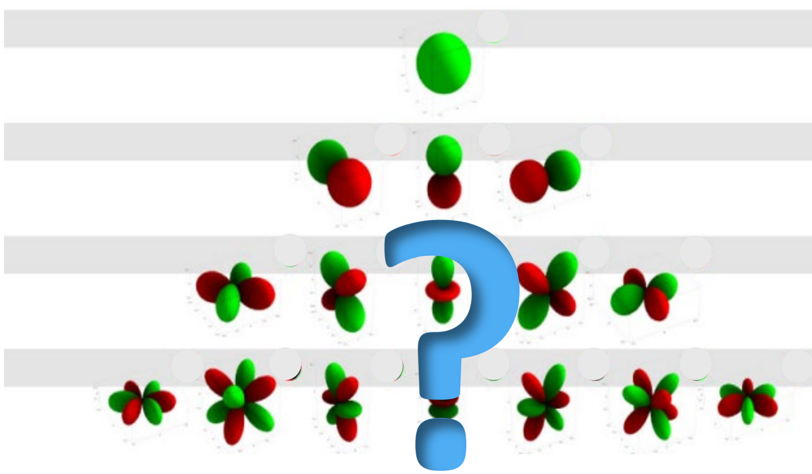
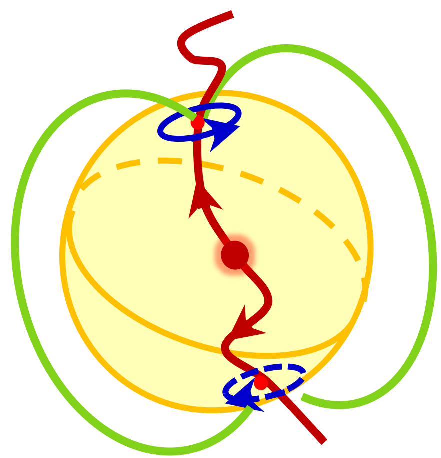
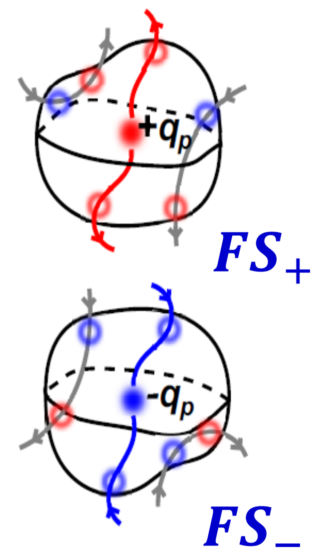
Monopole Harmonic Ordering in Weyl Semi-metals







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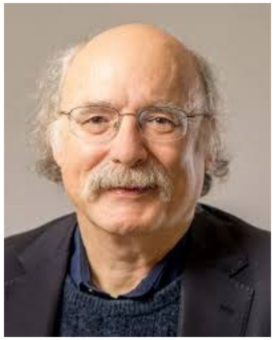
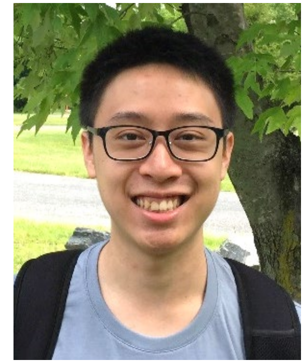
KITP, 9/30/2019

Collaborators:





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Acknowledgments:

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Collin Broholm (JHU)
Chia-Ling Chien (JHU)
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Liang Wu (U Penn)

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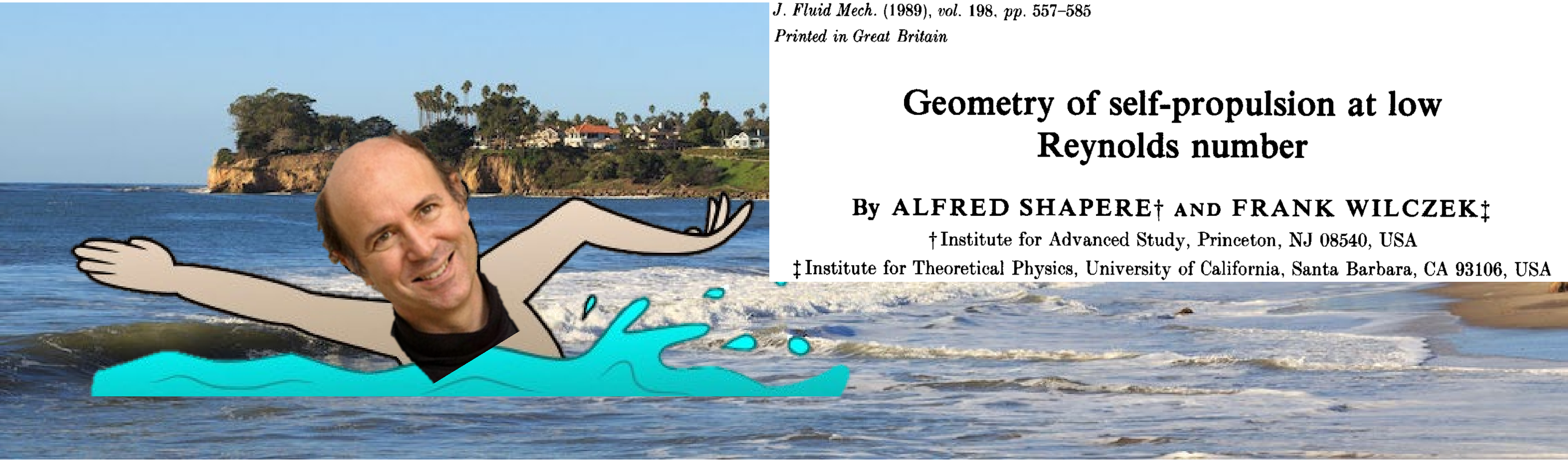
Geometric Phase – from Classical to Quantum



J. Fluid Mech. (1989), vol. 198, pp. 557–585
Printed in Great Britain

Geometry of self-propulsion at low Reynolds number

By ALFRED SHAPERE† AND FRANK WILCZEK‡
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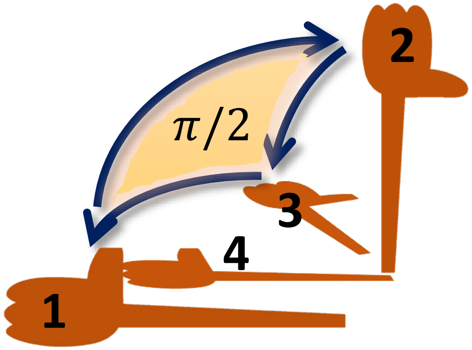
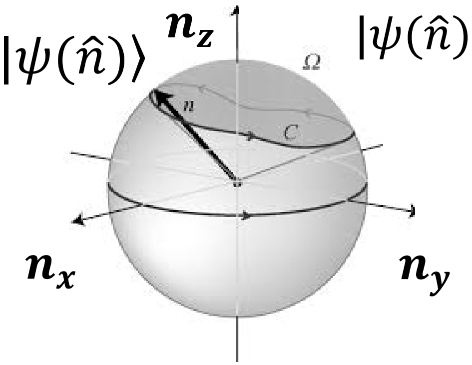
A "Thumb Trick" in the classical world

