{k}}$$

SrPtAs: hexagonal bilayer system with local lack of inversion symmetry



SrPtAs:
Nishikubo et al, JPSJ(2012)

checkerboard triangular lattice structure



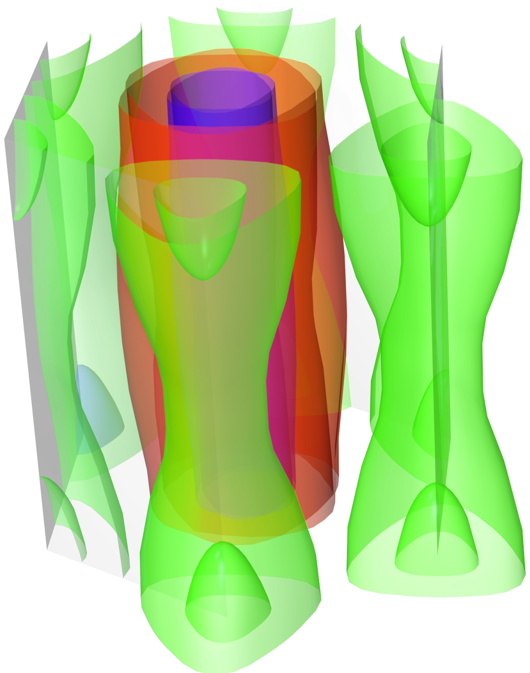
- *Globally* inversion symmetric
- ***No inversion center*** in each Pt-As sublayer
- staggered anti-symmetric SOC is expected

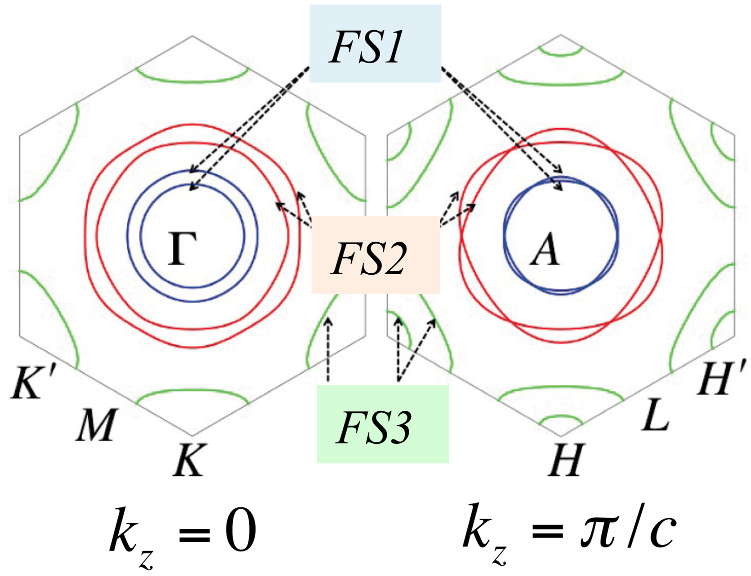
≠ staggered Rashba

Band structure calculation

Youn et al. PRB (2012)

Fermi Surfaces





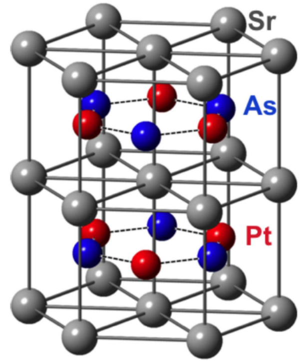
- ***Three Fermi surfaces with spin-orbit splitting***

  ⟶ *six* subsheets (five quasi-2d , one 3d)

5d orbitals of Pt ⇒ conduction bands

Tight-binding Hamiltonian

Youn et al (2012)



Pt-site hoppings only

TB fitting for a Fermi surface with spin-orbit splitting

$$H = \sum_{\boldsymbol{k}s_1 s_2} (u^\dagger_{\boldsymbol{k}s_1} d^\dagger_{\boldsymbol{k}s_1}) \begin{pmatrix} \xi_{\boldsymbol{k}}(\hat{\sigma}_0)_{s_1 s_2} + \lambda_{\boldsymbol{k}}(\hat{\sigma}_z)_{s_1 s_2} & \epsilon_{c\boldsymbol{k}}(\hat{\sigma}_0)_{s_1 s_2} \\ \epsilon^*_{c\boldsymbol{k}}(\hat{\sigma}_0)_{s_1 s_2} & \xi_{\boldsymbol{k}}(\hat{\sigma}_0)_{s_1 s_2} - \lambda_{\boldsymbol{k}}(\hat{\sigma}_z)_{s_1 s_2} \end{pmatrix} \begin{pmatrix} u_{\boldsymbol{k}s_2} \\ d_{\boldsymbol{k}s_2} \end{pmatrix}$$

Tight-binding Hamiltonian

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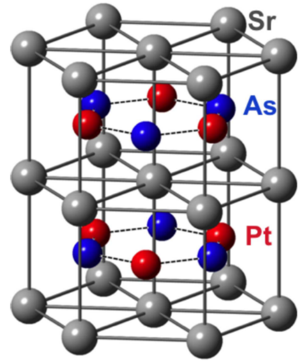

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$u^\dagger_{\boldsymbol{k}s}, u_{\boldsymbol{k}s}$ OPs of electrons in upper sublayer

$d^\dagger_{\boldsymbol{k}s}, d_{\boldsymbol{k}s}$ OPs of electrons in lower sublayer

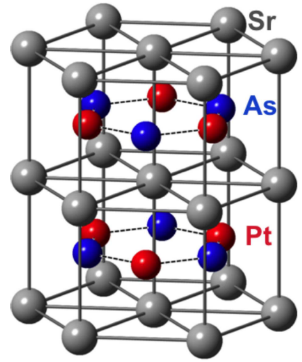
$\hat{\sigma}_0, \hat{\sigma}_z$ 2x2 unit matrix, and the z-component of Pauli matrix for spin

$$\xi_{\boldsymbol{k}} = -2t\sum_{i=1}^{3} \cos \boldsymbol{k}\cdot\boldsymbol{T}_i - 2t_{c2}\cos k_z c - \mu$$

$$\epsilon_{c\boldsymbol{k}} = -t_c(1 + e^{-i\boldsymbol{k}\cdot\boldsymbol{T}_2} + e^{i\boldsymbol{k}\cdot\boldsymbol{T}_3})(1 + e^{ik_zc})$$

Tight-binding Hamiltonian

Youn et al (2012)



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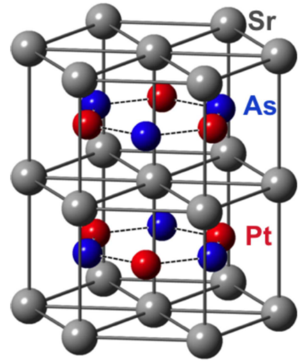
Tight-binding Hamiltonian

Youn et al (2012)



Pt-site hoppings only

TB fitting for a Fermi surface with spin-orbit splitting

$$H = \sum_{\boldsymbol{k}s_1s_2} (u^\dagger_{\boldsymbol{k}s_1} \, d^\dagger_{\boldsymbol{k}s_1}) \begin{pmatrix} \xi_{\boldsymbol{k}}(\hat{\sigma}_0)_{s_1s_2} + \lambda_{\boldsymbol{k}}(\hat{\sigma}_z)_{s_1s_2} & \epsilon_{c\boldsymbol{k}}(\hat{\sigma}_0)_{s_1s_2} \\ \epsilon^*_{c\boldsymbol{k}}(\hat{\sigma}_0)_{s_1s_2} & \xi_{\boldsymbol{k}}(\hat{\sigma}_0)_{s_1s_2} - \lambda_{\boldsymbol{k}}(\hat{\sigma}_z)_{s_1s_2} \end{pmatrix} \begin{pmatrix} u_{\boldsymbol{k}s_2} \\ d_{\boldsymbol{k}s_2} \end{pmatrix}$$

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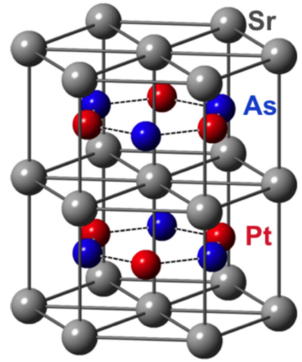
$$\xi_{\boldsymbol{k}} = -2t \sum_{i=1}^{3} \cos \boldsymbol{k} \cdot \boldsymbol{T}_i - 2t_{c2} \cos k_z c - \mu$$

