Topological superconductivity in doped nodal-line semimetals

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Intertwined program, KITP

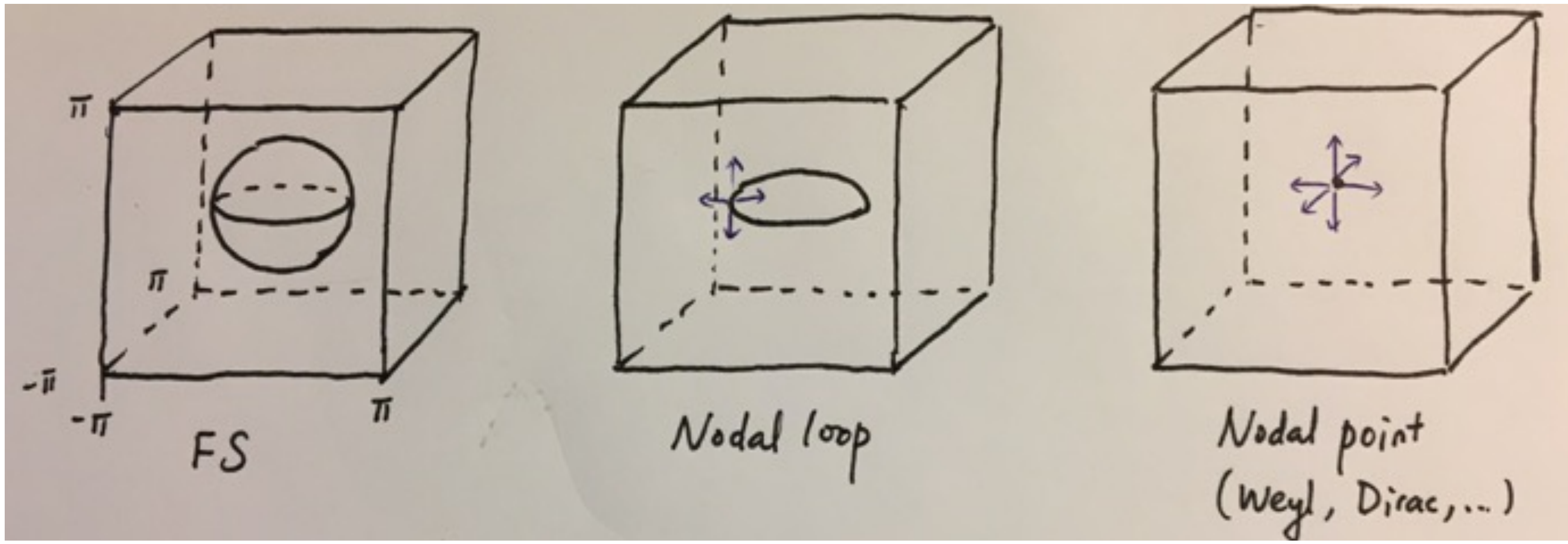
YW and Nandkishore, Phys. Rev. B **95**, 060506(R)
Shapourian, YW and Ryu, to appear

Outline

- Nodal-line semimetals/metals
- SC orders in the bulk and on the surface
- Odd parity pairing and its topology

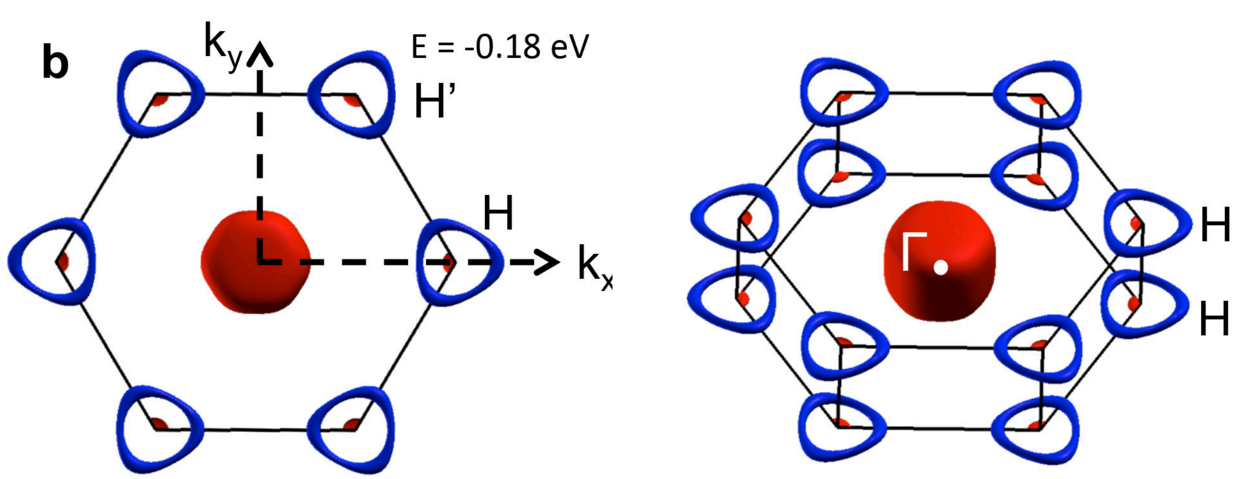
Nodal-line semimetals

- Low energy fermions in 3D band structures



Co-dimension =1 Co-dimension =2 Co-dimension =3

- Nodal lines, with FS co-dimension 2, proposed in Ca_3P_2, CaAgP, CaAgAs, and $TlTaSe_2$. Burkov, Hook, and Balents (2013) H. Weng, C. Fang, Z. Fang, B. A. Bernevig, and X. Dai (2015), Cava group (2015), Takenaka group (2016),



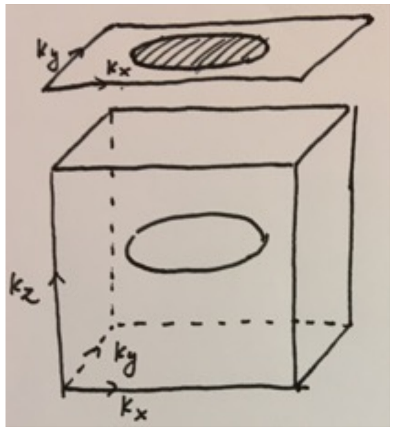
$TlTaSe_2$ (Proposed)
G. Bian et al, PRB (2016)

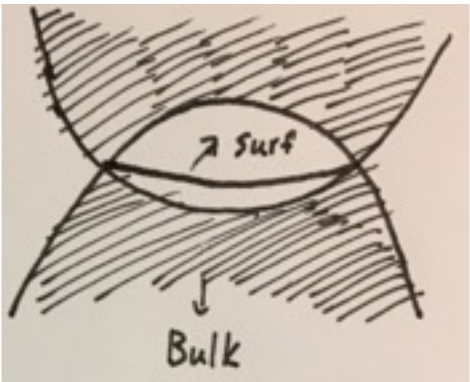
Nodal-line semimetals

- A minimal model is a two-band model ('Weyl loop')

$$\mathcal{H} = \sigma^x(k_x^2 + k_y^2 - k_F^2) + \sigma^y k_z$$

- We can use a mirror symmetry along z direction protects the nodal line, which is given by $M_z = \sigma^x$
- On the surface, *within* the momentum range of the projection of the line node, there exist bounds states with $\sigma^z = \pm 1$