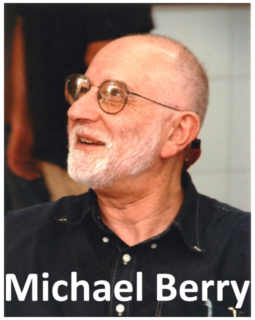


$\pi/2 =$ **solid angle spanned.**

A "Thumb Trick" played by a quantum state

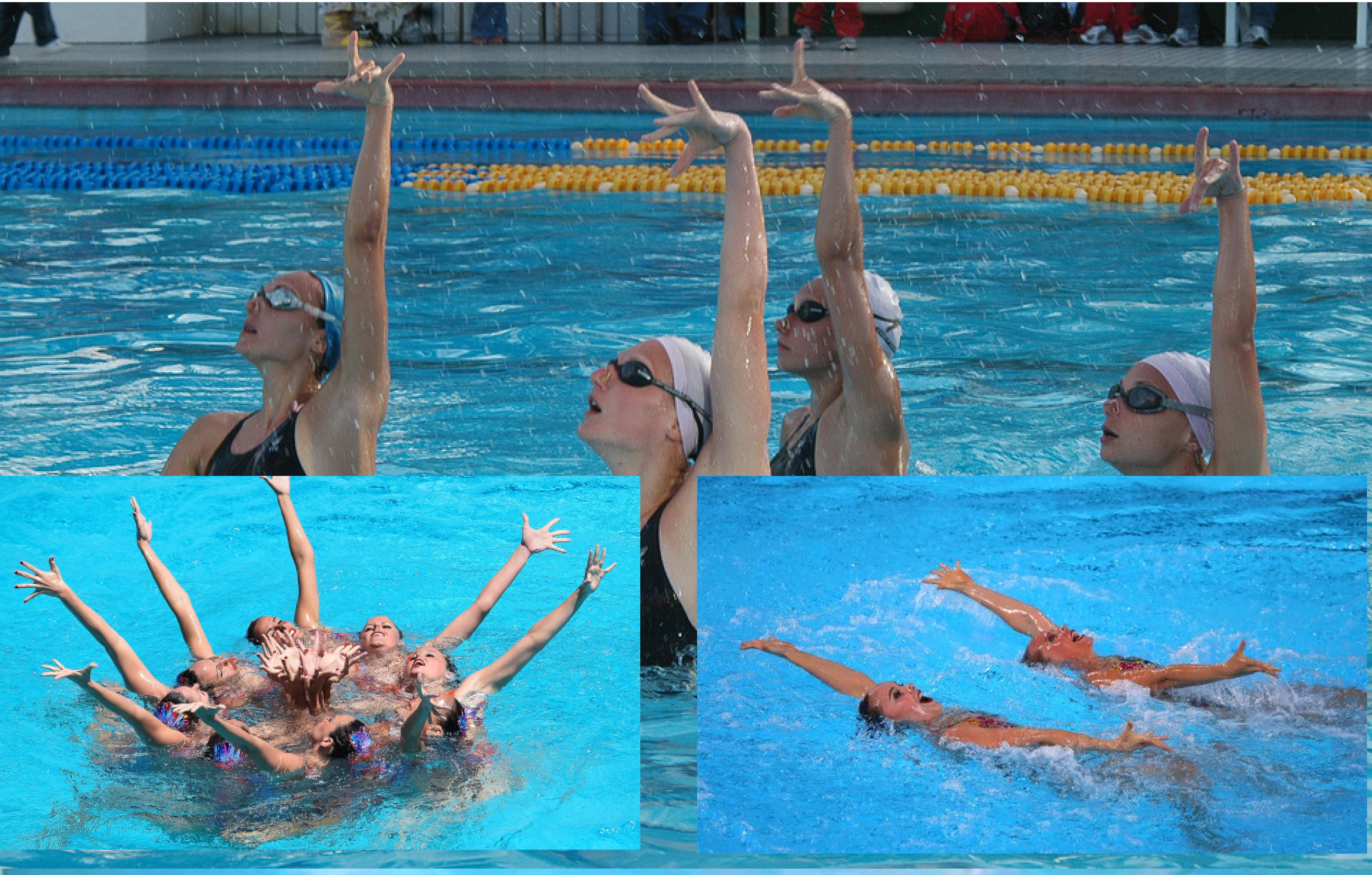


$|\psi(\hat{n})\rangle = e^{i\gamma}\,|\hat{n}\rangle$

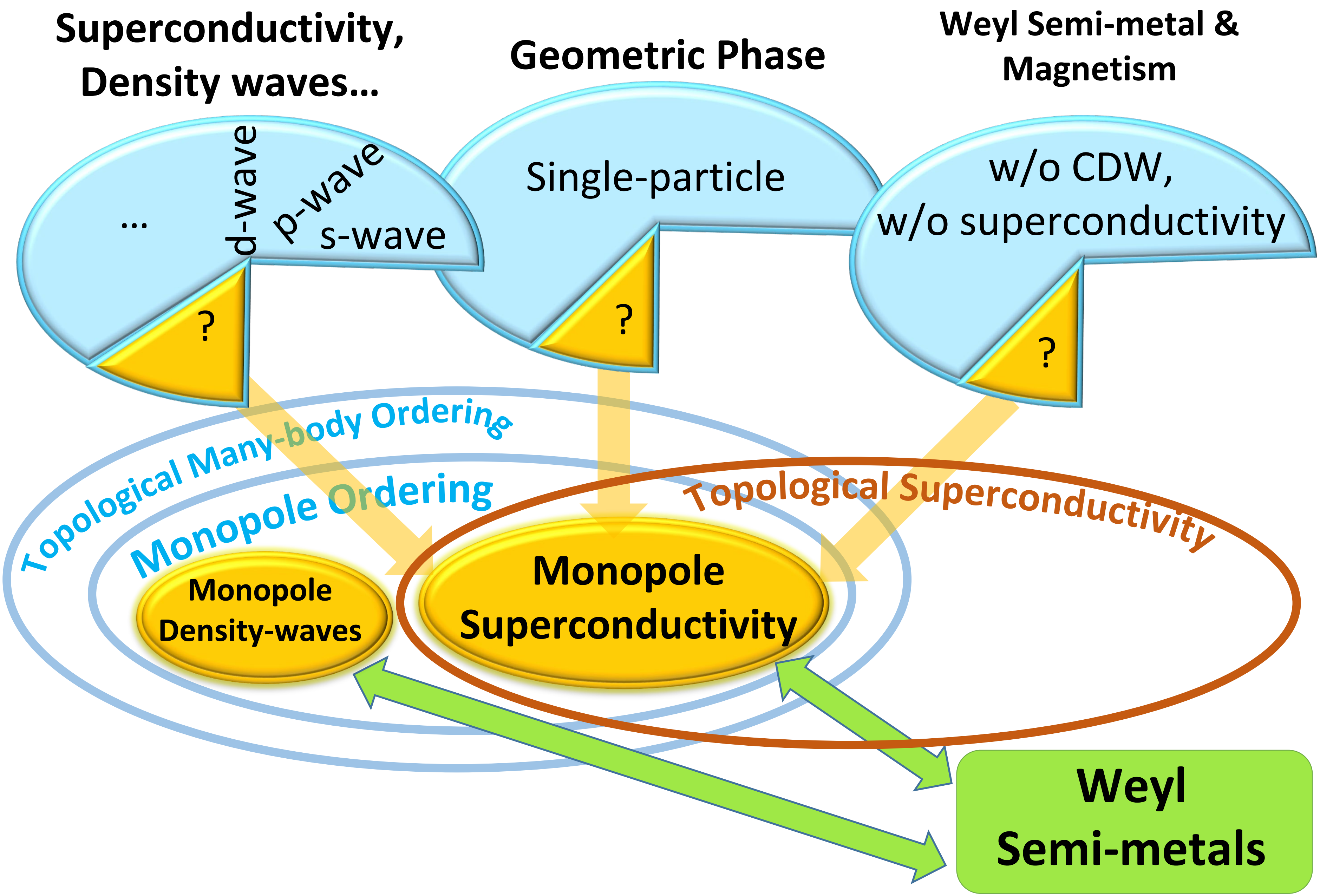


Geometric phase:
$\gamma = q \times$ **spanned solid angle**

Topological States from Many-body Geometric Phases



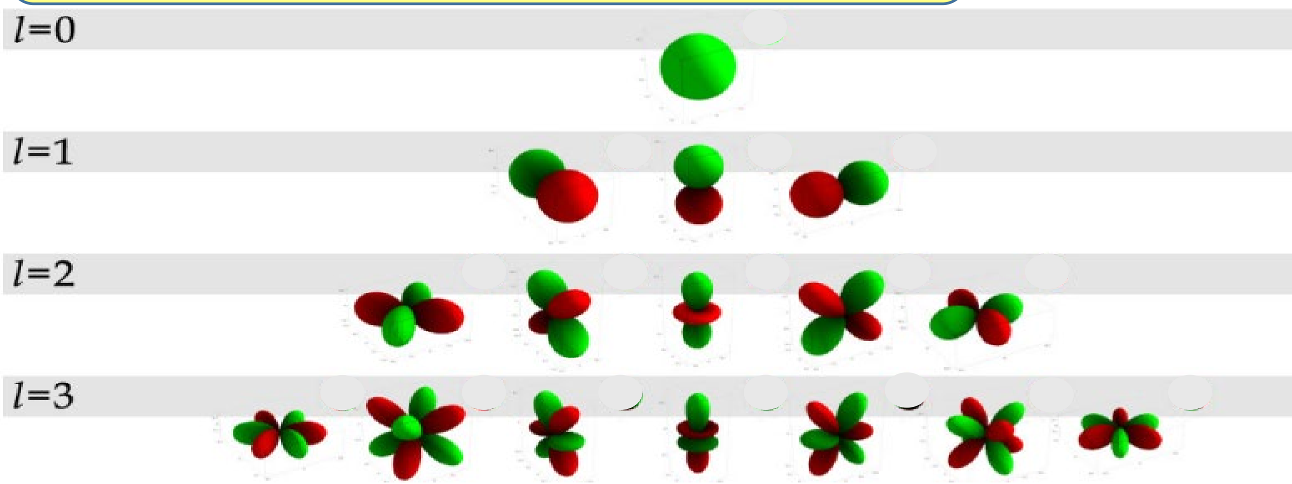
Overview

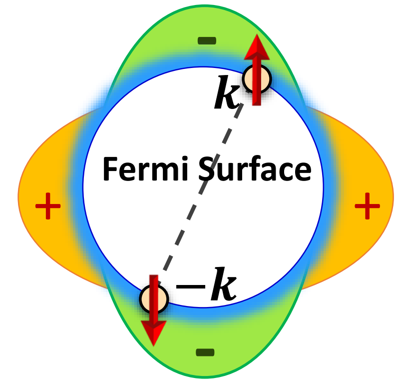

Superconductivity,
Density waves…
Geometric Phase
Weyl Semi-metal &
Magnetism
…
d-wave
p-wave
s-wave
?
Single-particle
?
w/o CDW,
w/o superconductivity
?
Topological Many-body Ordering
Monopole Ordering
Topological Superconductivity
Monopole
Density-waves
Monopole
Superconductivity
Weyl
Semi-metals

Superconducting/Superfluid 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: $\Delta(\boldsymbol{k}) = \sum_{l,m} \Delta_{lm} Y_{lm}(\Omega_{\boldsymbol{k}})$





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

Nobel prizes

l	Partial waves	Example		Year of Nobel prize
$l = 0$	(s-wave)	Hg	Onnes	1913
			Bardeen, Cooper, Schrieffer	1972
$l = 1$	(p-wave)	^3He	Lee, Osheroff, Richardson	1996
			Leggett	2003
$l = 2$	(d-wave)	$LaBaCuO_4$	Bednorz, Mueller	1987
⋮		⋮	⋮	⋮

Classes of 3D Topological superconductivity

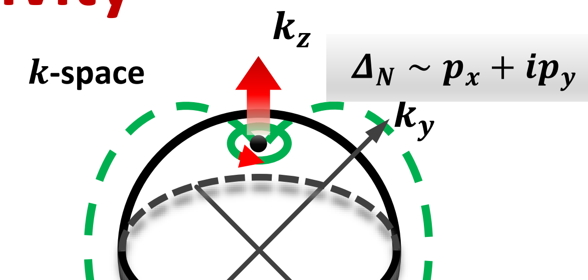
- **3D ^{3}He-A type $p_x + ip_y$**

  Time-reversal symmetry broken

  Non-trivial phase winding around each gap nodes.