(intra-sublayer hoppings)

$$\epsilon_{c\boldsymbol{k}} = -t_c(1 + e^{-i\boldsymbol{k}\cdot\boldsymbol{T}_2} + e^{i\boldsymbol{k}\cdot\boldsymbol{T}_3})(1 + e^{ik_zc})$$

Tight-binding Hamiltonian

Youn et al (2012)



Pt-site hoppings only

TB fitting for a Fermi surface with spin-orbit splitting

$$H = \sum_{\boldsymbol{k} s_1 s_2} (u^\dagger_{\boldsymbol{k} s_1} d^\dagger_{\boldsymbol{k} s_1}) \begin{pmatrix} \xi_{\boldsymbol{k}} (\hat{\sigma}_0)_{s_1 s_2} + \lambda_{\boldsymbol{k}} (\hat{\sigma}_z)_{s_1 s_2} & \underline{\epsilon_{c\boldsymbol{k}}} (\hat{\sigma}_0)_{s_1 s_2} \\ \underline{\epsilon^*_{c\boldsymbol{k}}} (\hat{\sigma}_0)_{s_1 s_2} & \xi_{\boldsymbol{k}} (\hat{\sigma}_0)_{s_1 s_2} - \lambda_{\boldsymbol{k}} (\hat{\sigma}_z)_{s_1 s_2} \end{pmatrix} \begin{pmatrix} u_{\boldsymbol{k} s_2} \\ d_{\boldsymbol{k} s_2} \end{pmatrix}$$

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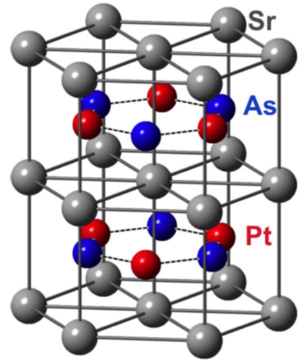
$$\boxed{\epsilon_{c\boldsymbol{k}} = -t_c (1 + e^{-i\boldsymbol{k}\cdot\boldsymbol{T}_2} + e^{i\boldsymbol{k}\cdot\boldsymbol{T}_3})(1 + e^{ik_z c})}$$

(inter sublayer hopping)

Tight-binding Hamiltonian

Youn et al (2012)



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staggered sign!

Staggered Anti-Symmetric Spin-Orbit Coupling

$$\lambda_{\boldsymbol{k}} \hat{\sigma_z} \hat{\tau_z} = \hat{\sigma_z} \hat{\tau_z} \sum_{i=1}^{3} \sin \boldsymbol{k} \cdot \boldsymbol{T}_i$$

Equivalent to the intrinsic spin-orbit coupling in Kane-Mele topological insulator

Kane-Mele, PRL('05)('05)

"Kane-Mele metal"

Note) S_z is conserved approximately (non-conserving term is negligible)

Staggered Anti-Symmetric
Spin-Orbit Coupling

$$\lambda_{\boldsymbol{k}}\hat{\sigma_z}\hat{\tau_z} = \hat{\sigma_z}\hat{\tau_z}\sum_{i=1}^{3}\sin \boldsymbol{k}\cdot\boldsymbol{T}_i$$

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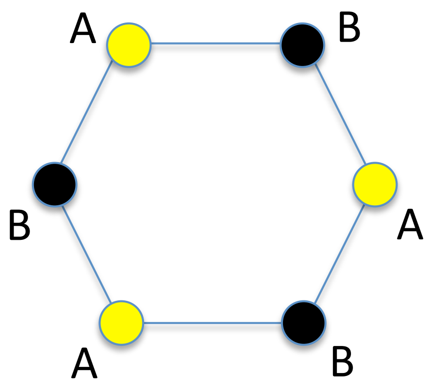
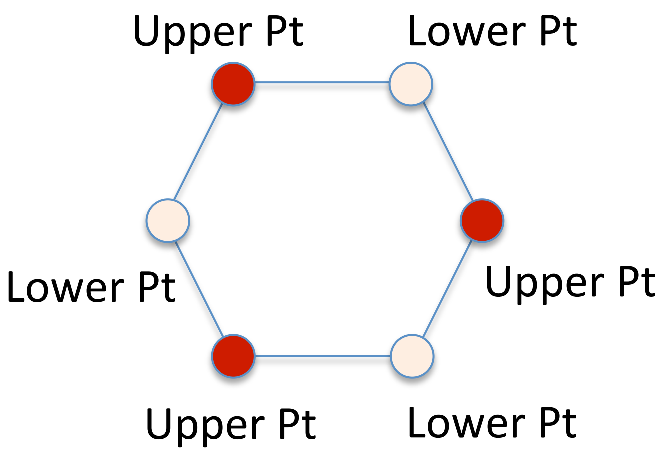
Kane-Mele model



Pt cites in our model



sublattice ⇄ sublayer

Staggered Anti-Symmetric
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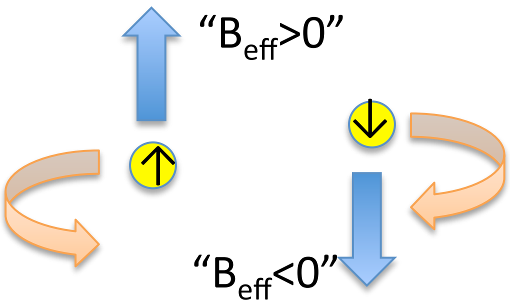
Kane-Mele, PRL('05)('05)

spin-dependent Aharonov-Bohm flux



- Quantized spin Hall effect in KM insulator
- spin Hall effect in our metallic model (non-quantized)

- Spin Hall conductivity（Kubo formula）

$$\sigma^s_{xy} = \frac{e}{2\pi}\int \frac{d^3k}{8\pi^2}\hat{\boldsymbol{g}}_{\boldsymbol{k}}\cdot(\partial_{k_x}\hat{\boldsymbol{g}}_{\boldsymbol{k}}\times\partial_{k_y}\hat{\boldsymbol{g}}_{\boldsymbol{k}})\left\{f(\xi^+_{\boldsymbol{k}})-f(\xi^-_{\boldsymbol{k}})\right\}$$

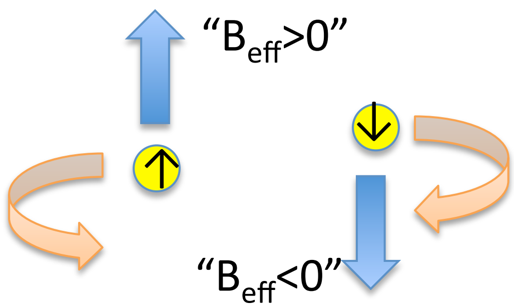
$$\boldsymbol{g}_{\boldsymbol{k}} = (\mathrm{Re}(\epsilon_{c\boldsymbol{k}}), -\mathrm{Im}(\epsilon_{c\boldsymbol{k}}), \lambda_{\boldsymbol{k}})$$

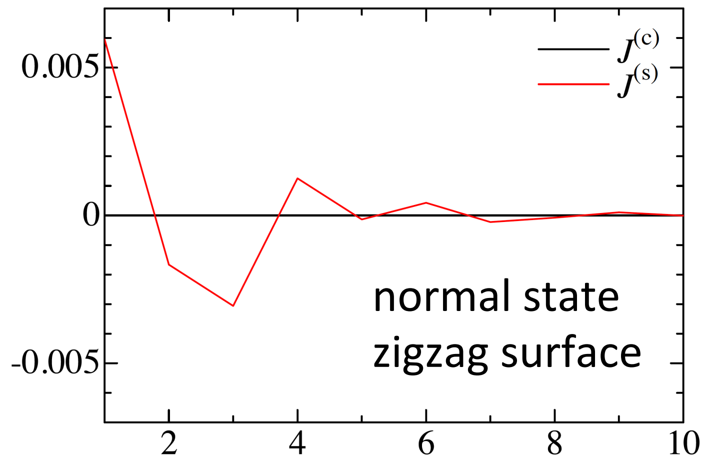
Both $\lambda_{\boldsymbol{k}}$ and $\varepsilon_{c\boldsymbol{k}}$ needed

$$\simeq -120\hbar/(e\Omega\mathrm{cm})$$

the same order of Pt (typical SH metal); T. Kimura et al, PRL (2007)