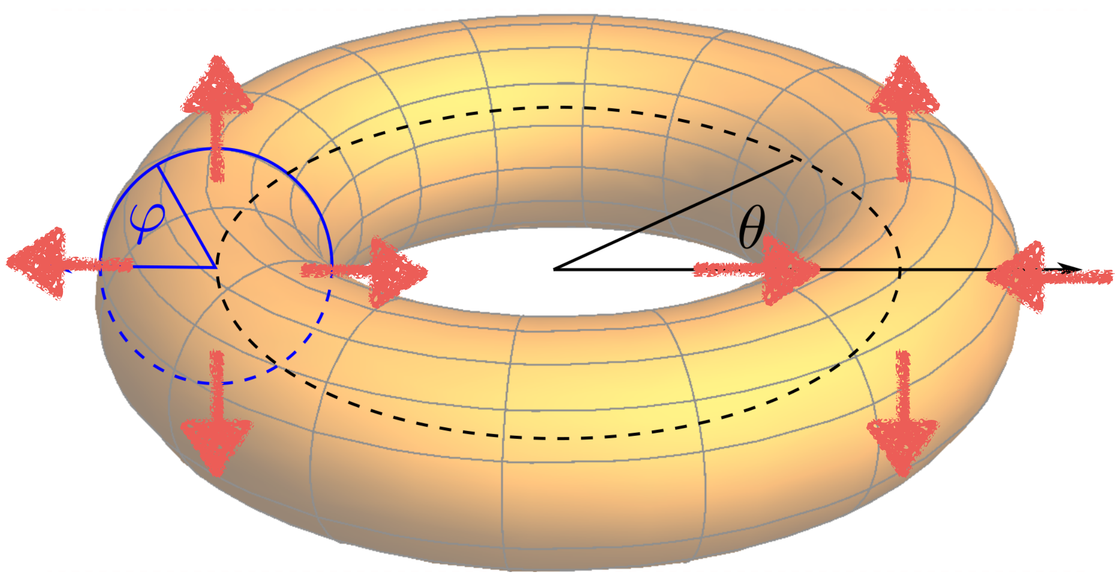


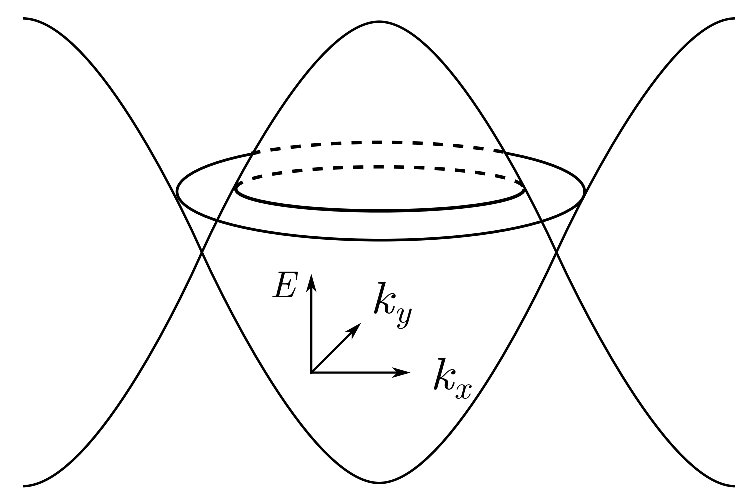
These so-called drumhead bands can lead to a topological polarization. Ramamurthy and Hughes 2015 Also its large density of states can lead to interesting correlation effects.

Nodal-line metals

- Today we focus on a Fermi surface obtained by 'doping a nodal line'.

$$\mathcal{H} = \sigma^x(k_x^2 + k_y^2 - k_F^2) + \sigma^y k_z - \mu$$





- The nontrivial properties of the nodal line now has been 'passed on' to the (pseudo)spin-textured Fermi surface.
- The torus-shaped FS naturally hosts superconducting instabilities.

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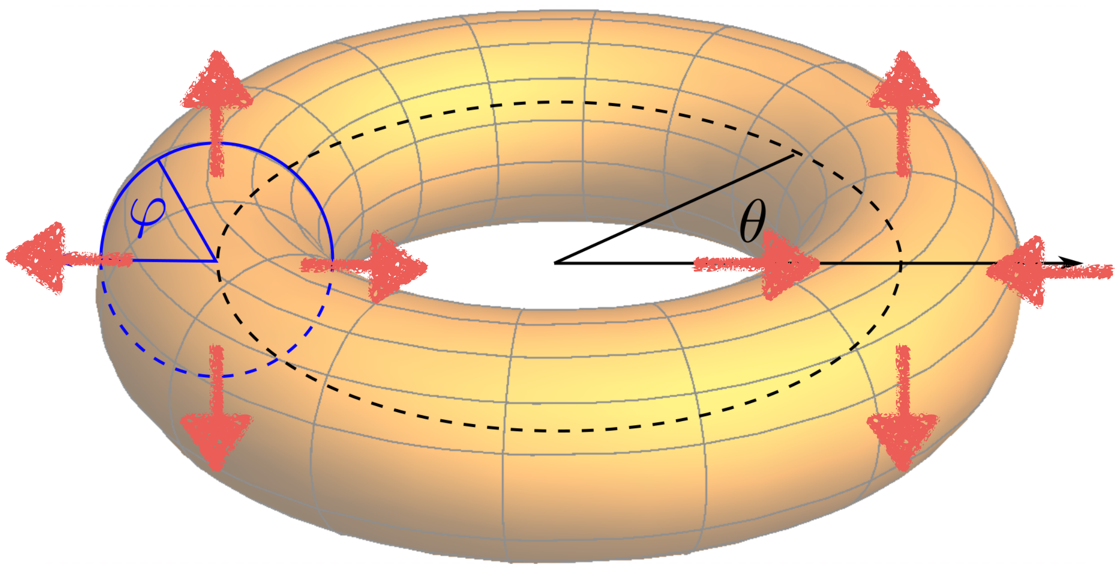
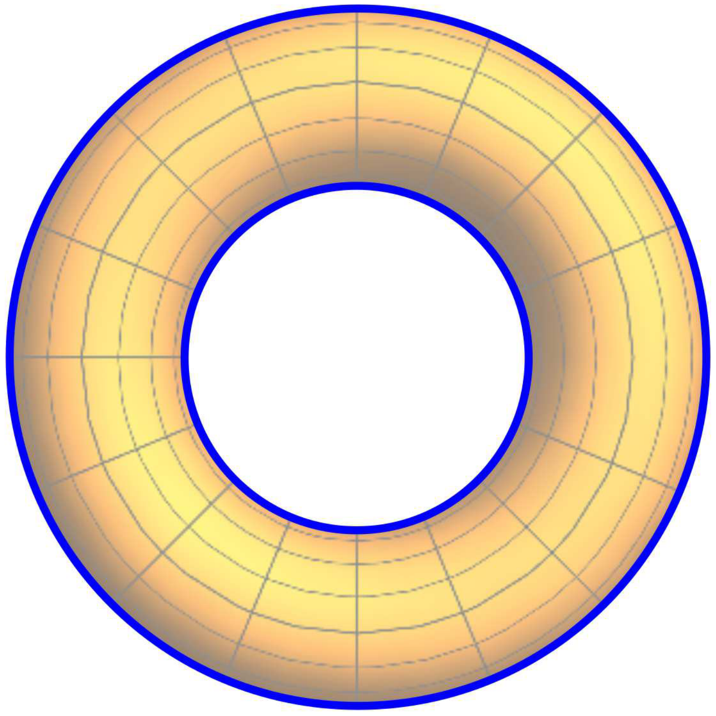
s-wave SC order

- The Fermi surface is spin-textured



- When projected to the Fermi surface, even *s*-wave order parameter can obtain nontrivial form factors (nodal lines).

