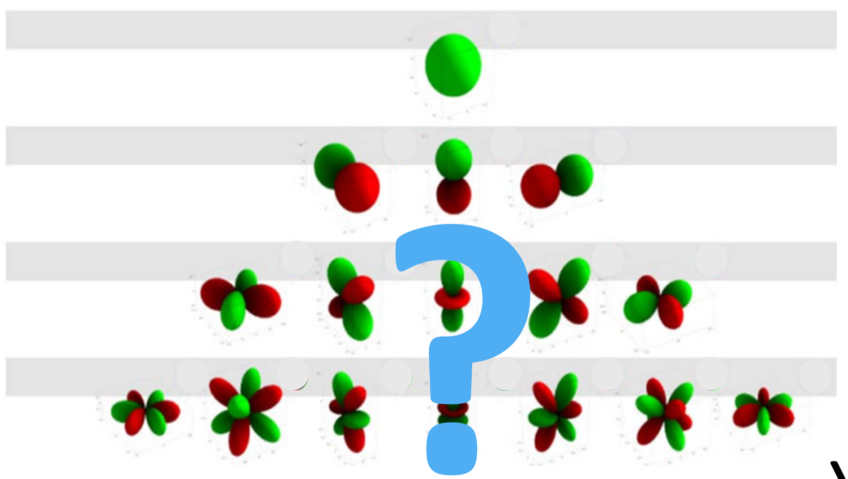
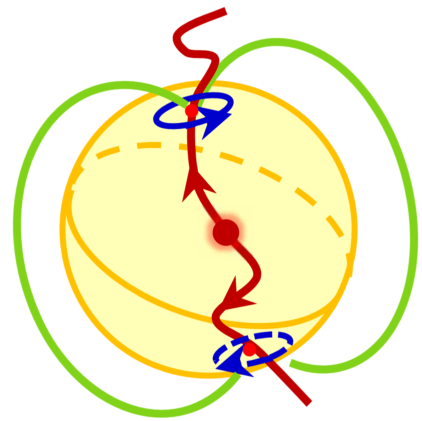
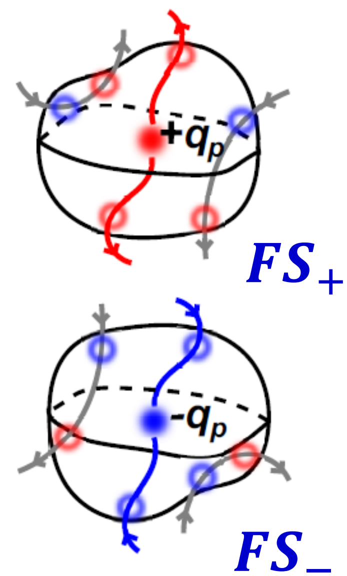
Monopole Harmonic Superconductivity







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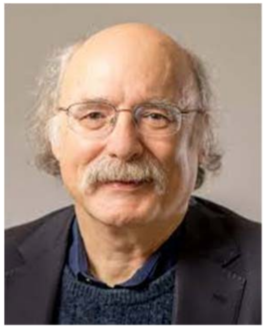

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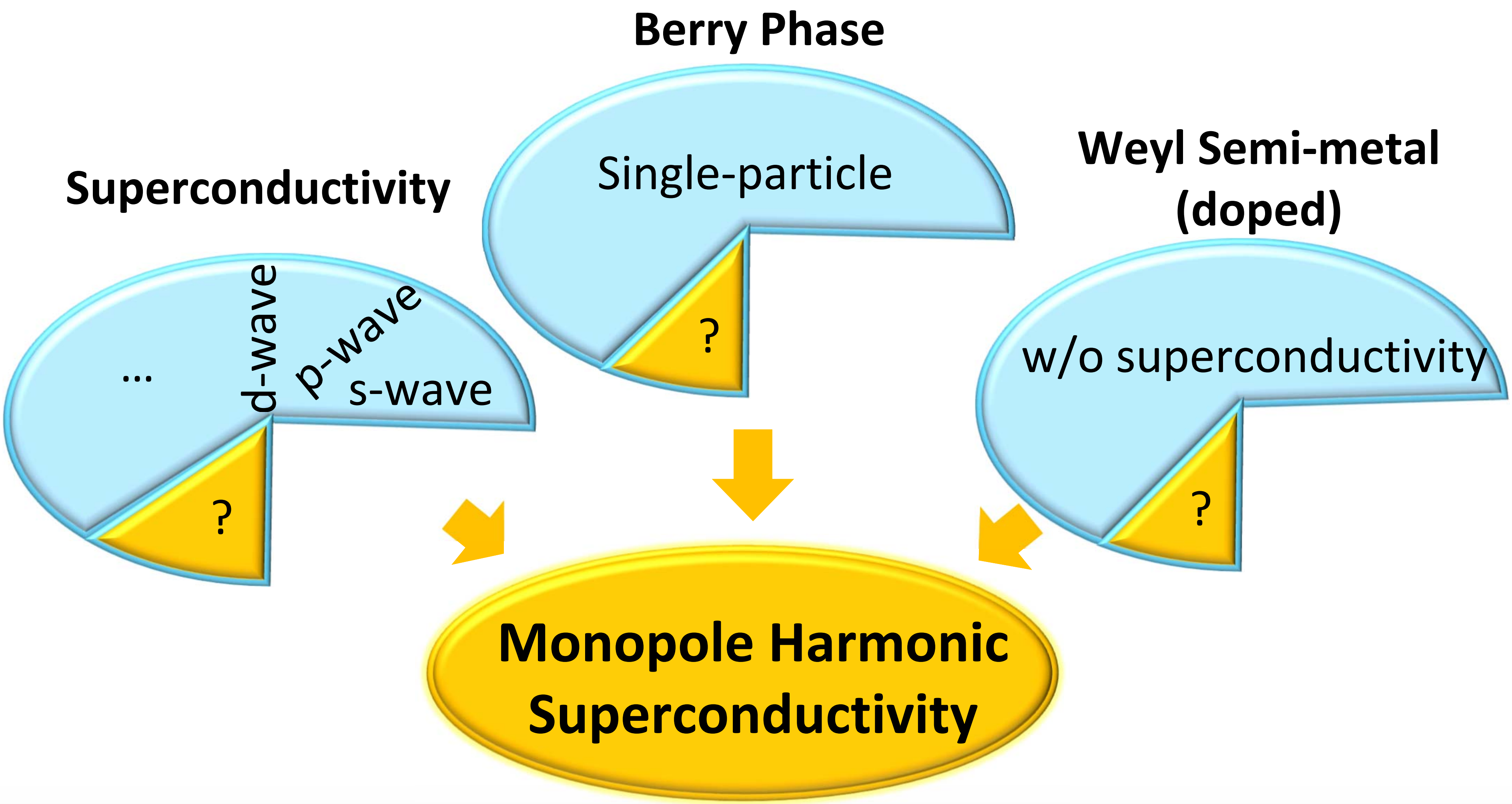
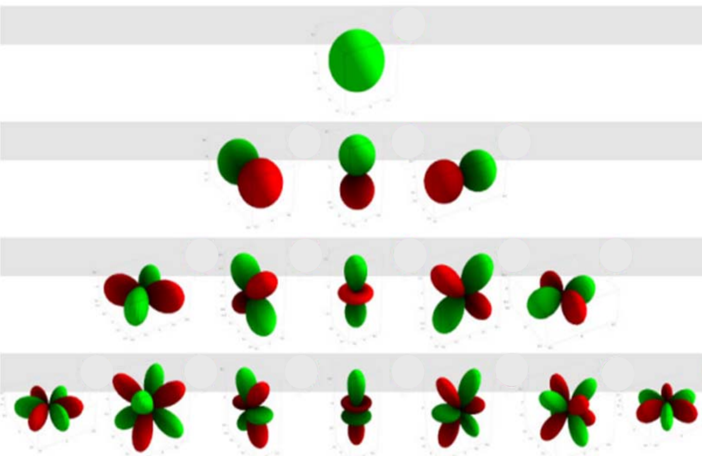

Berry Phase
Single-particle
?
Superconductivity
...
d-wave
p-wave
s-wave
?
Weyl Semi-metal
(doped)
w/o superconductivity
?
Monopole Harmonic
Superconductivity

Superconducting pairing symmetries

$$H_P(\boldsymbol{k}) = \Delta(\boldsymbol{k})P^+(\boldsymbol{k}) + \Delta^*(\boldsymbol{k})P(\boldsymbol{k}); \quad P^+(\boldsymbol{k}) = c_\uparrow^+(\boldsymbol{k})c_\downarrow^+(-\boldsymbol{k}).$$

Gap function: $\Delta(\boldsymbol{k}) = \sum_{l,m} \Delta_{lm} Y_{lm}(\Omega_{\boldsymbol{k}})$



$l = 0$ — s-wave: Hg, Pb, MgB_2 … singlet pairing

$l = 1$ — p-wave: ^3He, Sr_2RuO_4(?), … triplet pairing

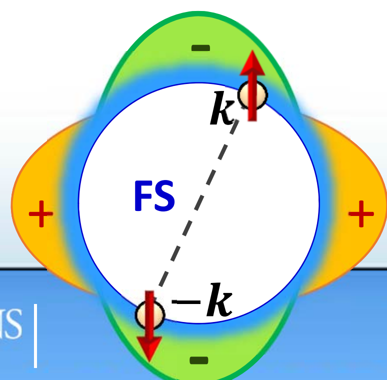
$l = 2$ — d-wave: $CeCu_2Si_2$, $LaBaCuO_4$ … singlet pairing

$l = 3$

⋮

Unconventional superconductivity

$d_{x^2-y^2}$-wave:

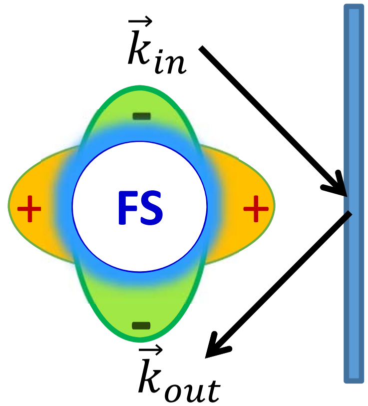


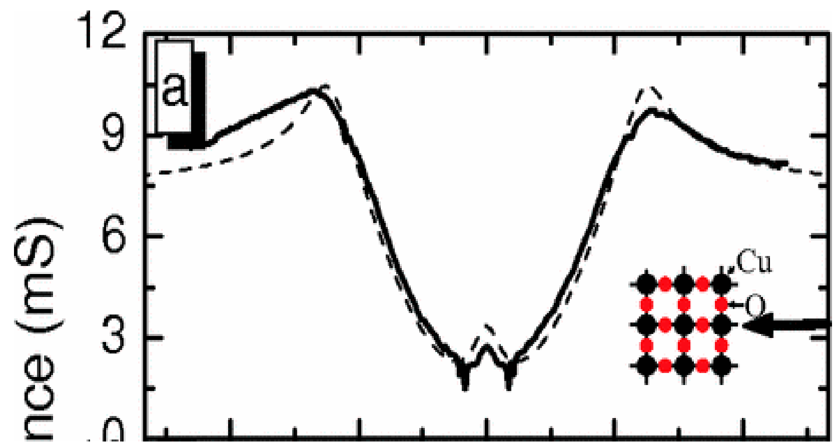
Van Harlingen, RMP (1995);
C. C. Tsuei et al., RMP (2000);
Leggett, RMP (1975); …

Zero-energy Andreev boundary states

[10] boundary:

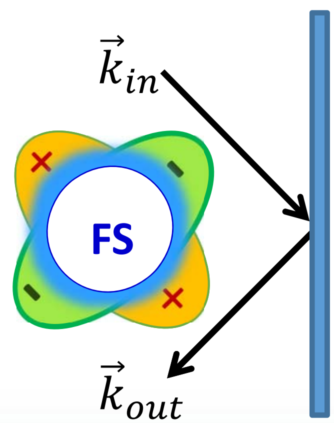
$\Delta\left(\vec{k}_{in}\right) = \Delta\left(\vec{k}_{out}\right)$

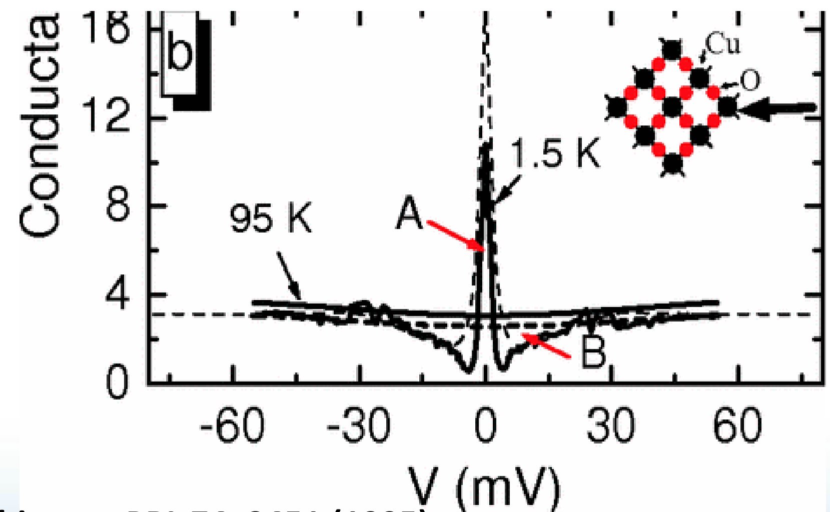




[11] boundary:

