Topological nonsymmorphic crystalline insulators and superconductors

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Chao-Xing Liu, Rui-Xing Zhang, and Brian K. VanLeeuwen, Phys. Rev. B 90, 085304 (2014).
Qing-Ze Wang and Chao-Xing Liu, arxiv: cond/1506.07938 (2015).

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Outline

- Introduction, symmetry and topology in the classification of states of matter
- Topological mirror insulators and superconductors
- Nonsymmorphic symmetry and topological phases
  - Topological non-symmorphic superconductors
  - Topological non-symmorphic insulators
- Conclusion and outlook

States of matter and Landau theory

- Landau theory: states of matter are classified by symmetry

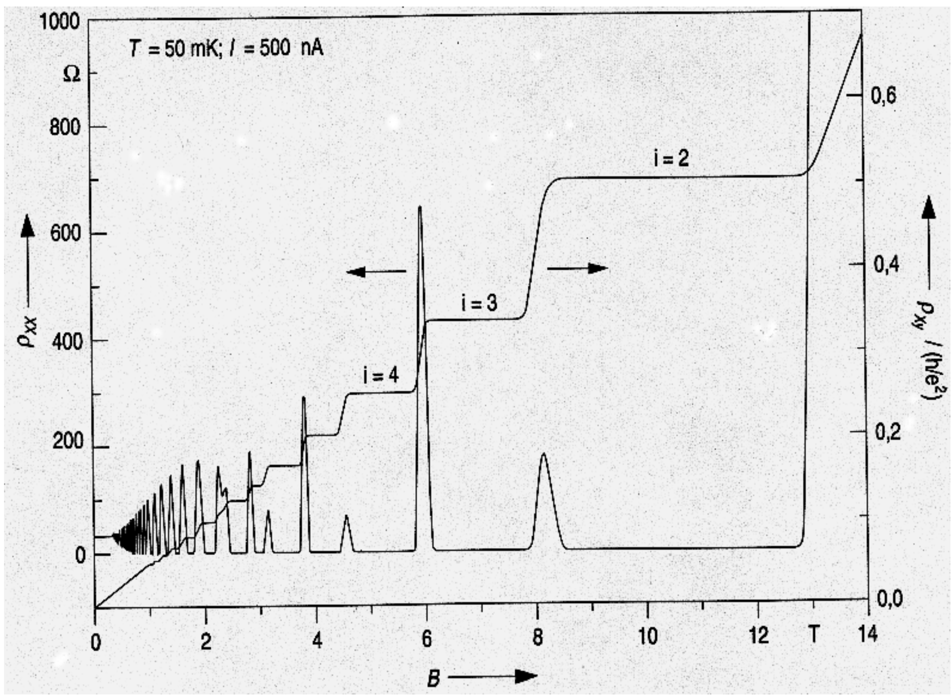
E.g. a solid is different from a gas because it breaks translational symmetry.

Solid

Gas

Quantum Hall Effect

- The quantum Hall effect: topological states, which is beyond Landau theory



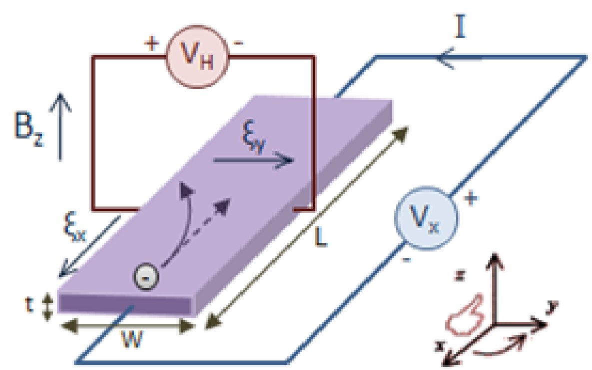
Klaus von Klitzing (1980)

$$\sigma_H = C\frac{e^2}{h}$$

$$C = 1,2,\dots,n$$

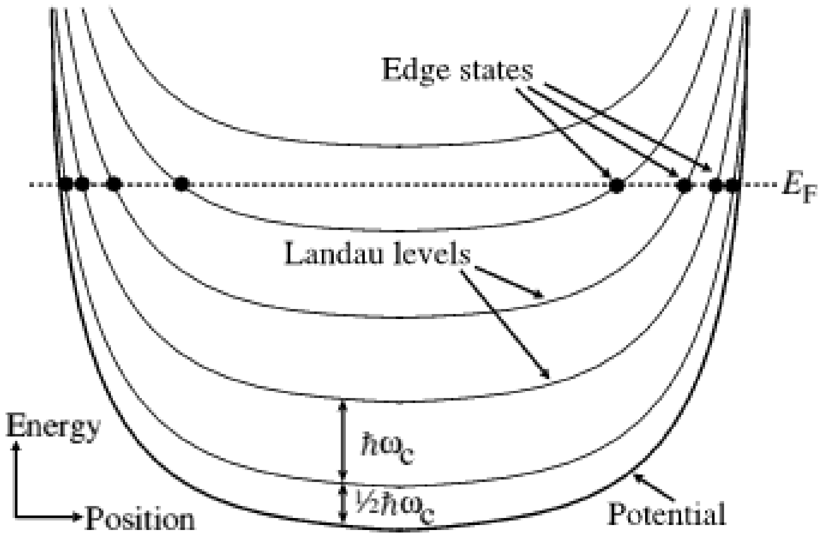
TKNN (1982)

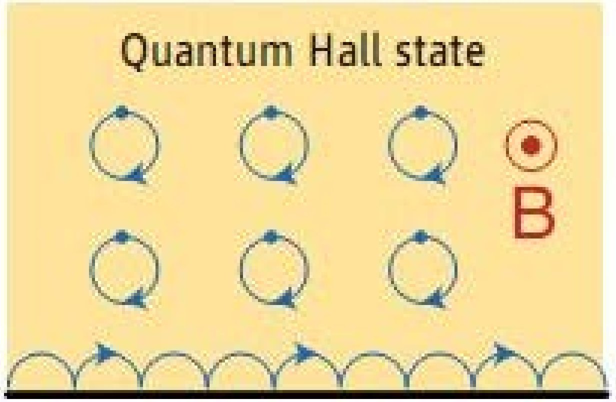
Klaus von Klitzing (1943-Present)

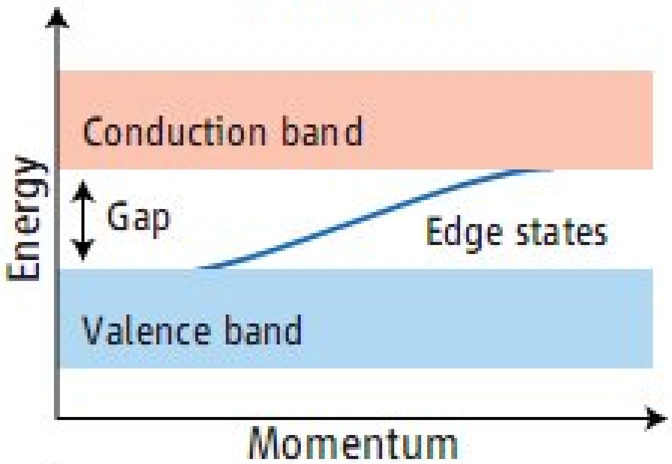


Quantum Hall effect

- The quantum Hall effect and chiral edge states

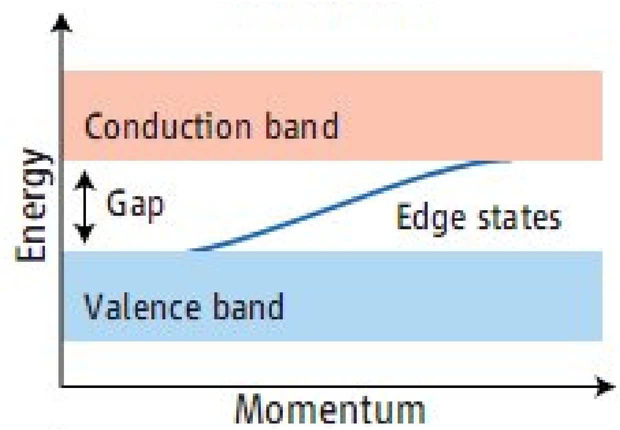






Topological states of matter

- Topological states for free fermions
  - Topological states cannot be adiabatically connected to normal states without gap closing even though sharing the same symmetry. E.g. Quantum Hall state with Landau gaps.
  - Topological states have edge/surface modes at the boundary (surface or interface). E.g. Chiral edge states of the QH effect



Symmetry and topological states of matter

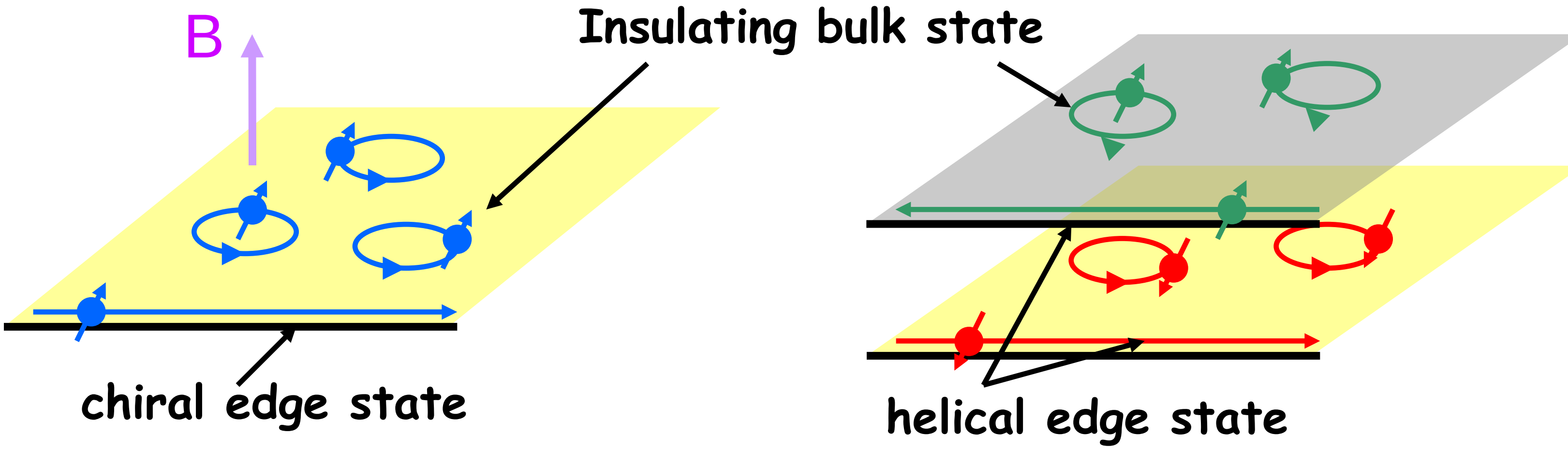
- Question: can we have more topological phases beyond the quantum Hall state?
- For a long time, people thought the QH state is the only example.
- Recent development has shown more topological states when there are additional symmetries.
  - Topological insulators: insulating bulk gap and helical edge states which are protected by time reversal symmetry.
  - Topological superconductors: superconducting bulk gap and Majorana zero modes
  - Topological crystalline insulators and superconductors
  - More topological states due to interaction.

Qi and Zhang, RMP (2011), Hasan and Kane, RMP (2010).

Topological insulators

Quantum Hall state
Magnetic fields

Quantum spin Hall state
(2D topological insulators)
Spin-orbit coupling



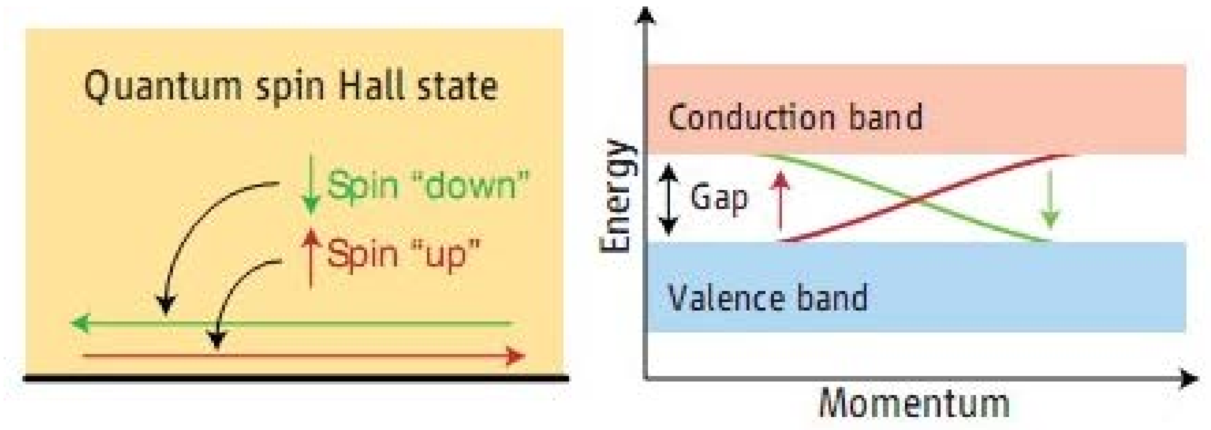
Break TR $\sigma_H \neq 0$

Preserve TR $\sigma_H^{\uparrow} = -\sigma_H^{\downarrow}$

Kane and Mele, PRL (2005) (2006), Bernevig and Zhang, PRL (2006)

Topological insulators

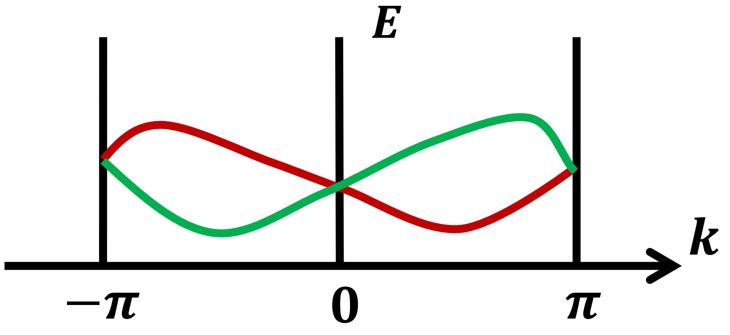
- Helical edge/surface states and time reversal symmetry



  - Krammers' theorem, time reversal can protect degeneracy of spinful fermions when $\Theta^2 = -1$.