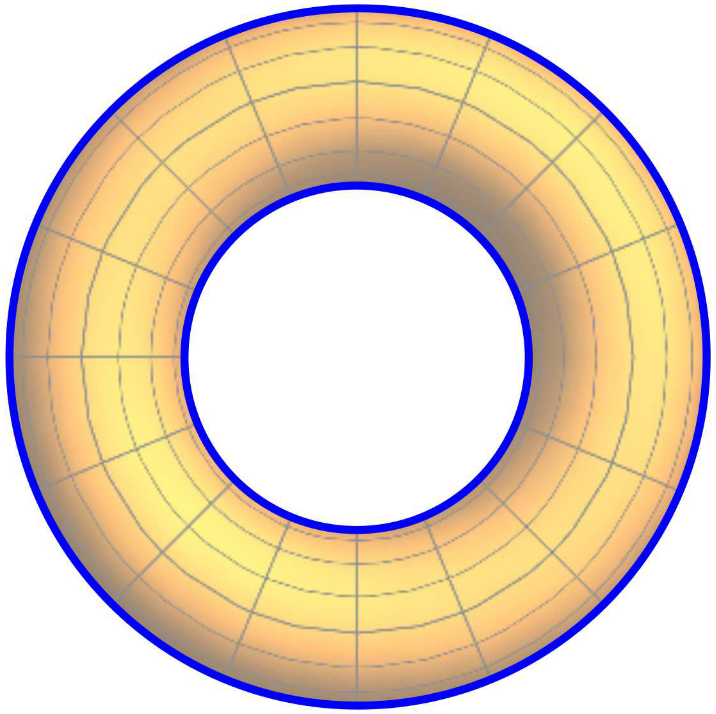


Surface states of *s*-wave SC order

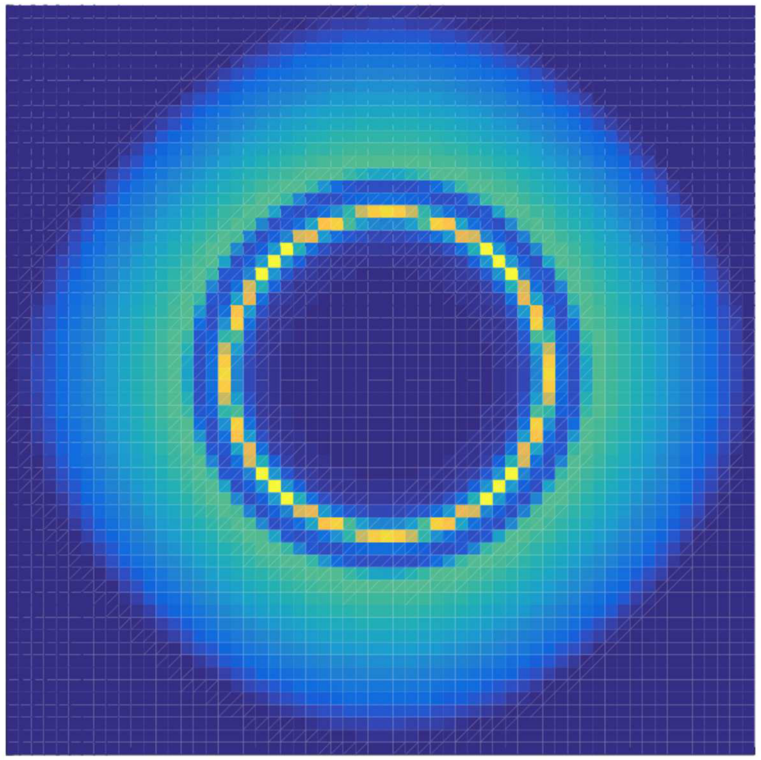
- The *s*-wave SC order also gets projected to the surface. However, the surface drumhead states are fully spin polarized, and hence is immune to *s*-wave pairing.

  SC bulk + Metallic surface!

- The 'new' nodal lines create their own surface states within the range of their surface projection. Due to a particle-hole symmetry they have strictly zero energy (Majorana flat band).



(a)

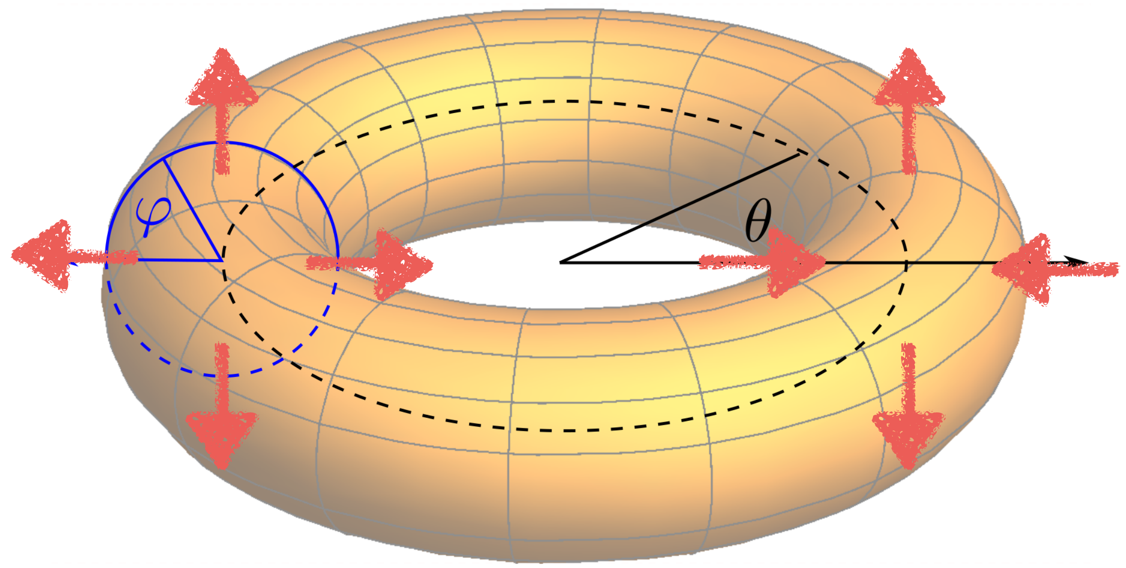


(b)

p-wave SC orders

- The torus-shaped FS with spin polarization is a natural host of a p-wave orders.

$$\mathcal{H}_p = e^{i\theta} c_{\mathbf{k}}^{\dagger} (\mathbf{d} \cdot \vec{\sigma})(i\sigma^y) c_{-\mathbf{k}}^{\dagger}$$



- Again, the bulk and the surface can behave differently.

d=d$_x$	metallic bulk	gapped surface
d=d$_y$	fully gapped bulk	fully gapped surface
d=d$_z$	bulk line-nodal SC	metallic surface

leading instability from a repulsive interaction! (→ row d=d$_y$)

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Topology of the fully-gapped SC state

- Fully gapped SC (both bulk and surface)with $\mathbf{d}=\mathbf{d}_y$.

$$\mathcal{H}_p = e^{i\theta} c^\dagger_{\mathbf{k}} (\mathbf{d} \cdot \vec{\sigma})(i\sigma^y) c^\dagger_{-\mathbf{k}}$$

- Found to be leading instability with short-range repulsion.
  Sur and Nandkishore (2016)
- What about its topology?