$\Delta\left(\vec{k}_{in}\right) = -\Delta\left(\vec{k}_{out}\right)$



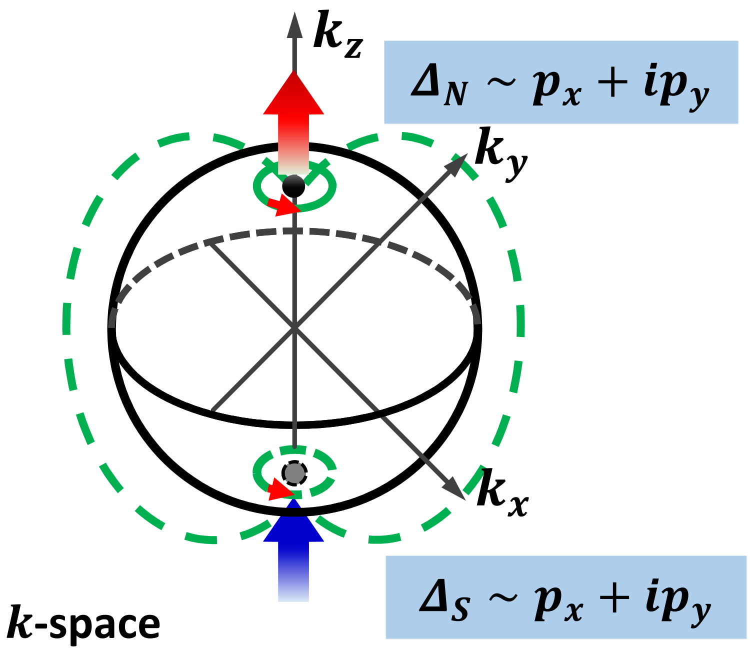


Theory: C.-R. Hu, PRL 72, 1526 (1994), Y. Tanaka, Kashiwaya, PRL 74, 3451 (1995)

Experiments: J. Wei, et al, PRL 81, 2542 (1998); L. H. Greene, et al, PRL 89, 177001 (2002), …

A new topological class of unconventional superconductivity in 3D – monopole harmonic symmetry

Known: ³He-A: $Y_{11}(\hat{\Omega}_k)$

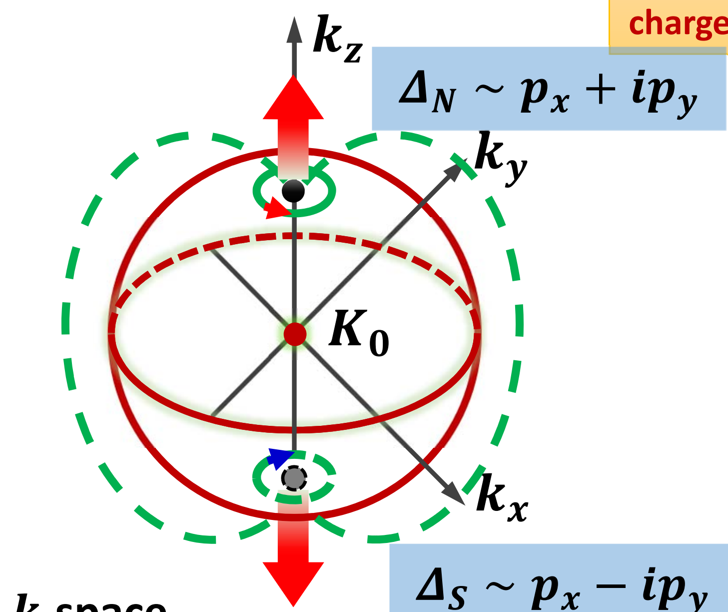


- **Total vorticity over FS**

  $1 - 1 = 0$

Doped Weyl Semi-metal: $Y_{q=1,10}(\hat{\Omega}_k)$

monopole charge

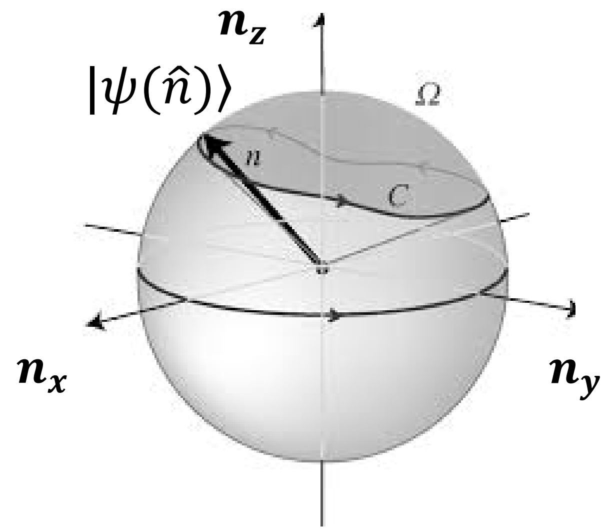


- **Total vorticity over FS**

  $1 + 1 = 2$

YL, FDM Haldane, PRL 120, 067003 (2018).

Single-particle Berry phase - “magnetic” monopole in parameter space



- **Bloch sphere of a 2−level system**

$$(\vec{\sigma}\cdot\hat{n})\,|\hat{n}\rangle=|\hat{n}\rangle \qquad \vec{A}(\hat{n}) = i\left\langle \hat{n}\middle|\vec{\nabla}_n\middle|\hat{n}\right\rangle$$

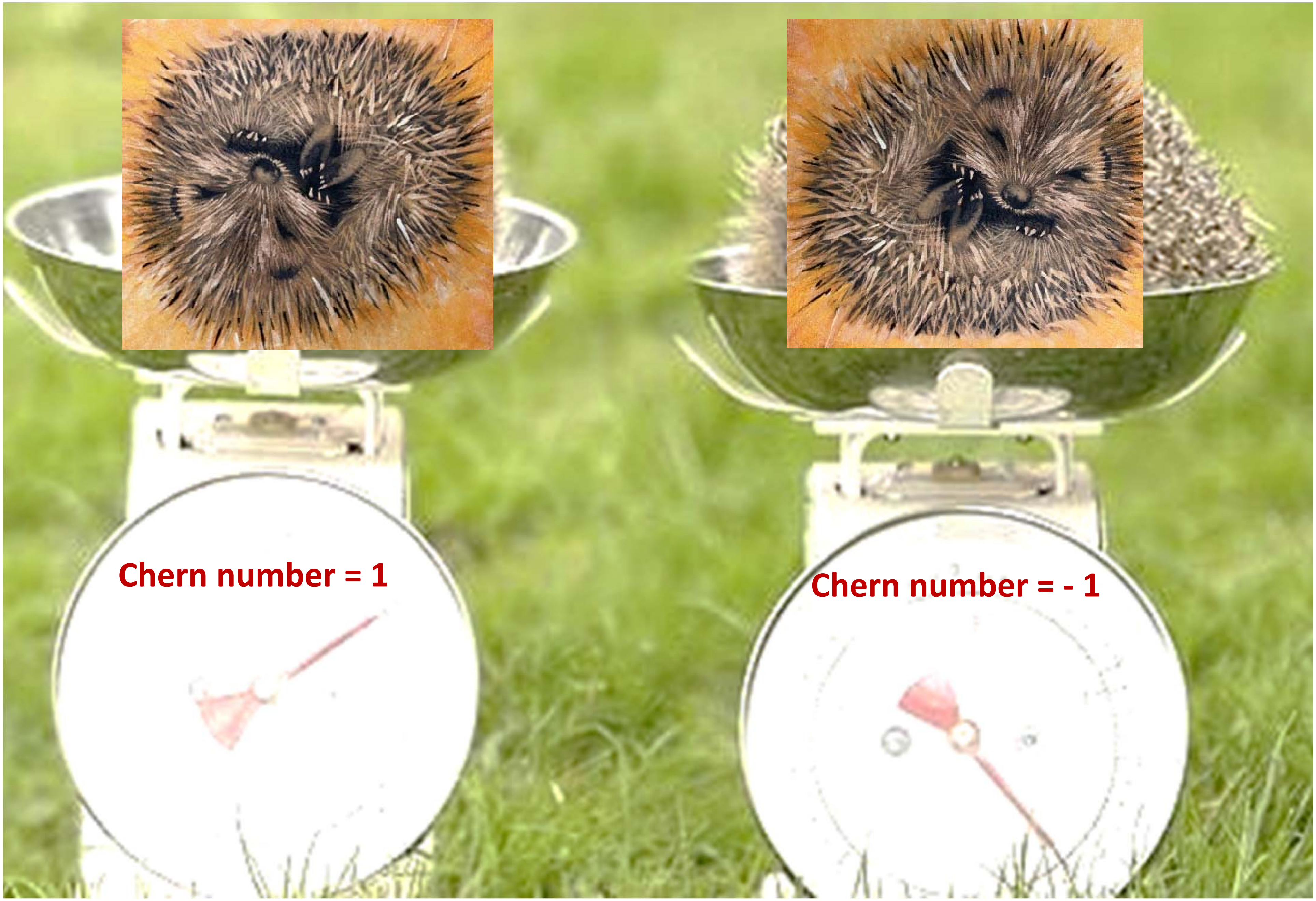
$$\vec{\nabla}_n \times \vec{A} = q\hat{n}$$

- **Adiabatic evolution around a loop:** $|\psi(\hat{n})\rangle = e^{i\gamma}\,|\hat{n}\rangle$

Geometric phase $\gamma = \oint d\vec{n}\cdot\vec{A}$ **=** $\boldsymbol{q}$ $\times$ **enclosed solid angle**

- **Monopole charge** $\boldsymbol{q} = \frac{\mathbf{1}}{\mathbf{2}}$ **-- Chern number** $\boldsymbol{C} = \mathbf{2}\boldsymbol{q} = \mathbf{1}.$

$$\frac{1}{2\pi}\oiint d\hat{n}\cdot\vec{\nabla}_n \times \vec{A}(\hat{n}) = 2q = C$$


Chern number = 1
Chern number = - 1

Berry phase of Cooper pairs – topologically protected nodal pairing

$$|\mathrm{BCS}\rangle = e^{\sum_k f_k c_1^+(\vec{k}) c_2^+(-\vec{k})}|0\rangle$$

$$= \prod_k \left(1 + f_k c_1^+\left(\vec{k}\right) c_2^+\left(-\vec{k}\right)\right)|0\rangle$$

Chern # = -1 $q_1 = -1/2$

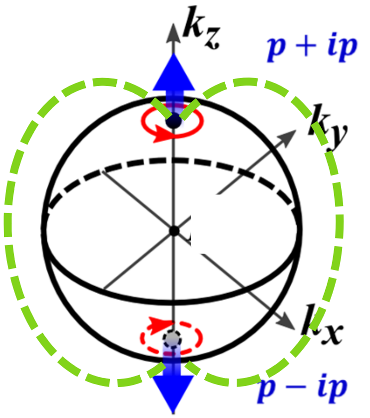
Chern # = 1 $q_2 = 1/2$

$$\frac{f_k}{1+|f_k|^2} = \frac{\Delta_k}{2E_k}$$

Δ_k: gap function

$$\boldsymbol{A}_p(\boldsymbol{k}) = i\langle\Psi_p(\boldsymbol{k})|\boldsymbol{\nabla}_k|\Psi_p(\boldsymbol{k})\rangle \neq 0$$

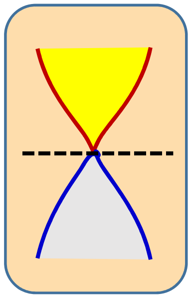
$$|\Psi_p(\boldsymbol{k})\rangle = c_1^+(\boldsymbol{k})c_2^+(-\boldsymbol{k})|0\rangle$$



$$\frac{1}{2\pi}\oiint d\hat{k}\cdot\vec{\nabla}_k\times\vec{A}_p\left(\hat{k}\right) = 2q_p$$

	Pair Berry phase	Phase of $\Delta\left(\vec{k}\right)$	Node protection
Spherical harmonics	trivial	well-defined	pairing mechanism total vorticity =0
Monopole harmonics	**monopole charge q_p**	**Not well-defined**	**topological protected total vorticity $2q_p$**

Weyl semi-metal



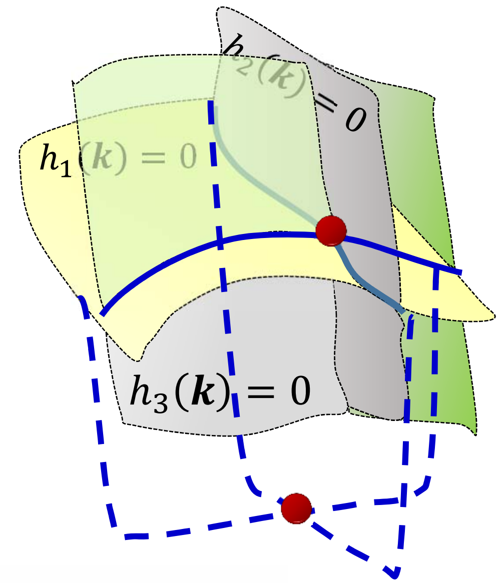
- **A general two-band system in 3D (without any symmetry)**

$$H(\boldsymbol{k}) = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} = h_0(\boldsymbol{k})I + \sum_{i=1}^{3} h_i(\boldsymbol{k})\sigma_i$$

$$E_{\pm}(\boldsymbol{k}) = h_0(\boldsymbol{k}) \pm \sqrt{\sum_{i=1}^{3} h_i^2(\boldsymbol{k})}$$

$$\sum_{i=1}^{3} h_i^2(\boldsymbol{k})\Big|_{\boldsymbol{k}\,=\,\boldsymbol{K}_0} = 0$$