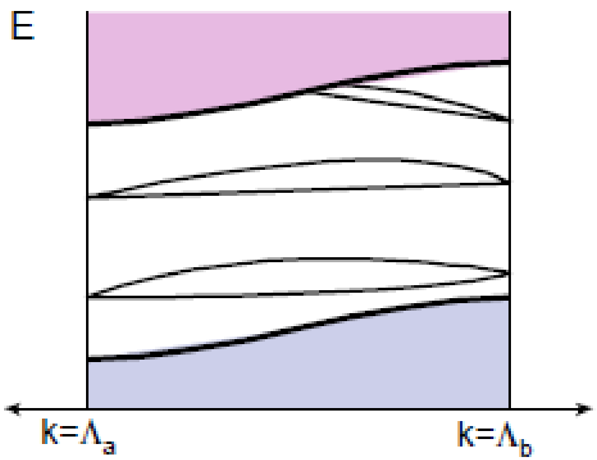
$$E(\vec{k},\uparrow) = E(-\vec{k},\downarrow)$$

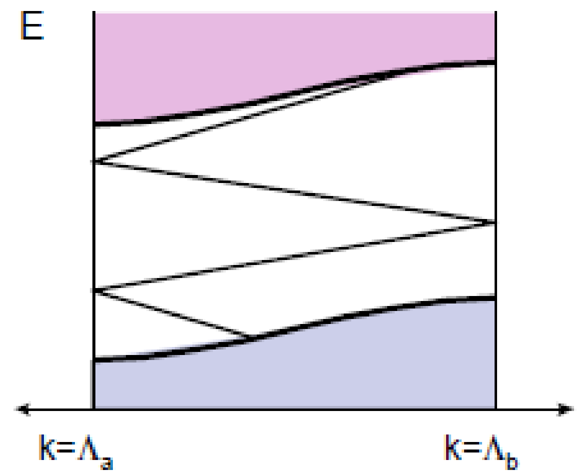
$$\vec{k} = -\vec{k} + \vec{G}$$



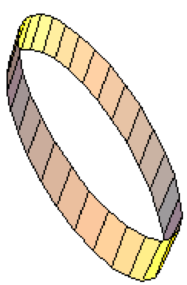
Topological insulators

- How does Kramers' degeneracy protect non-trivial surface states?

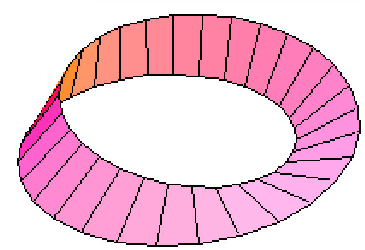




Trivial

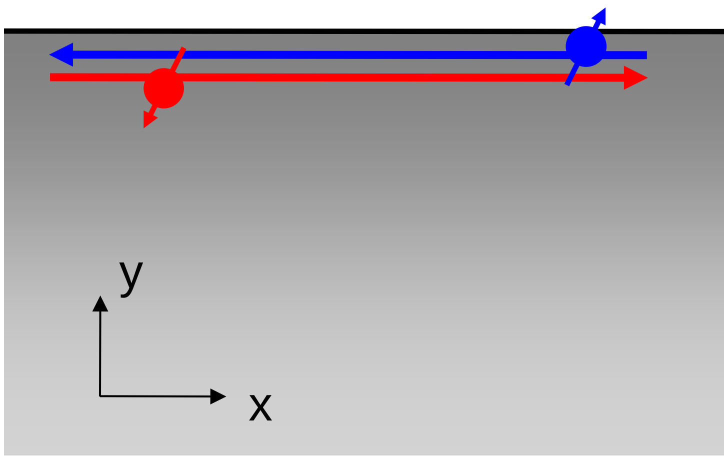


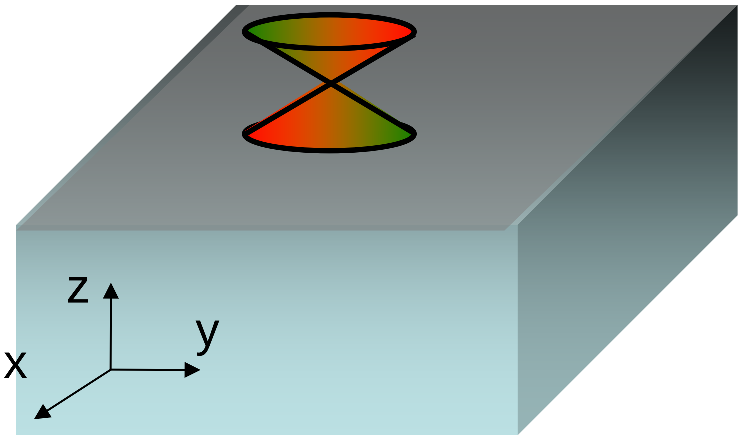
Non-trivial



Topological insulators

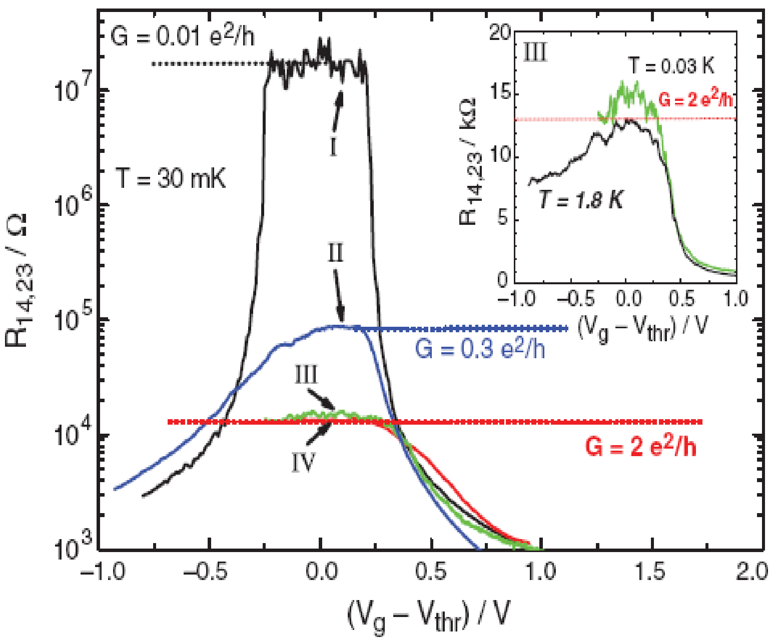
- Topological insulators in 3D: an odd number of Dirac cones at one surface.

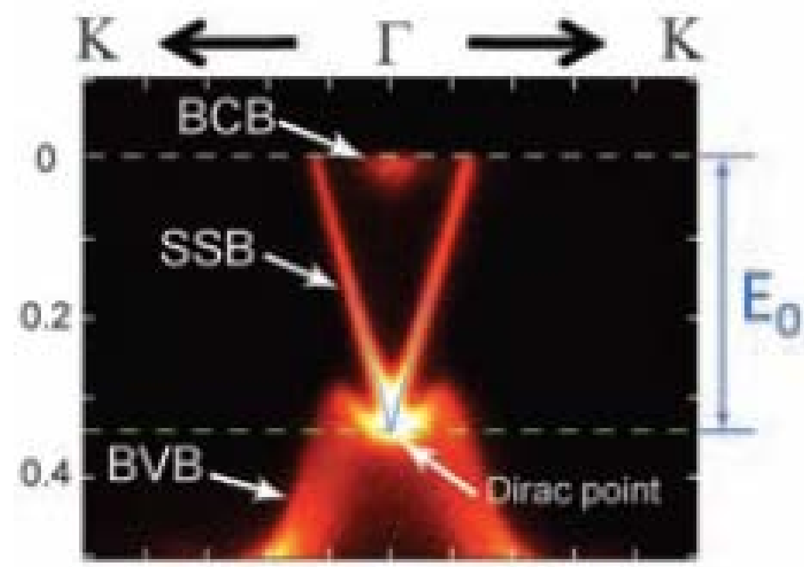




Topological insulators

- Experimental observation of helical edge states in topological insulators



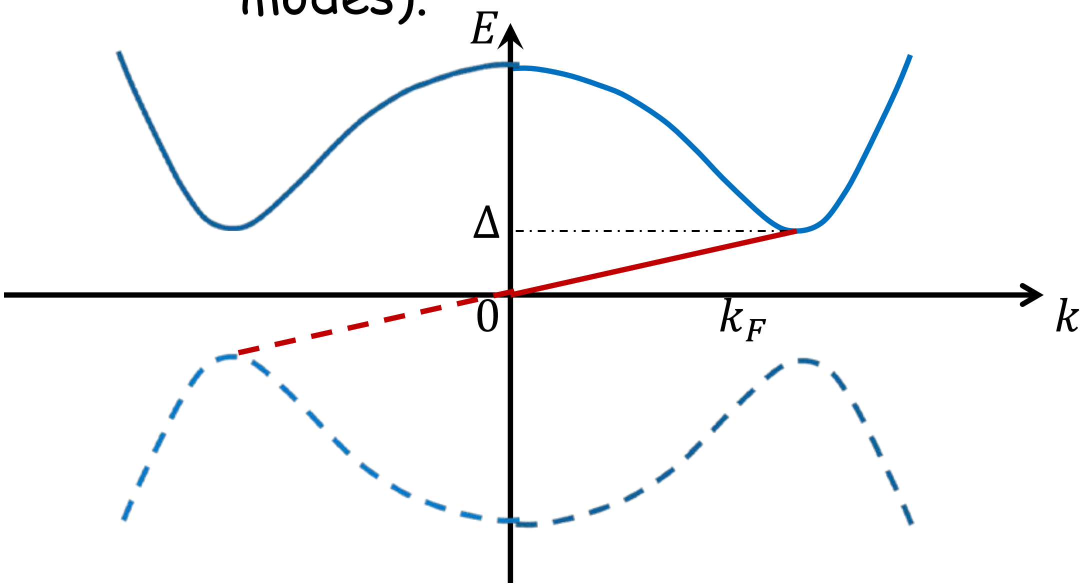


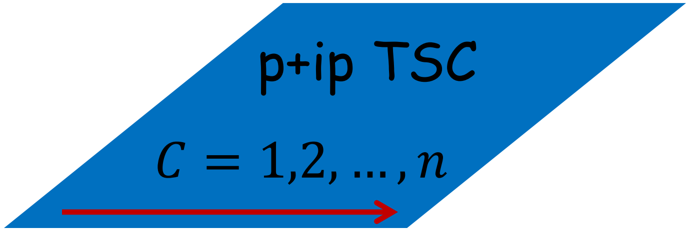
Bernevig, et al (2006), Konig, et al (2007)

Hsieh, *et al,* (2008), (2009); Roushan, et al, (2009), H.J. Zhang *et al* (2009); Xia *et al* (2009); Y. L. Chen (2009)

Topological superconductors

- Topological superconductors and particle-hole symmetry
  - Superconducting gap in the bulk
  - Gapless excitation at the boundary with zero energy at zero momentum (Majorana fermion or Majorana zero modes).



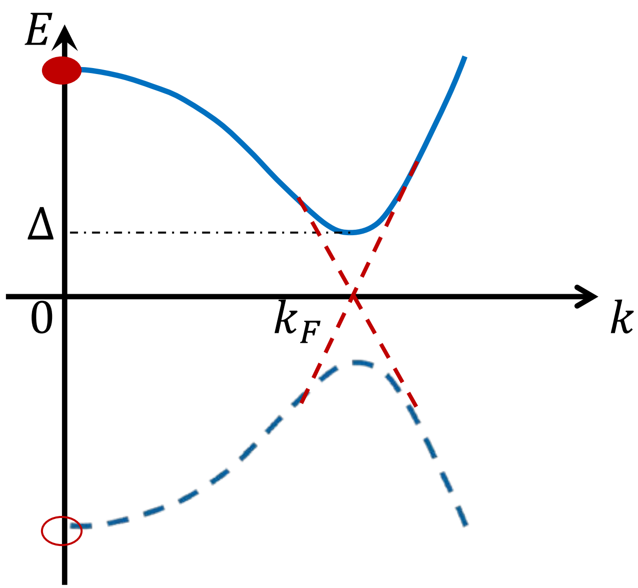


Read and Green (2000)

Topological superconductors

- Bogoliubov-de Gennes Hamiltonian and particle-hole symmetry (redundancy).

$$\hat{H} = \frac{1}{2}\sum_{k}\left(\psi_k^+ \quad \psi_{-k}\right) H_{BdG} \begin{pmatrix} \psi_k \\ \psi_{-k}^+ \end{pmatrix}$$



$$H_{BdG} = \begin{pmatrix} h(k) - \mu & \Delta(k) \\ \Delta^+(k) & -h^*(-k) + \mu \end{pmatrix}$$

Particle-hole symmetry

$$C H_{BdG} C^{-1} = -H_{BdG}$$

$$C = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} K$$

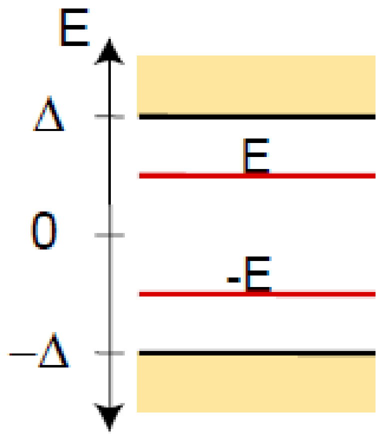
Topological superconductors

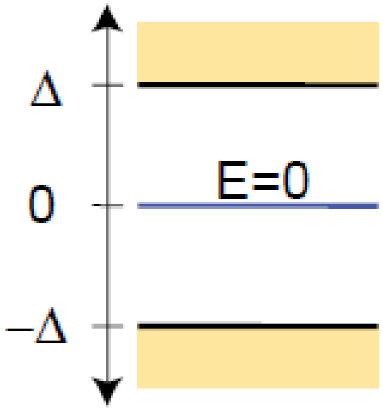
- Particle-hole symmetry and Majorana zero modes **Alicea (2012), Beenakker (2011)**
  - Particle-hole partner

$$\phi_{-E} = C\phi_E \quad \rightarrow \quad \gamma_E^+ = \gamma_{-E}$$

$$\phi_0 = C\phi_0 \quad \rightarrow \quad \gamma_0^+ = \gamma_0$$

Majorana fermions:
Particle=Antiparticle

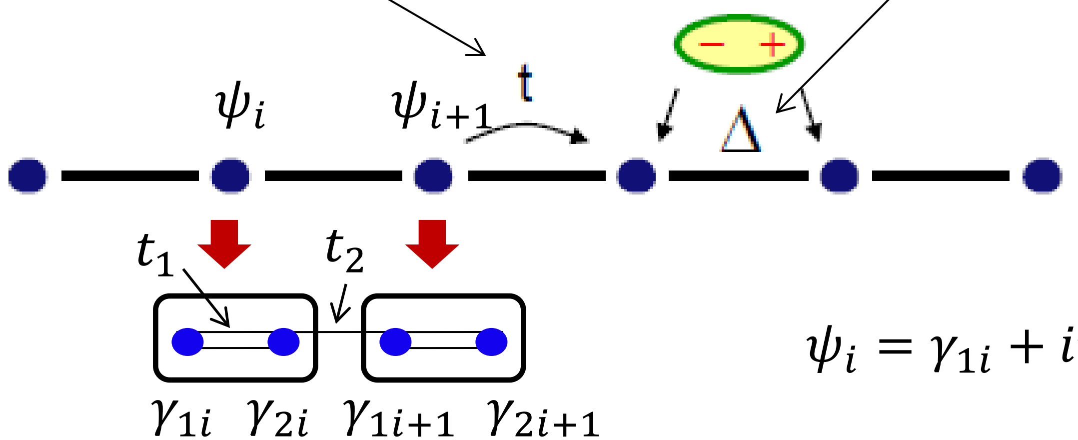




Topological superconductors

- Kitaev model for 1D p-wave superconductor

$$H - \mu N = \sum_i t(\psi_i^+ \psi_{i+1} + \psi_{i+1}^+ \psi_i) - \mu \psi_i^+ \psi_i + \Delta(\psi_i \psi_{i+1} + \psi_{i+1}^+ \psi_i^+)$$