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	Symmetry			Dimension							
AZ	T	C	S	1	2	3	4	5	6	7	8
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AI	1	0	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
BDI	1	1	1	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
DIII	-1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0
AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$
CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
C	0	-1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
CI	1	-1	1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

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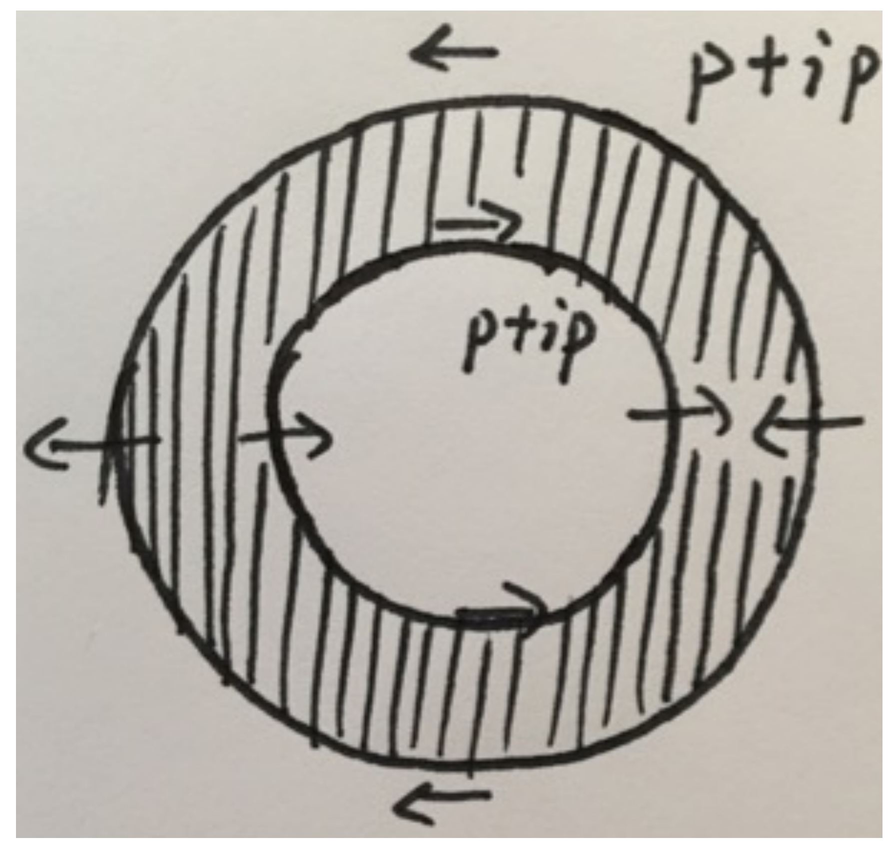
  Sur and Nandkishore (2016)
- What about its topology?
- At a given k_z, the Fermi surface slice is composed of two circles. One is an electron-like FS, and the other is an hole-like FS. Both of them are subject to *p+ip* pairing. The Chern numbers on the FS's are ±1, and cancel each other.



Topology of the fully-gapped SC state

- Mirror symmetry given by $M_z = \sigma^1$, which protects the nodal line in the normal state and is intact with SC.

$$h(\mathbf{k}) = \sigma_1 \tau_z (6 - t_1 - 2\cos k_x - 2\cos k_y - 2\cos k_z) + 2t_2 \sigma_2 \tau_z \sin k_z - \mu \sigma_0 \tau_z + \Delta \sigma_0 (\tau_x \sin k_x + \tau_y \sin k_y),$$

- It turns out that our system is a topological *crystalline* superconductor in Class 'D+Reflection'*, characterized by a mirror Chern number C_M=1.

*Needs M_z^2=1

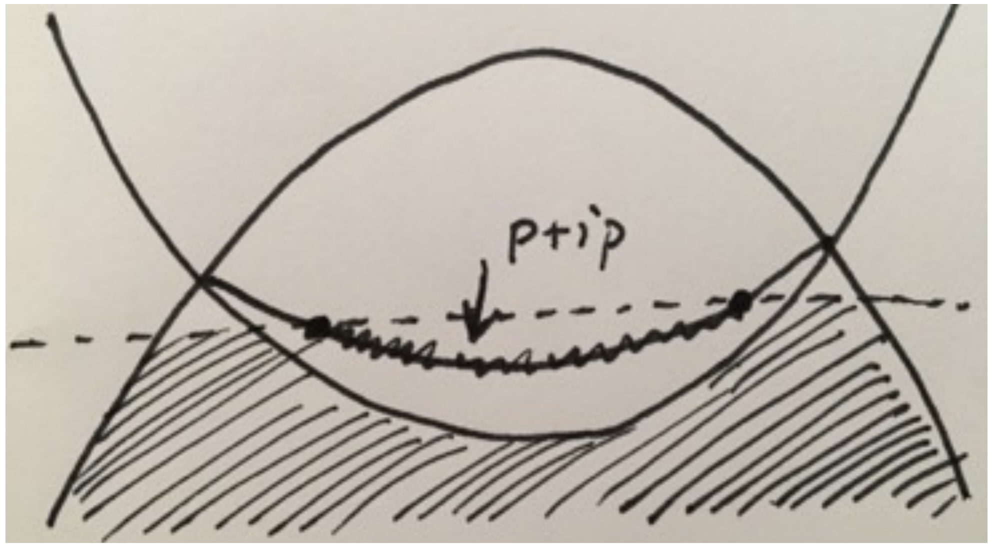
AZ Class	T	C	S	R operator	MSC	$d=1$	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$	$d=7$	$d=8$
AIII	0	0	1	R_+	$AIII^2$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$
				R_-	A	$\mathbb{Z}^1$	0	$\mathbb{Z}^1$	0	$\mathbb{Z}^1$	0	$\mathbb{Z}^1$	0
A	0	0	0	R	A^2	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0
AI	+	0	0	R_+^c	AI^2	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
				R_-	A	0	0	$2M\mathbb{Z}$	0	0	$\mathbb{Z}_2$	$M\mathbb{Z}$	0
BDI	+	+	1	R_{++}^c	BDI^2	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$\mathbb{Z}_2$
				R_{--}	AIII	0	0	0	$2M\mathbb{Z}$	0	0	$\mathbb{Z}_2$	$M\mathbb{Z}$
				R_{+-}	AI	$2\mathbb{Z}^1$	0	0	0	$\mathbb{Z}^1$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
				R_{-+}	D	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0
D	0	+	0	R_+^c	D^2	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
				R_-^d	A	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	0	$\mathbb{Z}_2$

Chiu-Yao-Ryu 2013

- The mirror Chern number protects the gapless yz and xz surfaces. What about xy surface that breaks mirror?