Gap closing

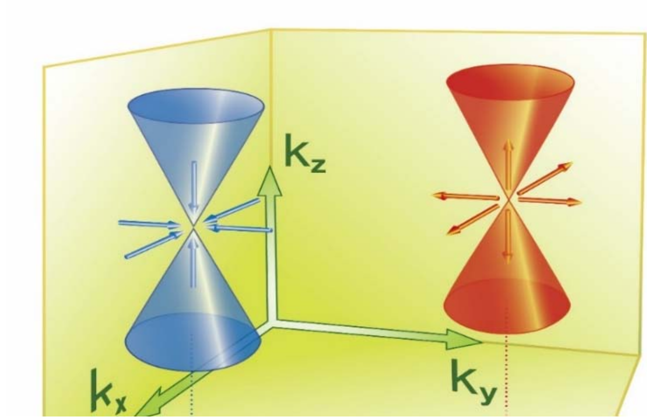


- **Linearized dispersion near isolated nodes ($det\left(\frac{\partial h_i}{\partial k_j}\right) \neq 0$)**

$$H(\boldsymbol{K}_0 + \boldsymbol{k}) = \pm\hbar v_F \boldsymbol{k}\cdot\boldsymbol{\sigma}$$

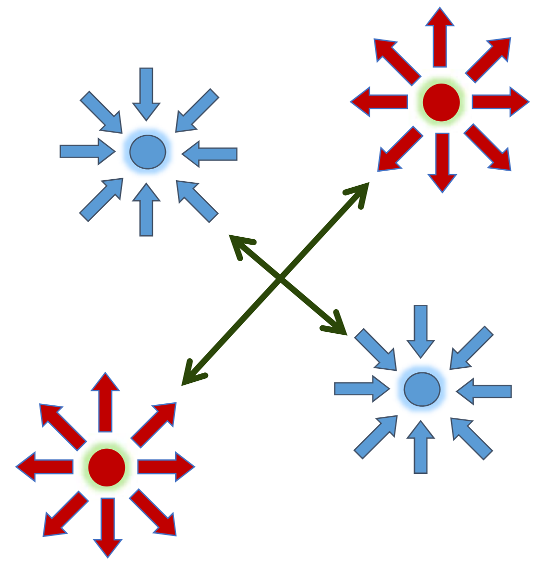
Weyl Node

- **"Weyl fermions" w/ $\pm$ chiralities appear in pairs (Nielsen-Ninomiya)**



Time-reversal (TR) and Inversion

TR, no Inversion



- **TR-related Weyl points have the same chirality.**

$$\vec{\boldsymbol{k}} \to -\vec{\boldsymbol{k}}, \vec{\boldsymbol{\sigma}} \to -\vec{\boldsymbol{\sigma}}$$

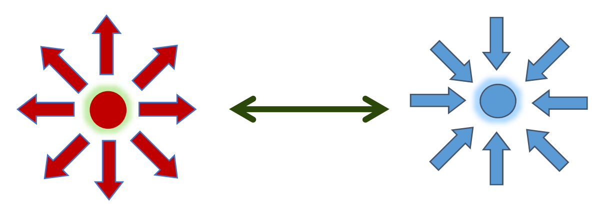
$$H\left(\vec{K}+\vec{k}\right)=\vec{k}\cdot\vec{\sigma} \qquad H\left(-\vec{K}+\vec{k}\right)=\vec{k}\cdot\vec{\sigma}$$

Minimal 4 Weyl points

- **Inversion-related Weyl points have opposite chiralities.**

$$\vec{\boldsymbol{k}} \to -\vec{\boldsymbol{k}}, \vec{\boldsymbol{\sigma}} \to \vec{\boldsymbol{\sigma}}$$

Inversion, no TR



$$H\left(\vec{K}+\vec{k}\right)=\vec{k}\cdot\vec{\sigma} \quad H\left(-\vec{K}+\vec{k}\right)=-\vec{k}\cdot\vec{\sigma}$$

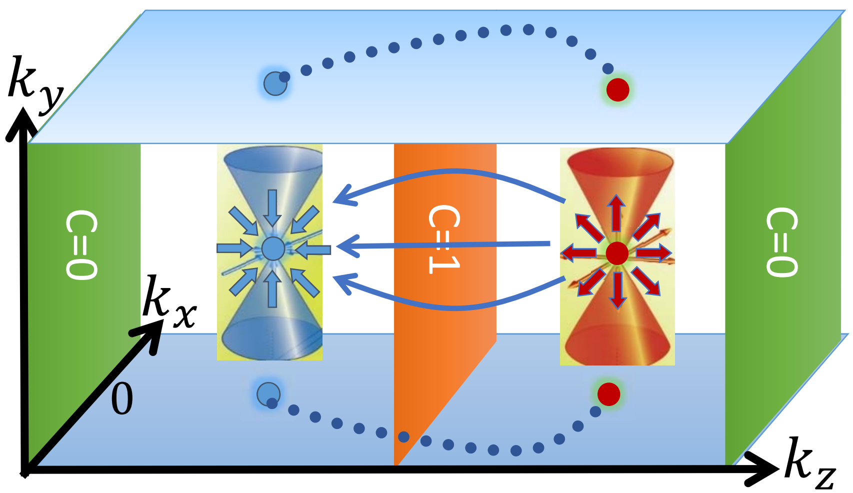
Minimal 2 Weyl points

- **Need to break at least one of TR and inversion symmetries.**

Weyl points as monopole pairs (k-space)

- Chern # $C(k_z)$ defined for each 2D crossing section at a fixed $\mathrm{k_z}$

$$\boldsymbol{A}(\boldsymbol{k}) = i\left\langle \psi_{-}(\boldsymbol{k}) \middle| \vec{\partial}_k \middle| \psi_{-}(\boldsymbol{k}) \right\rangle \qquad C(k_z) = \oiint \frac{d^2\vec{k}}{2\pi}\Omega_z\left(\vec{k}\right)$$

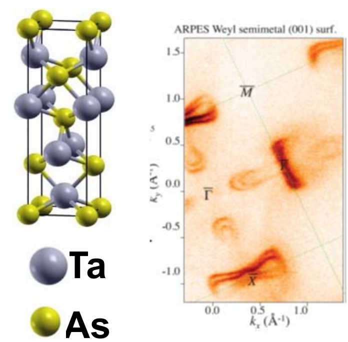


Theory: Wan, Turner, Vishwanath, Savrasov, PRB (2011); …
(Murakami 2007)

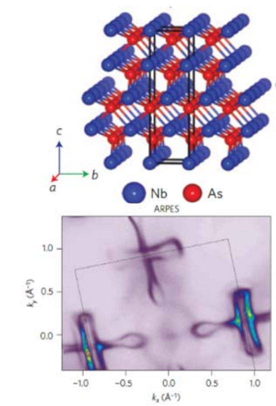
- Fermi arcs connect projections of Weyl point pairs on the surface

Observed in TR invariant Weyl semi-metals

TaAs



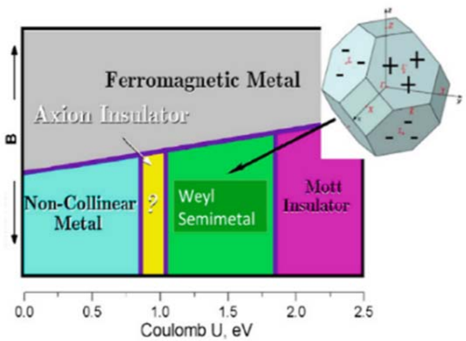
NbAs

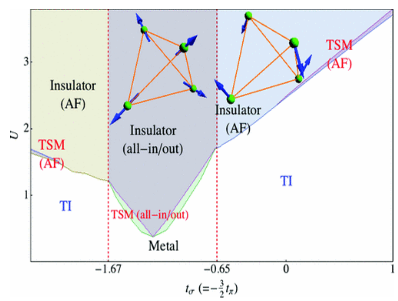


ARPES: Hasan's group, Ding's group (2015); …

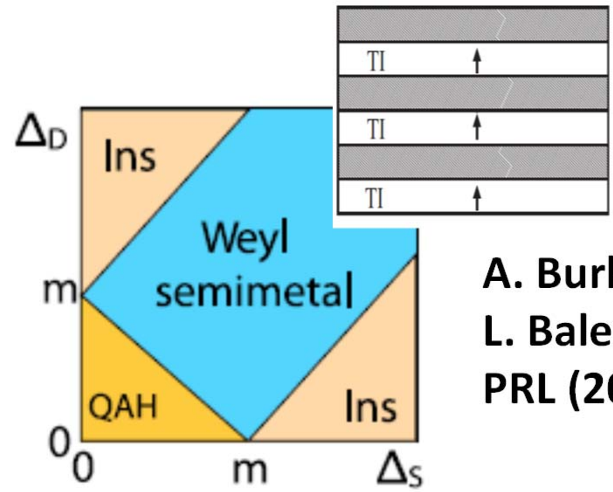
TR breaking Weyl semi-metals

- Magnetism and topology

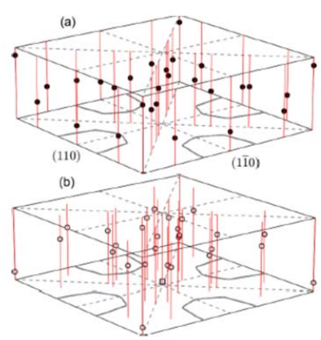




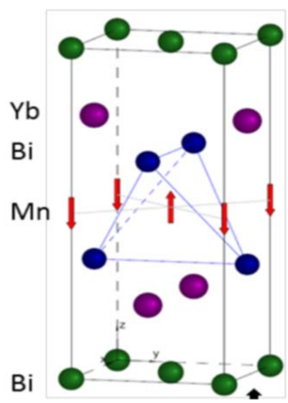
Wan, Turner, Vishwanath, Savrasov, PRB (2011),
Witczak-Krempa, Kim, PRB (2012)



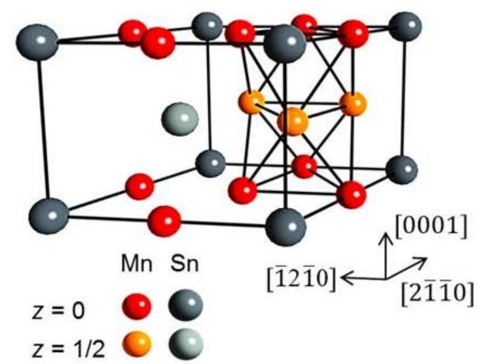
A. Burkov,
L. Balents
PRL (2011)



bcc Fe
Gosalbez-Martinez,
Souza, Vanderbilt
PRB (2015)



$YbMnBi_2$
Cava's group
arXiv:1507.04847
…



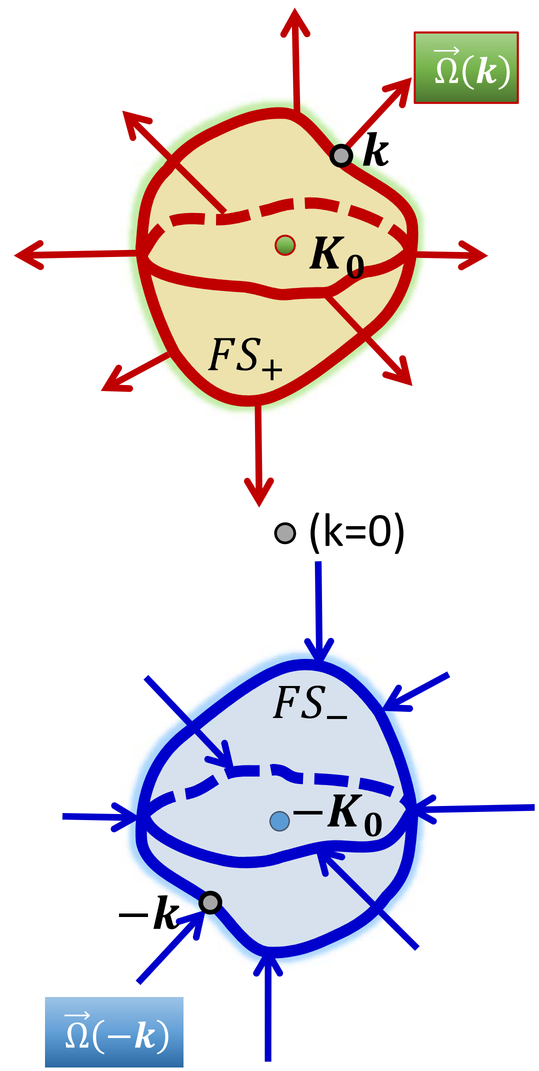
Mn_3Sn
S. Nakatsuji's group
Nature 2015

First principle:
C. Felser's group (2013)
B. Yan's group (2016)

L. Balents' group (2017)

Doped TR-breaking Weyl semi-metal (with parity)

- **Fermi surfaces appear at $\mu \neq 0$.**
- **Fermi surfaces generally not spherical.**
- **Inversion-related Fermi surfaces carry the opposite Chern #'s.**



odd $\vec{A}(\boldsymbol{k}) = i\langle \boldsymbol{k}|\nabla_{\boldsymbol{k}}|\boldsymbol{k}\rangle \quad \vec{A}(\boldsymbol{k}) = -\vec{A}(-\boldsymbol{k})$

even $\vec{\Omega}(\boldsymbol{k}) = \vec{\Omega}(-\boldsymbol{k})$

odd $\oiint_{FS_+} d\vec{S}_k \cdot \vec{\Omega}(\boldsymbol{k}) = -\oiint_{FS_-} d\vec{S}_k \cdot \vec{\Omega}(\boldsymbol{k})$