Kitaev (2001)

$$\psi_i = \gamma_{1i} + i\gamma_{2i}, \qquad \gamma_{\alpha i}^+ = \gamma_{\alpha i}$$

$$t_1 = \mu, \qquad t_2 = 2t = 2\Delta$$

$$H = 2i \sum_i t_1 \gamma_{1i}\gamma_{2i} + t_2 \gamma_{2i}\gamma_{1i+1}$$

Su, Schrieffer and Heeger (1979)

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Topological superconductors

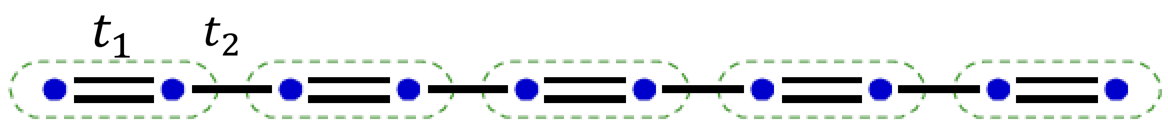
- Kitaev model for 1D p wave superconductor

Kitaev (2001)

$$H = 2i \sum_i t_1 \gamma_{1i}\gamma_{2i} + t_2 \gamma_{2i}\gamma_{1i+1}$$

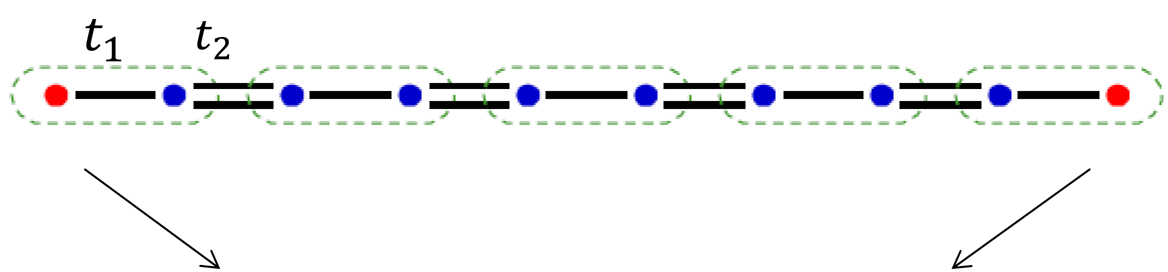
Trivial phase

$t_1 > t_2$



Topological phase

$t_1 < t_2$



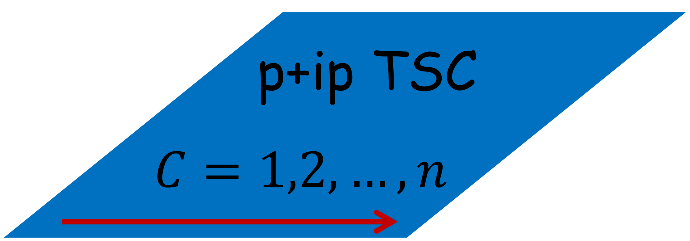
Unpaired end Majorana zero modes

Topological superconductors

o P+ip chiral topological superconductors

1d p wave TSC with 0d (bound) majorana end mode

2d p+ip TSC with 1d Majorana edge mode



Read and Green (2000)

Topological classification

- Schnyder-Ryu-Furusaki-Ludwig (SRFL) classification **Schnyder, Ryu, Furusaki, Ludwig (2008)**

		TRS	PHS	SLS	$d=1$	$d=2$	$d=3$
Standard	A (unitary)	0	0	0	-	$\mathbb{Z}$	-
(Wigner-Dyson)	AI (orthogonal)	+1	0	0	-	-	-
Topological insulators	AII (symplectic)	−1	0	0	-	$\mathbb{Z}_2$	$\mathbb{Z}_2$
Chiral	AIII (chiral unitary)	0	0	1	$\mathbb{Z}$	-	$\mathbb{Z}$
(sublattice)	BDI (chiral orthogonal)	+1	+1	1	$\mathbb{Z}$	-	-
	CII (chiral symplectic)	−1	−1	1	$\mathbb{Z}$	-	$\mathbb{Z}_2$
BdG	D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	-
P-wave topological superconductors	C	0	−1	0	-	$\mathbb{Z}$	-
	DIII	−1	+1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
	CI	+1	−1	1	-	-	$\mathbb{Z}$

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  - Topological non-symmorphic insulators
- Conclusion and outlook

Topological states and crystalline symmetry

- Topological surface states protected by other symmetries? (beyond SRFL classification)
- Yes, crystalline symmetry Timothy, et al, (2012)

➢ Anti-unitary, magnetic crystalline TIs.

Fu (2011), Mong, et al (2010), Fang, et al (2013), Liu (2013), RXZ, CXL, (2014)

➢ Different irreducible representations, mirror TIs and non-symmorphic TSCs.

Timothy, et al, (2012), SYX, et al (2012), Dziawa, et al (2012), Tanaka, et al (2012)

➢ Non-commutation, non-symmorphic TIs, C4v TIs.

CXL, RXZ, BV, (2013), A. Alexandradinata, et al (2014)

Topological states and crystalline symmetry

- Example: topological mirror insulators.
  - Two subspaces with opposite mirror parities are decoupled.

$m_z|\psi_+\rangle = |\psi_+\rangle \qquad m_z|\psi_-\rangle = |\psi_-\rangle$

$m_z V m_z^+ = V$

$$
\begin{aligned}
&\langle\psi_+|V|\psi_-\rangle \\
&= \langle\psi_+|m_z^+ m_z V m_z^+ m_z|\psi_-\rangle \\
&= -\langle\psi_+|V|\psi_-\rangle \\
&\rightarrow \langle\psi_+|V|\psi_-\rangle = 0
\end{aligned}
$$

Mirror invariant plane

$m_z\colon (x, y, z) \rightarrow (x, y, -z)$

Topological states and crystalline symmetry

- Example: topological mirror insulators.
  - Two subspaces with opposite mirror parities are decoupled.

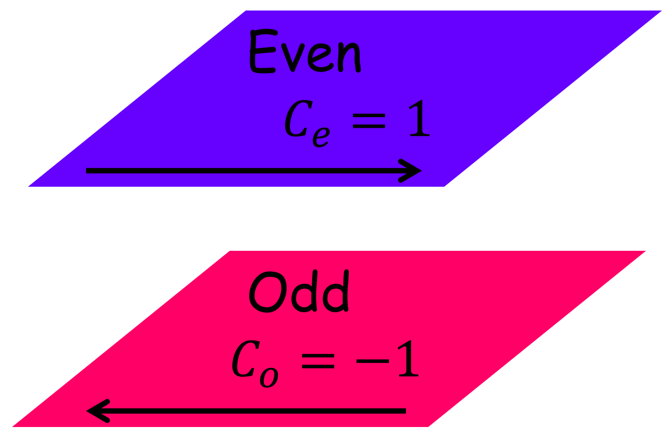
Mirror invariant plane

$$m_z: (x, y, z) \to (x, y, -z)$$

$$C = C_e + C_o = 0$$

$$C_M = C_e - C_o \neq 0$$

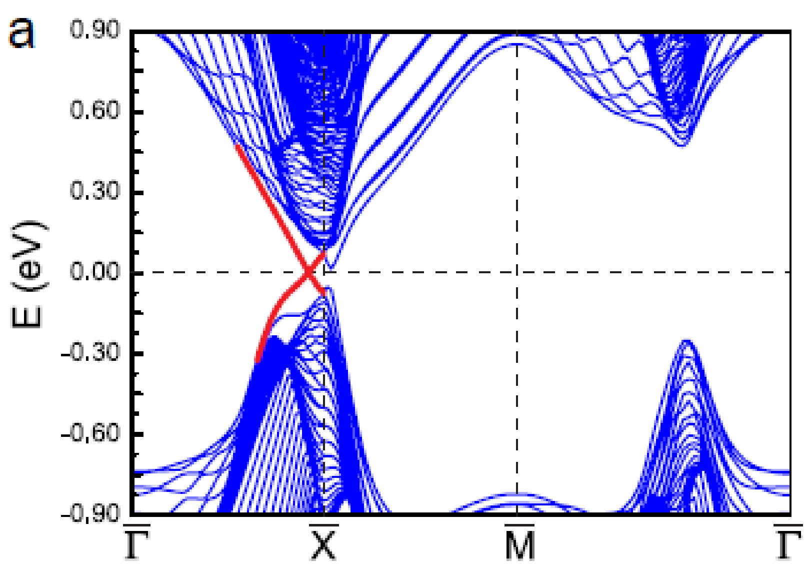
Mirror subspace

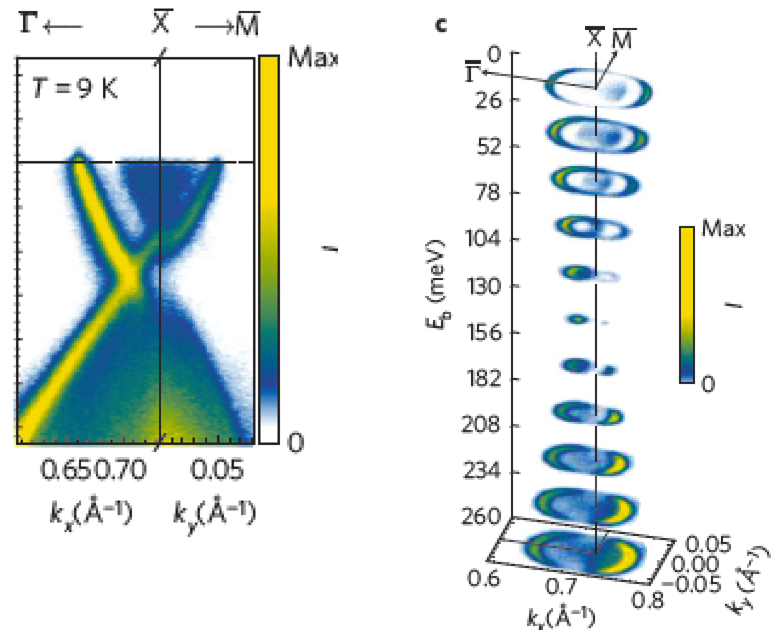


Topological mirror insulators

- Theoretical prediction and experimental observation of topological mirror insulators in SnTe family of materials

Fu (2011); Timothy, et al, (2012)



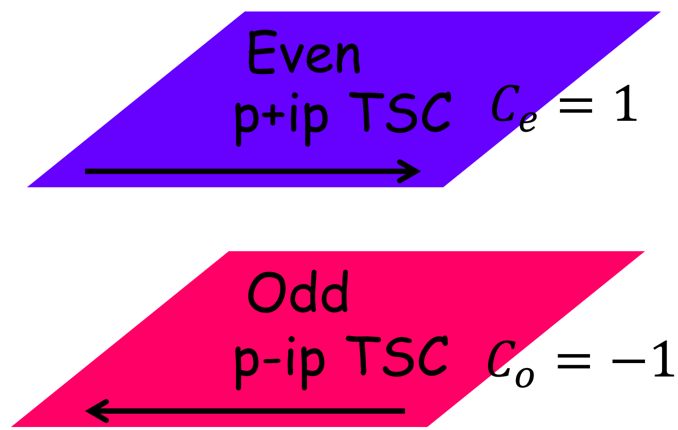


SuYang Xu, et al (2012); Dziawa, et al (2012); Tanaka, et al (2012)

Topological mirror Superconductors

- Can similar idea be applied to superconducting states? (Topological mirror superconductors)
  - Key question: will particle-hole symmetry still exist in one mirror parity subspace? Equivalently, do a state ψ and its particle-hole partner $\tilde{\psi} = C\psi$ have the same mirror parity or not?

Zhang (2013), Ueno (2013)



Topological mirror Superconductors

- In a mirror superconductor, particle-hole symmetry might exist in one mirror parity subspace or not, depending on gap function.
  - Gap function is classified by irreducible representations of symmetry group.

$$D(m)\Delta(k)D^T(m) = \eta\Delta(k), \qquad \eta = \pm$$

$$\Delta(k) = V_0\langle\psi_{-k}\psi_k\rangle$$

  - The $\eta = -$ means that superconducting phase spontaneously breaks mirror symmetry.