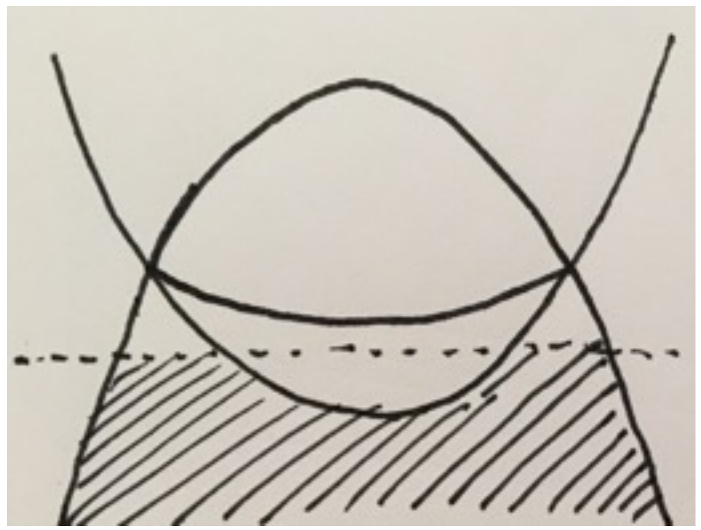
Topology of the surface states

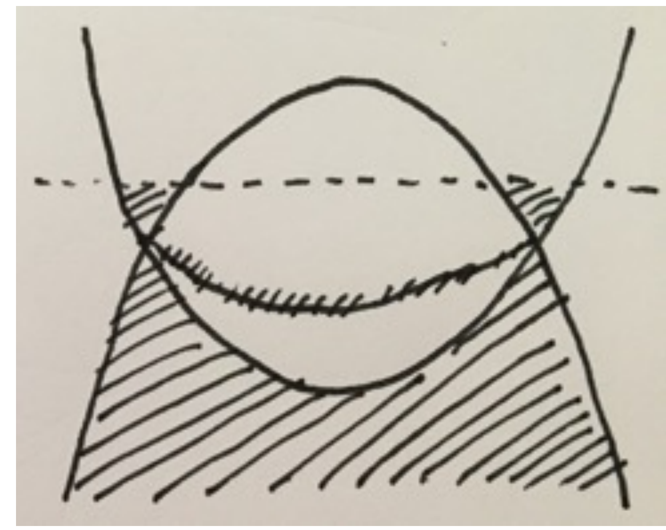
- What about the xy surface states in a slab geometry?
- First, suppose we allow a dispersion to the surface bands; they can have a 'surface Fermi surface'.
- The surface drumhead bands are subject to a *p+ip* pairing, and thus mimics a two-dimensional topological superconductor.
- Guess: Vortex lines in z-direction may trap Majorana modes



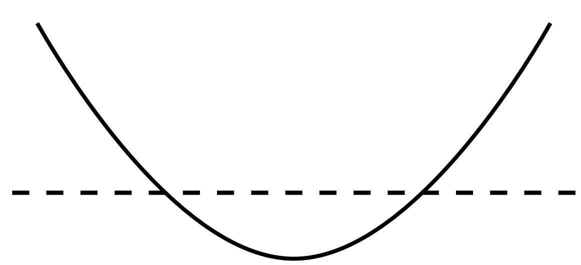
Topology of the surface states

- But what about the following cases?

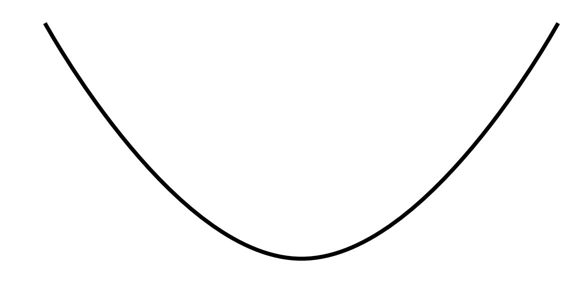




- These states don't have a 'surface Fermi surface'. (Let's call these 'strong' phases, for the lack of a better name)
- For the 2D *p+ip* state, there are two phases, a trivial phase and a topological phase. Moore-Read 1991



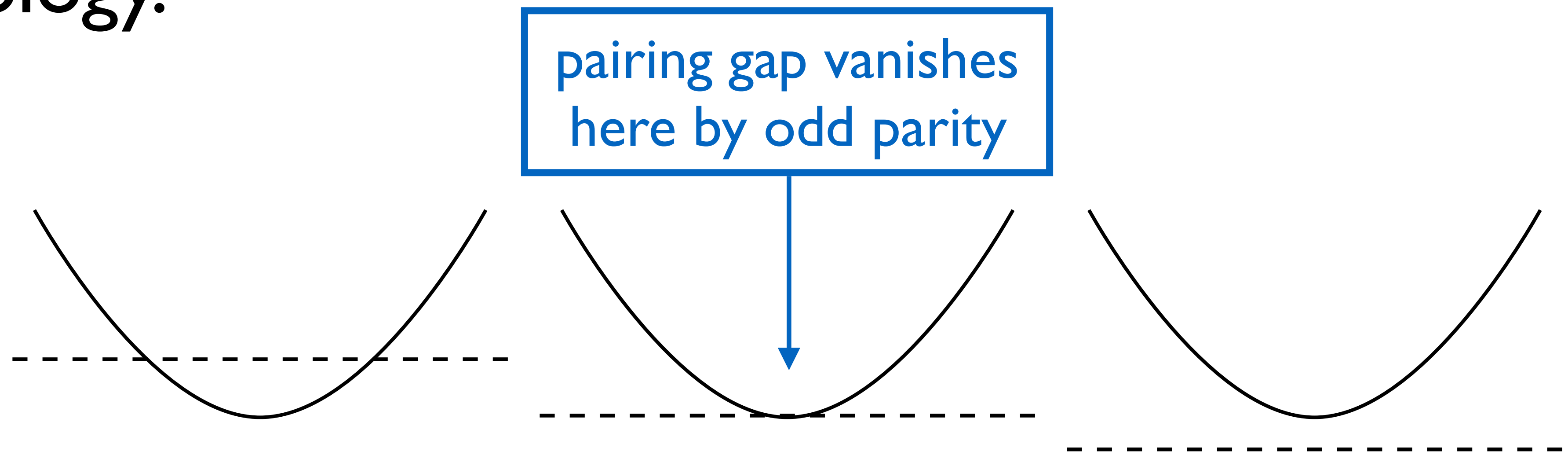
'weak' pairing phase, topological



'strong' pairing phase, trivial

Gap closing argument

- For a 2D *p*+*ip* state, going from weak to strong pairing phase, the bulk gap has to close, signifying a change in topology.