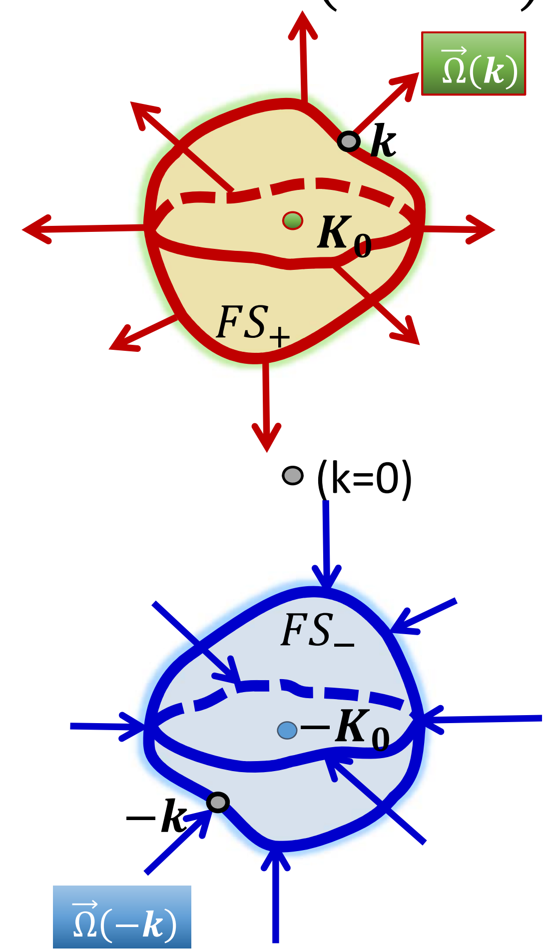
Pair Berry phase from Fermi surface topology

- **Inter-Fermi surface pairing is favored (common center-of-mass momentum)**

$$\Psi_p\left(\vec{k}\right) = |k\rangle_+ \otimes |-k\rangle_-$$

$$\vec{A}_p\left(\vec{k}\right) = i\left\langle \Psi_p(\vec{\boldsymbol{k}}) \middle| \vec{\partial}_k \middle| \Psi_p(\vec{\boldsymbol{k}}) \right\rangle$$

$$|k\rangle_+ = \alpha_+^+\left(\vec{K}_0 + \vec{k}\right)|0\rangle$$



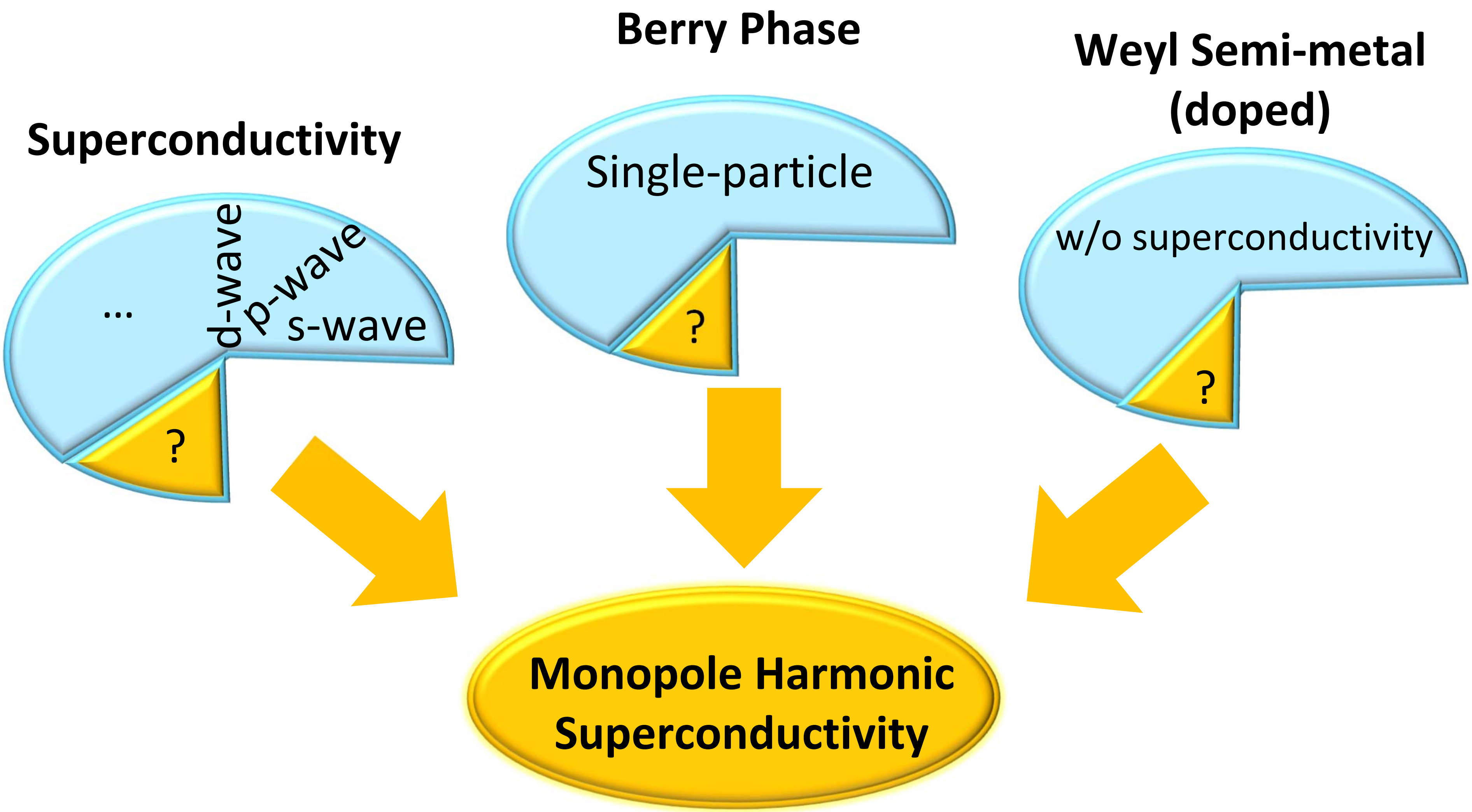
$$|-k\rangle_- = \alpha_-^+\left(-\vec{K}_0 - \vec{k}\right)|0\rangle$$

- **Contributions from $|\boldsymbol{k}\rangle_+$ and $|-\boldsymbol{k}\rangle_-$ add up.**

$$\boldsymbol{A}_P(\boldsymbol{k}) = i\left\langle \vec{k}_+ \middle| \vec{\partial}_k \middle| \vec{k}_+ \right\rangle + i\left\langle -\vec{k}_- \middle| \vec{\partial}_k \middle| -\vec{k}_- \right\rangle$$
$$= \boldsymbol{A}_+(\boldsymbol{k}) - \boldsymbol{A}_-(-\boldsymbol{k}) = 2\boldsymbol{A}_+(\boldsymbol{k})$$

$$\frac{1}{2\pi}\oiint_{\boldsymbol{S}_+} \boldsymbol{dS_k}\cdot\boldsymbol{\Omega_p}(\boldsymbol{k}) = \frac{2}{2\pi}\oiint_{FS_+} \boldsymbol{dS_k}\cdot\boldsymbol{\Omega}(\boldsymbol{k})$$

- **Pair monopole charge** $q_p = 2q = 1$



Previous work on superconducting Weyl semimetals:

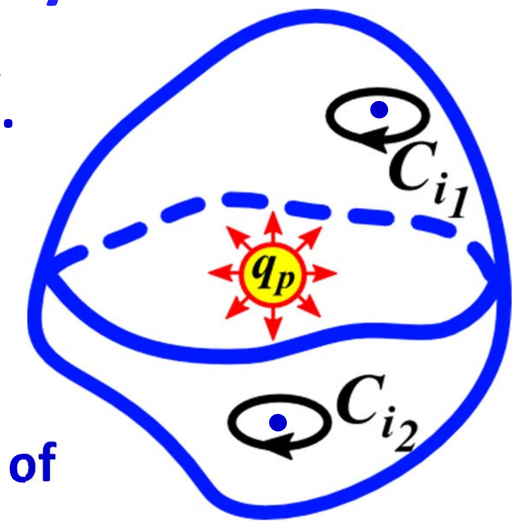
- **Meng and Balents (2012);**
- **Cho, Bardarson, Lu, Moore (2012);**
- **Hosur, Dai, Fang, Qi (2014)…**

Pair Berry phase leads to nodal vorticity

- **General pairing Hamiltonian: smooth w.r.t. $\vec{k}$.**

$$H_P\left(\vec{k}\right) = \Delta\left(\vec{k}\right) P^{+}\left(\vec{k}\right) + \Delta^{*}\left(\vec{k}\right) P\left(\vec{k}\right)$$

$$P^{+}\left(\vec{k}\right) = \alpha_{+}^{\dagger}\left(\vec{K}_0 + \vec{k}\right) \alpha_{-}^{\dagger}\left(-\vec{K}_0 - \vec{k}\right)$$



- **The gap nodes of $\Delta(\boldsymbol{k})$ possess total vorticity of $2q_p$ on S_+**

1) Gauge invariant "velocity". Performing integrals along small loops around all nodes .

$$\vec{v}\left(\vec{k}\right) = \vec{\nabla}_k \phi\left(\vec{k}\right) - \vec{A}_p\left(\vec{k}\right) \Rightarrow \frac{1}{2\pi}\oint_{C_i} d\vec{k}\cdot\vec{v} = g_i$$

2) Reverse the direction of each loop and apply Stokes theorem.

$$-\sum_i g_i = \frac{1}{2\pi}\sum_i \oint_{\bar{C}_i} d\vec{k}\cdot\vec{v} = -\oiint \frac{d\vec{k}}{2\pi}\cdot(\vec{\nabla}_k \times \vec{A}_p) = -2q_p.$$

YL, FDM Haldane, PRL 120, 067003 (2018).
Related previous work: Murakami, Nagaosa (2003);
H. Yao, private communication.

Monopole harmonics instead of spherical harmonics

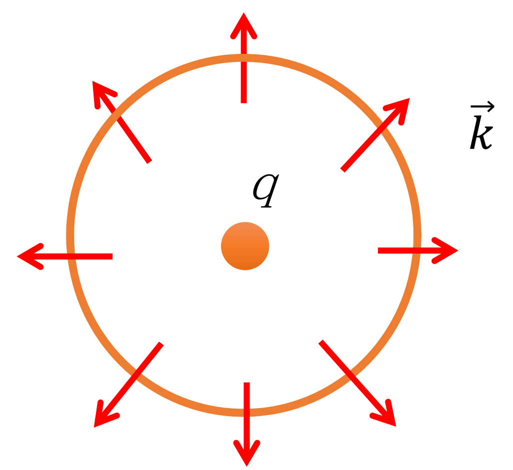
- **Angular momentum eigenstates $Y_{q;jj_z}(\hat{k})$ in the presence of a monopole with charge q.**

Yang and Wu 1976, Haldane 1983

$$\vec{L} = \hbar\vec{k} \times \left(-i\vec{\partial}_k - \frac{1}{k}\vec{A}(\hat{k})\right) - q\hbar\hat{k}$$

$$L^2 Y_{q;jj_z}(\hat{k}) = \hbar^2 j(j+1)\, Y_{q;jj_z}(\hat{k})$$

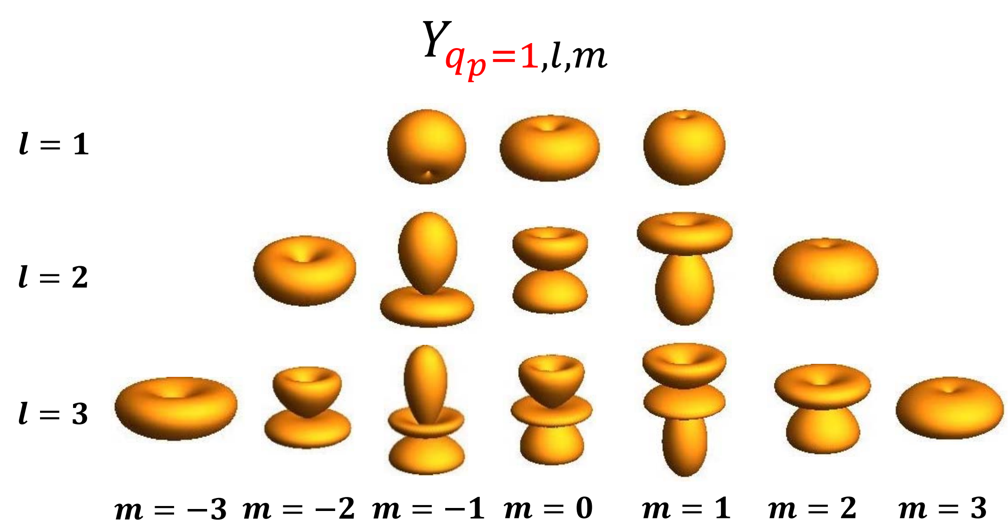
$$L_z Y_{q;jj_z}(\hat{k}) = \hbar j_z Y_{q;jj_z}(\hat{k}), j \geq |q|$$