- Spontaneous surface spin current





Symmetry breaking
& topology
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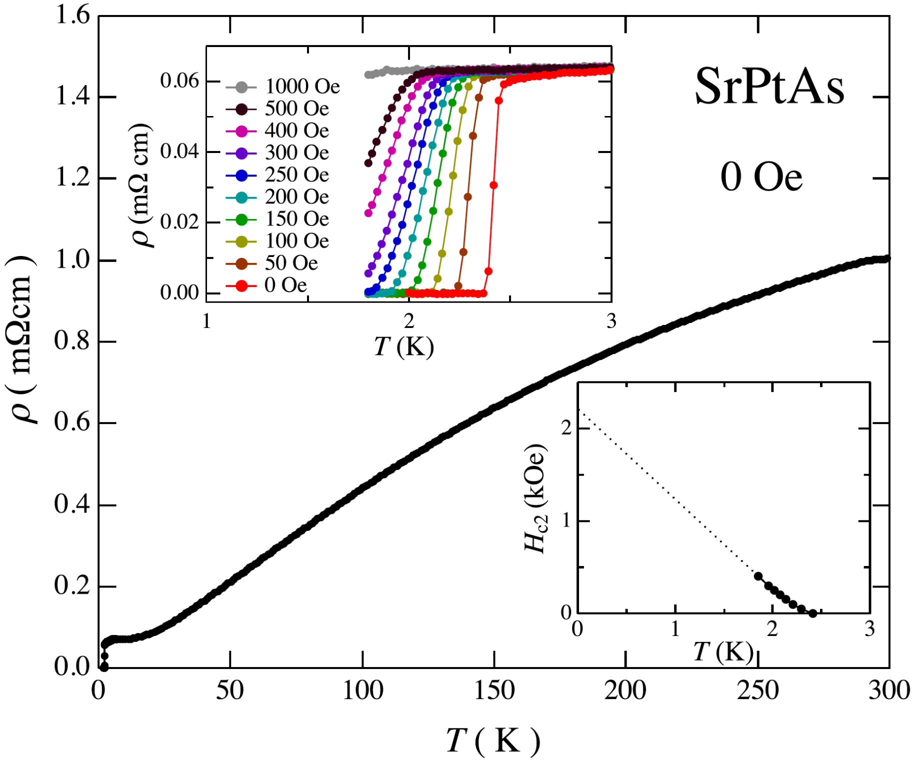
Superconductivity of SrPtAs

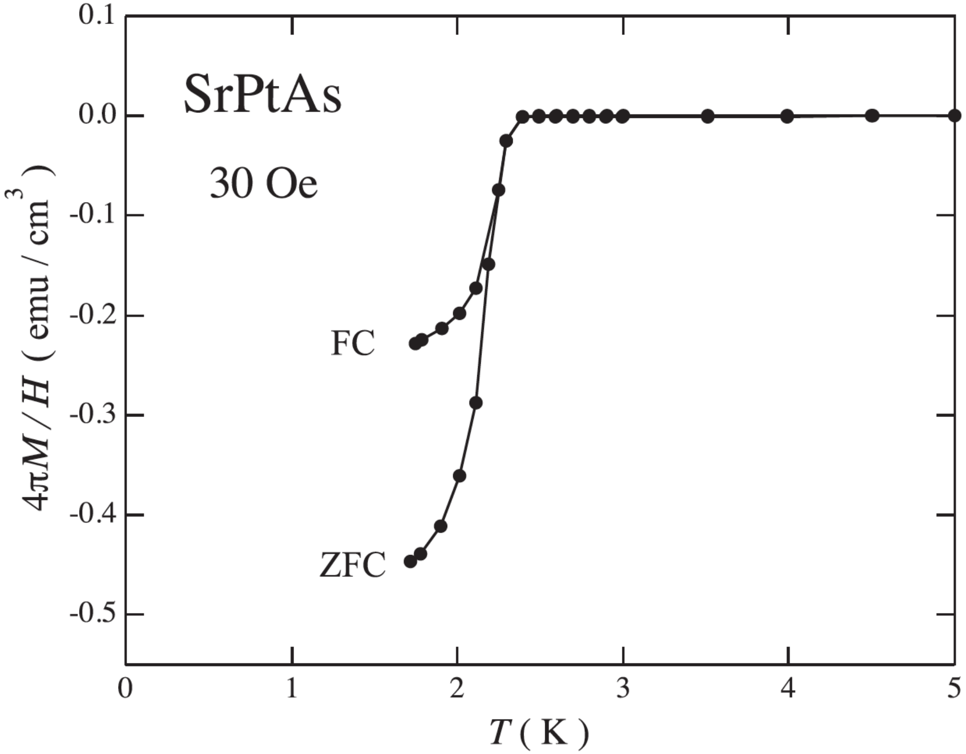
Y.Nishikubo, K.Kudo, M.Nohara, JPSJ **80**, 055002 (2011)

T_c=2.4K

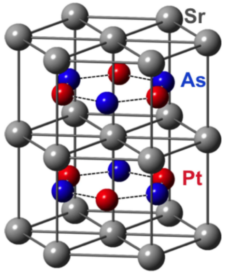
ρ vs T



M vs T



Possible pairing symmetry



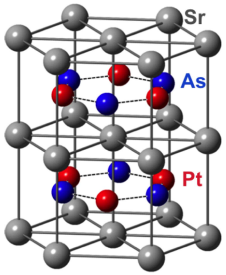
（in-plane pairing ）

Goryo, Fischer, Sigrist, PRB (2012); D_{3d}
Fischer, Goryo, JPSJ (2015); D_{6h}

Γ	Parity	(a) spin-singlet $\hat{\Delta}^{\Gamma,m}_{\boldsymbol{k}l} = i\hat{\sigma}_y \psi^{\Gamma,m}_{\boldsymbol{k}l}$	(b) spin-triplet $\hat{\Delta}^{\Gamma,m}_{\boldsymbol{k}l} = i\left[\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{d}^{\Gamma,m}_{\boldsymbol{k}l}\right]\hat{\sigma}_y$
A_{1g}		$\psi^{A_{1g}}_{l} = 1,\ \psi^{A_{1g}}_{\boldsymbol{k}l} = e_{\boldsymbol{k}}$	$\boldsymbol{d}^{A_{1g}}_{\boldsymbol{k}l} = (-1)^l o_{\boldsymbol{k}}\hat{\boldsymbol{z}}$
A_{2g}	Even		$\boldsymbol{d}^{A_{2g}}_{\boldsymbol{k}l} = (-1)^l o_{\boldsymbol{k}}\hat{\boldsymbol{x}}_{\pm}$
E_g		$\psi^{E_g,1}_{\boldsymbol{k}l} = e^{+}_{\boldsymbol{k}}$	$\boldsymbol{d}^{E_g,1}_{\boldsymbol{k}l} = (-1)^l o^{+}_{\boldsymbol{k}}\hat{\boldsymbol{z}}$
		$\psi^{E_g,2}_{\boldsymbol{k}l} = e^{-}_{\boldsymbol{k}}$	$\boldsymbol{d}^{E_g,2}_{\boldsymbol{k}l} = (-1)^l o^{-}_{\boldsymbol{k}}\hat{\boldsymbol{z}}$
A_{1u}			$\boldsymbol{d}^{A_{1u}}_{\boldsymbol{k}l} = o_{\boldsymbol{k}}\hat{\boldsymbol{x}}_{\pm}$
A_{2u}	Odd	$\psi^{A_{2u}}_{l} = (-1)^l,\ \psi^{A_{2u}}_{\boldsymbol{k}l} = (-1)^l e_{\boldsymbol{k}}$	$\boldsymbol{d}^{A_{2u}}_{\boldsymbol{k}l} = o_{\boldsymbol{k}}\hat{\boldsymbol{z}}$
E_u		$\psi^{E_u,1}_{\boldsymbol{k}l} = (-1)^l e^{+}_{\boldsymbol{k}}$	$\boldsymbol{d}^{E_u,1}_{\boldsymbol{k}l} = o^{+}_{\boldsymbol{k}}\hat{\boldsymbol{z}}$
		$\psi^{E_u,2}_{\boldsymbol{k}l} = (-1)^l e^{-}_{\boldsymbol{k}}$	$\boldsymbol{d}^{E_u,2}_{\boldsymbol{k}l} = o^{-}_{\boldsymbol{k}}\hat{\boldsymbol{z}}$

singlet-triplet mixing

Possible pairing symmetry

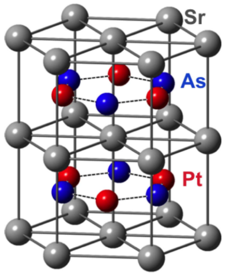


(in-plane pairing)