Topological mirror Superconductors

- Key step: mathematically, we can still define a new "mirror" symmetry operation for the BdG Hamiltonian.

$$D(m)\Delta(k)D^T(m) = \eta\Delta(k), \qquad \eta = \pm$$

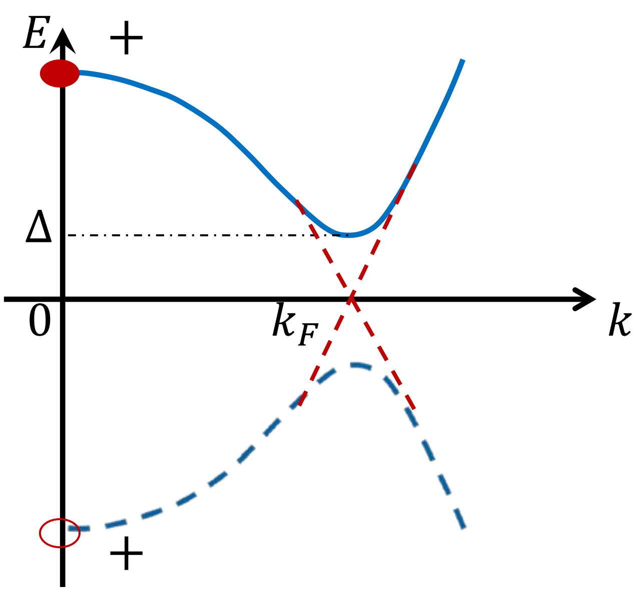
$$\mathcal{D}(m) = \begin{pmatrix} D(m) & 0 \\ 0 & \eta D^*(m) \end{pmatrix} \qquad H_{BdG} = \begin{pmatrix} h(k)-\mu & \Delta(k) \\ \Delta^+(k) & -h^*(-k)+\mu \end{pmatrix}$$

$$\mathcal{D}(m)H_{BdG}\mathcal{D}^+(m) = H_{BdG}$$

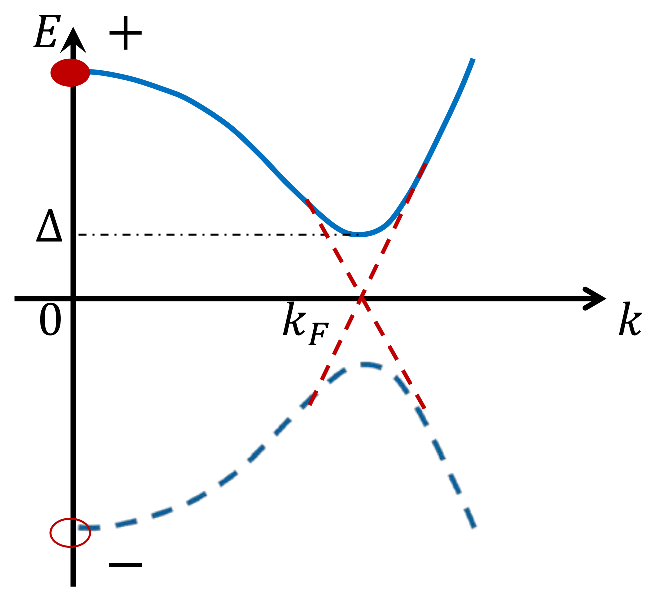
Topological mirror superconductors

- Physical meaning of the new "mirror" symmetry operator $D(m)$. The parity of hole band is determined by $\Delta(k)$.

$$D(m)\Delta(k)D^T(m) = \Delta(k)$$



$$D(m)\Delta(k)D^T(m) = -\Delta(k)$$



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Topological mirror Superconductors

- Any eigen-state of the BdG Hamiltonian can have the definite mirror parity.

$$\mathcal{D}(m)H_{BdG}\mathcal{D}^{+}(m) = H_{BdG}$$

$$H_{BdG}\psi = E\psi, \qquad \mathcal{D}(m)\psi = \delta_m\psi, \qquad \delta_m = \pm$$

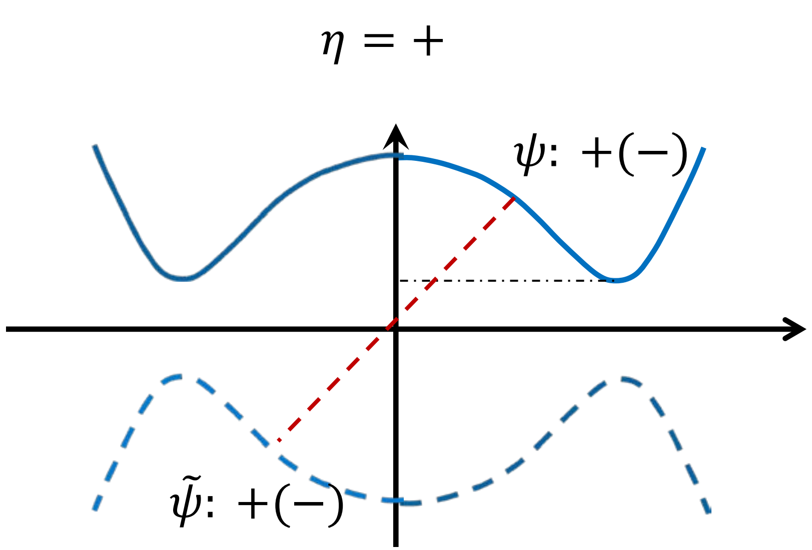
- The mirror parities of ψ and $\tilde{\psi}$ are determined by η.

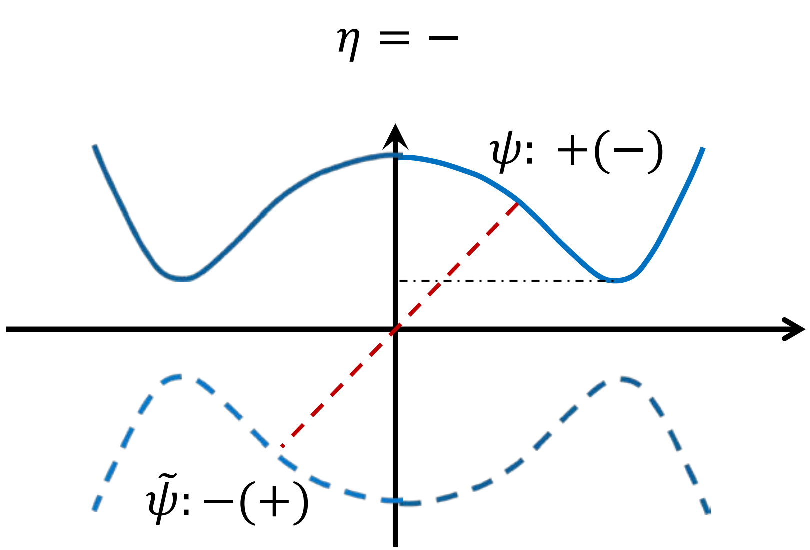
$$C\mathcal{D}(m)C^{-1} = \eta\mathcal{D}(m)$$

$$\tilde{\psi} = C\psi, \qquad H_{BdG}\tilde{\psi} = -E\tilde{\psi}, \qquad \mathcal{D}(m)\tilde{\psi} = \eta\delta_m\tilde{\psi}$$

Topological mirror Superconductors

- When $\eta = +$, ψ and $\tilde{\psi}$ have the same mirror parity, while $\eta = -$, ψ and $\tilde{\psi}$ have opposite mirror parities.





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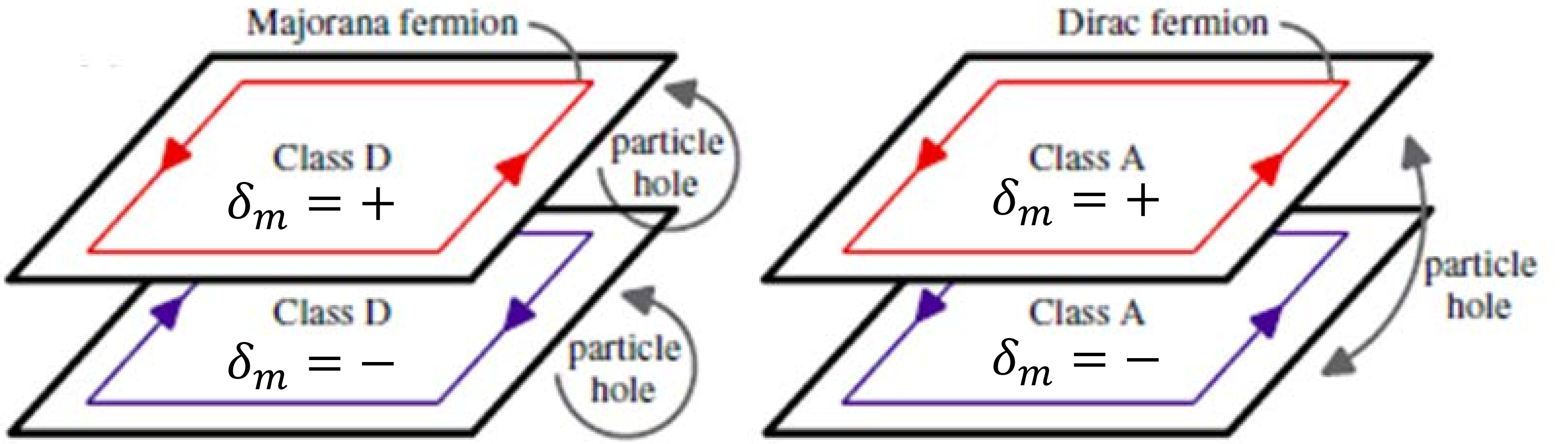
Topological mirror Superconductors

- Different topological classifications for different types of gap functions.

$$D(m)\Delta(k)D^T(m) = \eta\Delta(k), \qquad \eta = \pm$$

D class $\quad \eta = + \qquad\qquad \eta = -$



Zhang (2013), Ueno (2013)

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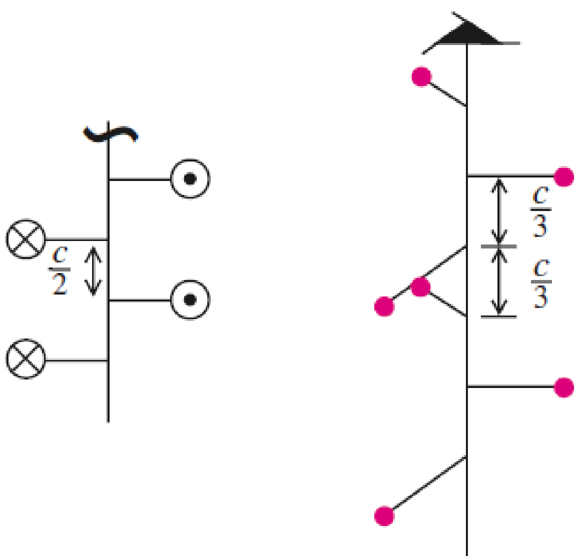
Non-symmorphic symmetry

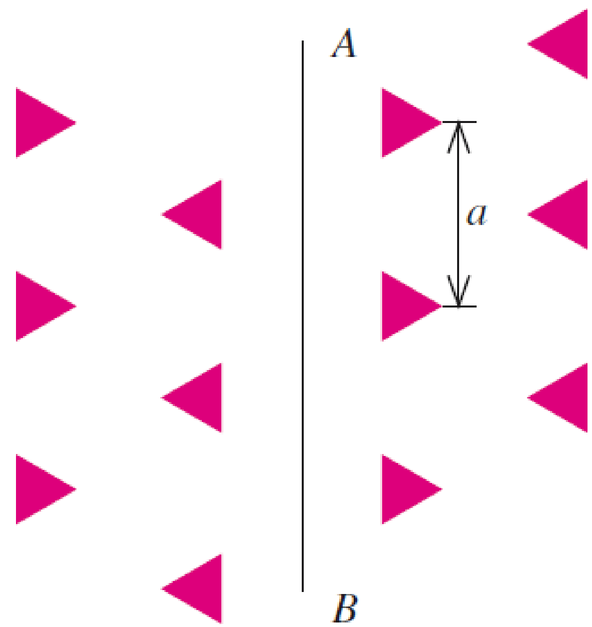
- Non-symmorphic symmetry: glide reflection and screw axis

Screw axis



$(C_n|\vec{\tau})$

Glide reflection

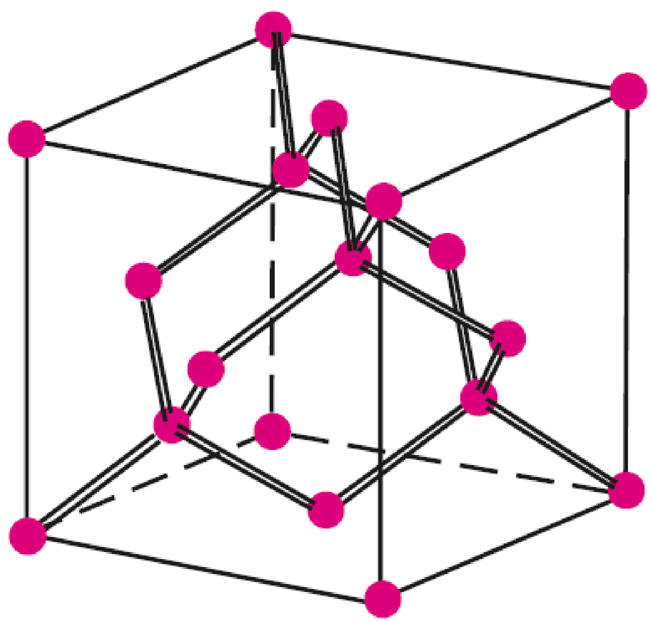


$(m|\vec{\tau})$

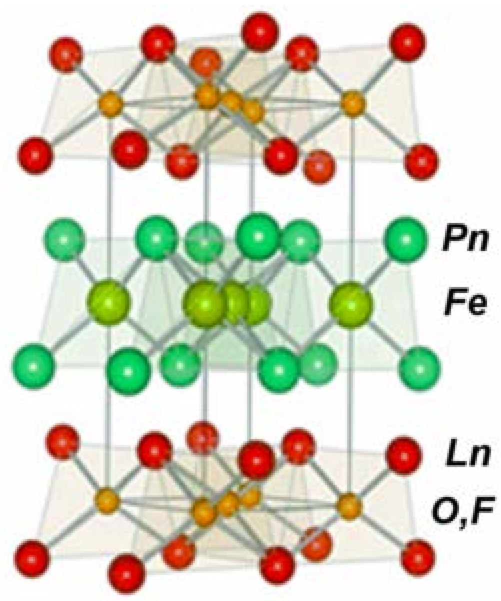
Non-symmorphic materials

- 157 of 230 space groups are non-symmorphic
- Examples of non-symmorphic systems

Diamond



Iron-based superconductors



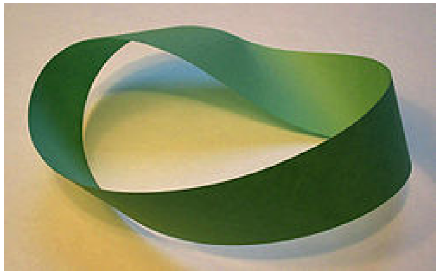
Electronic states in a non-symmorphic crystal