- **Example:**

$$Y_{q_p=1,l=1,m} = u^2, uv, v^2$$

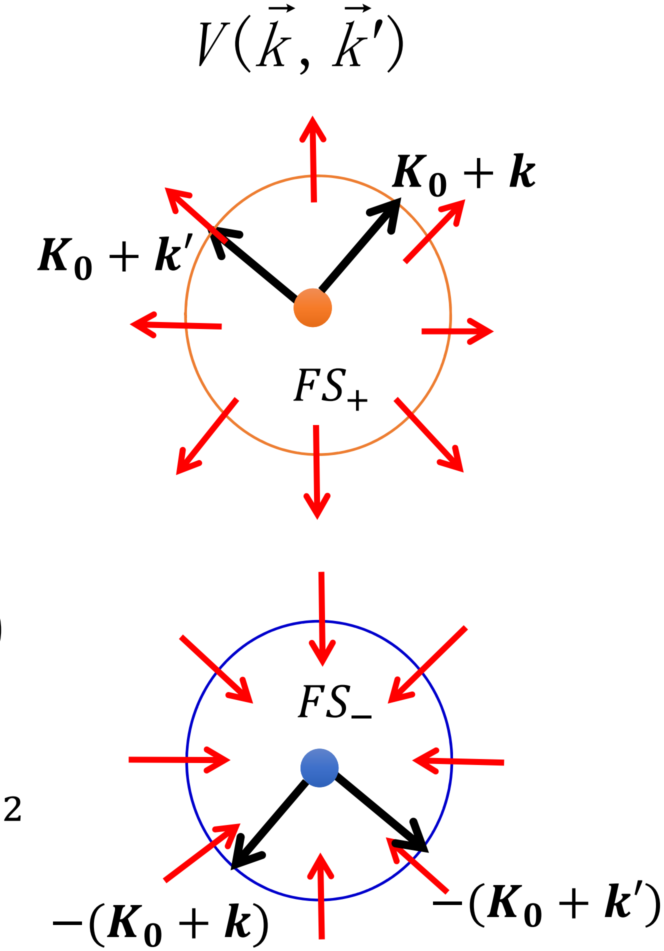
$$\begin{pmatrix} u_k \\ v_k \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta_k}{2} \\ \sin\frac{\theta_k}{2} e^{i\phi_k} \end{pmatrix}$$



Monopole Harmonic Pairing

- If $FS_{\pm}$ can be approximated by spheres, partial wave decomposition of bare scattering before projection.

$$V\left(\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{k}}'\right)=\sum_{lm}4\pi g_l\, Y^*_{lm}(\widehat{\boldsymbol{k}})Y_{lm}(\widehat{\boldsymbol{k}}')$$



- After projection onto $\mathrm{FS}_{\pm}$

$$\widetilde{H}_{pair}=\sum_{\vec{k},\vec{k}'}\tilde{V}\left(\vec{\boldsymbol{k}},\vec{\boldsymbol{k}}'\right)P^{\dagger}\left(\vec{\boldsymbol{k}}\right)P\left(\vec{\boldsymbol{k}}'\right)+h.c.$$

$$\tilde{V}\left(\vec{\boldsymbol{k}},\vec{\boldsymbol{k}}'\right)=\sum_{jm}4\pi\,\tilde{g}_j Y^*_{-1,jm}(\widehat{\boldsymbol{k}})Y_{-1,jm}(\widehat{\boldsymbol{k}}')$$

$$\widetilde{g_j}=\frac{1}{2j+1}\sum_{l=j,j\pm1}(2l+1)g_l|\langle l0;11|j1\rangle|^2$$

- In general, $\Delta(\boldsymbol{k})=|\Delta(\vec{k})|\sum_{j\geq q_p,m}c_{jm}Y_{q_p;jm}(\widehat{\boldsymbol{k}})$.

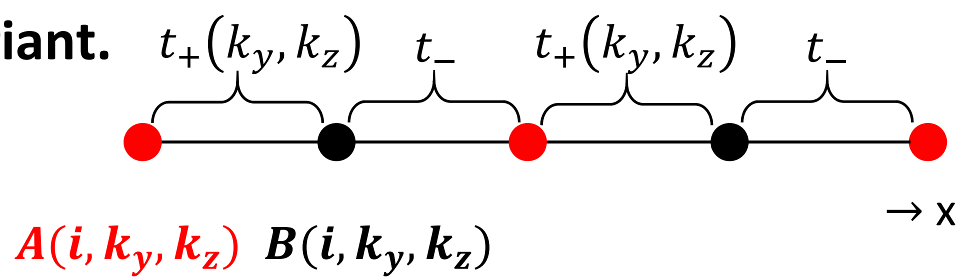
Example: Weyl semi-metal of spinless fermions

$$H_K = \sum_{\vec{k}} c_a^\dagger\left(\vec{k}\right)\{V(k_y)\sigma_3 + \left[t_- \cos(2k_x) + t_+(k_y,k_z)\right]\sigma_1$$
$$+ \sin(2k_x)\sigma_2 - \mu\}_{ab} c_b\left(\vec{k}\right) + h.c.$$

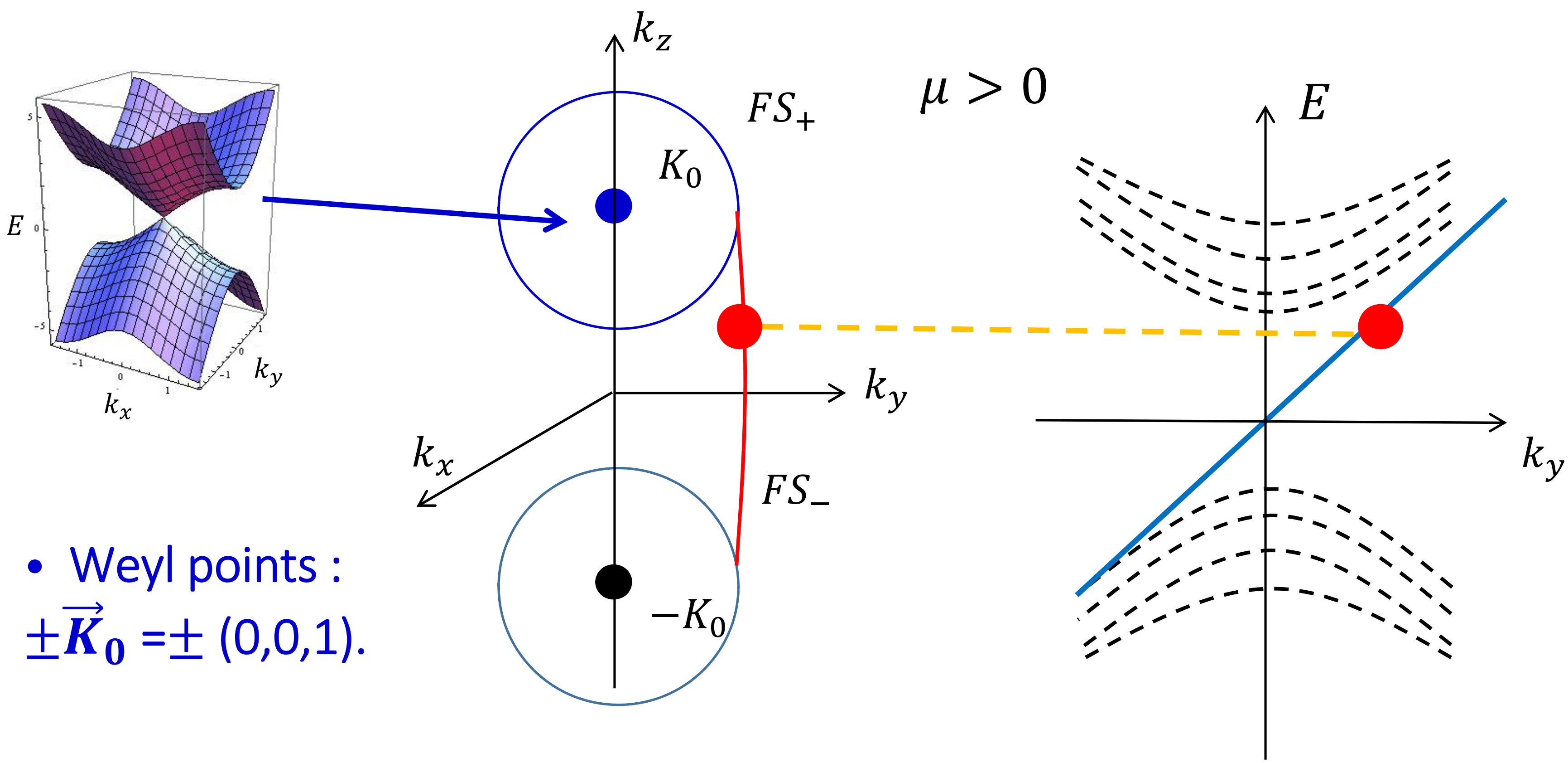
Modified Rice-Mele model: Pavan Hosur; FDM Haldane.

$$V(k_y) = 2k_y, \quad t_+(k_y,k_z) = -(k_y^2 + k_z^2), \quad t_- = 1.$$

- σ_z**-eigenstates refer to A-, B-sublattice.**
- **Inv. operation A⟷B** $(\boldsymbol{\sigma_1 \longrightarrow \sigma_1, \sigma_{2,3} \longrightarrow -\sigma_{2,3}})$ **and** $\boldsymbol{k \rightarrow -k}$.
- **TR** $(\boldsymbol{\sigma_{1,3} \longrightarrow \sigma_{1,3}, \sigma_2 \longrightarrow -\sigma_2})$ **and** $\boldsymbol{k \rightarrow -k}$.
- **TR breaking but inversion invariant.**



Weyl points, helical Fermi surfaces, surface modes



- Weyl points :

$\pm\vec{K}_0 = \pm\ (0,0,1)$.

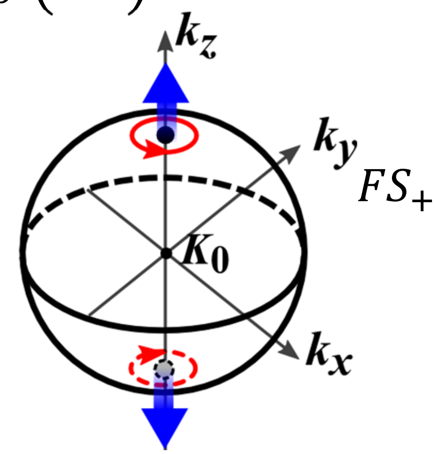
- $\boldsymbol{FS_\pm}$ carry non-zero monopole charges $\pm \boldsymbol{q} = \pm\ \frac{1}{2}$.
- Chiral surface Fermi arcs (the yz–boundary plane) $-\boldsymbol{K_0} < \boldsymbol{k_z} < \boldsymbol{K_0}$

Universal nodal vorticity - regardless of pairing patterns

$$H_\Delta\left(\vec{k}\right) = \sum_{\vec{k}} c_a^\dagger\left(\vec{k}\right)\{2i\Delta_x \sin(2k_x) + 2i\Delta_y \sin k_y\, \sigma_1\}_{ab} c_b^\dagger\left(-\vec{k}\right) + h.c.$$

A) If $\Delta_y = -i\Delta_x$, $p + ip$ at north pole and $p - ip$ at south pole.

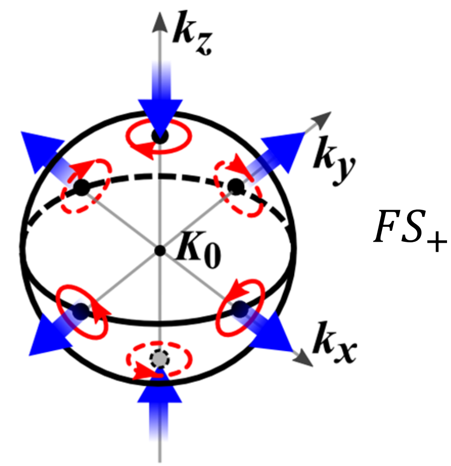
- **1+1=2 (fundamental nodes)**



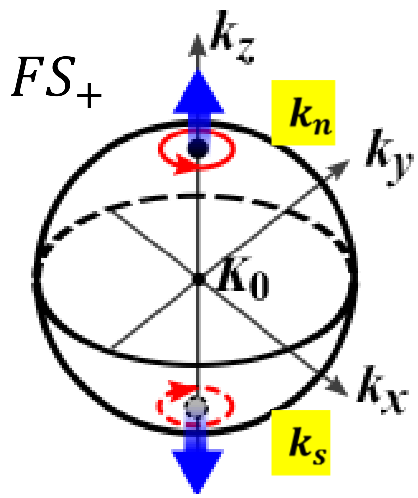
B) If $\Delta_y = i\Delta_x$, $p - ip$ at north pole and $p + ip$ at south pole contributing vorticity -2;

Four nodes appear around the equator contributing vorticity +4.