Goryo, Fischer, Sigrist, PRB (2012); D_{3d}
Fischer, Goryo, JPSJ (2015); D_{6h}

Γ		
A_{1g}	s-wave	$\Delta_{\boldsymbol{k}} = const.$
A_{2g}		
E_g	chiral d-wave *TRSB*	$\Delta_{\boldsymbol{k}} = \Delta(k_x \pm i k_y)^2$
A_{1u}		
A_{2u}	f-wave	$\Delta_{\boldsymbol{k}} = \Delta\left(3k_x^2 - k_y^2\right) k_y$
E_u		

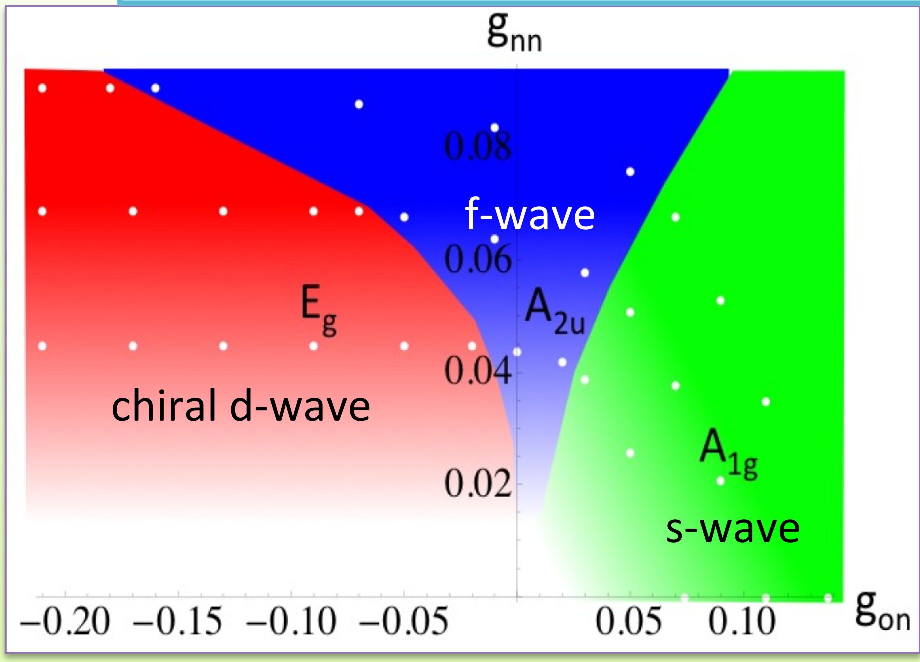
Possible pairing symmetry



(in-plane pairing)

Goryo, Fischer, Sigrist, PRB (2012); D_{3d}
Fischer, Goryo, JPSJ (2015); D_{6h}

Linearized gap eq. with extended Hubbard interaction
=> Pairing instability



- attractive g_{on}

  s-wave or f-wave

- repulsive g_{on}

  f-wave or chiral d

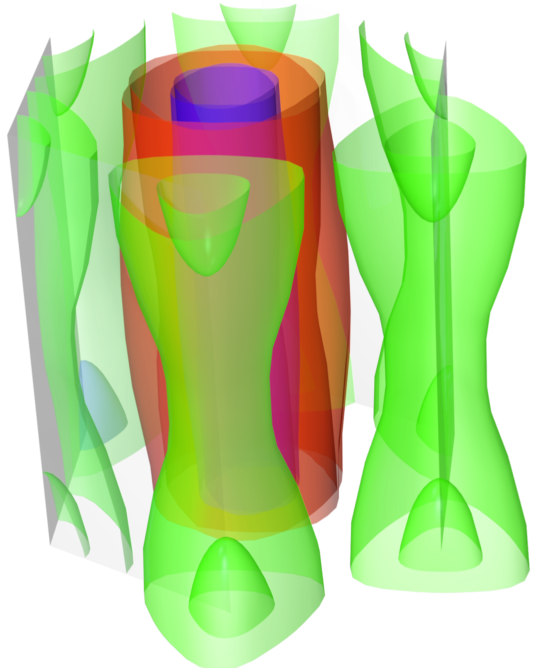
- Small S-T mixing except for the phase boundaries

iplet
g

Functional RG analysis

Fischer et al, PRB (2014)

Wang et al, PRB (2015)



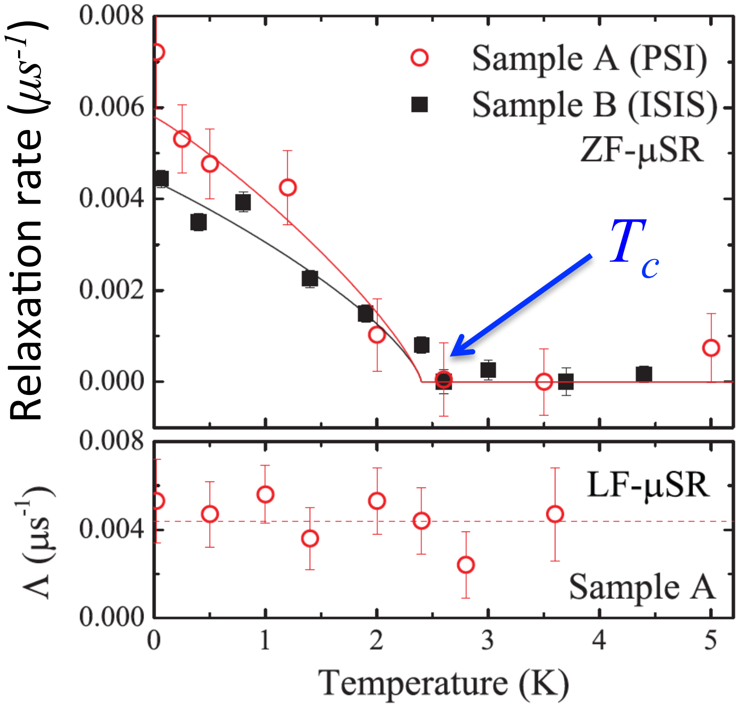
DOSs of *inner* FSs

negligible $\Rightarrow$ *f*-wave
comparable $\Rightarrow$ chiral *d*-wave

FS		f-wave	chiral d-wave
inner	four quasi-2D	***line nodes***	full gap
corner	one quasi-2D	full gap	full gap
	one 3D	full gap	***point nodes***

μSR measurement

P. K. Biswas et al, PRB (2013)



spontaneous magnetization
⇒ chiral d-wave with TRSB

Note)

- large HS peak of $1/T_1$

  Matano et. al. PRB (2014)
- T-dependence of λ_L

  Landaeta et al, PRB (2016)

⇒ s-wave

$d_{x^2-y^2} + id_{xy}$

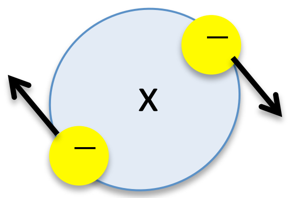
chiral d-wave state

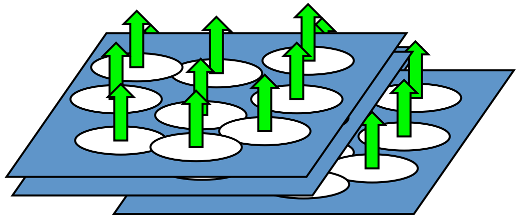
Cf)
chiral *d* has never been observed

d-wave version of chiral p-wave (^{3}He-A, Sr_2RuO_4)

L_{rel} is ordered ***ferromagnetically***

$\Rightarrow$ ***spontaneous breaking of TRS***

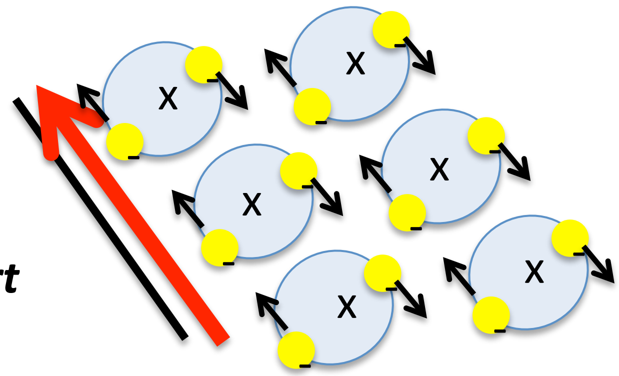




class D(= Chern SC) Schnyder et al, PRB (2008)

(quasi-)1D chiral surface states

surface transport



Volovik('88)('97),
Haldane & Rezayi('88)
Laughlin('94)('98)
Goryo & Ishikawa('99)
Read & Green('00)
Furusaki & Matsumoto & Sigrist('00)
...etc

Vanishing surface charge current in non-p-wave chiral state?