  Volovik's book (1992), JETP (1999); Read, Green, PRB (2000), … …

  2D: Ivanov, PRL (2001), Fu, Kane, PRL (2008), Lutchyn, Sau, Das Sarma, PRL
  Nayak, Simon, Stern, Freedman, Das Sarma, RMP (2008)…

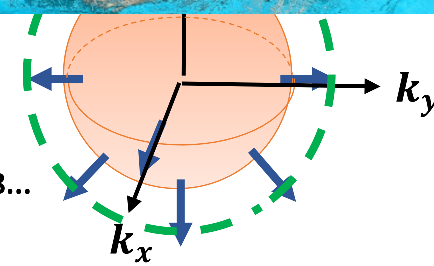


- **3D ^{3}He-B type p-wave**

  Time-reversal invariant.

  Nontrivial real d-vector configuration over Fermi surface characterized by Pontryagin number.

  Volovik's book (1992), Schnyder, Ryu, Furusaki, Ludwig, PRB (2008);
  Qi, Hughes, Raghu, Zhang, PRL (2009), Chung, Zhang, PRL (2009), R. Roy, arXiv:0803.2868…



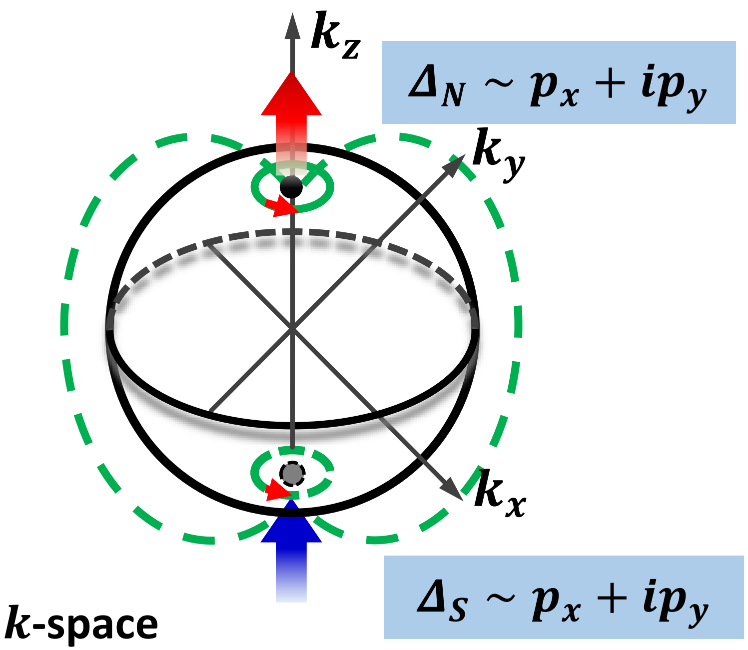
- **Monopole harmonic Cooper pairing:**

  Time-reversal symmetry broken

  Nodal pairing gap characterized monopole harmonics, indep. of pairing mechanisms. Non-trivial complex d-vector characterized by the Chern number.

An overview of Monopole Harmonic Orderings

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

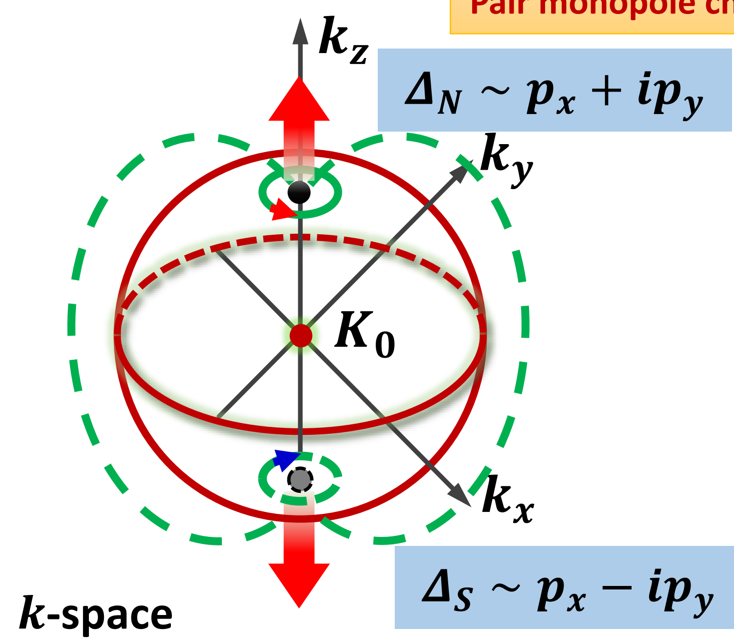


- **Total vorticity over FS**

$$1 - 1 = 0$$

Monopole Ordering: $Y_{q=1,10}(\hat{\Omega}_k)$

Pair monopole charge



- **Total vorticity over FS**

$$1 + 1 = 2$$

Monopole Superconductivity: Yi Li, F.D.M. Haldane, PRL 120, 067003 (2018).

Monopole Charge Density Waves: Eric Bobrow, Canon Sun, Yi Li, arXiv:1810.08715.

Pair Berry phase from Fermi surface topology

- **Inversion-related Fermi surfaces have opposite Chern #'s in TR broken Weyl.**

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

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

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

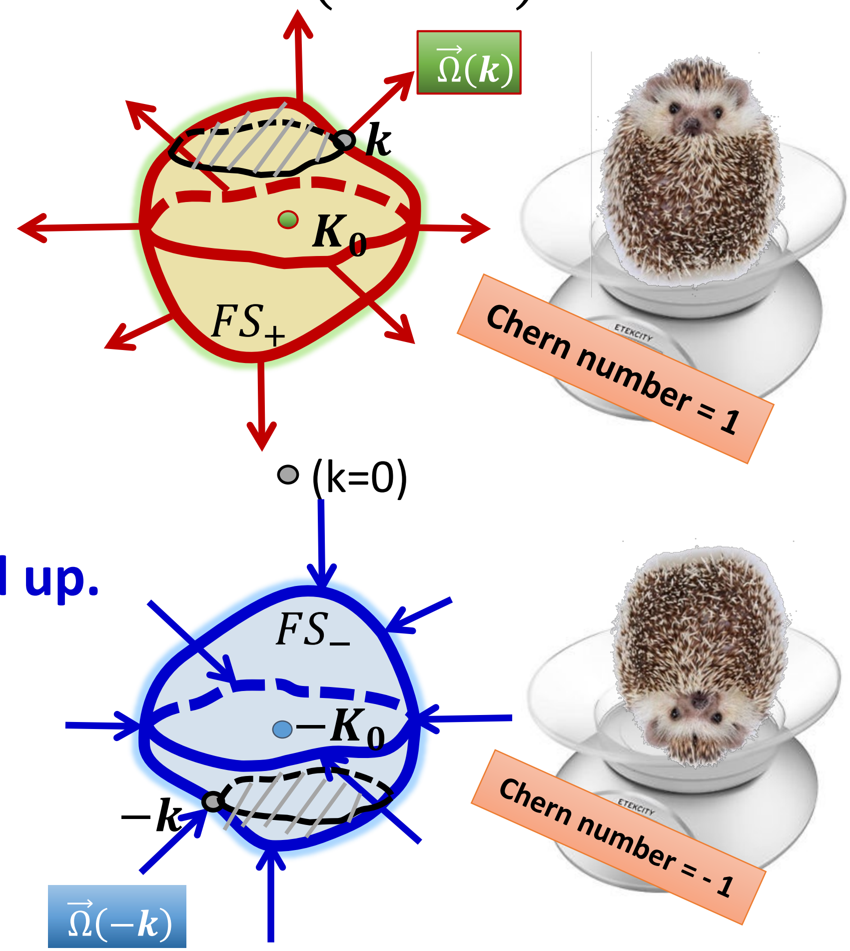
- **Contributions from $|\boldsymbol{k}\rangle_+$ and $|-\boldsymbol{k}\rangle_-$ add up.**

$$\boldsymbol{A}_{Pair}(\boldsymbol{k}) = \boldsymbol{A}_+(\boldsymbol{k}) - \boldsymbol{A}_-(-\boldsymbol{k}) = 2\boldsymbol{A}_+(\boldsymbol{k})$$

- **Pair monopole charge**

$$\boldsymbol{q}_{pair} = \frac{1}{4\pi}\oiint_{S_+} \boldsymbol{dS}_k \cdot \boldsymbol{\Omega}_{pair}(\boldsymbol{k}) = 2q$$

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



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

Pair Berry phase protected nodal vorticity

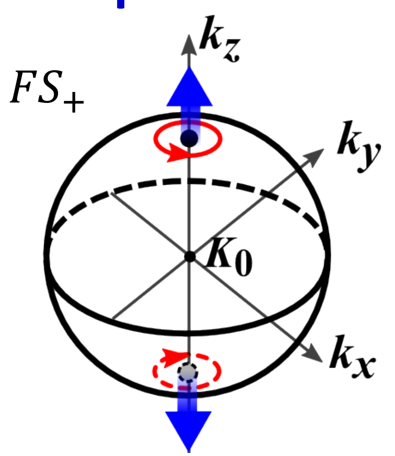
Yi Li, F.D.M. Haldane, PRL 120, 067003 (2018).

- **The total vorticity over one Fermi surface**

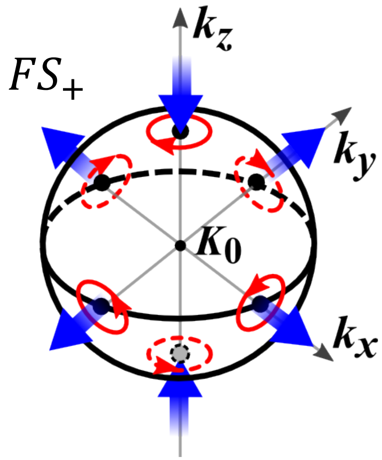
$$Total\ vorticity = \oiint \frac{d\vec{k}}{2\pi} \cdot (\vec{\nabla}_k \times \vec{A}_p) = 2q_p.$$

A related interesting work: Murakami, Nagaosa, PRL 90, 057002 (2003).