- **-1-1+1+1+1+1=2**



Surface spectra: Majorana meets Weyl

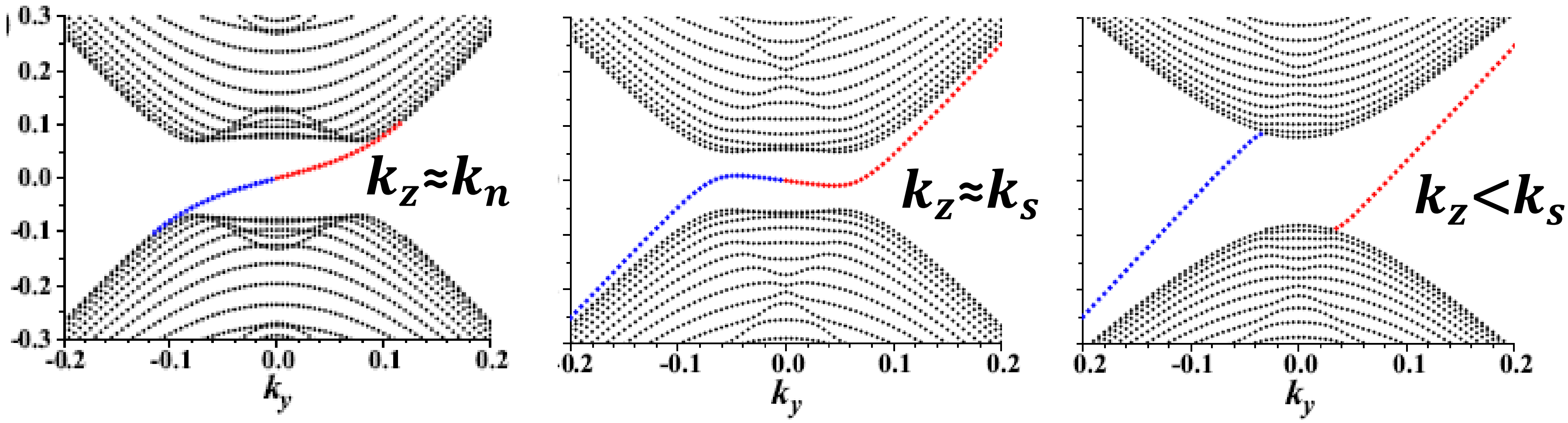


$$\Delta_{\mathbf{y}} = -\mathbf{i}\Delta_{\mathbf{x}}$$

- **Majorana modes : positive → negative chirality as k_z from N → S-hemisphere.**

- **Connect to surface modes from the Weyl band structure.**

- **Chirality : 0** $(k_z > k_n)$ **→ 1** $(k_n > k_z > k_s)$ **→ 2** $(k_z < k_s)$ **.**



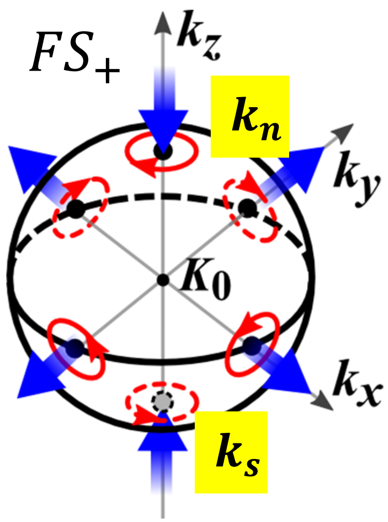
$+1$ $\qquad$ $+1 - 1 + 1 = +1$ $\qquad$ $+2$

YL, FDM Haldane, PRL 120, 067003 (2018).

Related previous work based on mirror symmetry:

SA Yang, H. Pan, F. Zhang (2014); Lu, Yada, Sato, Tanaka (2015)

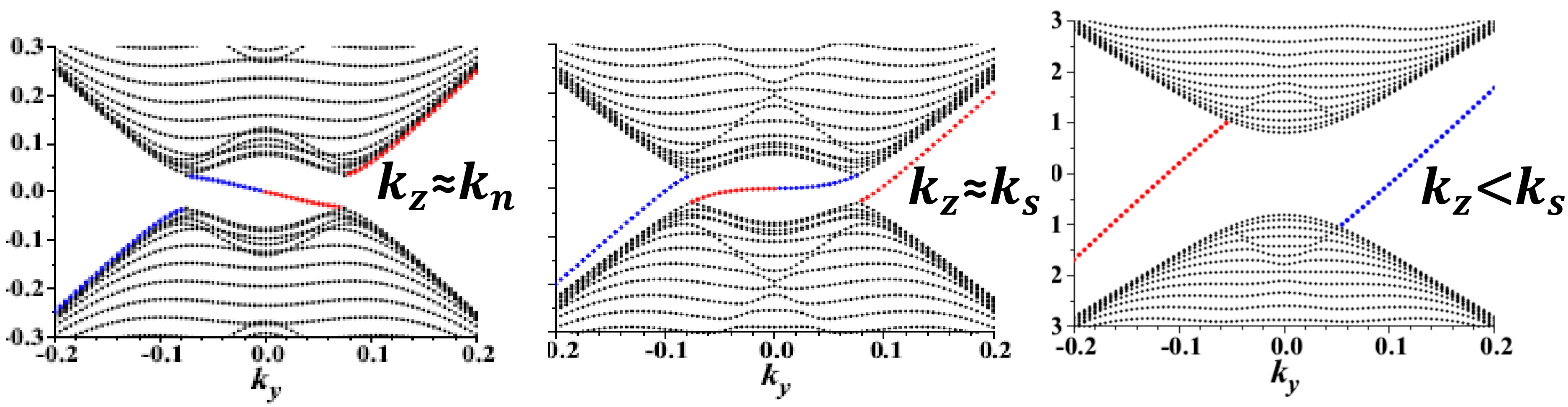
Surface spectra: Majorana meets Weyl



$$\Delta_y = i\Delta_x$$

- Majorana modes: negative → positive chirality as k_z from N → S-hemisphere.

- Chirality : 0 $(k_z > k_n)$ → 1 (north herm-sphere) → 3(south hemi-sphere) → 2 $(k_z < k_s)$



YL, FDM Haldane, PRL 120, 067003 (2018).

Low energy excitations determined by high energy topo.

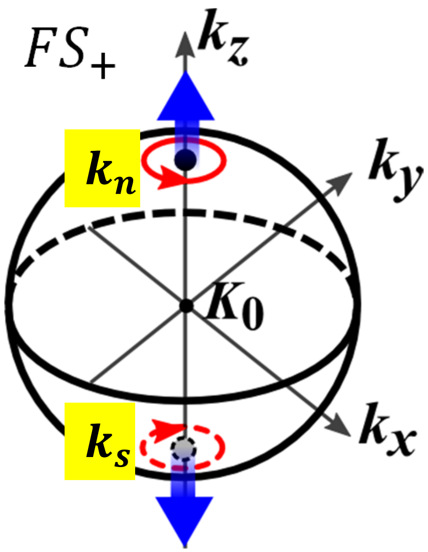
- High energy scale: band structure Weyl nodes.

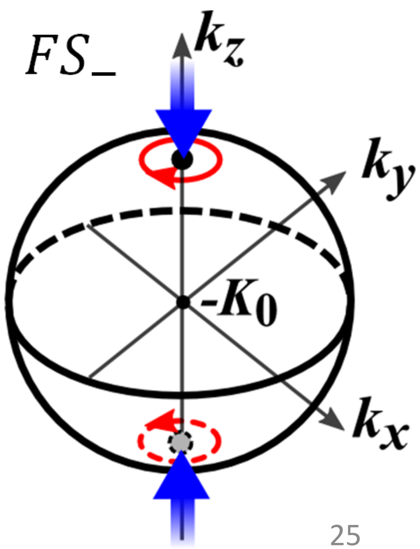
- Low energy physics: emergent Majorana nodes on $\boldsymbol{FS_\pm}$ in the Nambu spinor Rep.

$$H_{\text{eff}} = \begin{bmatrix} v_F(k_z - k_n) & |\Delta|(k_x + ik_y) \\ |\Delta|(k_x - ik_y) & -v_F(k_z - k_n) \end{bmatrix}$$

- Vortex of $\Delta\left(\vec{k}\right)$ on FS $\longleftrightarrow$ Majorana-Weyl monopole in the $\vec{k}$-space

- Topology threads all the energy scales





Half-integer angular momentum pairing

- Integer partial-wave symmetries: $\boldsymbol{Y_{q,jm}(\hat{\Omega}_k)}$

Conventional: $\boldsymbol{q = 0, j = 0}$ Unconventional: $\boldsymbol{q = 0, j \neq 1, 2, \ldots}$

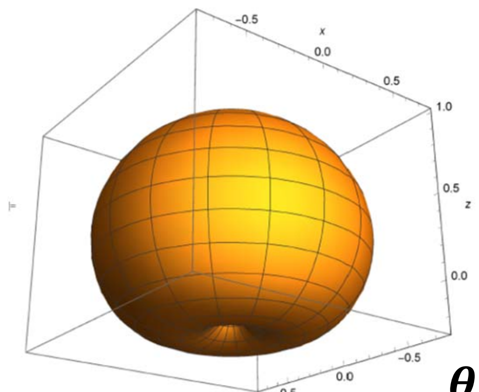
Monopole harmonics (integer $\boldsymbol{q = 1, 2, ..}$): $\boldsymbol{j = |q|, |q| + 1, \ldots}$.

- Half-integer monopole charge q: spinor representation of SU(2) group.

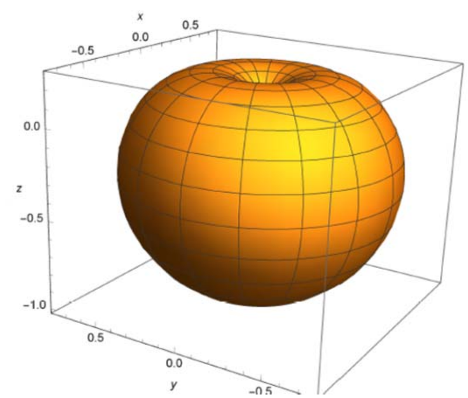
$$Y_{q;j,j_z}(\theta,\varphi) = \sqrt{\frac{2j+1}{4\pi}}\, e^{i(q+j_z)\varphi} d^{\,j}_{m,-q}(\theta), \qquad j \geq |q|.$$

Example: $\boldsymbol{q = -\frac{1}{2}}$.

$\boldsymbol{j = \frac{1}{2}, j_z = \pm\frac{1}{2}}$



$$\boldsymbol{u} \equiv Y_{-\frac{1}{2};\frac{1}{2},\frac{1}{2}}(\theta,\varphi) = \boldsymbol{\cos\frac{\theta}{2}}$$

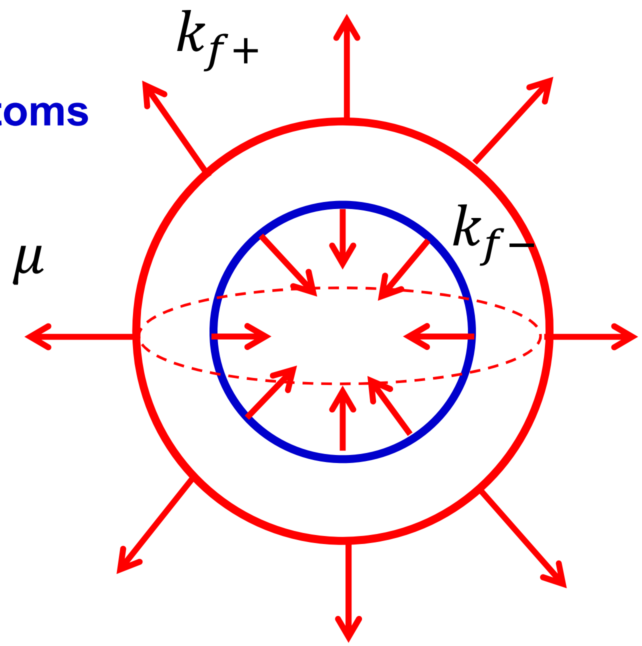


$$\boldsymbol{v}^* \equiv Y_{-\frac{1}{2};\frac{1}{2},-\frac{1}{2}}(\theta,\varphi) = \boldsymbol{\sin\frac{\theta}{2}\, e^{-i\phi}}$$

3D Weyl type spin-orbit coupling

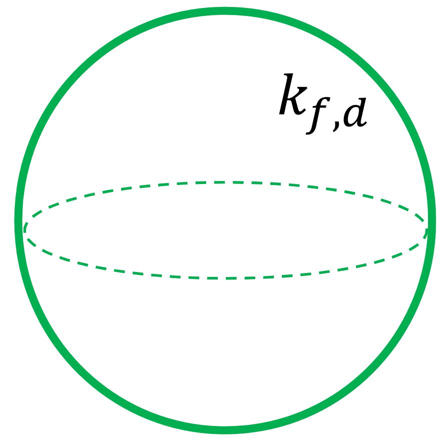
- 3D synthetic Weyl type spin-orbit coupling **in cold atoms**

$$H_c^0(\boldsymbol{k}) = c_\alpha^+(\boldsymbol{k})\left(\frac{k^2}{2m} - \boldsymbol{\lambda_{soc}\sigma}\cdot\boldsymbol{k}\right)_{\alpha\beta} c_\beta(\boldsymbol{k}) - \mu$$



- Split-Fermi surfaces with opposite monopole charges $\boldsymbol{q} = \pm\frac{\boldsymbol{1}}{\boldsymbol{2}}$

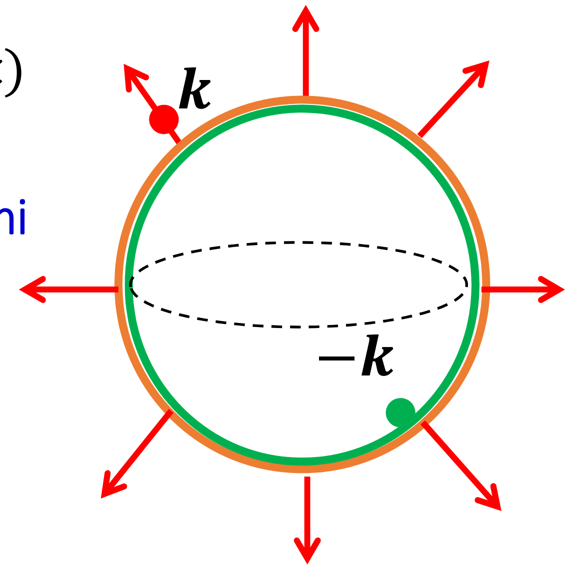
- Another spinless fermion with Fermi surface matching with a split one, e.g. $\boldsymbol{k_{f,d}} = \boldsymbol{k_{f+}}$



$$H_d^0(\boldsymbol{k}) = \frac{k^2}{2m}\, d^+(\boldsymbol{k})d(\boldsymbol{k})$$

Paring between two Fermi surfaces with $\boldsymbol{C} = \mathbf{1}$ and $\boldsymbol{C} = \mathbf{0}$

$$H_\Delta(\boldsymbol{k}) = \Delta_\alpha(\boldsymbol{k}) c_\alpha^+(\boldsymbol{k}) d^+(-\boldsymbol{k}) + \Delta_\alpha^*(\boldsymbol{k}) d(\boldsymbol{k}) c_\alpha(-\boldsymbol{k})$$



- Pairing between positive helicity (C=1) and spinless Fermi surfaces (C=0).