- survives only for chiral p-wave state in the *rot. sym. system*

  Huang-Taylor-Kalline, PRB ('14); Tada et al, PRL ('15)

- some varieties in the *lattice systems*

  Huang-Taylor-Kalline, PRB ('14)

chiral

OP symmetry; lattice	Integrated current?	Degenerate?
p wave; continuum	yes	yes
d wave; continuum	no	yes
p wave; square	yes	yes
d wave; square	no	no
p wave; triangle	yes	yes
d wave; triangle	yes	yes
f wave; triangle	no	no

We can have the surface charge current even in the chiral *d*-wave state,
if it belongs to the 2D irr. rep. of the crystal point group

Symmetry breaking & topology } *Exotic Phenomena*

Pnictide superconductor SrPtAs

Y.Nishikubo, K.Kudo, M.Nohara, JPSJ **80**, 055002 (2011)

Contents:

- SrPtAs normal state

  local lack of inversion symmetry

  ⇒ spin-orbit coupling of Kane-Mele type "KM metal"

- Superconductivity and its pairing symmetry

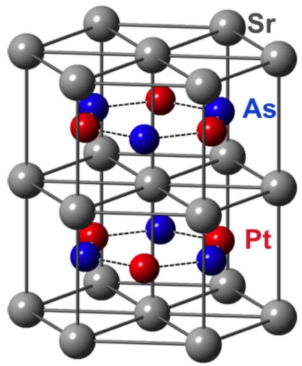
  Topological chiral d-wave with Time Rev. Sym. Breaking (?)

- Surface properties

  Spontaneous ***charge*** & ***spin currents***, and ***spin polarization***

  Goryo,Imai,Rui,Sigrist, and Schnyder, PRB (2017)

BdG analysis

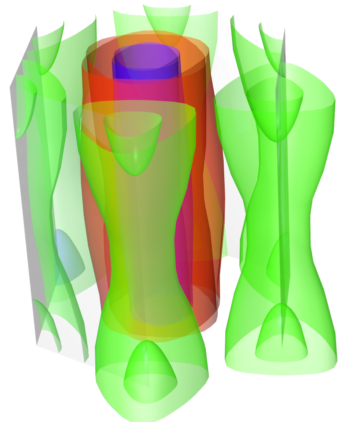


One-body Hamiltonian

Intra-layer hopping
- NN cites t
- Spin-orbit coupling λ
  (spin-dependent NN hopping)

Inter-layer hopping
- NN layers t_c
- NNN layers t_{c2}

…fitted to the ***dominant FS*** (green)



Youn et al PRB(2012)

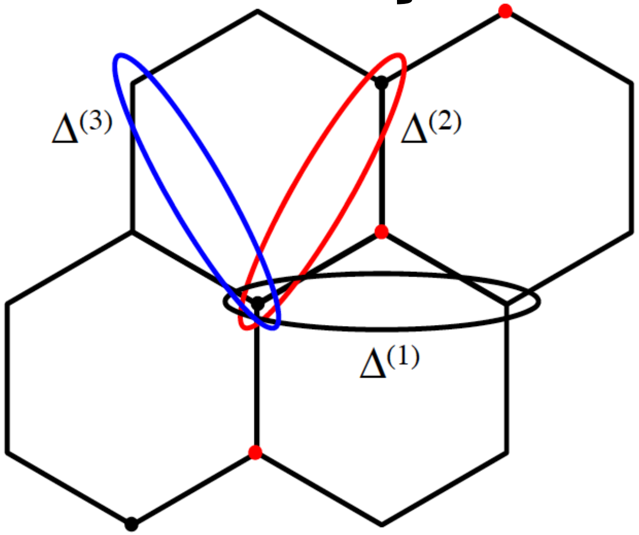
Pairing interaction

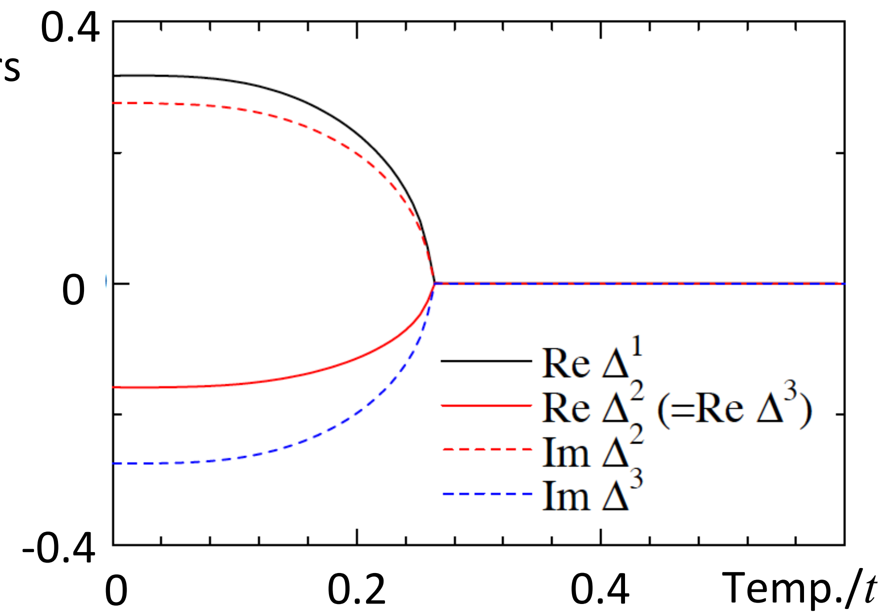
- density-density type attractive int.
- between in-plane NN cites
- U=-2.0t

BdG equation … solved selfconsistently

Stable pairing symmetry in bulk

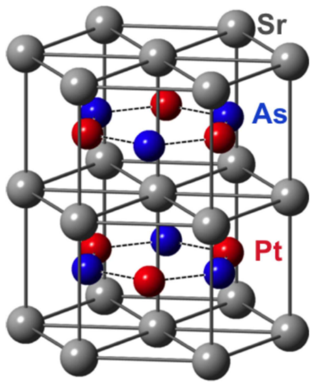
spin-singlet channels of in-plane NN pairing } 3 order parameters