(a)

Gap closing argument

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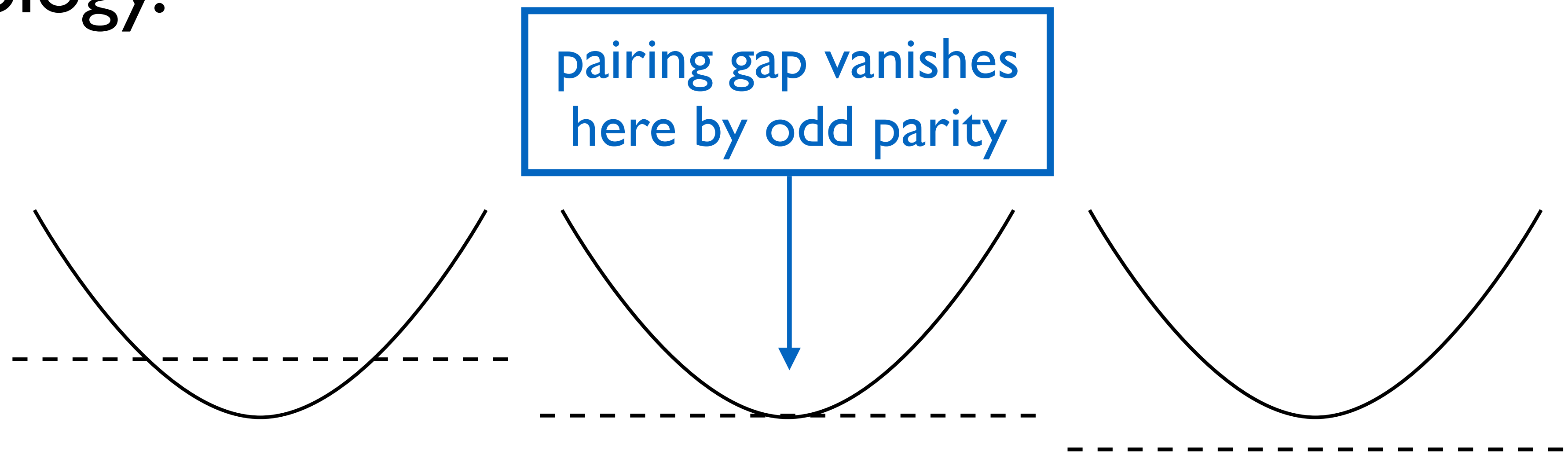
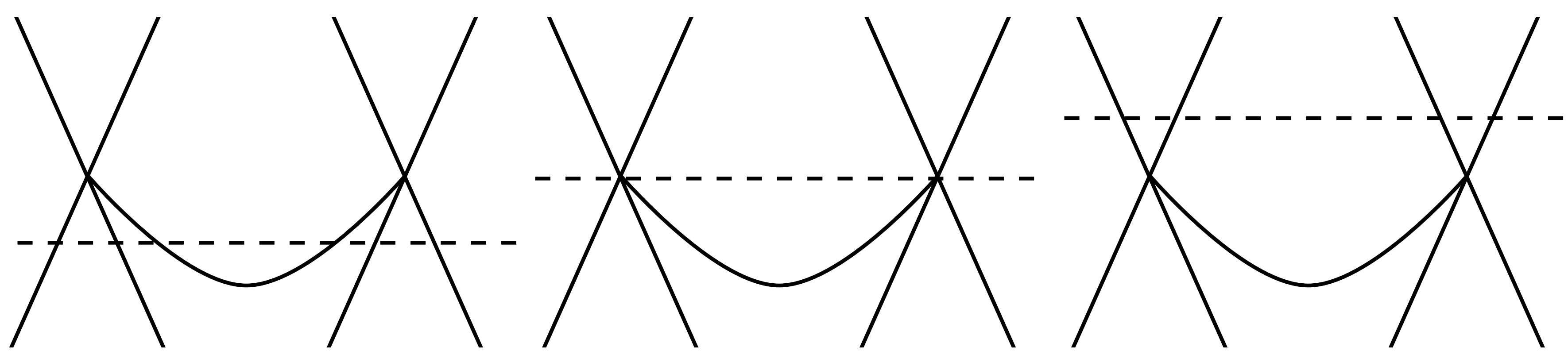


(a)

- For the drumhead bands, going from 'weak' to 'strong' case doesn't require such a gap closing! (Both are topo.?)



Layer-resolved Chern number

- The two surfaces are *not* stand-alone 2D systems, and one cannot use a homotopy to define a quantized Chern number.
- One can nevertheless define a layer-resolved Chern number Essin-Moore-Vanderbilt 2009

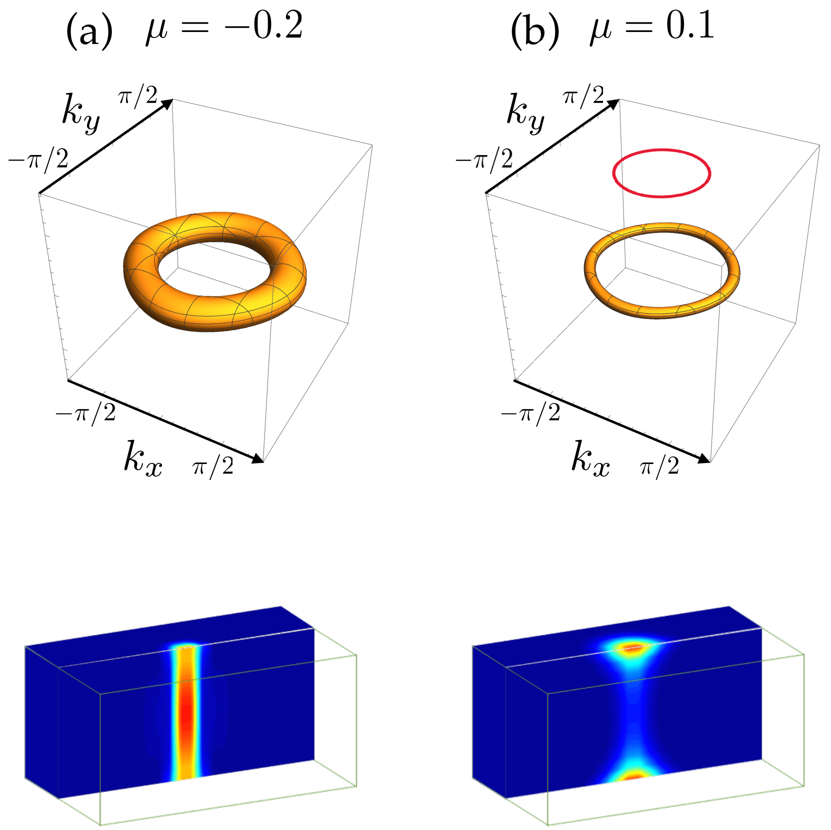
$$C = \frac{2\pi}{iL^2} \sum_{\mathbf{k}} \mathrm{Tr}\left[\mathcal{P}_{\mathbf{k}} \epsilon_{ij} (\partial_i \mathcal{P}_{\mathbf{k}})(\partial_j \mathcal{P}_{\mathbf{k}})\right]$$

$$C_z = \frac{2\pi}{iL^2} \sum_{\mathbf{k}} \mathrm{Tr}\left[\mathcal{P}_{\mathbf{k}} \epsilon_{ij} (\partial_i \mathcal{P}_{\mathbf{k}}) |z\rangle\langle z| (\partial_j \mathcal{P}_{\mathbf{k}})\right]$$

- It turns out layers from each surface contributes to a layer Chern number 1/2, which comes from drumhead bands subject to p+ip pairing, for both "strong" and "weak" cases
- Total Chern number =1, meaning *one* Majorana mode for a vortex line. Different from a Fu-Kane SC where there are two.