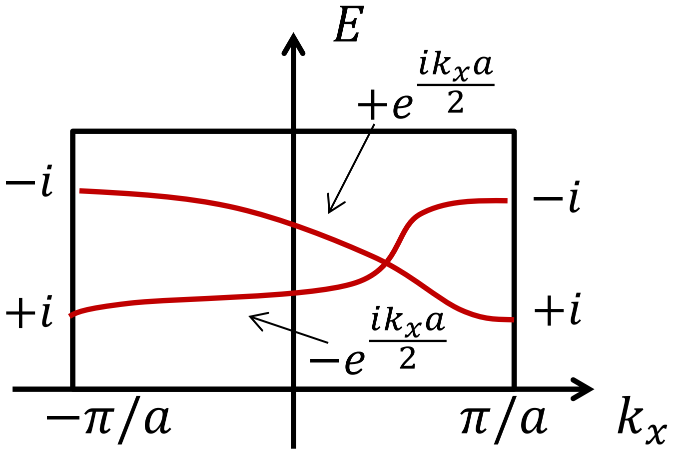
- Electronic states in a system with glide symmetry (glide parity)

$$D(g)\psi_{\vec{k}} = \delta_m e^{i\vec{k}\cdot\vec{\tau}}\psi_{\vec{k}} = \delta_m e^{ik_x a/2}\psi_{\vec{k}}, \qquad \delta_m = \pm, \vec{\tau} = \left(\frac{a}{2}, 0,0\right)$$

- All the bands appear in pairs.

$$D(g)\psi_{\vec{k}+2\pi/a} = \delta_m e^{\frac{ik_x a}{2}+i\pi}\psi_{\vec{k}+2\pi/a}$$
$$= -\delta_m e^{\frac{ik_x a}{2}}\psi_{\vec{k}+2\pi/a}$$





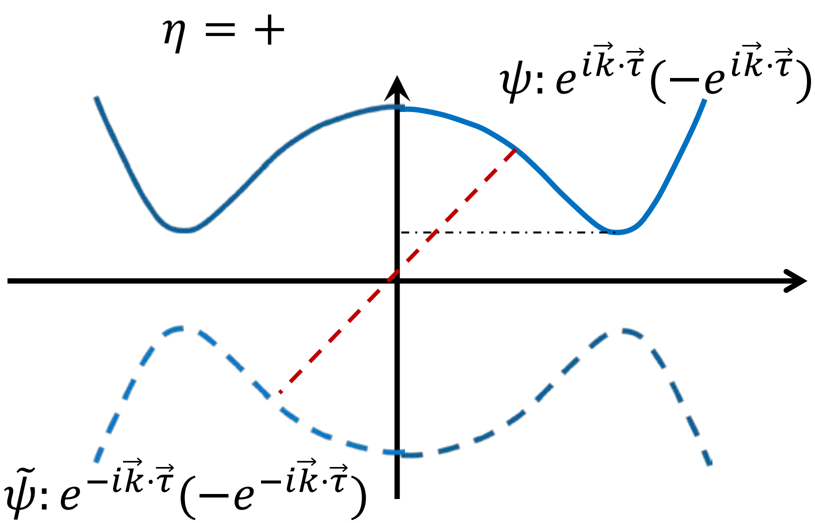
Fang and Fu (2015)

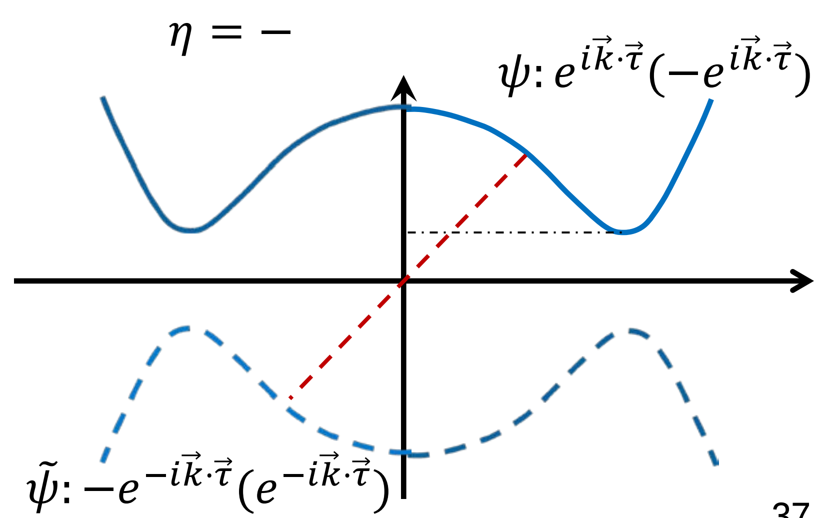
Glide parity

- We can follow the logic of topological mirror superconductors and identify glide parity for the states ψ and $\tilde{\psi}$. (Homework???)

$$D_{\vec{k}}(g)\Delta(\vec{k})D^{T}_{-\vec{k}}(g) = \eta\Delta(\vec{k}), \qquad \eta = \pm$$

$$G(g)\psi = \delta_\eta e^{i\vec{k}\cdot\vec{\tau}}\psi, \qquad G(g)\tilde{\psi} = \eta\delta^*_\eta e^{-i\vec{k}\cdot\vec{\tau}}\tilde{\psi}, \qquad \delta_\eta = \pm$$

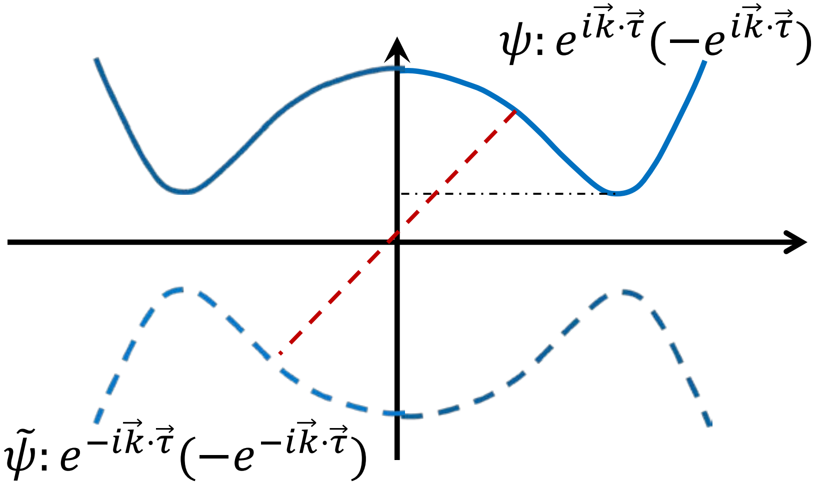




Glide parity

- Glide parities of ψ and $\tilde{\psi}$ depend on the momentum

$\eta = +$



$\vec{k}\cdot\vec{\tau} = 0$

$\psi: +,\quad \tilde{\psi}: +$ Same

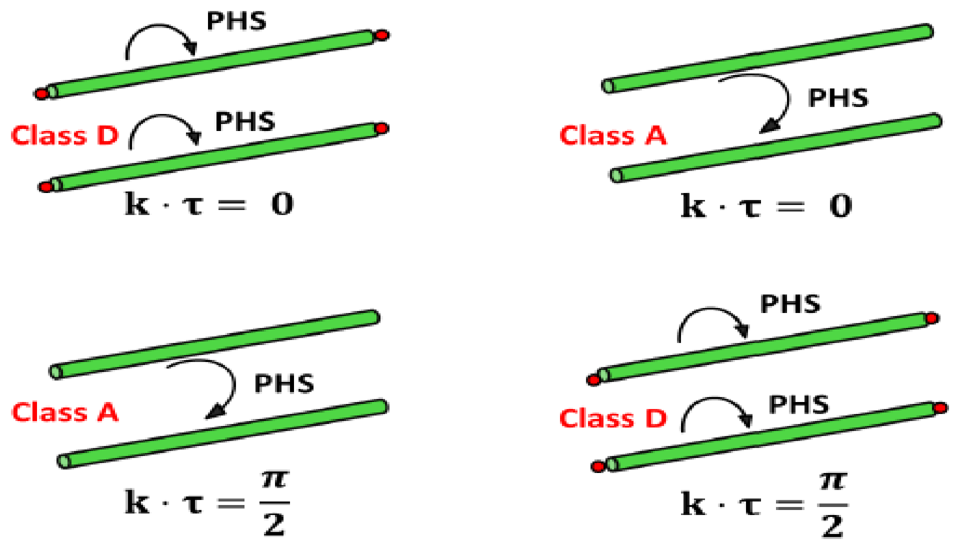
$\vec{k}\cdot\vec{\tau} = \frac{\pi}{2}$

$\psi: +i,\quad \tilde{\psi}: -i$ Opposite

Glide parity and particle-hole symmetry

- Particle-hole symmetry only exists in one line in the 2D Brillouin zone for one glide parity subspace.
- Topological invariant can be only defined in 1D line, but not in 2D plane.

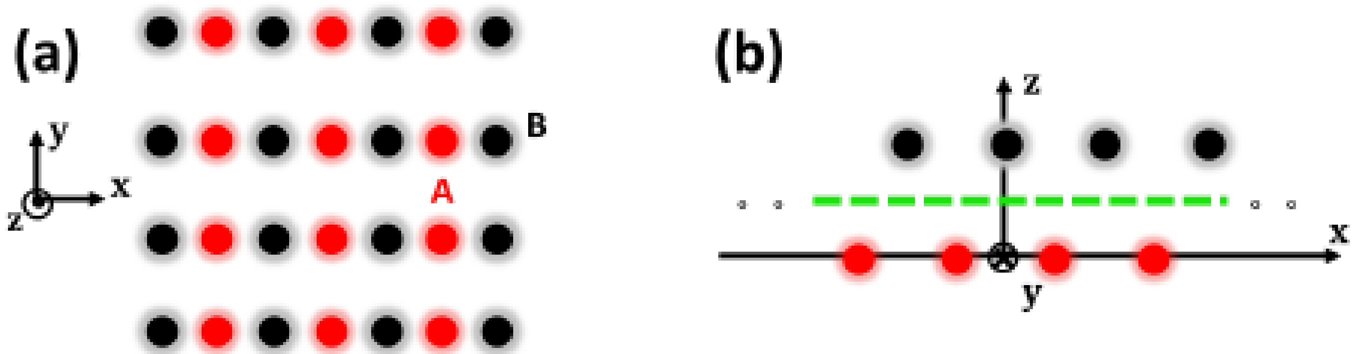
$\eta = +$



$\eta = -$

Topological glide superconductors

- There is a Z_2 classification for the D class, the Kitaev model.
- Our model for topological glide superconductors in a distorted square lattice



Topological glide superconductors

- Model Hamiltonian

$$h(\mathbf{k}) = \epsilon(\mathbf{k})\sigma_0 + t_3 cos(\frac{(k_x-\phi)a}{2})cos(\frac{k_x a}{2})\sigma_1 + t_3 cos(\frac{(k_x-\phi)a}{2})sin(\frac{k_x a}{2})\sigma_2$$

σ is for A and B sublattices

Glide symmetry

$$D_{\mathbf{k}}(g) = e^{i\frac{k_x a}{2}}(cos(\frac{k_x a}{2})\sigma_1 + sin(\frac{k_x a}{2})\sigma_2)$$

$$D_k(g)h(k_x,k_y)D_k^{-1}(g) = h(k_x,k_y)$$

Gap function

$$\Delta_+ = \Delta_0 sin(k_y a)\sigma_0$$

$$\Delta_- = \Delta_0 sin(k_y a)\sigma_3$$

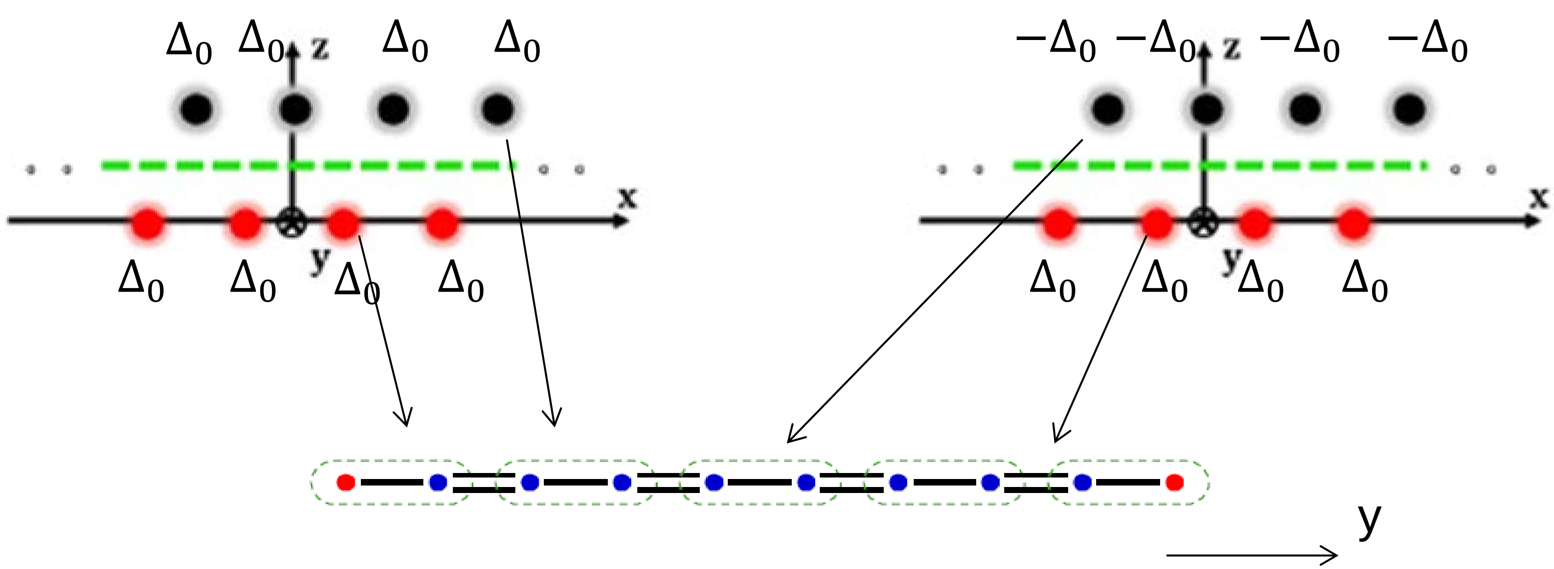
$$D_{\vec{k}}(g)\Delta_\pm(\vec{k})D^T_{-\vec{k}}(g) = \pm\Delta_\pm(\vec{k}),$$

Qing-Ze Wang and Chao-Xing Liu, arxiv: cond/1506.07938 (2015).