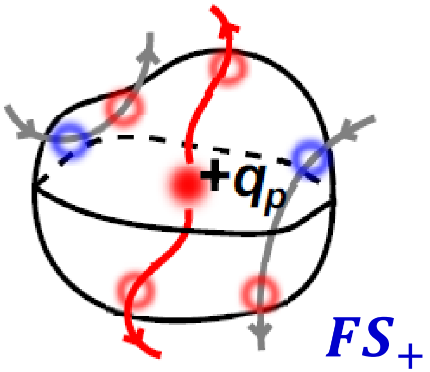
- **Examples in a Weyl-semimetal models:**

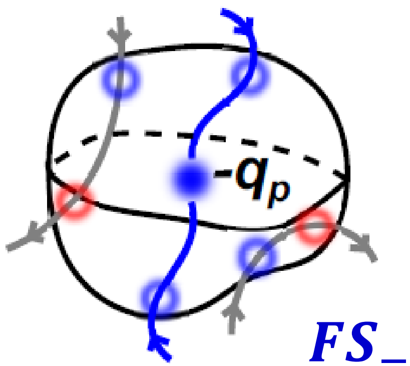


1+1=2 (fundamental nodes)



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





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

Monopole harmonics functions

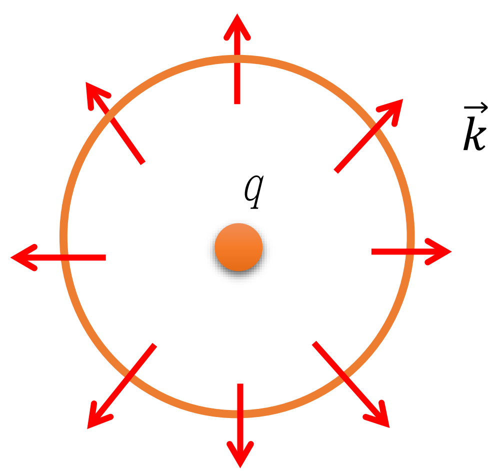
Poincaré 1896, Yang and Wu 1976, Haldane 1983.

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

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

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

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

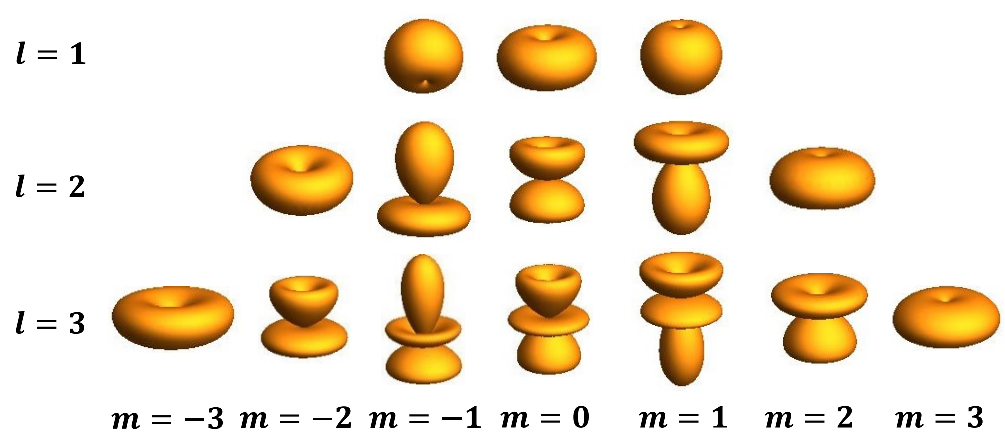


- **Example:**

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

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

$Y_{q_p=1,l,m}$



Monopole harmonic pairing

Yi Li, F.D.M. Haldane, PRL 120, 067003 (2018).

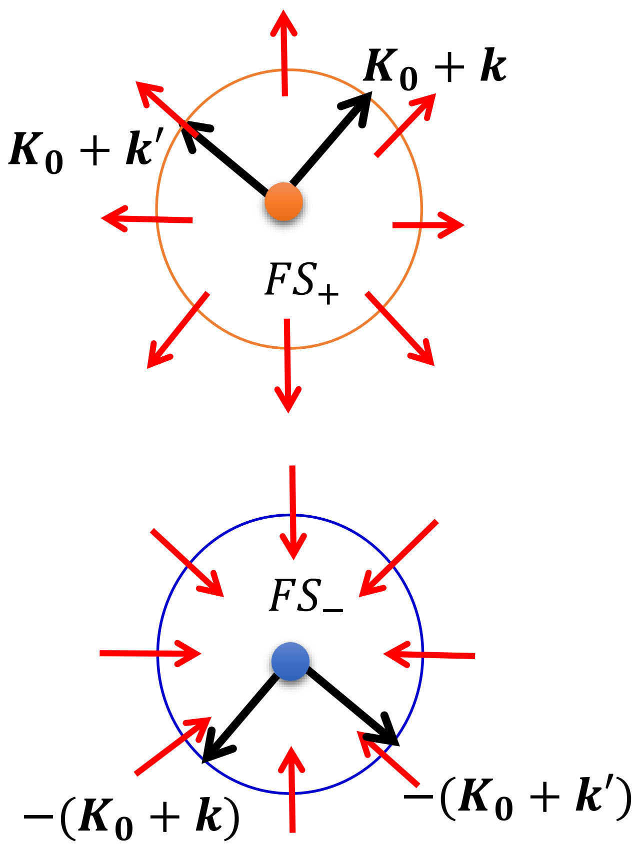
- If $FS_{\pm}$ can be approximated by spheres, partial wave decomposition of bare scattering before projection.

$V(\vec{k},\ \vec{k}')$

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

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

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



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

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

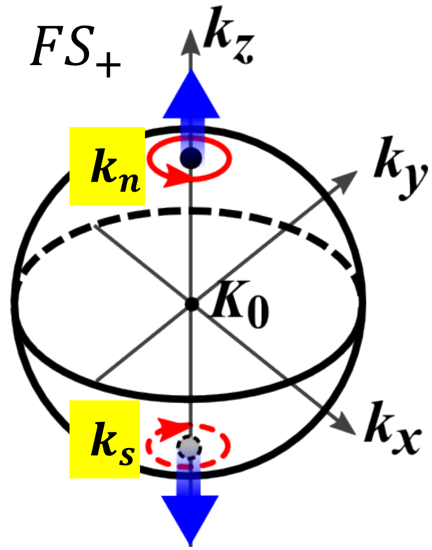
- In general, $\Delta(\boldsymbol{k})=|\Delta(\vec{k})|\sum_{j\geq q_p,m}c_{jm}Y_{q_p;jm}(\widehat{\boldsymbol{k}})$.

Low-energy excitations determined by high-energy topology

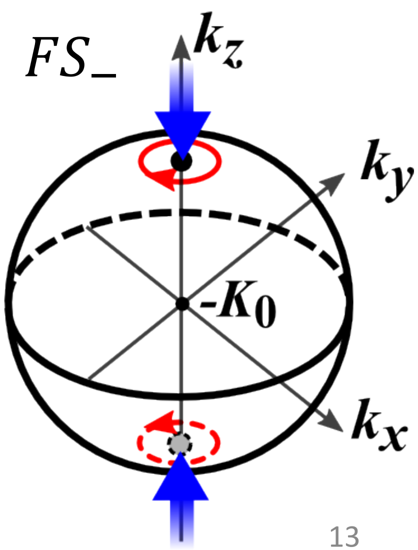
- **High energy scale: band structure Weyl nodes.**

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

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

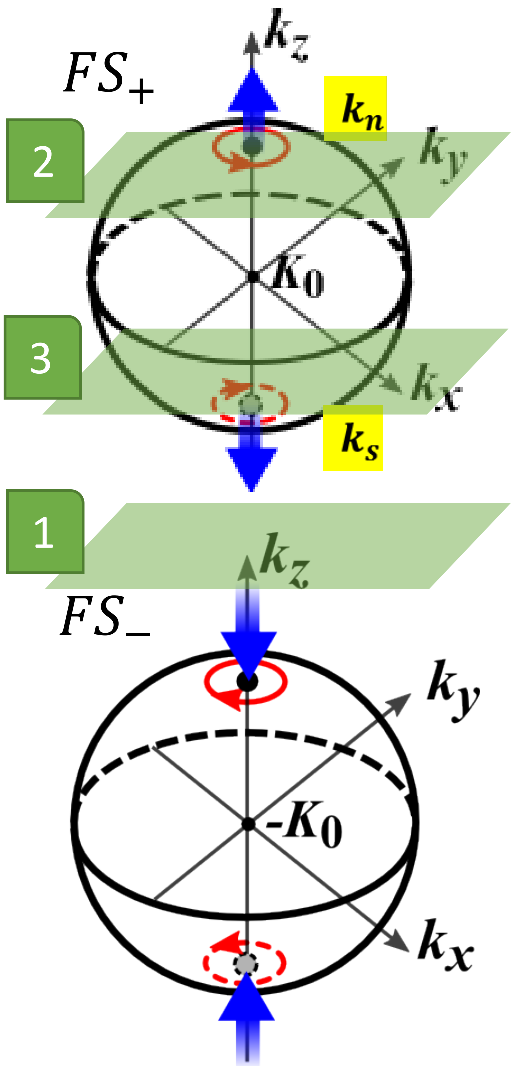


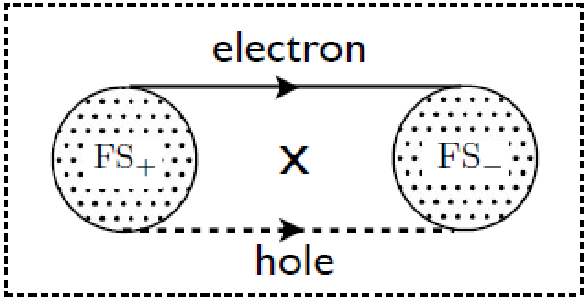
- **Vortex of $\Delta\left(\vec{k}\right)$ on FS $\longleftrightarrow$ BdG-Weyl monopole in the $\vec{k}$-space with a non-zero total monopole charge in a Fermi Surface.**