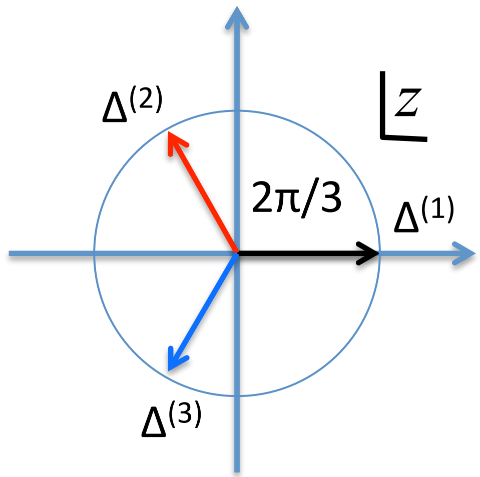




A sublattice … Pt cites in the upper sublayer

B sublattice … Pt cites in the lower sublayer

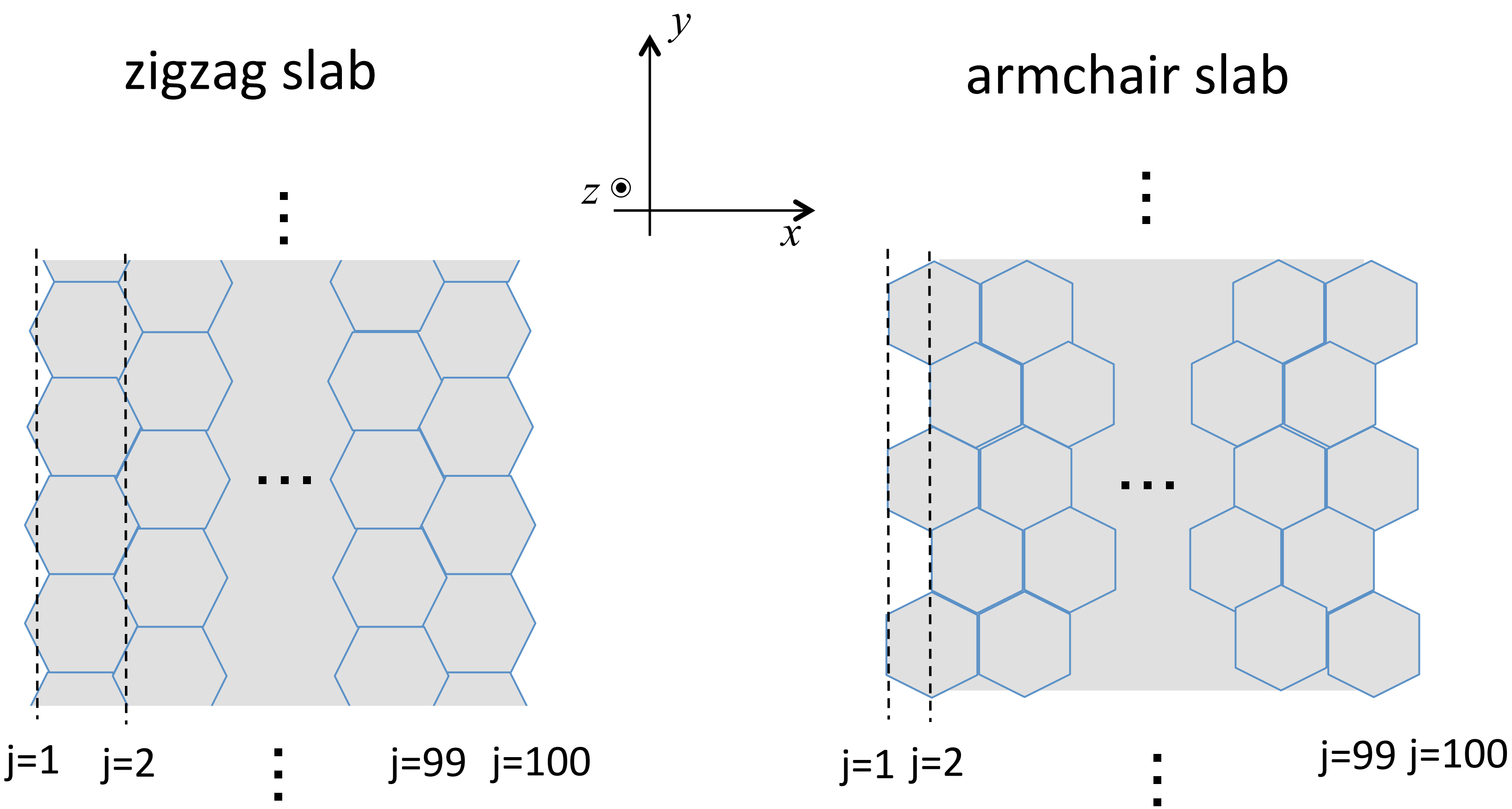




chiral d-wave is indeed stabilized

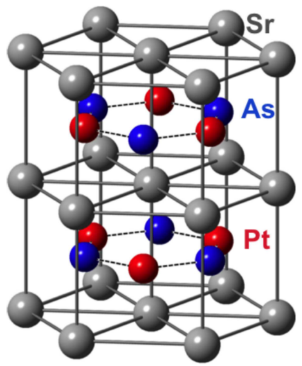
Slab geometries

x: open, y,z: periodic



Mirror symmetry

Cf) Sato & Ando. Rep. Prog. Phys. ('17)



sublayer -> mirror plane

$$\mathcal{M}_{xy};k_z \to -k_z,\ \sigma_x \to -\sigma_x,\ \sigma_y \to -\sigma_y,$$

$$D\left(\{\mathcal{M}_{xy}\}\right) \propto \sigma_z$$

At k_z=0,

$$\Psi_{\boldsymbol{k}\uparrow} = \begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} \in \mathcal{M}_{xy} = +i; \quad \Psi_{\boldsymbol{k}\downarrow} = \begin{pmatrix} c_{\boldsymbol{k}\downarrow} \\ c^\dagger_{-\boldsymbol{k}\uparrow} \end{pmatrix} \in \mathcal{M}_{xy} = -i$$

The chiral d-wave gap function … even under $\mathcal{M}_{xy}$

$\Psi_{\boldsymbol{k}\uparrow}$ ⟺ $\Psi_{\boldsymbol{k}\downarrow}$

particle-hole transf.

While entire system is p-h symmetric, each QP sector can break p-h sym.

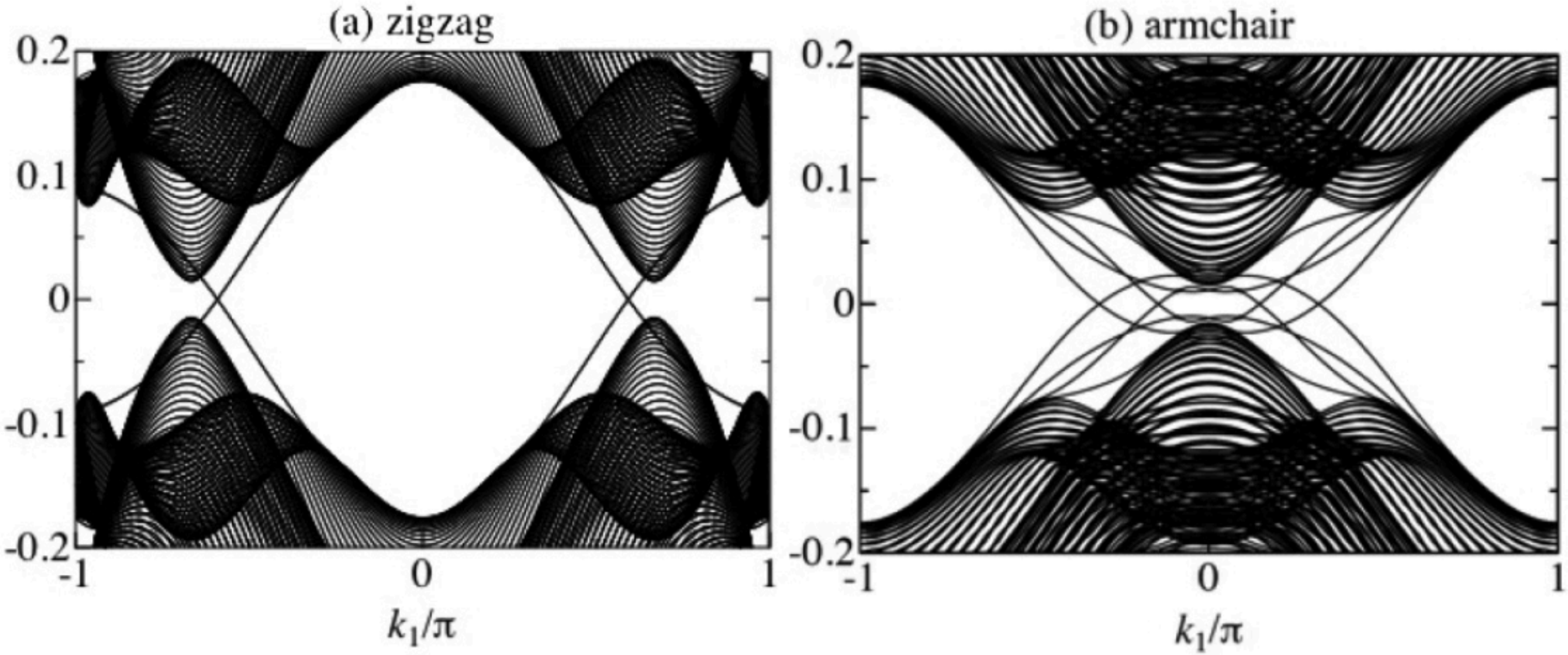
$$\therefore\ E_{\boldsymbol{k}\uparrow} \text{ and } E_{\boldsymbol{k}\downarrow} \text{ may split.}$$

Energy spectrum(k_z=0)

$\Psi_{\boldsymbol{k}\uparrow}$; 2 chiral states / a boundary

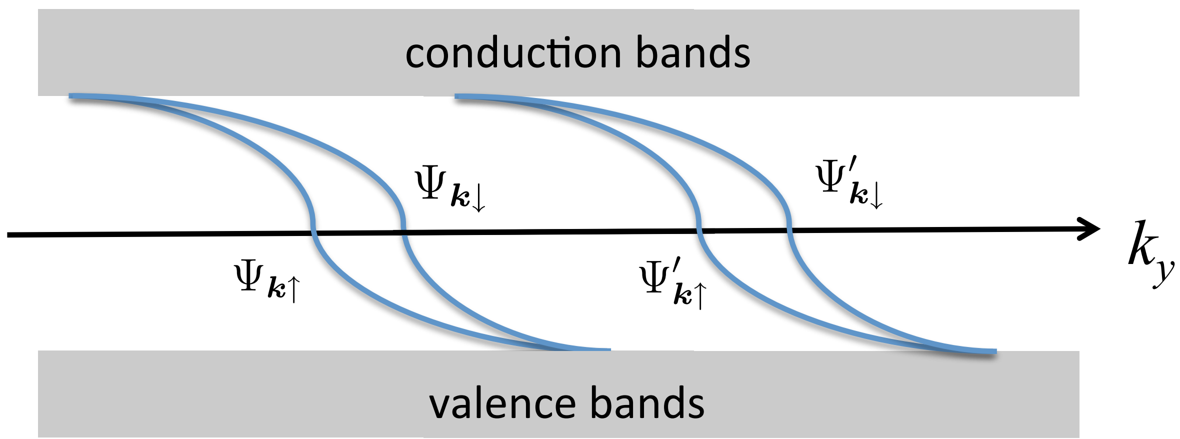
$\Psi_{\boldsymbol{k}\downarrow}$; 2 chiral states / a boundary

→ 4 chiral states / a boundary



The splitting vanishes, when $\lambda_{\boldsymbol{k}}=0$ *or* $\varepsilon_{c\boldsymbol{k}}=0$.