Topological glide superconductors

- Our model Hamiltonian can be viewed as a generalization of Kitaev model

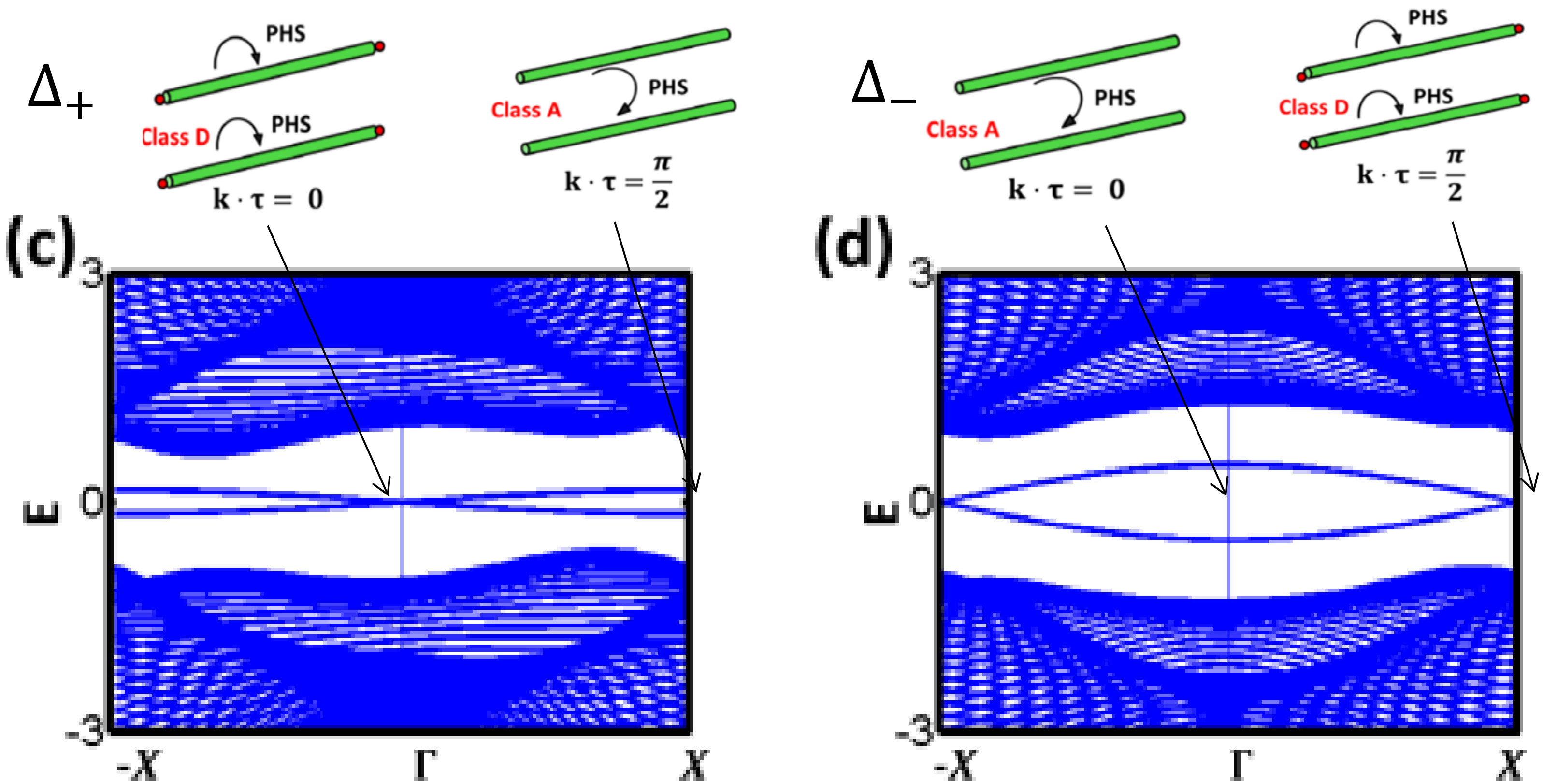
$$\Delta_+ = \Delta_0 sin(k_y a)\sigma_0 \qquad \Delta_- = \Delta_0 sin(k_y a)\sigma_3$$



Qing-Ze Wang and Chao-Xing Liu, arxiv: cond/1506.07938 (2015).

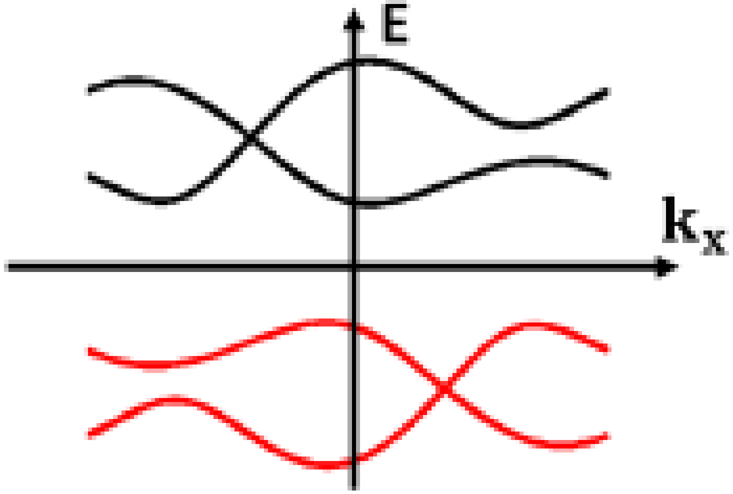
Topological glide superconductors

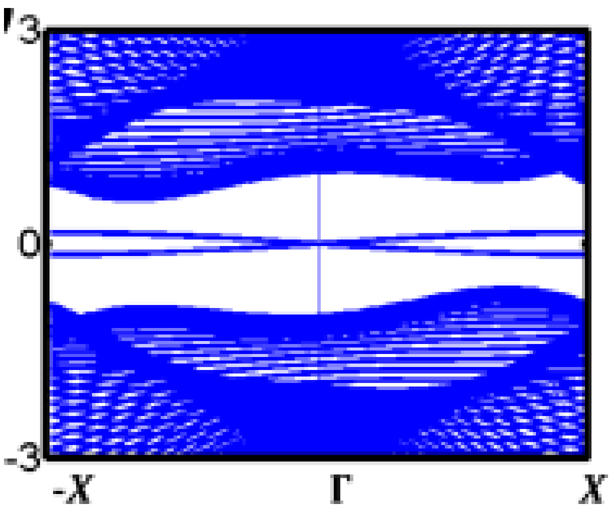
- Energy spectrum for a slab configuration



No-go theorem for topological glide superconductors

- In a 1D glide superconductors, there should be $4N$ bands for BdG Hamiltonian due to the glide symmetry and particle-hole symmetry.





Topological classification

- Topological classification with and without time reversal symmetry

No TR	spinless		spin-$\frac{1}{2}$	
NoGS(2D)	BDI, $\mathbb{Z}$		DIII, $\mathbb{Z}$	
	$\mathbf{k}\cdot\tau=0$	$\mathbf{k}\cdot\tau=\frac{\pi}{2}$	$\mathbf{k}\cdot\tau=0$	$\mathbf{k}\cdot\tau=\frac{\pi}{2}$
G_+	BDI, $\mathbb{Z}$	AIII, $\mathbb{Z}$	AIII, $\mathbb{Z}$	DIII, $\mathbb{Z}_2$
G_-	AI, -	D, $\mathbb{Z}_2$	D, $\mathbb{Z}_2$	AII, -

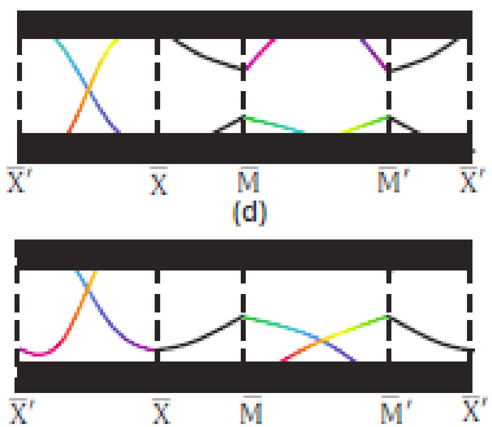
TR	spinless		spin-$\frac{1}{2}$	
NoGS(2D)	D, $\mathbb{Z}$		D, $\mathbb{Z}$	
	$\mathbf{k}\cdot\tau=0$	$\mathbf{k}\cdot\tau=\frac{\pi}{2}$	$\mathbf{k}\cdot\tau=0$	$\mathbf{k}\cdot\tau=\frac{\pi}{2}$
G_+	D, $\mathbb{Z}_2$	A, -	A, -	D, $\mathbb{Z}_2$
G_-	A, -	D, $\mathbb{Z}_2$	D, $\mathbb{Z}_2$	A, -

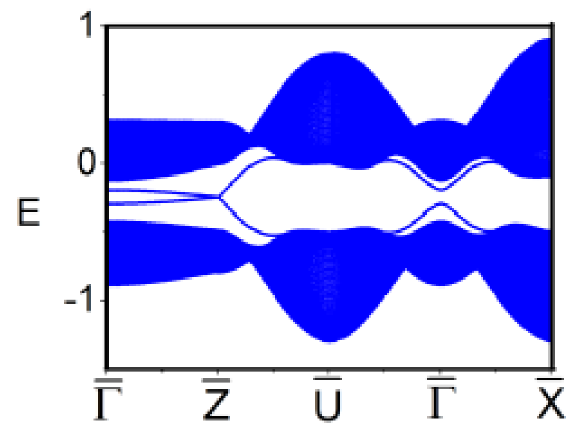
Outline

- Introduction, symmetry and topology in the classification of states of matter
- Topological crystalline insulators and superconductors
- Nonsymmorphic symmetry and topological phases
  - Topological non-symmorphic superconductors
  - Topological non-symmorphic insulators
- Conclusion and outlook

Topological non-symmorphic insulators

- Topological insulating phase protected by non-symmorphic symmetry does not exist in 2D, but only in 3D.
- Two types of topological non-symmorphic insulators



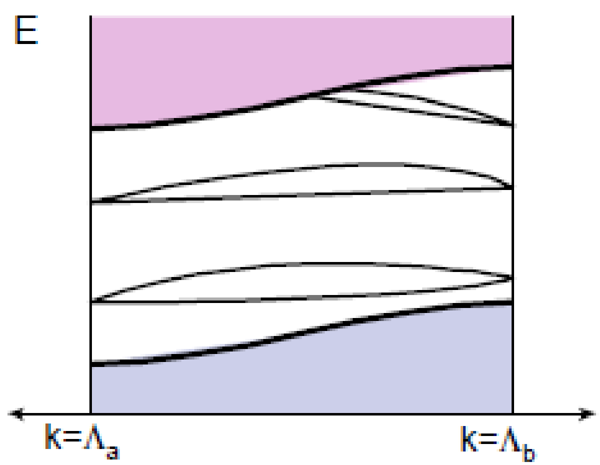


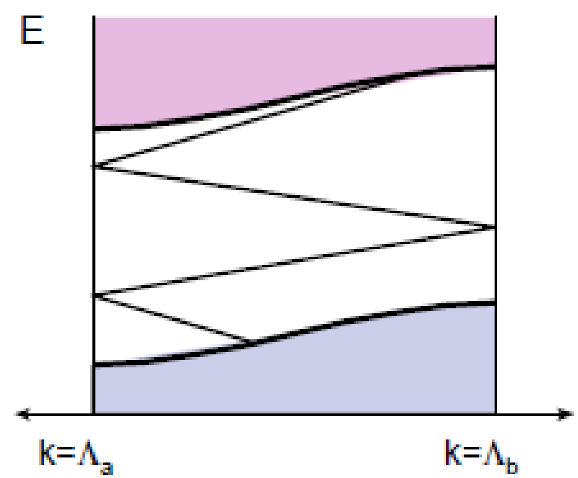
pg: Fang and Fu (2015)

pmg, pgg and p4g: Liu's group (2014), (2015)

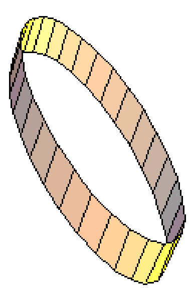
Degeneracy and topological surface states

- Degeneracy can lead to non-trivial surface states. E.g. TI due to time reversal symmetry

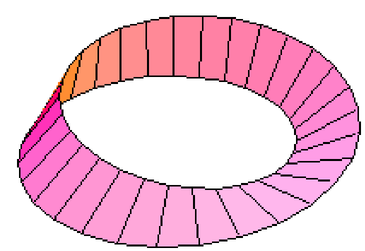




Trivial



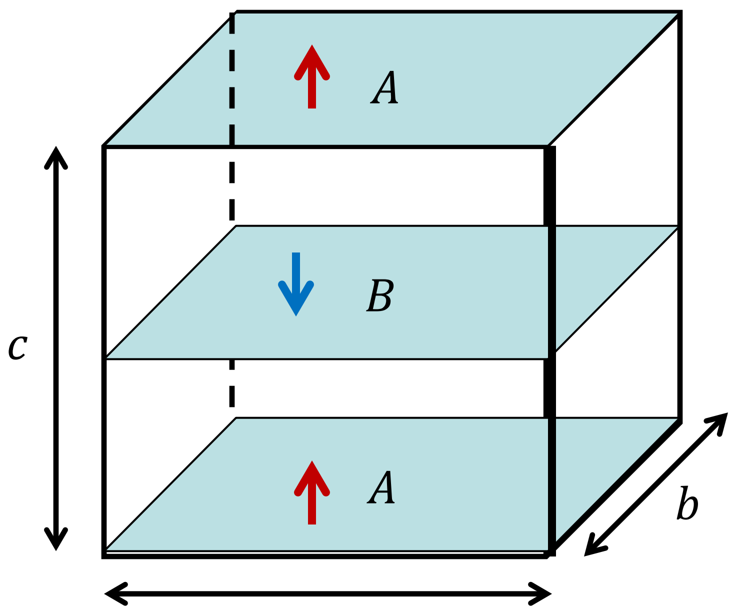
Non-trivial

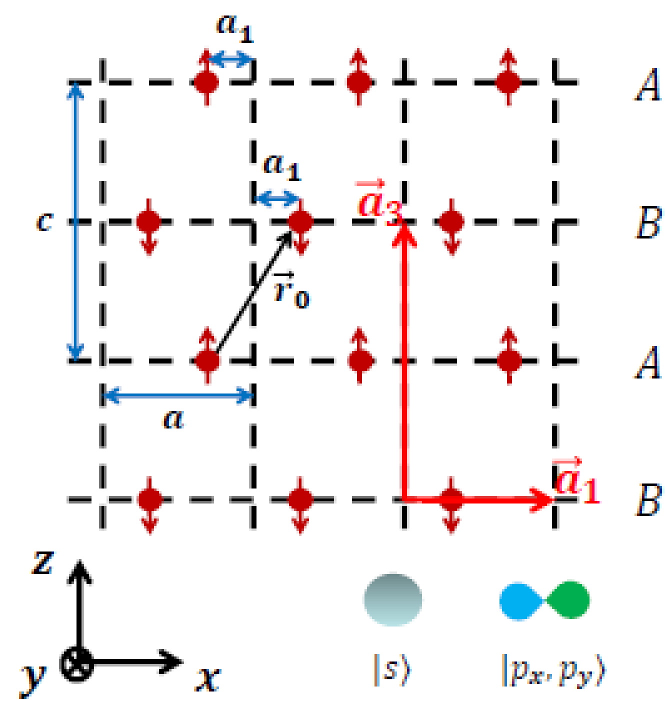


Topological non-symmorphic insulators

- Non-symmorphic symmetry can induce degeneracy
- An example in pmg group

Liu's group (2014)