Wave function of Majorana zero modes

- Numerically, the wave function profile for strong and weak cases are different, but in both cases there is only one Majorana zero mode.



- For weak case, despite the resemblance with two p+ip SC's, the wave function of the Majorana mode *cannot* be split into two.

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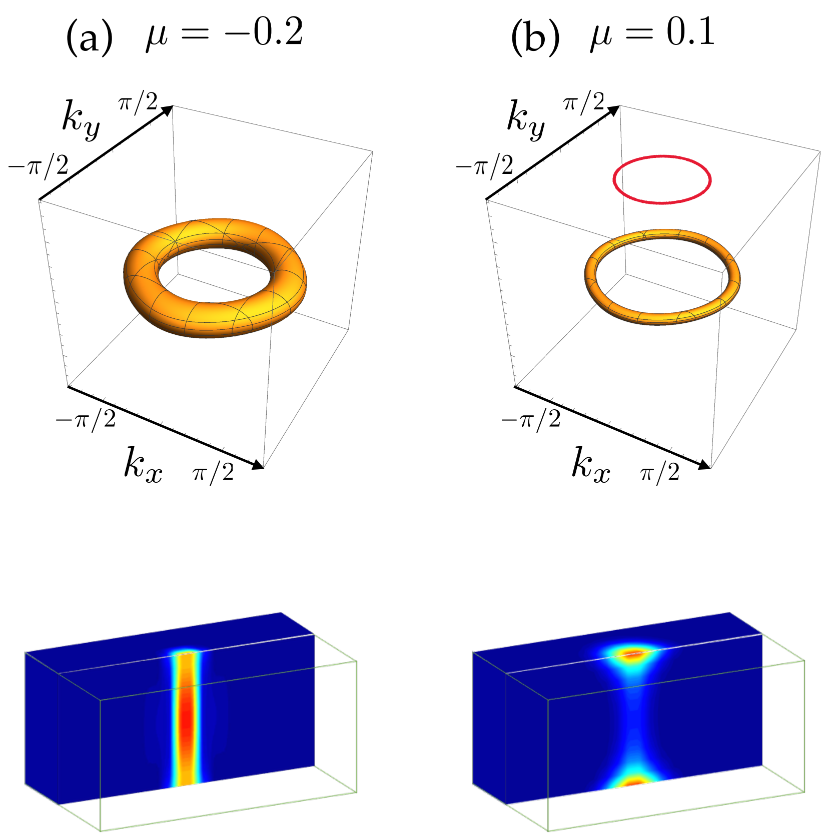

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- The MZM is localized on surface if mirror is broken.

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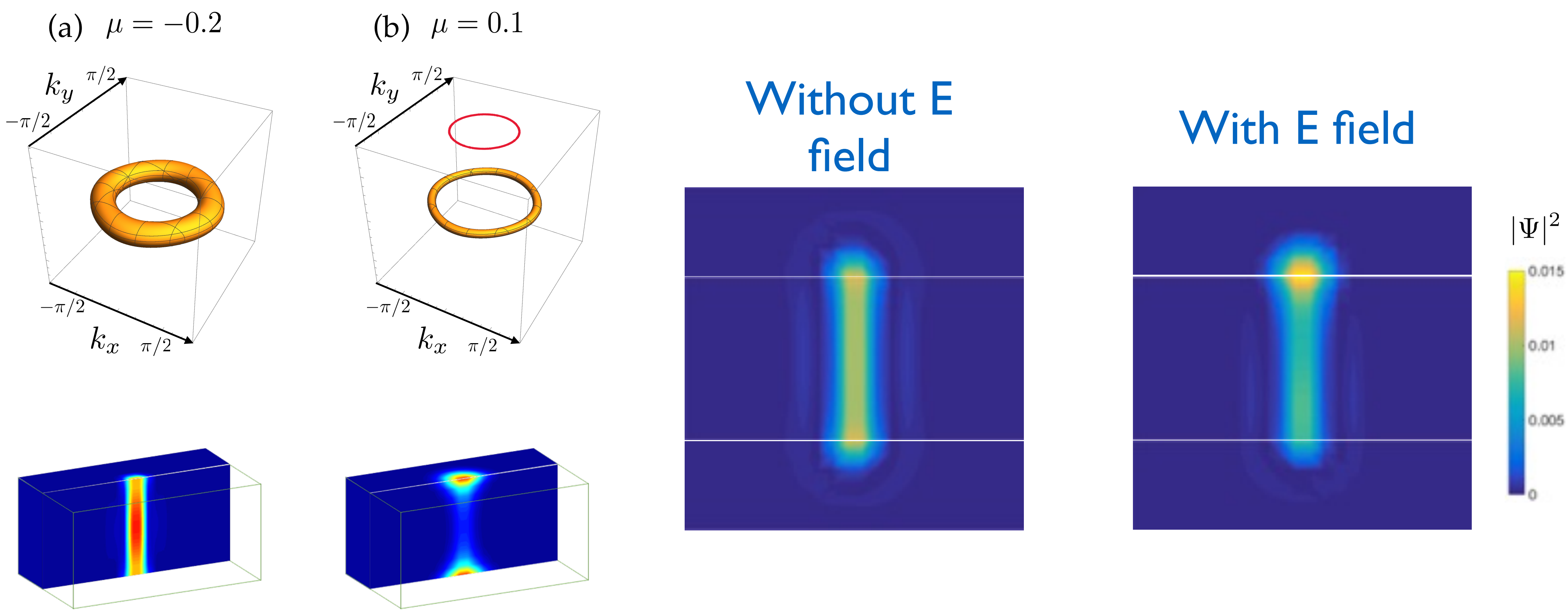

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Where does the Chern number come from

- The lattice BdG Hamiltonian:

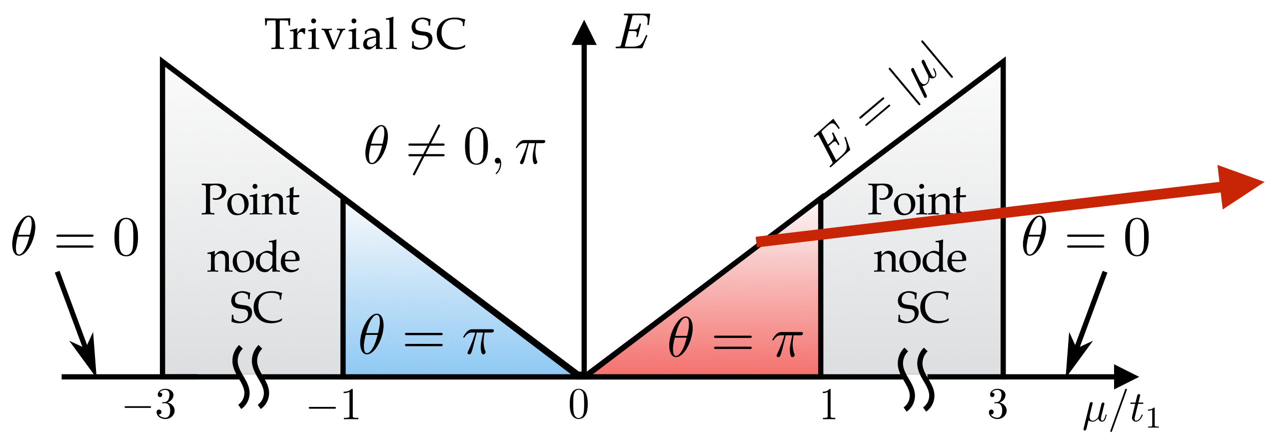
$$h(\mathbf{k}) = \sigma_1 \tau_z (6 - t_1 - 2\cos k_x - 2\cos k_y - 2\cos k_z) + 2t_2 \sigma_2 \tau_z \sin k_z - \mu \sigma_0 \tau_z + \Delta \sigma_0 (\tau_x \sin k_x + \tau_y \sin k_y),$$

- Viewed as an insulator, the EM response is given by:

$$\mathcal{S} = \frac{\theta}{8\pi^2} \int d^3x dt\, \epsilon^{\mu\nu\rho\sigma} F_{\mu\nu} F_{\rho\sigma}$$

  where $\theta = \pi$. At the surface this action gives rise to the half (layer-resolved) Chern number.