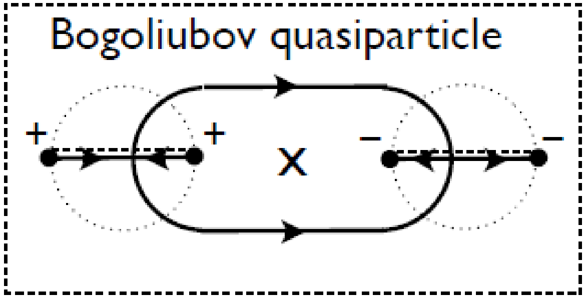


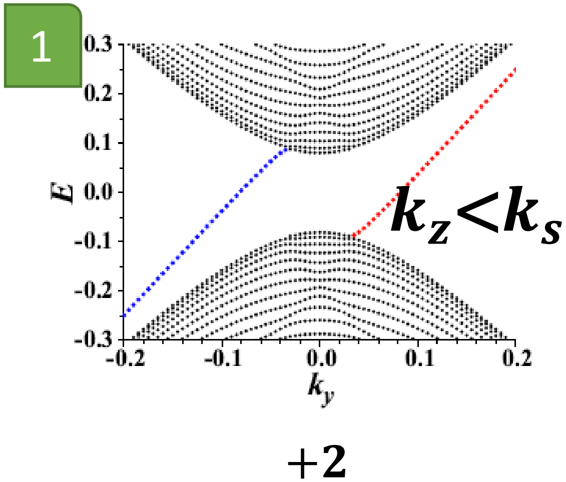
- **Topology threads all the energy scales**

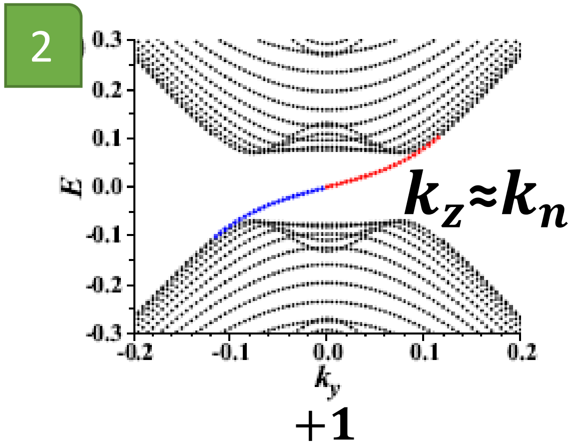
Surface spectra: Majorana meets Weyl

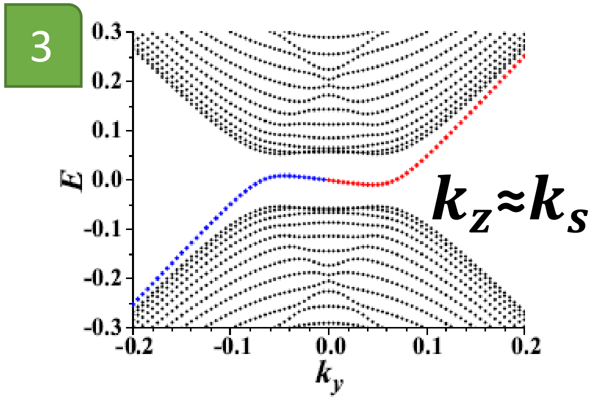








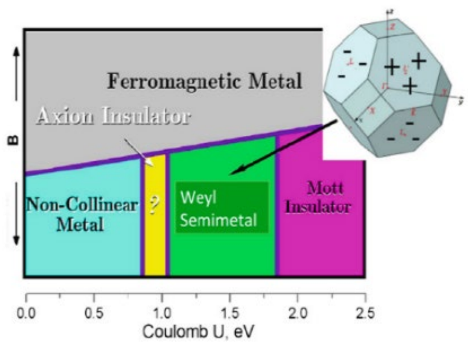


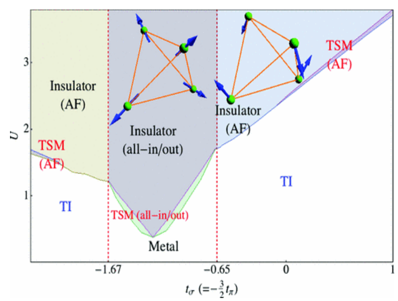


$+1-1+1=+1$

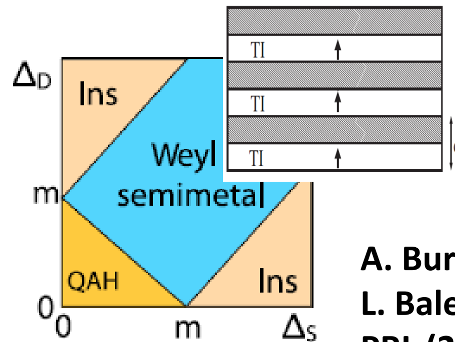
YL, FDM Haldane, PRL 120, 067003 (2018).
Related previous work based on mirror symmetry:
SA Yang, H. Pan, F. Zhang (2014); Lu, Yada, Sato, Tanaka (2015)

TR breaking Weyl semi-metals

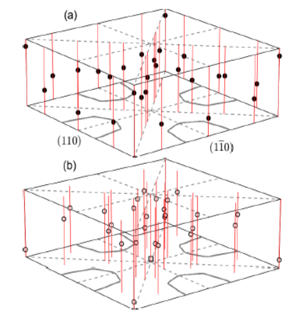




Wan, Turner, Vishwanath, Savrasov, PRB (2011),
Witczak-Krempa, Kim, PRB (2012)…



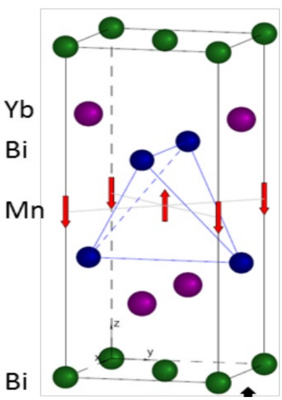
A. Burkov,
L. Balents,
PRL (2011)



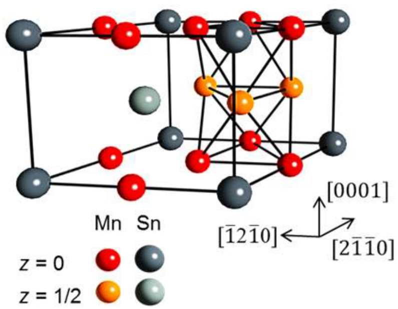
bcc Fe

Vanderbil's group,
PRB (2015)

First-Principle: Z. Wang, Bernevig and collaborators, PRL (2016)…



$YbMnBi_2$
Cava's group
arXiv:1507.04847
…

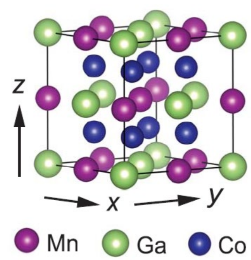


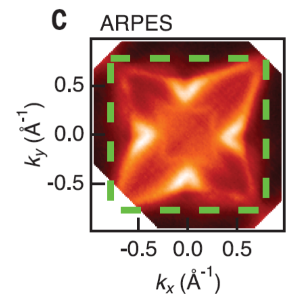
Mn_3Sn

S. Nakatsuji's group (2015)

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

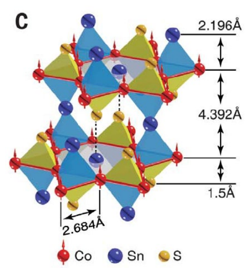
Other Theory:
H. Chen, Q. Niu, A. H. MacDonald (2014)
L. Balents' group (2017)…

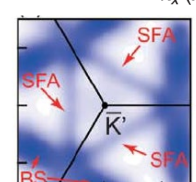




Co_2MnGa

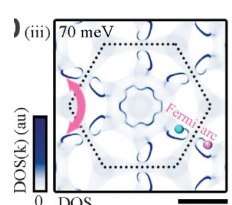
Hasan & collaborators,
Science (2019).

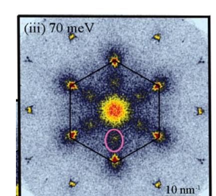




$Co_3Sn_2S_2$

YL Chen & collaborators,
Science (2019).