The schematic spectra of chiral surface states at a boundary



unbalance

$$\langle j_\uparrow \rangle \neq \langle j_\downarrow \rangle$$

$$\langle \rho_\uparrow \rangle \neq \langle \rho_\downarrow \rangle$$

⇒

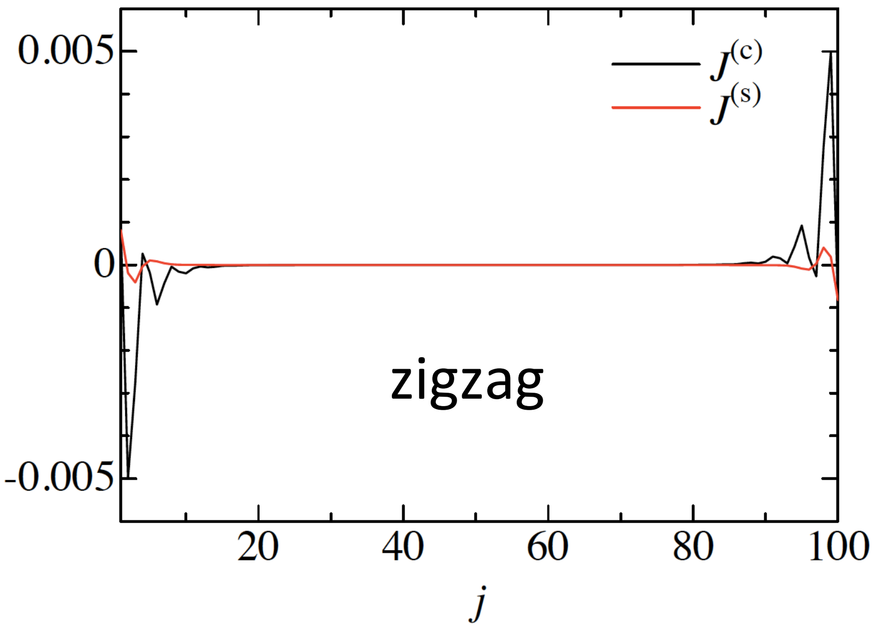
Besides the charge current,

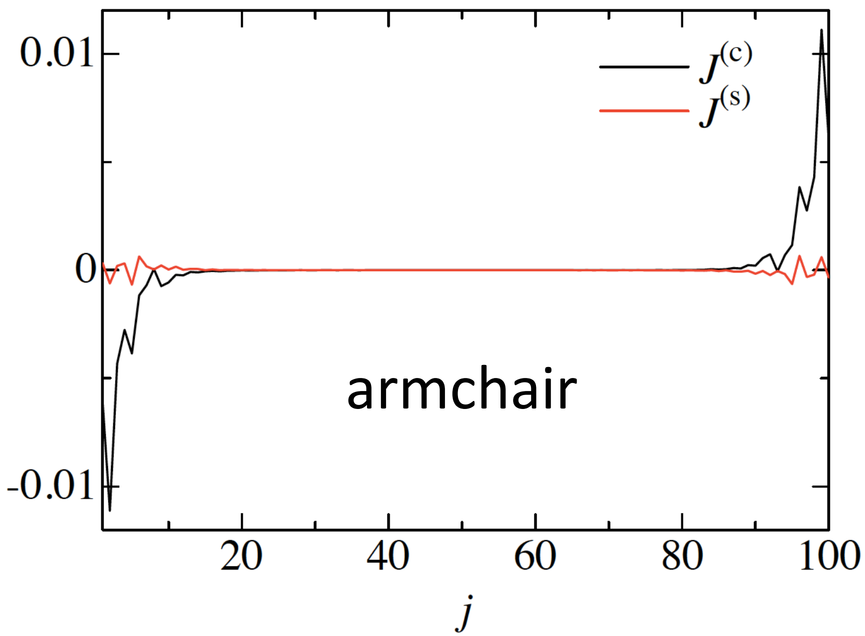
$$\langle J_s \rangle = \langle j_\uparrow \rangle - \langle j_\downarrow \rangle \neq 0$$

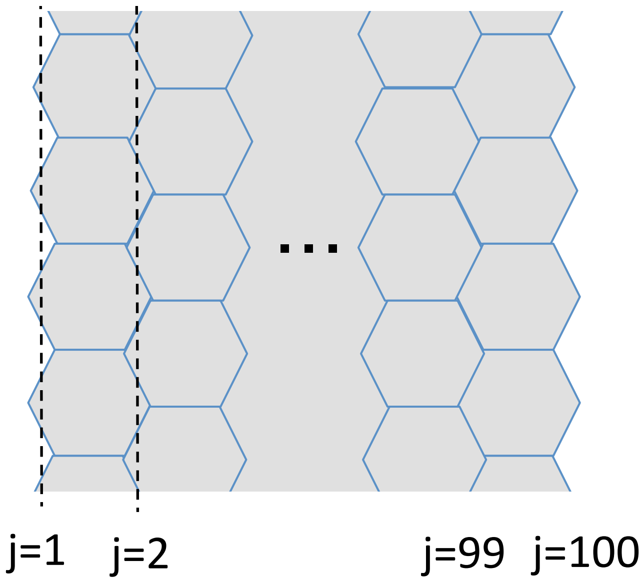
$$\langle S_z \rangle = \langle \rho_\uparrow \rangle - \langle \rho_\downarrow \rangle \neq 0$$

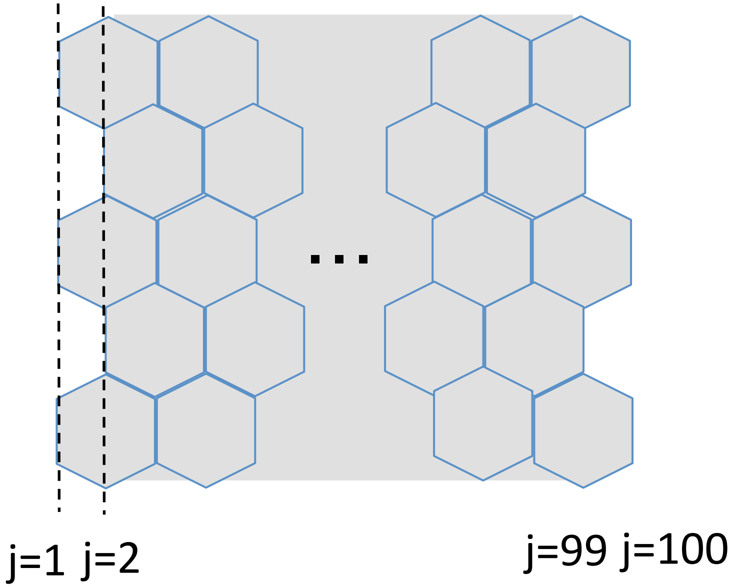
Distributions of charge and spin currents