- Here the quantization $\theta = \pi$ is protected by mirror symmetry. $\theta = \pi$ *can even* survive a small mirror breaking field, as long as the torus FS is intact.



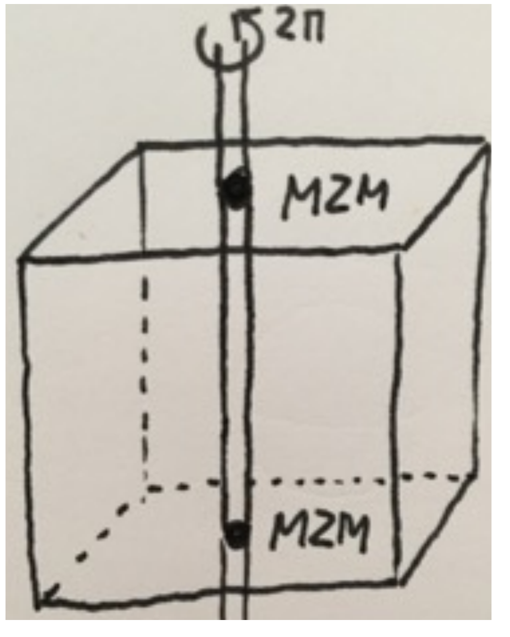
The mirror breaking field eliminates the torus FS

Extension to Dirac loop case

- In real materials the nodal loop is four-fold degenerate, which, without spin-orbit coupling, can be viewed as the spin double of a Weyl loop. (Weyl loop is still desirable!)
- The same *p*-wave order can still be the leading instability for a repulsive interaction.
- It is a topological crystalline superconductor in the same class with C_M=2.
- Top and bottom surfaces combine to Chern number C=2. This typically does not lead to two vortex core Majorana modes, as they can gap out each other.

Extension to Dirac loop case

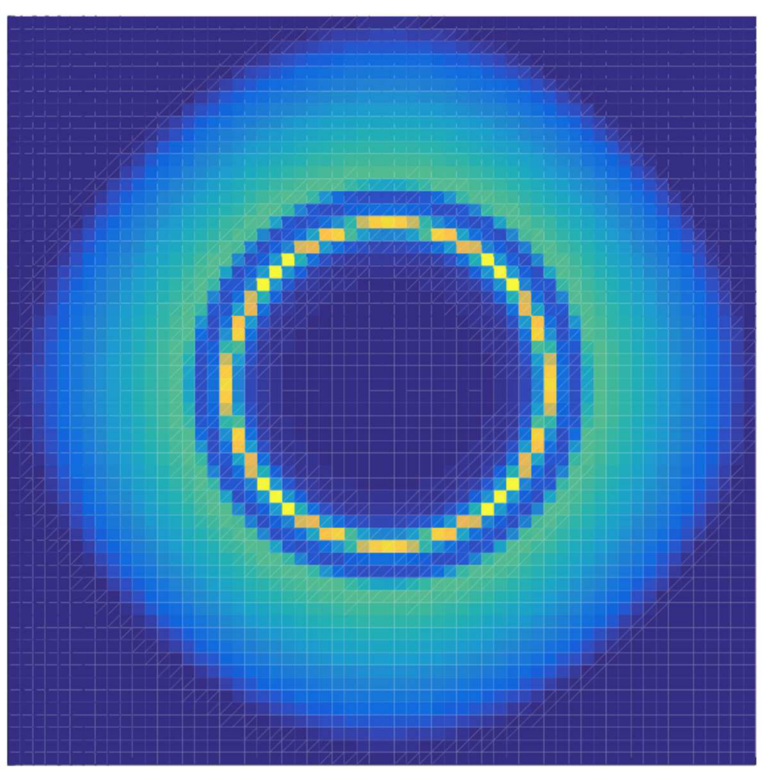
- However, consider a spin-orbit coupling term which couples like a $+E$ field for spin up, and a $-E$ field for spin down.
- With such a spin-orbit coupling the two Majorana modes can be spatially separated onto top and bottom surfaces and thus remain at zero energy.

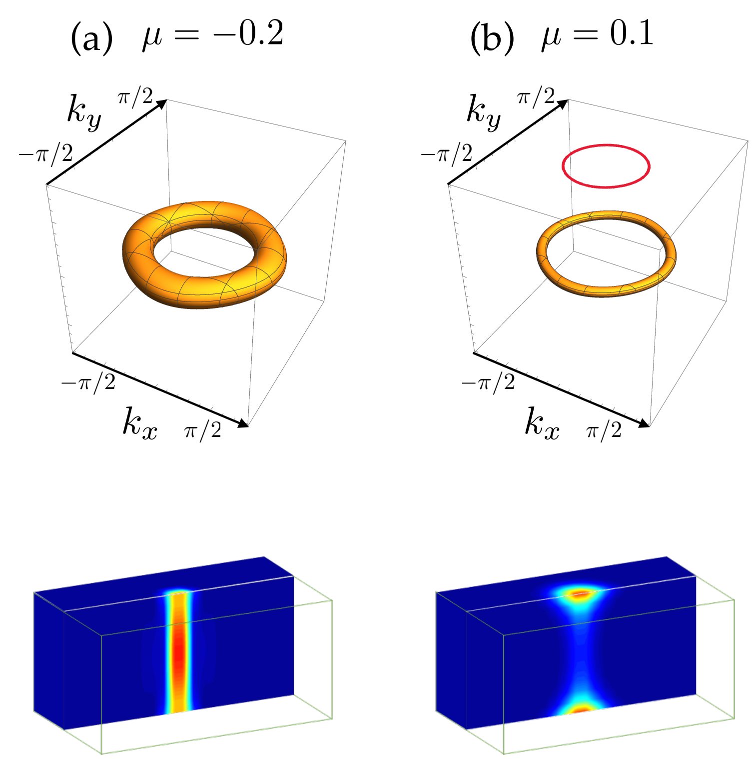


- Spin-orbit coupling does exist in candidate materials such as CaAgAs.

Summary

- The torus-shaped FS is a natural host of many unconventional SC.
- The *s*-wave state features metallic surface bands, Majorana flat bands, and bulk nodal-line superconductivity.
- The *p*-wave state is a topological crystalline superconductor hosting MZM's. This result can be extended to four-band Dirac loop case.





Thank You!