$Co_3Sn_2S_2$

Beidenkopf & collaborators,
Science (2019) …

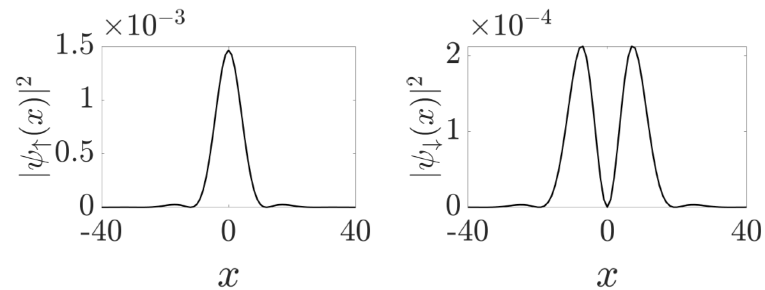
Vortices and Josephson Junctions of Monopole Superconductors

- **Monopole superconductors from time-reversal broken Weyl semi-metal with proximity-induced superconductivity.**
- **Zero-energy vortex bound states protected by the index theorem.**

$$\psi_{0,k_z}(\rho,\phi) = e^{-\frac{1}{\hbar v_F}\int_0^\rho d\rho' \Delta(\rho')}\chi_{k_z}(\rho,\phi)$$

$$\chi_{K_0+q_z}(\rho,\phi) = \begin{bmatrix} Ae^{-i\frac{\pi}{4}}J_0(k\rho) \\ Be^{i\frac{\pi}{4}}e^{i\phi}J_1(k\rho) \\ Ae^{i\frac{\pi}{4}}J_0(k\rho) \\ Be^{-i\frac{\pi}{4}}e^{-i\phi}J_1(k\rho) \end{bmatrix}$$

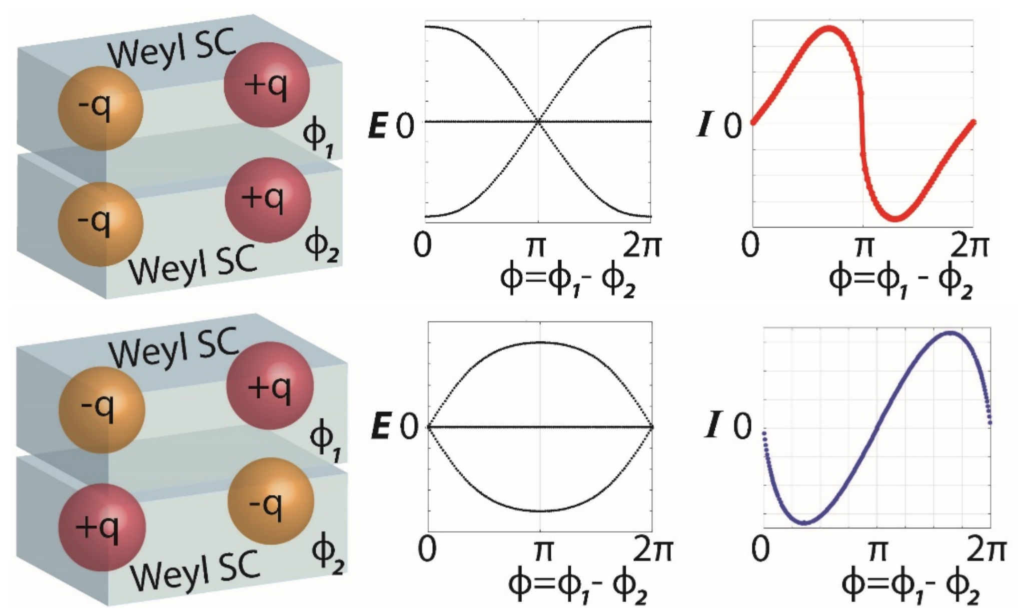
$$A = \sqrt{1+q_z/q_F} \quad B = \sqrt{1-q_z/q_F} \quad k = \sqrt{|q_F^2 - q_z^2|}$$



ArXiv: 1909.04179. Canon Sun, Shu-Ping Lee, Yi Li.

- **Josephson junctions of Monopole superconductors**

(Preliminary: Shu-Ping Lee, Yi Li)



CDW Berry Phase

E. Bobrow, C. Sun, Y. Li, arXiv:1810.08715.

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

$$H_{density-wave}(\boldsymbol{k}) = \Delta(\boldsymbol{k})c_1^{+}(\boldsymbol{k})c_2(\boldsymbol{k}+\boldsymbol{Q}) + h.c.$$

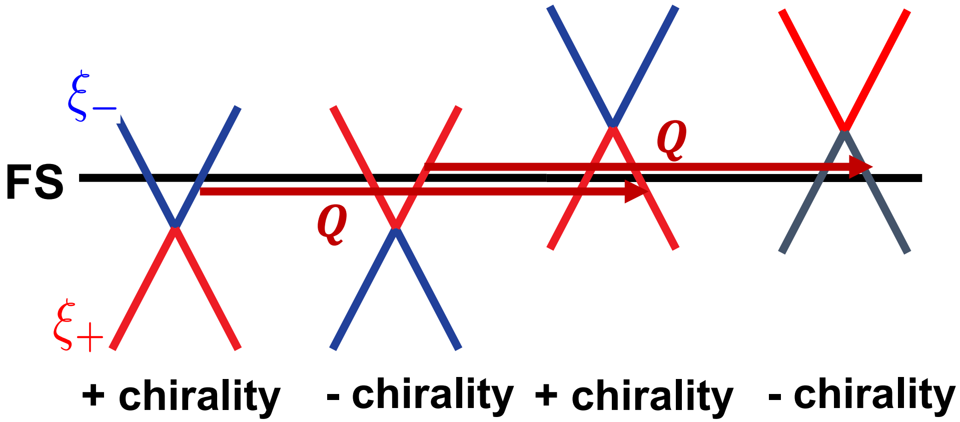
- **Particle-hole Berry phase**

$$\hat{\rho}^{\dagger}_{CDW}(\mathbf{k}) = \alpha^{\dagger}_{+}(\mathbf{k}+\mathbf{Q})\alpha_{-}(\mathbf{k}) \qquad \alpha^{\dagger}_{\pm}(\mathbf{k}) = \sum_i \xi_{\pm,i}(\mathbf{k})c^{\dagger}_i(\mathbf{k})$$

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

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

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

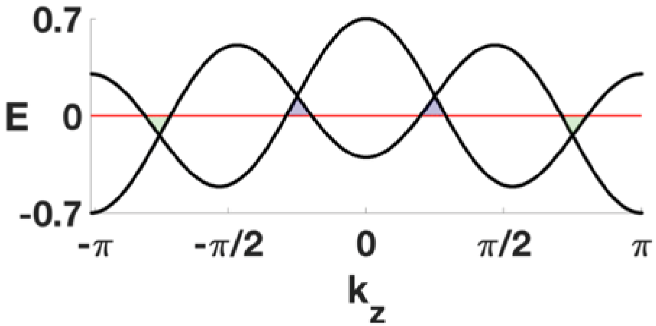


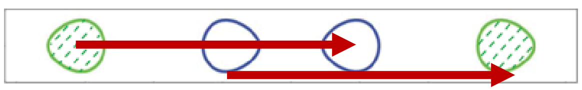
Model Hamiltonian

Weyl Hamiltonian

$$h_{\mathrm{Weyl}}(\mathbf{k}) = \left(\frac{3}{2} - \cos k_x - \cos k_y + \cos^2 k_z\right)\tau_z + \sin k_x \tau_x + \sin k_y \tau_y + V_0 \cos k_z \mathbb{1}$$

Invariant under $k_z \mapsto -k_z$





$\boldsymbol{Q} = (0,0,\pi)$

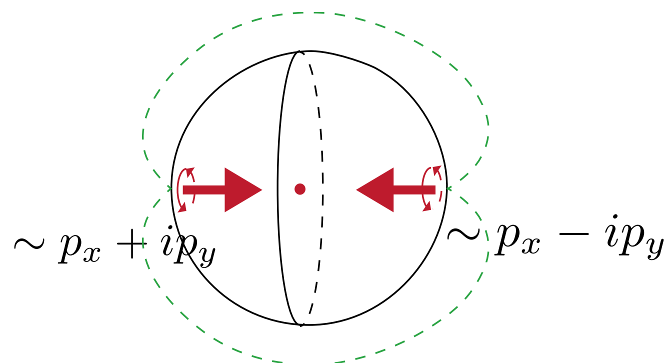
Weyl Nodes	$k_z = -\frac{3\pi}{4}$	$k_z = -\frac{\pi}{4}$	$k_z = \frac{\pi}{4}$	$k_z = \frac{3\pi}{4}$
Chirality of Weyl Nodes	$\chi = +1$	$\chi = -1$	$\chi = +1$	$\chi = -1$
Electron/hole pockets	e	h	h	e
FS Chern #	$C = -1$	$C = -1$	$C = +1$	$C = +1$

$$H = \underbrace{\sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}} h_{\mathrm{Weyl}}(\mathbf{k}) c_{\mathbf{k}}}_{\mathrm{Weyl}} + \underbrace{\sum_{\mathbf{k}} \left(c^{\dagger}_{\mathbf{k}+\mathbf{Q}} \rho(\mathbf{k}) c_{\mathbf{k}} + \mathrm{h.c.}\right)}_{\mathrm{CDW}}$$

Density-wave order

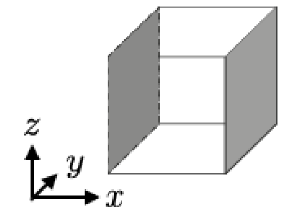
$$\rho(\mathbf{k}) = \rho_0 \tau_z$$

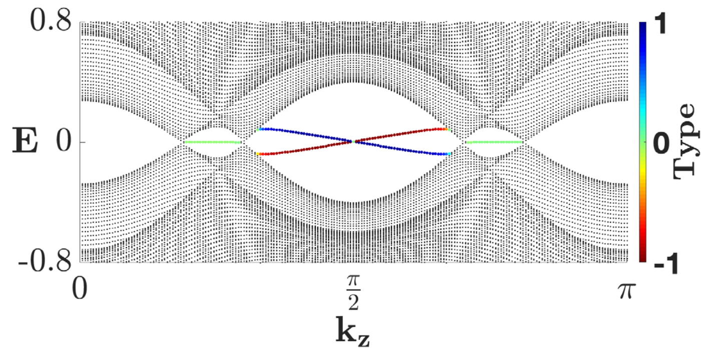
Monopole Density-wave State

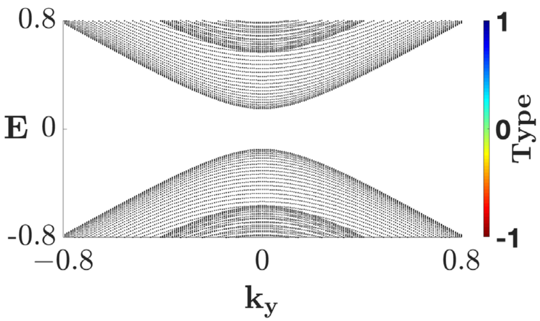


$$\tilde{\rho}(\hat{\mathbf{p}}) = \rho_0 \mathcal{Y}_{q_p=-1, l=1, m=0}(\theta_{\mathbf{p}}, \phi_{\mathbf{p}})$$