Note) Meissner effect is neglected



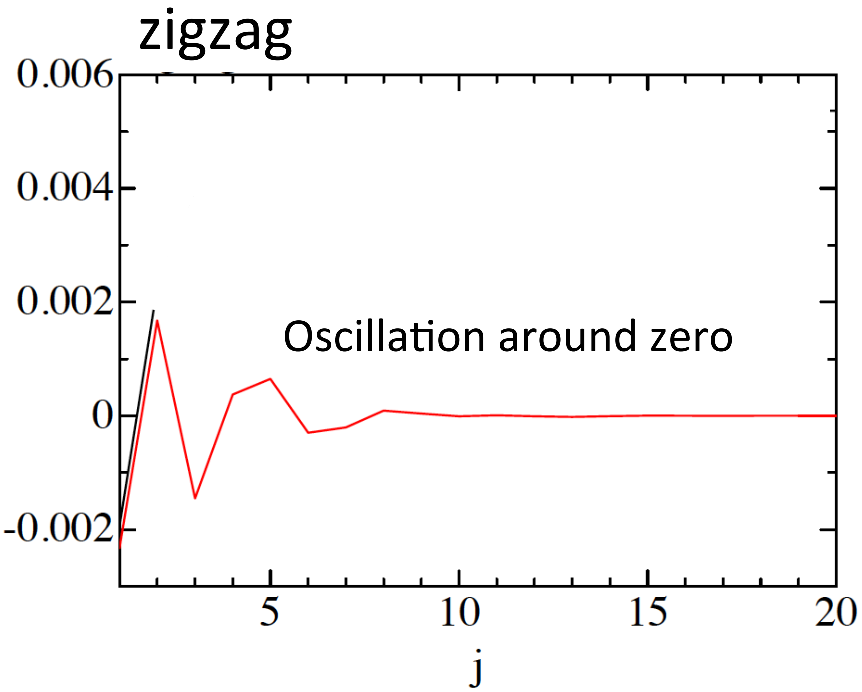


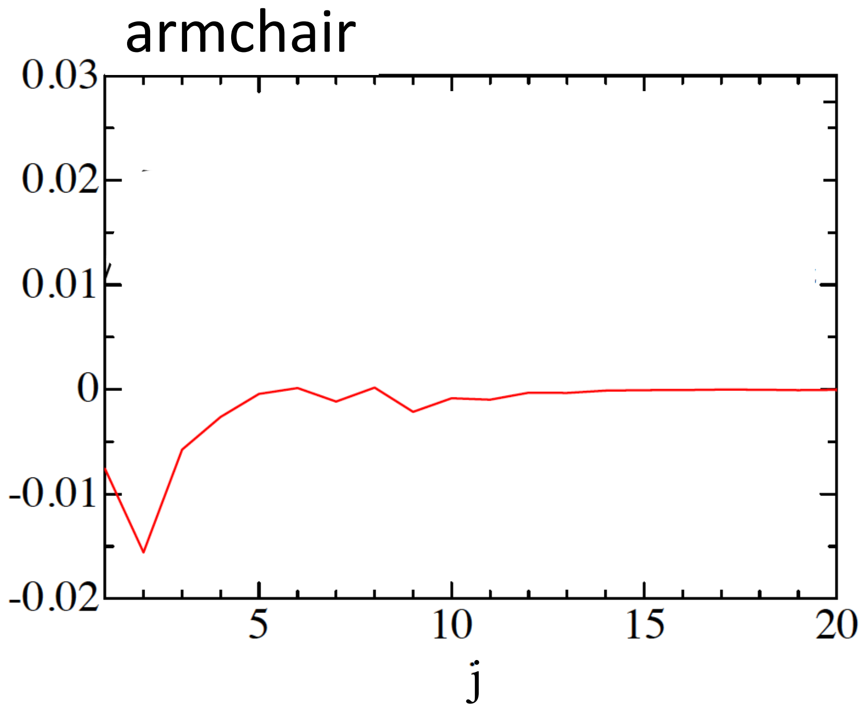




Distribution of spin polarization

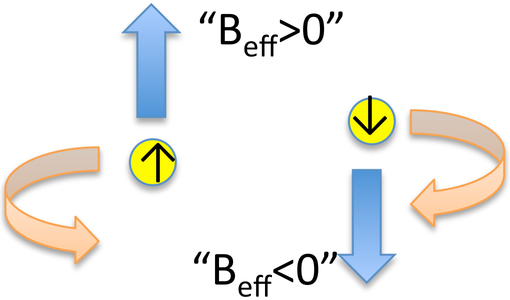
$$\langle S_{zj}\rangle = \langle n_{j\uparrow}\rangle - \langle n_{j\downarrow}\rangle$$



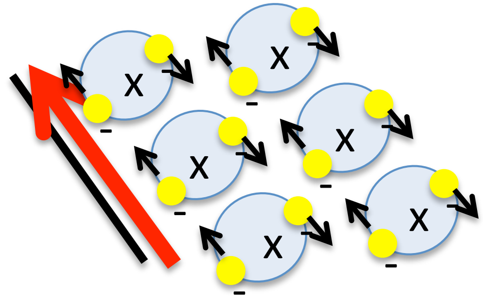


armchair … more suitable for the measurement spin-resolved STM ?

sign of the chiral d-wave pairing



Conclusions

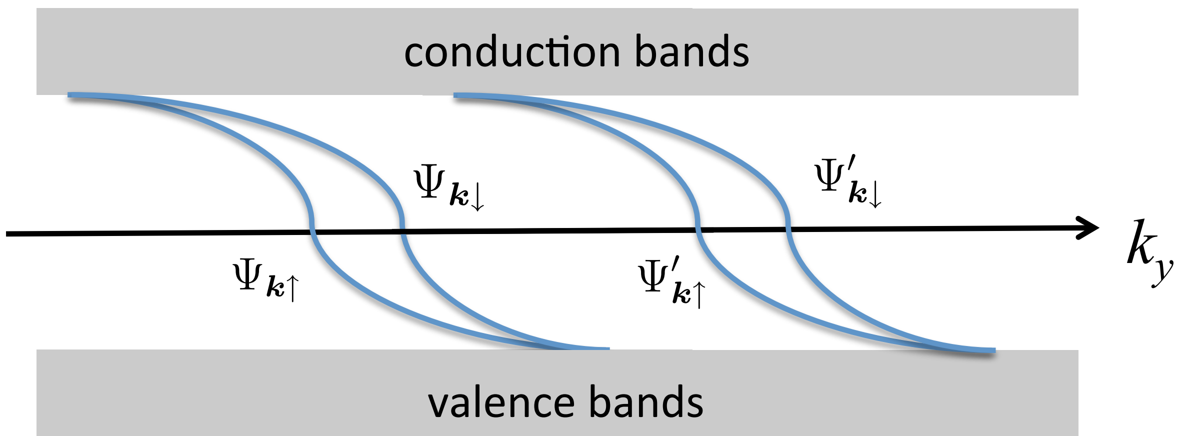


chiral d-wave pairing in Kane-Mele metal

symmetry breaking & topology

(local inversion, time-reversal & chiral pairing)

Spontaneous ***charge*** and ***spin currents***, and ***spin polarization*** @ surface



Interactions in FRG analysis

M. H. Fischer et. al. Phys. Rev. B. (2014)

band structure. We then introduce the interaction Hamiltonian,

$$\mathcal{H}' = G_1 \sum_{\beta<\beta'} \sum_{\boldsymbol{k},s} \psi^\dagger_{\beta \boldsymbol{k}_1 s} \psi^\dagger_{\beta' \boldsymbol{k}_2 s'} \psi_{\beta' \boldsymbol{k}_3 s'} \psi_{\beta \boldsymbol{k}_4 s}$$

β, β'; Fermi surface

$$+ G_2 \sum_{\beta<\beta'} \sum_{\boldsymbol{k},s} \psi^\dagger_{\beta \boldsymbol{k}_1 s} \psi^\dagger_{\beta' \boldsymbol{k}_2 s'} \psi_{\beta \boldsymbol{k}_3 s'} \psi_{\beta' \boldsymbol{k}_4 s}$$

$$+ G_3 \sum_{\beta<\beta'} \sum_{\boldsymbol{k},s} \psi^\dagger_{\beta \boldsymbol{k}_1 s} \psi^\dagger_{\beta \boldsymbol{k}_2 s'} \psi_{\beta' \boldsymbol{k}_3 s'} \psi_{\beta' \boldsymbol{k}_4 s}$$

$$+ G_4 \sum_{\beta} \sum_{\boldsymbol{k},s} \psi^\dagger_{\beta \boldsymbol{k}_1 s} \psi^\dagger_{\beta \boldsymbol{k}_2 s'} \psi_{\beta \boldsymbol{k}_3 s'} \psi_{\beta \boldsymbol{k}_4 s},$$

containing interband (G_1) and intraband (G_4) density-density interactions, an exchange interaction (G_2), and a pair-hopping term (G_3). Note that the sum $\sum_{\boldsymbol{k},s}$ runs over all spins