Topological non-symmorphic insulators

- Two symmetry operations

  z-direction mirror operation $m_z: (x, y, z) \to (x, y, -z)$

  x-direction glide operation $g_x = \{\sigma_x|\vec{\tau}\} : (x, y, z) \to \left(-x, y, z + \frac{c}{2}\right)$, $\vec{\tau} = \left(0,0,\frac{c}{2}\right)$

CXL, RXZ and BV (2014)

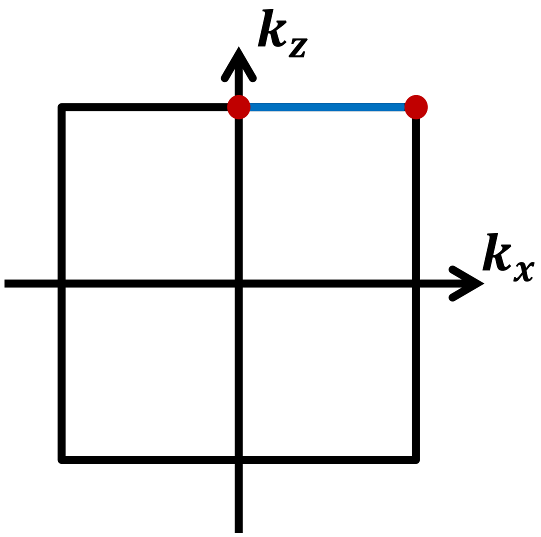
- Anti-commutation relation

$$g_x m_z = m_z g_x + \boldsymbol{t}, \qquad \boldsymbol{t} = (0,0,c)$$

When $\vec{k} = \left(0, k_y, \frac{\pi}{c}\right) = \left(\frac{\pi}{a}, k_y, \frac{\pi}{c}\right)$,

$$g_x m_z|\phi_k\rangle = e^{i\boldsymbol{k}\cdot\boldsymbol{t}} m_z g_x|\phi_k\rangle$$

$$\to \{m_z, g_x\} = 0$$ at $\bar{Z}$ and $\bar{U}$



Degeneracy due to non-symmorphic symmetry

- Degeneracy due to the anti-commutation relation in a symmetry group

$$[R,H]=0, \qquad [S,H]=0, \qquad \{R,S\}=0$$

If $H|\phi\rangle = E|\phi\rangle$ and $R|\phi\rangle = r|\phi\rangle$, $S|\phi\rangle$ and $|\phi\rangle$ are two orthogonal and degenerate eigen states.

$HS|\phi\rangle = SH|\phi\rangle = ES|\phi\rangle \;\; \rightarrow \;\; S|\phi\rangle$ is an eigen-state

$RS|\phi\rangle = -SR|\phi\rangle = -rS|\phi\rangle \;\; \rightarrow \;\; S|\phi\rangle$ is different from $|\phi\rangle$.

Mathematically, all high dimensional irreducible representations in a space symmetry group are due to non-commutation relations.

Surface states in TNCIs

- Non-symmorphic symmetry

  Anti-commutation relation requires the degeneracy at $\bar{Z}$ and $\bar{U}$.

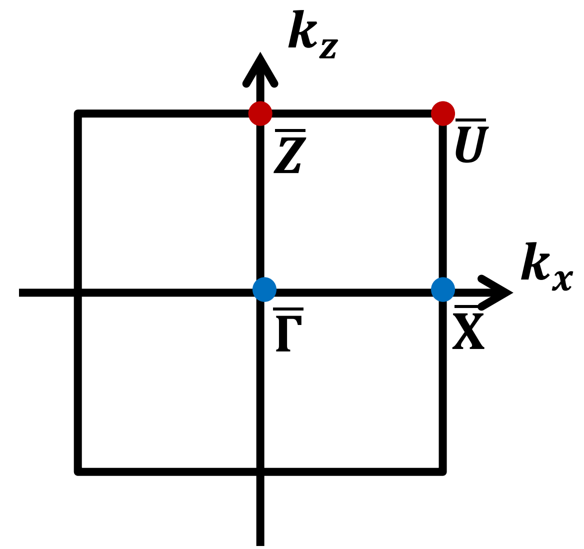
  CXL, RXZ and BV (2014)

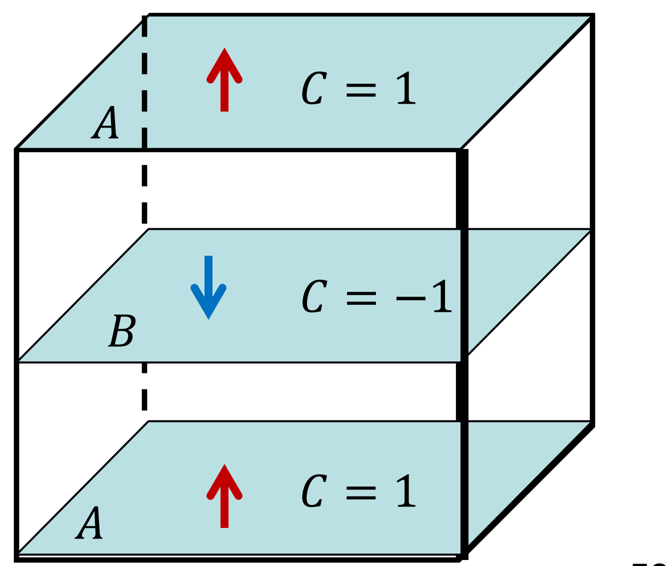
- Model Hamiltonian

$$H = H_A + H_B + H_{AB}$$

$$H_\eta = \sum_{\langle \vec{n}\vec{m}\rangle_{in},\alpha\beta} t^{\alpha\beta}_{\vec{n}\vec{m}} c^\dagger_{\alpha\vec{n}\eta} c_{\beta\vec{m}\eta} + \sum_{\vec{n},\alpha} \epsilon_\alpha c^\dagger_{\alpha\vec{n}\eta} c_{\alpha\vec{n}\eta}$$
$$+ \sum_{\vec{n}} \delta_\eta M_1 \left(-i c^\dagger_{\vec{n}p_x\eta} c_{\vec{n}p_y\eta} + \mathrm{H.c.} \right),$$

$$H_{AB} = \sum_{\langle \vec{n}\vec{m}\rangle_{AB},\alpha\beta} \left(r^{\alpha\beta}_{\vec{n}\vec{m}} c^\dagger_{\alpha\vec{n}A} c_{\beta\vec{m}B} + \mathrm{H.c.} \right),$$

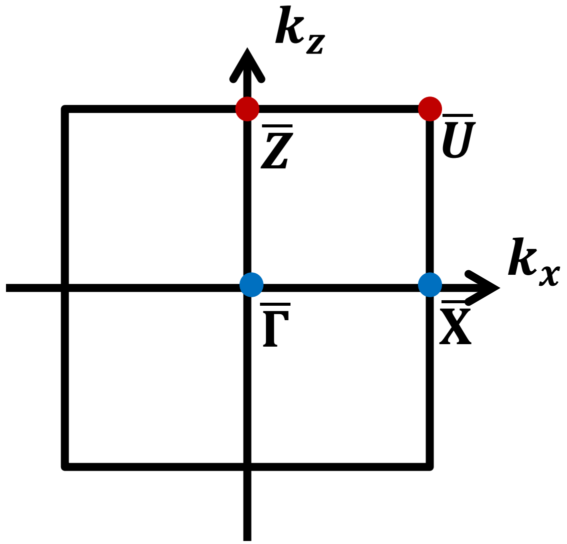


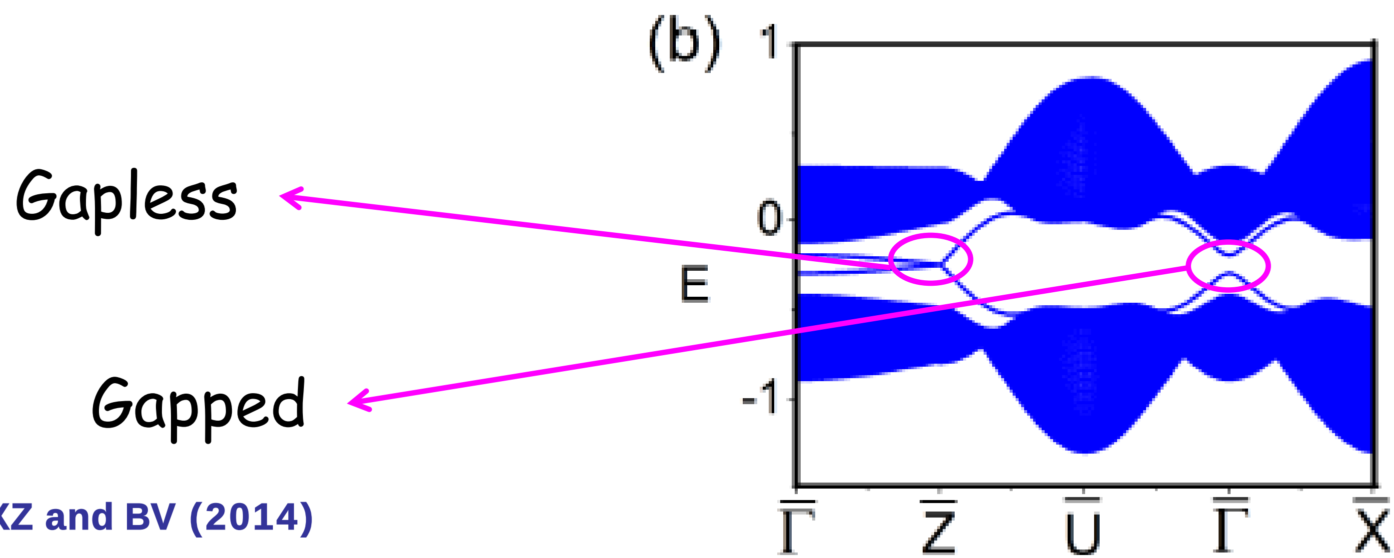


Surface states in TNCIs

- Gapless surface states

Perform calculation of this Hamiltonian on a slab configuration.

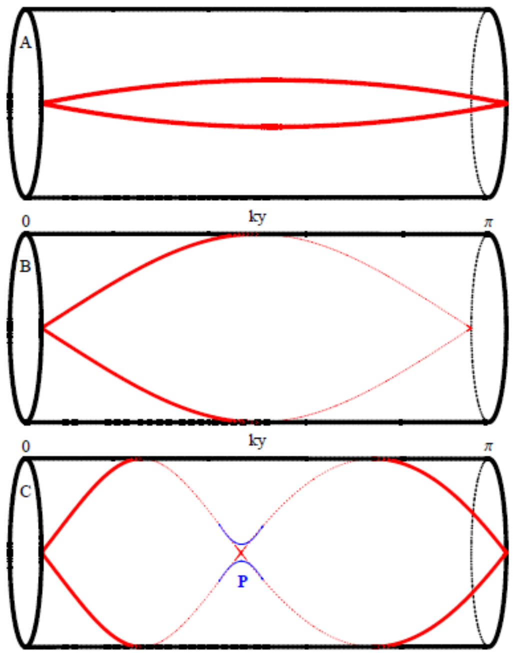




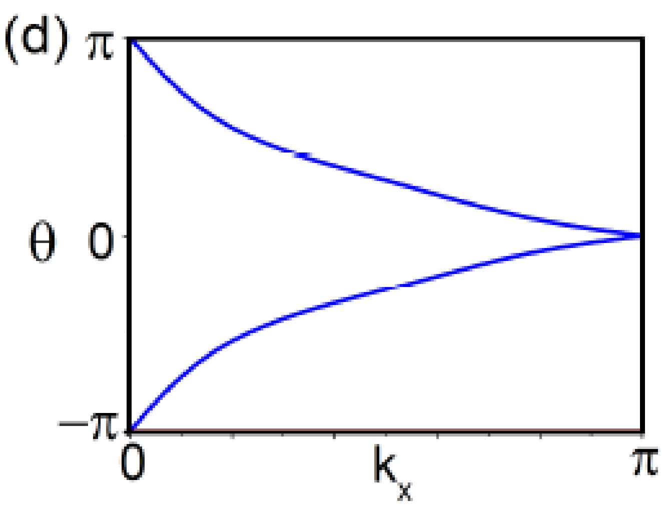
CXL, RXZ and BV (2014)

Topological non-symmorphic insulators

- Bulk topological invariants can be defined by Wannier function centers. (Pfaffian does not work).



Flow of Wannier function centers



Fu (2008), RY, XLQ, AB, ZF, XD, (2011)

CXL, RXZ and BV (2014)

More topological non-symmorphic insulators

- Here we only focus on non-symmorphic symmetry, but there are more crystalline symmetries.
- There are 17 2D space groups and 230 3D space groups.
- Our classification of all possible topological crystalline insulators.