Energy spectrum

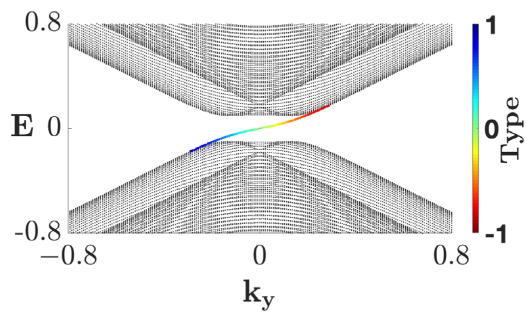






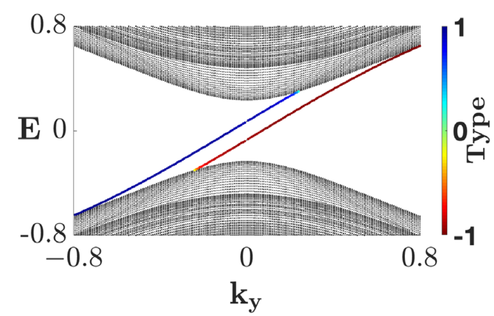
Trivial insulator

No surface states



Topological CDW

Quasiparticle surface states

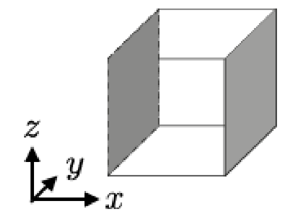


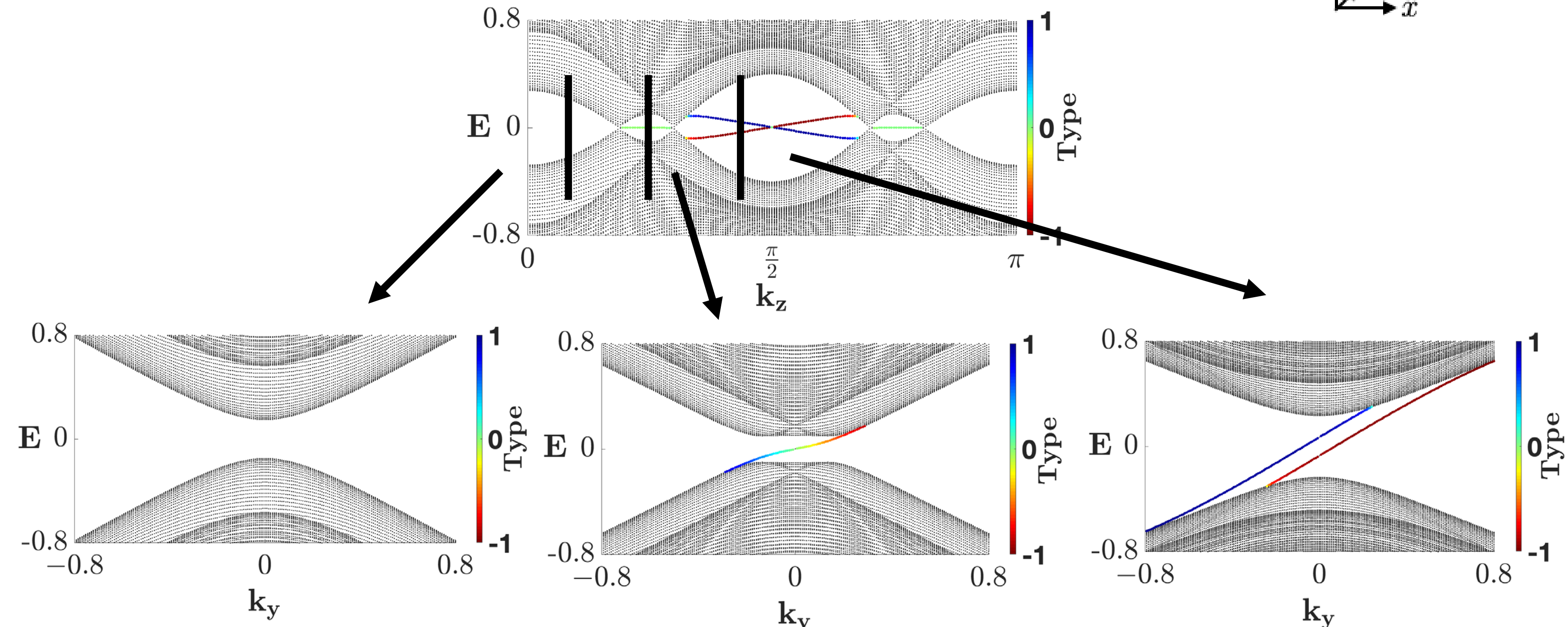
(CDW doubled)

Chern insulator

Fermi arc states

Energy spectrum





Trivial insulator

No surface states

Topological CDW

Quasiparticle surface states

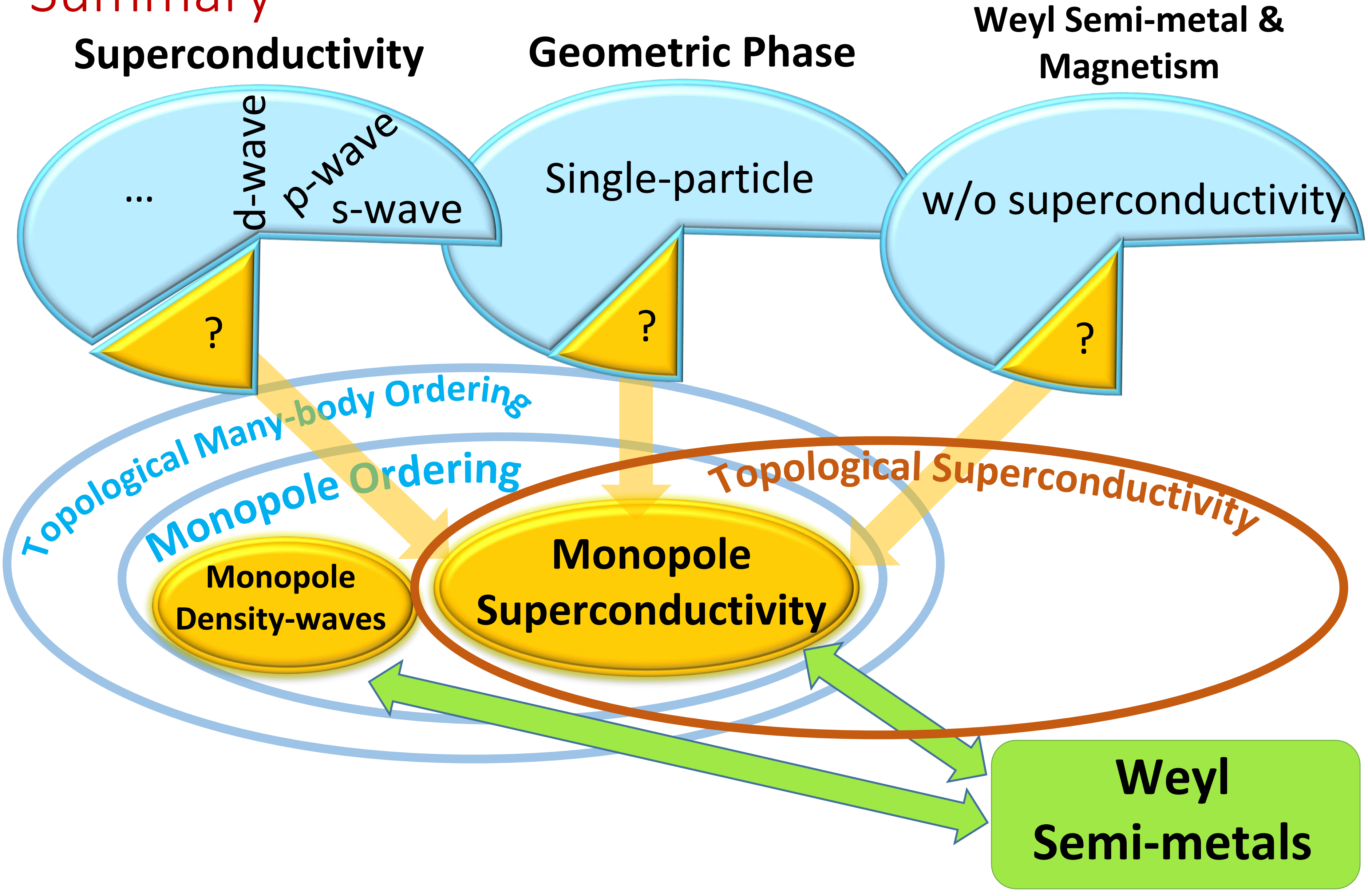
$$\gamma_{\mathbf{k}} = u c_{\mathbf{k}} + v c_{\mathbf{k}+\mathbf{Q}}$$

(CDW doubled)

Chern insulator

Fermi arc states

Summary


Superconductivity
Geometric Phase
Weyl Semi-metal &
Magnetism
…
d-wave
p-wave
s-wave
?
Single-particle
?
w/o superconductivity
?
Topological Many-body Ordering
Monopole Ordering
Topological Superconductivity
Monopole
Density-waves
Monopole
Superconductivity
Weyl
Semi-metals