- Inversion symmetry is broken but rotation symmetry is preserved.

- Spinor gap function $\boldsymbol{\Delta}_\alpha(\boldsymbol{k}) = \begin{pmatrix} \boldsymbol{\Delta}_\uparrow(\boldsymbol{k}), \\ \boldsymbol{\Delta}_\downarrow(\boldsymbol{k}) \end{pmatrix}$

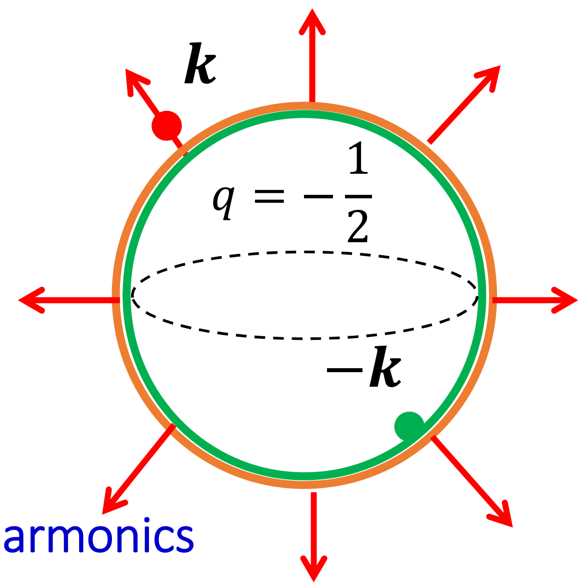
Spin-orbit coupled spherical harmonic gap functions (mixing opposite parity eigenstates)

$$\boldsymbol{\Delta}_{1,\alpha}{}^{j,l,j_z}(\boldsymbol{k}) = \boldsymbol{\Delta}\boldsymbol{\phi}_{j=l+\frac{1}{2},\, l,\, j_z,\alpha}(\hat{\boldsymbol{k}}) \qquad \boldsymbol{\Delta}_{2,\alpha}{}^{j,l+1,j_z}(\boldsymbol{k}) = \boldsymbol{\Delta}\boldsymbol{\phi}_{j=l+\frac{1}{2},\, l+1,\, j_z,\alpha}(\hat{\boldsymbol{k}})$$

Projection to the helicity basis

Helicity basis $\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}}|\boldsymbol{\lambda}_{\pm}(\hat{\boldsymbol{k}})\rangle = \pm|\boldsymbol{\lambda}_{\pm}(\hat{\boldsymbol{k}})\rangle$ ⇨ $\chi^{+}(\boldsymbol{k}) = \lambda_{+,\alpha}(\hat{k})c_{\alpha}^{+}(\boldsymbol{k})$

$$H_{\Delta}(\boldsymbol{k}) = \Delta(\hat{\boldsymbol{k}})\chi^{+}(\boldsymbol{k})d^{+}(-\boldsymbol{k}) + \Delta^{*}(\hat{\boldsymbol{k}})d(-\boldsymbol{k})\chi(\boldsymbol{k})$$



- **Project** $\boldsymbol{J} = \boldsymbol{L} + \frac{\boldsymbol{\sigma}}{2}$ **to the subspace of** $\boldsymbol{\Delta}(\hat{\boldsymbol{k}})\boldsymbol{\lambda}_{+}(\hat{\boldsymbol{k}})$:

$$\boldsymbol{J} = \hat{\boldsymbol{k}} \times (-\boldsymbol{i}\boldsymbol{\nabla}_{\boldsymbol{k}} - \boldsymbol{A}_{\boldsymbol{k}}) + \frac{\hat{\boldsymbol{k}}}{\mathbf{2}}, \qquad \boldsymbol{A}_{\boldsymbol{k}} = \boldsymbol{i}\langle\boldsymbol{\lambda}_{+}|\boldsymbol{\nabla}_{\mathbf{k}}|\boldsymbol{\lambda}_{+}\rangle$$

- Spin-orbit coupled spherical harmonics → monopole harmonics

$$\boldsymbol{\phi}_{j=l+\frac{1}{2},\,l,\,j_z,\alpha}(\hat{\boldsymbol{k}}) = \frac{\mathbf{1}}{\sqrt{2}}\left(\boldsymbol{Y}_{-\frac{1}{2},j,j_z}(\hat{\boldsymbol{k}})\boldsymbol{\lambda}_{+}(\hat{\boldsymbol{k}}) + \boldsymbol{Y}_{\frac{1}{2},j,j_z}(\hat{\boldsymbol{k}})\boldsymbol{\lambda}_{-}(\hat{\boldsymbol{k}})\right)$$

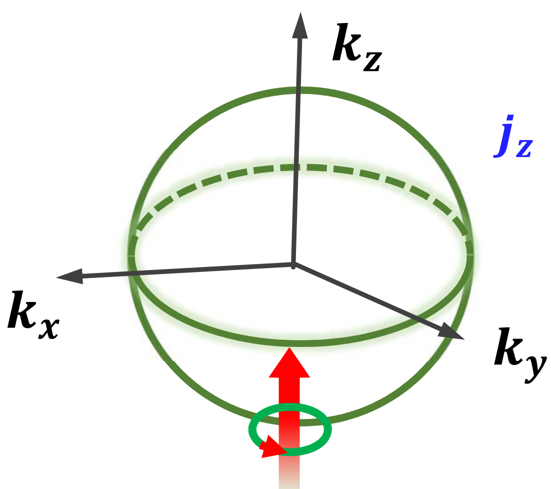
$$\boldsymbol{\phi}_{j=l+\frac{1}{2},\,l+1,\,j_z,\alpha}(\hat{\boldsymbol{k}}) = \frac{\mathbf{1}}{\sqrt{2}}\left(-\boldsymbol{Y}_{-\frac{1}{2},j,j_z}(\hat{\boldsymbol{k}})\boldsymbol{\lambda}_{+}(\hat{\boldsymbol{k}}) + \boldsymbol{Y}_{\frac{1}{2},j,j_z}(\hat{\boldsymbol{k}})\boldsymbol{\lambda}_{-}(\hat{\boldsymbol{k}})\right)$$

⇨ $\Delta(\hat{k}) = \Delta Y_{-\frac{1}{2},j,j_z}(\hat{k})$

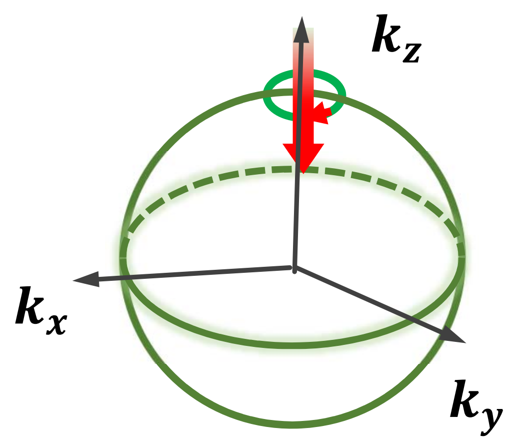
Gap node as vortex on pairing surface $\left(q=-\frac{1}{2}, j=\frac{1}{2}\right)$

Gap symmetry: $Y_{-\frac{1}{2},\frac{1}{2},\frac{1}{2}}$ $\qquad$ $Y_{-\frac{1}{2},\frac{1}{2},-\frac{1}{2}}$

$$\Delta(\hat{k}) = \Delta\cos\frac{\theta_k}{2} \xrightarrow{\text{Time-reversal}} \Delta sin\frac{\theta_k}{2}\, e^{-i\phi}$$



$j_z = \frac{1}{2}$



$j_z = -\frac{1}{2}$

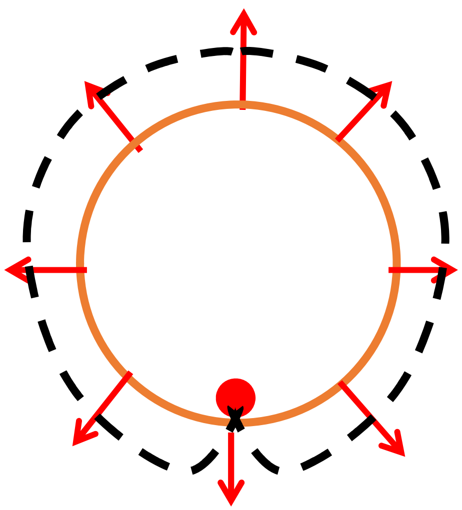
$$\vec{v}\left(\vec{k}\right) = \vec{\nabla}_k\phi\left(\vec{k}\right) - \vec{A}_p\left(\vec{k}\right)$$

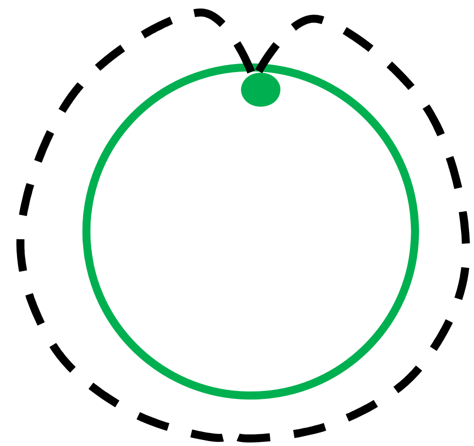
$$\frac{1}{2\pi}\sum_{C_i}\oint_{C_i} d\vec{k}\cdot\vec{v} = 2q = -1$$

Bogoliubov quasi-particles ($\boldsymbol{q} = \frac{1}{2}, \boldsymbol{j} = \boldsymbol{j_z} = \frac{1}{2}$)

$$H(k) = (\epsilon_k - \mu)\tau_3 + \Delta \cos\frac{\theta_k}{2}\tau_1 \qquad \psi(\boldsymbol{k}) = \begin{pmatrix} \chi(\boldsymbol{k}) \\ d^+(-\boldsymbol{k}) \end{pmatrix} \qquad tan\theta'_k = \frac{\Delta \cos\frac{\theta_k}{2}}{\epsilon_k - \mu}$$

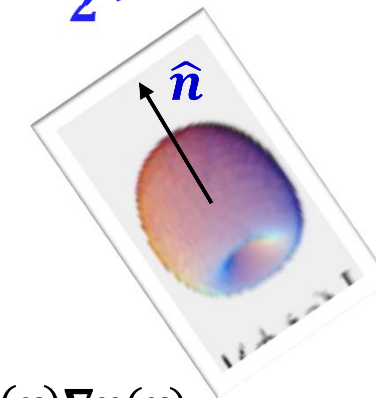
$$\gamma_1^+(\boldsymbol{k}) = \cos\frac{\theta'_k}{2}\chi^+(\boldsymbol{k}) + \sin\frac{\theta'_k}{2}d(-\boldsymbol{k}) \qquad \gamma_2^+(\boldsymbol{k}) = \sin\frac{\theta'_k}{2}d^+(\boldsymbol{k}) - \cos\frac{\theta'_k}{2}\chi(-\boldsymbol{k})$$





$$E_1^2(k) = (\epsilon_k - \mu)^2 + \Delta^2 \cos^2\frac{\theta_k}{2} \qquad E_2^2(k) = (\epsilon_k - \mu)^2 + \Delta^2 \sin^2\frac{\theta_k}{2}$$

Real space texture: curvature → vortex ($q = \frac{1}{2}, j = \frac{1}{2}$)



- Gap symmetry: spinor $\eta = \binom{w}{t}$

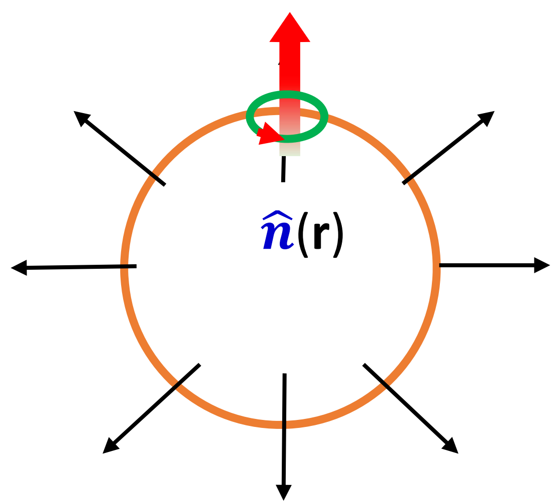
→ Hopf map $\hat{n} = \eta^{+}\sigma\eta$

$$\Delta(r) = \Delta e^{i\phi(r)}\,\eta(r)$$

- Super-current: $v(r) = \frac{\hbar}{2m}\left(\nabla\phi(r) - A_g(r)\right), \quad A_g(r) = i\eta^{+}(r)\nabla\eta(r)$

$$\nabla \times v(r) = -\frac{\hbar}{2m}\nabla \times A_g(r) \qquad \frac{2m}{\hbar}\oint dl \cdot \nabla \times v(r) = \frac{1}{2}\iint n \cdot \partial_i n \times \partial_j n \; dx_i \wedge dx_j = 2\pi$$