Back up

Berry phase of Cooper pairs and topologically protected nodal pairing

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

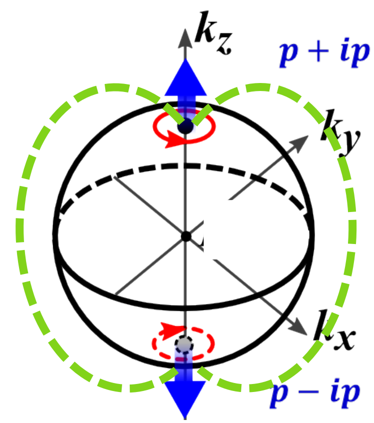
$$\frac{f_k}{1+|f_k|^2} = \frac{\Delta_k}{2E_k}$$

Δ_k: gap function

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

Chern # = 1 $q_2 = 1/2$

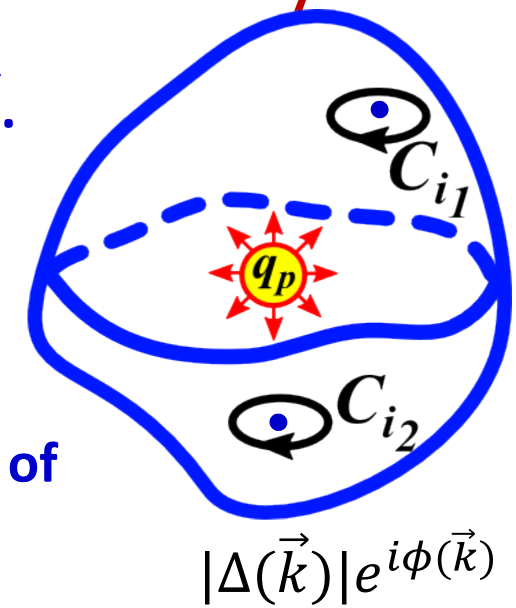
$$\boldsymbol{A}_p(\boldsymbol{k}) = i\langle\Psi_p(\boldsymbol{k})|\boldsymbol{\nabla}_k|\Psi_p(\boldsymbol{k})\rangle \neq 0$$
$$|\Psi_p(\boldsymbol{k})\rangle = c_1^+(\boldsymbol{k}) c_2^+(-\boldsymbol{k})|0\rangle$$



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

	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 $2q_p$**

Pair Berry phase protected nodal vorticity



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

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

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

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

1) k-space vorticity from gauge invariant “circulation field”.

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

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.

Example: Weyl semi-metal of spinless fermions

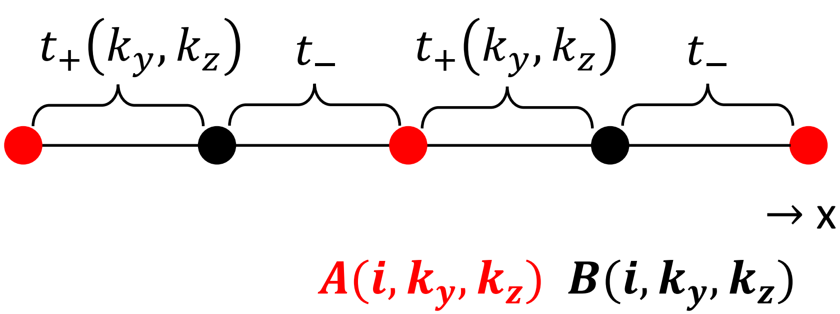
$$H_K = \sum_{\vec{k}} c_a^\dagger\left(\vec{k}\right)\{V(k_y)\sigma_3 + \left[t_- \cos(2k_x) + t_+(k_y,k_z)\right]\sigma_1$$

$$+\sin(2k_x)\sigma_2 - \mu\}_{ab} c_b\left(\vec{k}\right) + h.c.$$

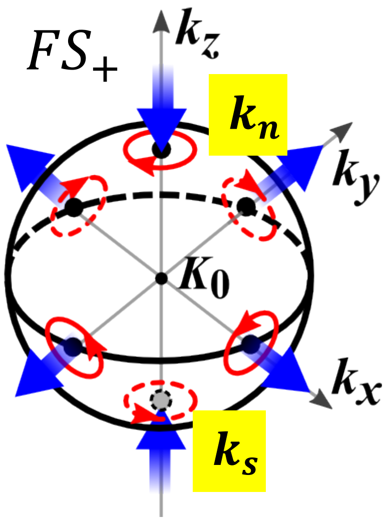
Modified Rice-Mele model: Pavan Hosur; FDM Haldane.

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

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

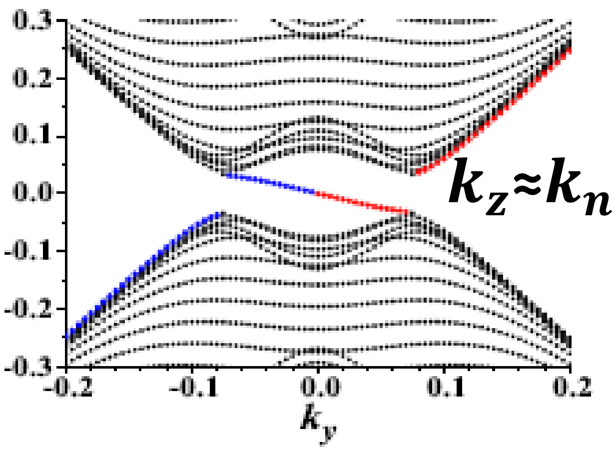


Surface spectra: Majorana meets Weyl

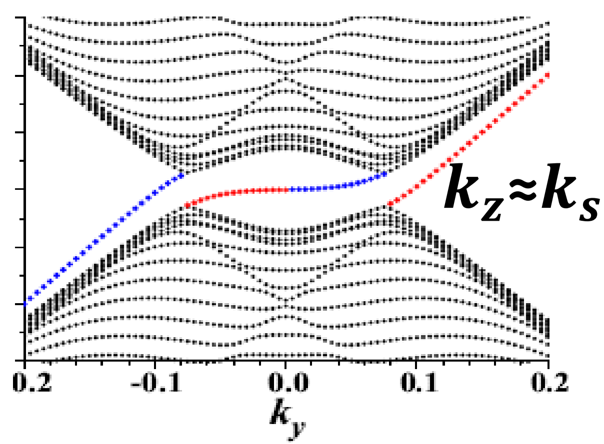


$$\Delta_y = i\Delta_x$$

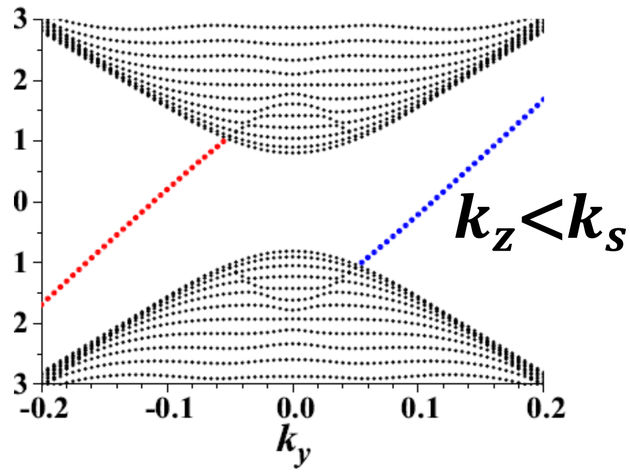
- Majorana modes: negative → positive chirality as k_z from N → S-hemisphere.
- Chirality : 0 $(k_z > k_n)$ → 1 (north herm-sphere) → 3(south hemi-sphere) → 2 $(k_z < k_s)$



-1



$-1 + 4 = +3$



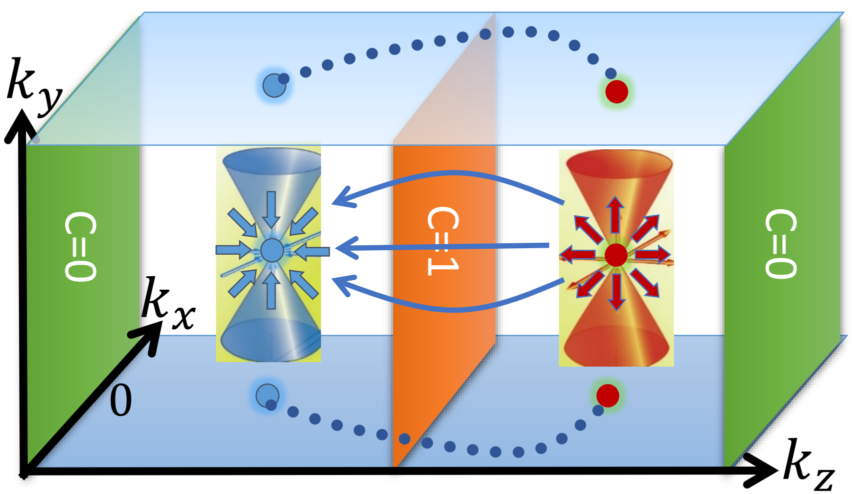
$-2 + 4 = +2$

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

Weyl points as pairs of monopoles (k-space)

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

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

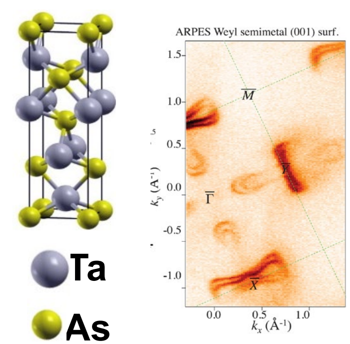


Theory: Wan, Turner, Vishwanath, Savrasov, PRB (2011); …
(Murakami 2007)

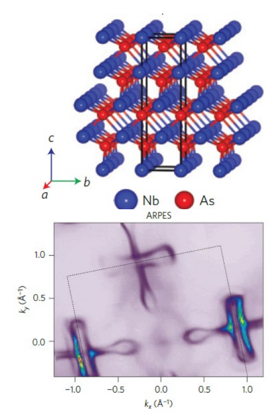
- **Fermi arcs connect projections of Weyl point pairs on the surface**

Observed in TR invariant Weyl semi-metals

TaAs



NbAs



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