- Single vortex appears for a hedgehog n(r)



real space

CDW Berry Phase

(Eric Bobrow, Canon Sun, YL, in preparation)

- **Charge/spin density wave: condensate in the particle-hole channel**

$$H_D(\boldsymbol{k}) = \Delta(\boldsymbol{k}) W^+(\boldsymbol{k}) + \Delta^*(\boldsymbol{k}) W(\boldsymbol{k}); \quad W^+(\boldsymbol{k}) = c_1^+(\boldsymbol{k}) c_2(\boldsymbol{k}+\boldsymbol{Q}).$$

- **Particle-hole Berry phase**

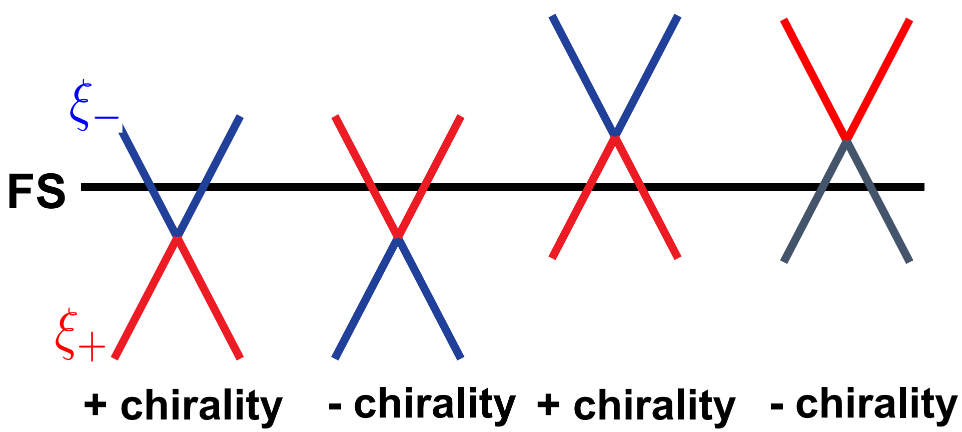
- $\hat{\rho}^\dagger_{CDW}(\mathbf{k}) = \alpha^\dagger_+(\mathbf{k}+\mathbf{Q})\alpha_-(\mathbf{k})$

  $\alpha^\dagger_\pm(\mathbf{k}) = \sum_i \xi_{\pm,i}(\mathbf{k}) c^\dagger_i(\mathbf{k})$

- **CDW Berry connection difference of single-particle connections**

$$A_{CDW}(\mathbf{k}) = A_+(\mathbf{k}+\mathbf{Q}) - A_-(\mathbf{k})$$

$$\oiint_{FS} dS_{\mathbf{k}} \cdot \Omega_{CDW} = 4\pi q_{CDW}$$



The Model

$$H = \sum_{\substack{\mathbf{k} \\ i,j=A,B}} c_i^\dagger(\mathbf{k})[h(\mathbf{k}) + \mu(k_z))]_{ij} c_j(\mathbf{k}) + (c_i^\dagger(\mathbf{k}+\mathbf{Q})\rho(\mathbf{k})_{ij} c_j(\mathbf{k}) + h.c.)$$

- Kinetic terms $h(\mathbf{k}) = t_z(2 - \cos k_x - \cos k_y - \frac{1}{2} + \cos^2 k_z)\tau_z$
  $+ t_x \sin k_x \tau_x + t_y \sin k_y \tau_y$

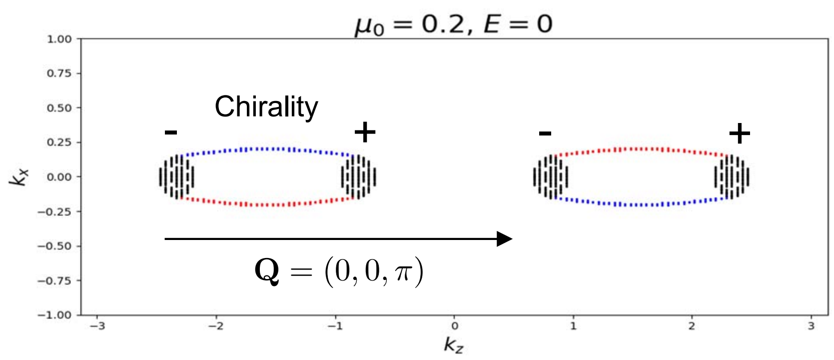
  $\tau_i \longrightarrow$ Pseudospin Pauli matrix

  - Weyl nodes along k_z axis at $k_z = \pm\frac{\pi}{4}, \pm\frac{3\pi}{4}$
  - Satisfies nesting condition $E_+(\mathbf{k}) = -E_-(\mathbf{k}+\mathbf{Q})$

- Spatially-varying potential

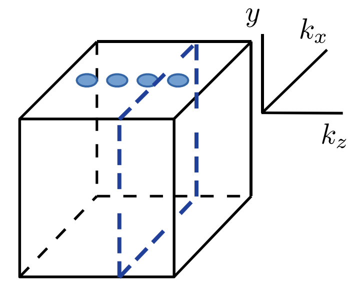
  $$\mu(k_z) = \mu_0 \sin k_z I$$

- CDW order parameter $\rho(\mathbf{k}) = \rho\tau_z$

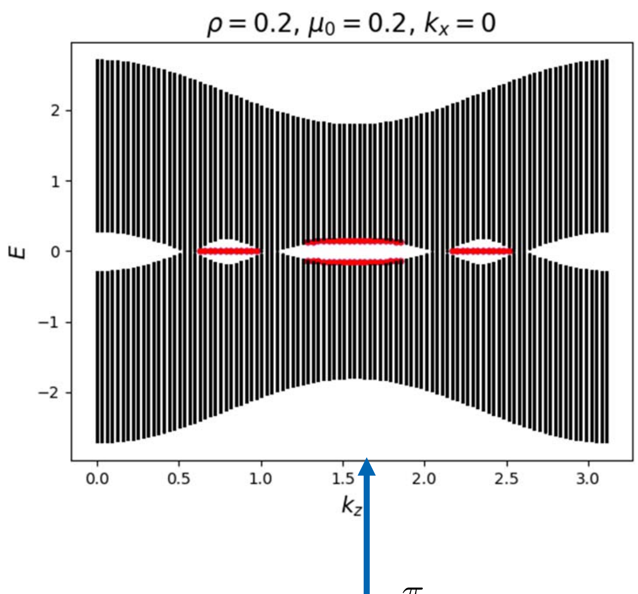


- Open boundary in y
- Periodic in x, z
- $\rho = 0$

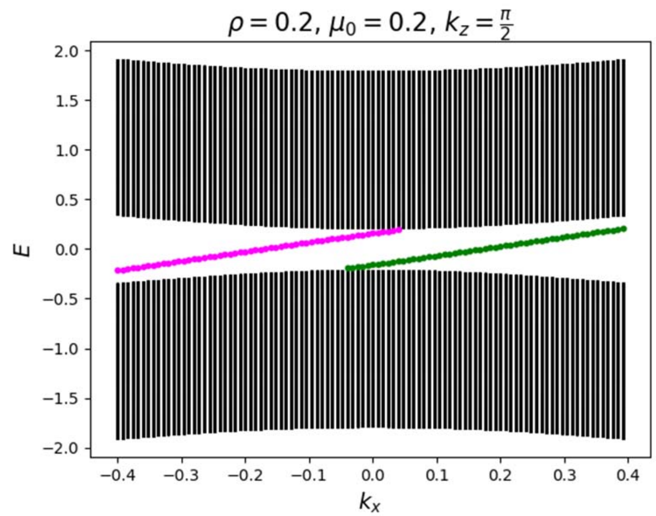
$k_z = \frac{\pi}{2}$ cut (Fermi arcs)



$k_z = \frac{\pi}{2}$ cut



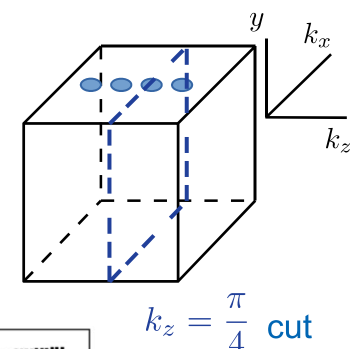
$k_z = \frac{\pi}{2}$

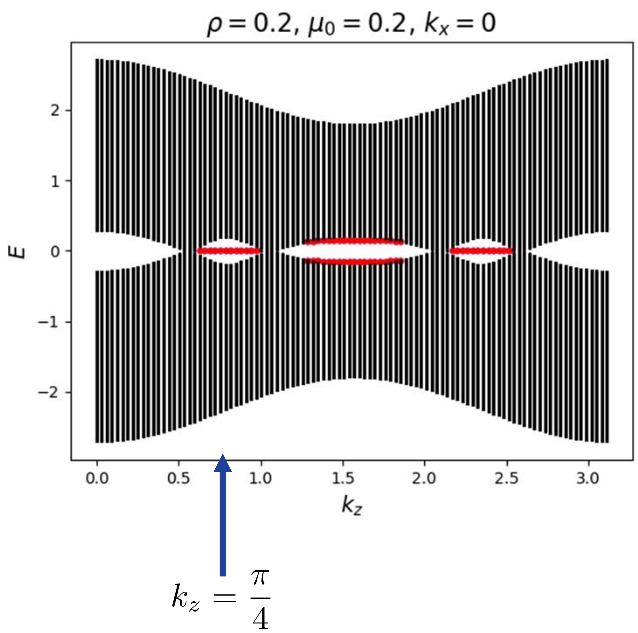


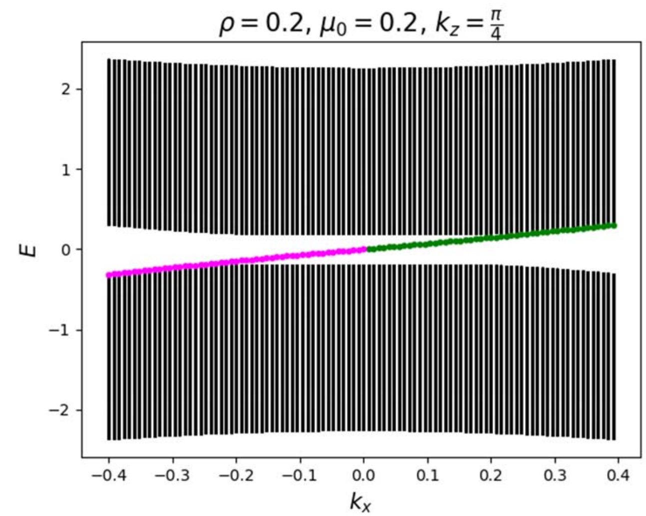
Basis $\begin{pmatrix} c_A(\mathbf{k}) \\ c_B(\mathbf{k}) \\ c_A(\mathbf{k}+\mathbf{Q}) \\ c_B(\mathbf{k}+\mathbf{Q}) \end{pmatrix}$

- Green – mostly k type
- Magenta – mostly k+Q type
- y = 0 edge

$k_z = \frac{\pi}{4}$ cut (new surface states)





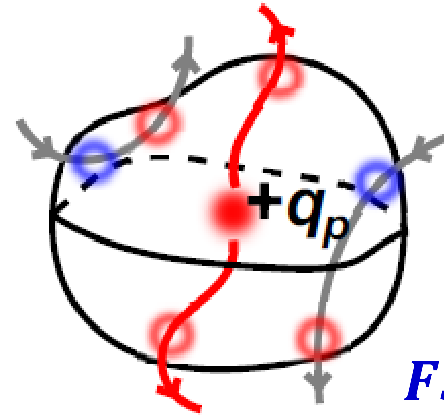


Basis $\begin{pmatrix} c_A(\mathbf{k}) \\ c_B(\mathbf{k}) \\ c_A(\mathbf{k}+\mathbf{Q}) \\ c_B(\mathbf{k}+\mathbf{Q}) \end{pmatrix}$

- Green – mostly k type
- Magenta – mostly k+Q type
- y = 0 edge

Summary and Outlook

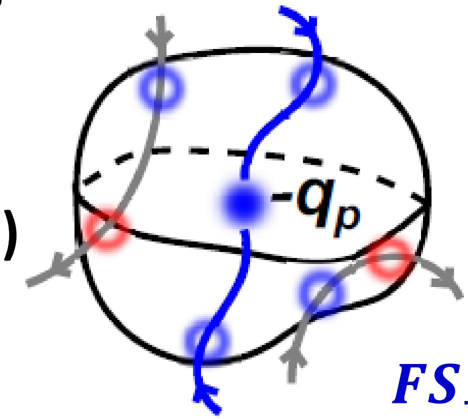
- Non-trivial pair Berry phase → Topological protected nodal structure determined by FS topology instead of interaction and symmetry.



FS_+

- Monopole harmonic superconductivity -- spherical symmetry is insufficient .

- Nodal lines of $\Delta(\vec{k})$ as vortex lines in 3D k-space, where Weyl points are the source and drain.



FS_-

- Fundamental nodes on $FS_\pm$ contribute total vorticity $\pm 2q_p$ (independent of pairing mechanism)

- Non-fundamental nodes appear in pairs (can be affected by specific pairing mechanism)

- Half-integer harmonic superconductivity: Texture in real space: geometric curvature induced vortex

- Monopole harmonic superconductivity by proximity? Phase sensitive measurements? …

Thank you!