The classification of topological crystalline insulators based on representation theory

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[2] *Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802-6300, USA;*

Classification of topological crystalline insulators

Group	SBZ	HSP	HSL	Topological Classification	
				spinless	spinful
pm	re		$\bar{\Gamma}$-$\bar{X}$,$\bar{Y}$-$\bar{M}$:m_y	$\mathbb{Z}^2 \equiv \mathbb{Z} \times \mathbb{Z}$	$\mathbb{Z}^2$
$p3m1$	h	$\bar{\Gamma}$: C_{3v}	$\bar{\Gamma}$-$\bar{M}$:m	$\mathbb{Z}$	$\mathbb{Z}$
cm	rh		$\bar{\Gamma}$-$\bar{X}$:m_y	$\mathbb{Z}$	$\mathbb{Z}$
pmm	re	$\bar{\Gamma}$,$\bar{X}$,$\bar{M}$,$\bar{Y}$:C_{2v}	$\bar{\Gamma}$-$\bar{X}$,$\bar{Y}$-$\bar{M}$:m_y $\bar{\Gamma}$-$\bar{Y}$,$\bar{X}$-$\bar{M}$:m_x	None	$\mathbb{Z}^4$
cmm	rh	$\bar{\Gamma}$,$\bar{X}$,$\bar{Y}$:C_{2v}	$\bar{\Gamma}$-$\bar{X}$:m_y; $\bar{\Gamma}$-$\bar{Y}$:m_x	None	$\mathbb{Z}^2$
pg	re		$\bar{\Gamma}$-$\bar{X}$,$\bar{Y}$-$\bar{M}$:g_y	$\mathbb{Z}_2$	$\mathbb{Z}_2$
$p4m$	s	$\bar{\Gamma}$,$\bar{M}$:C_{4v} $\bar{X}$:C_{2v}	$\bar{\Gamma}$-$\bar{X}$:m_y; $\bar{X}$-$\bar{M}$:m_x; $\bar{\Gamma}$-$\bar{M}$:m_d	$\mathbb{Z}^2(\bar{\Gamma}, \bar{M} \in E)$ None ($\bar{\Gamma}$ or $\bar{M} \notin E$)	$\mathbb{Z}^3$
$p31m$	h	$\bar{\Gamma}$,$\bar{K}$,$\bar{K}'$:C_{3v}	$\bar{\Gamma}$-$\bar{K}$:m_1 $\bar{K}$-$\bar{K}'$:m_2 $\bar{K}'$-$\bar{\Gamma}$:m_3	$\mathbb{Z}^3$(3 HSPs $\notin E$) $\mathbb{Z}^2$(2 HSPs $\notin E$) $\mathbb{Z}$(general case)	$\mathbb{Z}^3$(3 HSPs $\notin E$) $\mathbb{Z}^2$(2 HSPs $\notin E$) $\mathbb{Z}$(general case)
$p6m$	h	$\bar{\Gamma}$:C_{6v} $\bar{K}$:C_{3v} $\bar{M}$:C_{2v}	$\bar{\Gamma}$-$\bar{K}$:m_1 $\bar{\Gamma}$-$\bar{M}$:m_2 $\bar{K}$-$\bar{M}$:m_3	$\mathbb{Z}^2(\bar{\Gamma} \in E_i(i=1,2), \bar{K} \in E, \bar{M} \in A_i(B_i))$ $\mathbb{Z}(\bar{\Gamma} \in E_i(i=1,2), \bar{K} \in E)$ None ($\bar{\Gamma} \notin E_i(i=1,2)$ or $\bar{K} \notin E$)	$\mathbb{Z}^3(\bar{K} \in E)$ $\mathbb{Z}^2(\bar{K} \notin E)$
pgg	re	$\bar{\Gamma}$,$\bar{X}$,$\bar{Y}$,$\bar{M}$:C_{2v}	$\bar{\Gamma}$-$\bar{X}$,$\bar{Y}$-$\bar{M}$:g_y; $\bar{\Gamma}$-$\bar{Y}$,$\bar{X}$-$\bar{M}$:g_x	$\mathbb{Z}^2(\bar{\Gamma}, \bar{M} \in A_i(B_i);\ \bar{\Gamma} \in A_i(B_i), \bar{M} \in B_i(A_i))$ $\mathbb{Z}(\bar{\Gamma}$ or $\bar{M} \in A_i; \bar{\Gamma}$ or $\bar{M} \in B_i)$ $\mathbb{Z}_2$(general case)	$\bar{\Gamma}, \bar{M} \to \bar{X}, \bar{Y}$
pmg	re	$\bar{\Gamma}$,$\bar{X}$,$\bar{Y}$,$\bar{M}$:C_{2v}	$\bar{\Gamma}$-$\bar{X}$,$\bar{Y}$-$\bar{M}$:g_y; $\bar{\Gamma}$-$\bar{Y}$,$\bar{X}$-$\bar{M}$:m_x	$\mathbb{Z}^2(\bar{Y}, \bar{\Gamma} \in A_i; \bar{Y}, \bar{\Gamma} \in B_i;$ $\bar{Y} \in A_i(B_i), \bar{\Gamma} \in B_i(A_i))$ $\mathbb{Z}$(general case)	$\bar{Y}, \bar{\Gamma} \to \bar{X}, \bar{M}$
$p4g$	s	$\bar{\Gamma}$,$\bar{M}$:C_{4v} $\bar{X}$:C_{2v}	$\bar{\Gamma}$-$\bar{X}$:g_y; $\bar{X}$-$\bar{M}$:g_x; $\bar{\Gamma}$-$\bar{M}$:g_d	$\mathbb{Z}^3(\bar{\Gamma}, \bar{M} \in E)$ $\mathbb{Z}^2(\bar{M} \in E, \bar{\Gamma} \in A_i(B_i); \bar{\Gamma} \to \bar{M})$ $\mathbb{Z}(\bar{M} \in E, \bar{\Gamma}$ general; $\bar{\Gamma} \to \bar{M})$ None$(\bar{\Gamma}, \bar{M} \notin E)$	$\mathbb{Z}^2(\bar{X} \in A_i(B_i))$ $\mathbb{Z}$(general case)

XY Dong and CX Liu (2015)

Conclusion and outlook

- We have shown the existence of new topological superconducting and insulating phases in non-symmorphic crystals.
- Possible material realization? Photonic crystals? Iron pnictide superconductors?

MIT group (2015) **Shen's group (2015)**

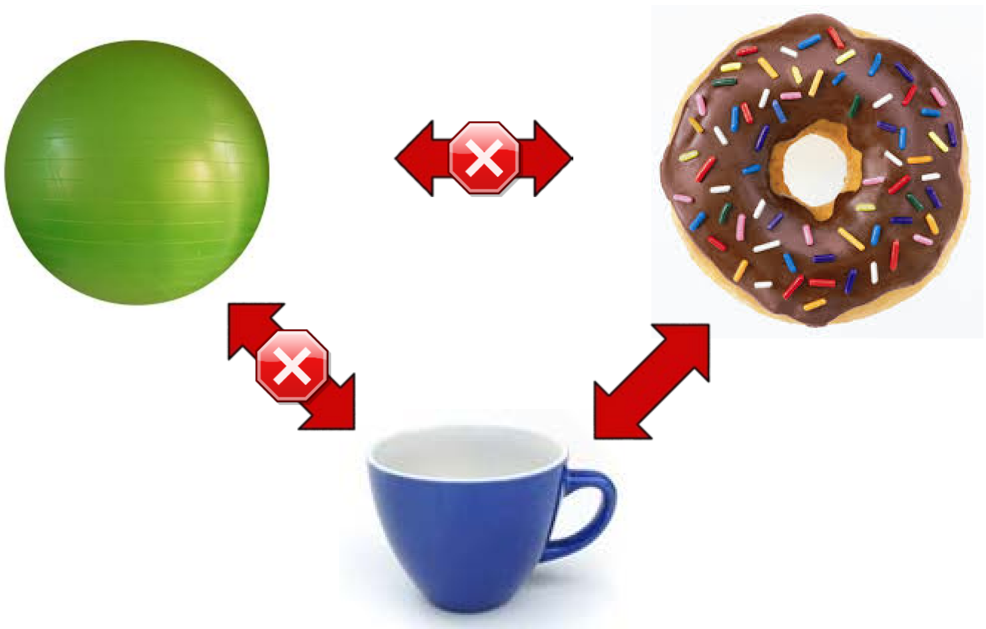
- More topological phases
  - Classification of topological crystalline superconductors
  - Classification of topological crystalline semi-metal phases (e.g. Dirac semi-metals)
  - Interacting topological phases and crystalline symmetry

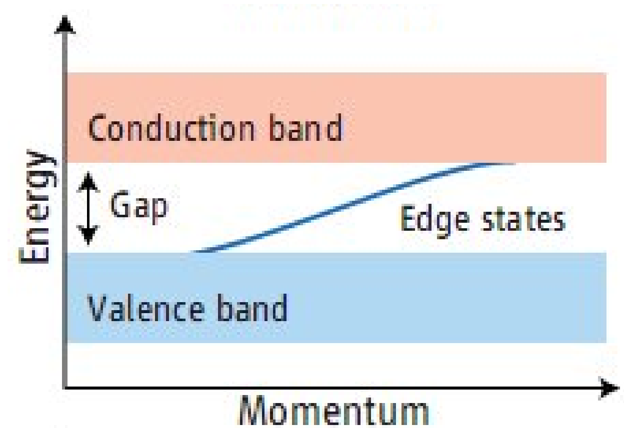
Fu (2015)

Thanks for your attention!

Topological states of matter

- Topological states for free fermions
  - Topological states cannot be adiabatically connected to normal states without gap closing even though sharing the same symmetry.
  - Topological states have edge/surface modes at the boundary (surface or interface).





Gap functions

- The gap function is classified by glide reflection

$$D_{\vec{k}}(g)\Delta(\vec{k})D^T_{-\vec{k}}(g) = \eta\Delta(\vec{k}), \qquad \eta = \pm$$

$$\Delta_{\alpha\beta}(k) = V_0\langle\psi_{\alpha,-k}\psi_{\beta,k}\rangle$$

- Glide symmetry for BdG Hamiltonian

$$\mathcal{G}_\eta(\vec{k}) = \begin{pmatrix} D_{\vec{k}}(g) & 0 \\ 0 & \eta D^*_{-\vec{k}}(g) \end{pmatrix}$$

$$\mathcal{G}_\eta(\vec{k})H_{BdG}\mathcal{G}^+_\eta(\vec{k}) = H_{BdG}$$

Glide parity

- Glide parities of particle-hole partners

$$H_{BdG}\psi = E\psi, \qquad G(g)\psi = \delta_\eta e^{i\vec{k}\cdot\vec{\tau}}\psi, \qquad \delta_\eta = \pm$$

$$\tilde{\psi} = C\psi, \qquad H_{BdG}\tilde{\psi} = -E\tilde{\psi}, \qquad G(g)\tilde{\psi} = \eta\delta_\eta^* e^{-i\vec{k}\cdot\vec{\tau}}\tilde{\psi}$$

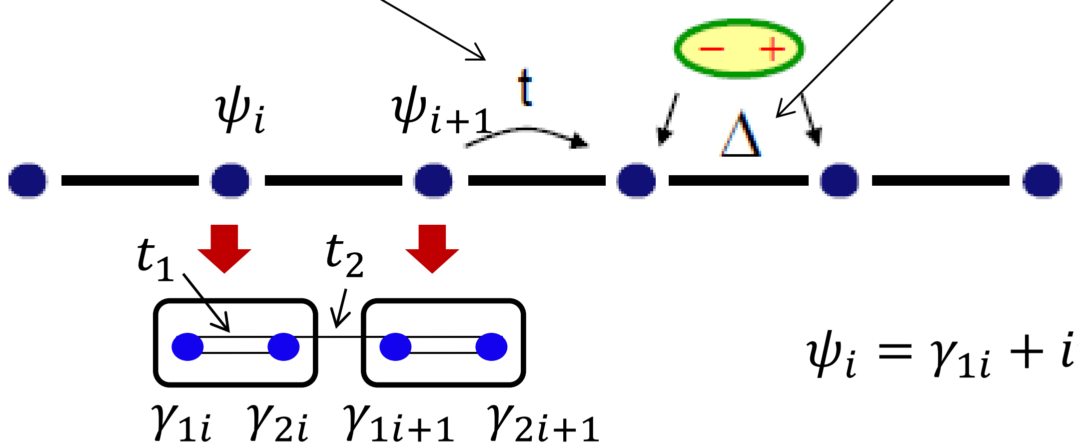
- Glide parities depend on the momentum

For example, for $\eta = +$, the glide parities for ψ and $\tilde{\psi}$ are $e^{i\vec{k}\cdot\vec{\tau}}$ and $e^{-i\vec{k}\cdot\vec{\tau}}$, respectively. They can be the same ($\vec{k}\cdot\vec{\tau} = 0$) or different ($\vec{k}\cdot\vec{\tau} = \frac{\pi}{2}$).

Topological superconductors

- Kitaev model for 1D p-wave superconductor

$$H-\mu N=\sum_i t(\psi_i^+\psi_{i+1}+\psi_{i+1}^+\psi_i)-\mu\psi_i^+\psi_i+\Delta(\psi_i\psi_{i+1}+\psi_{i+1}^+\psi_i^+)$$



Kitaev (2001)

$$\psi_i=\gamma_{1i}+i\gamma_{2i},\qquad \gamma_{\alpha i}^+=\gamma_{\alpha i}$$

$$t_1=\mu,\qquad t_2=2t=2\Delta$$

$$H=2i\sum_i t_1\gamma_{1i}\gamma_{2i}+t_2\gamma_{2i}\gamma_{1i+1}$$

Su, Schrieffer and Heeger (1979)

PENNSTATE 1855

Topological superconductors

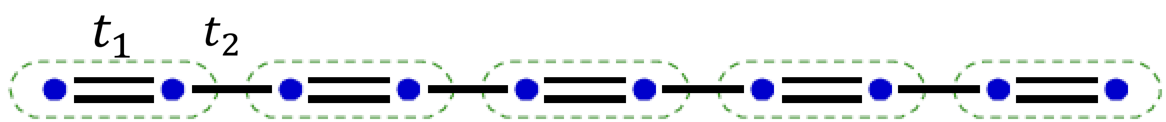
- Kitaev model for 1D p wave superconductor

Kitaev (2001)

$$H = 2i \sum_i t_1 \gamma_{1i}\gamma_{2i} + t_2 \gamma_{2i}\gamma_{1i+1}$$

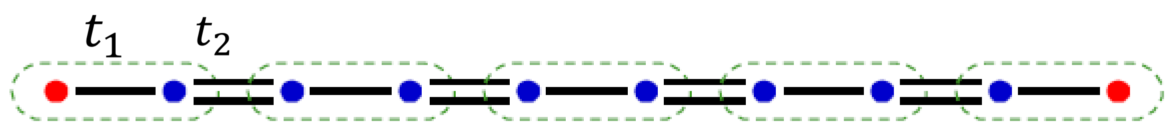
Trivial phase

$t_1 > t_2$



Topological phase

$t_1 < t_2$



Unpaired end Majorana zero modes

Topological mirror Superconductors

- Key step: mathematically, we can still define a new "mirror" symmetry operation for the BdG Hamiltonian.

$$D(m)\Delta(k)D^T(m) = \eta\Delta(k), \qquad \eta = \pm$$

$$\mathcal{D}(m) = \begin{pmatrix} D(m) & 0 \\ 0 & \eta D^*(m) \end{pmatrix} \qquad H_{BdG} = \begin{pmatrix} h(k)-\mu & \Delta(k) \\ \Delta^+(k) & -h^*(-k)+\mu \end{pmatrix}$$

$$\mathcal{D}(m)H_{BdG}\mathcal{D}^+(m) = H_{BdG}$$

Topological mirror Superconductors

- Any eigen-state of the BdG Hamiltonian can have the definite mirror parity.

$$\mathcal{D}(m) H_{BdG} \mathcal{D}^{+}(m) = H_{BdG}$$

$$H_{BdG}\psi = E\psi, \qquad \mathcal{D}(m)\psi = \delta_m \psi, \qquad \delta_m = \pm$$

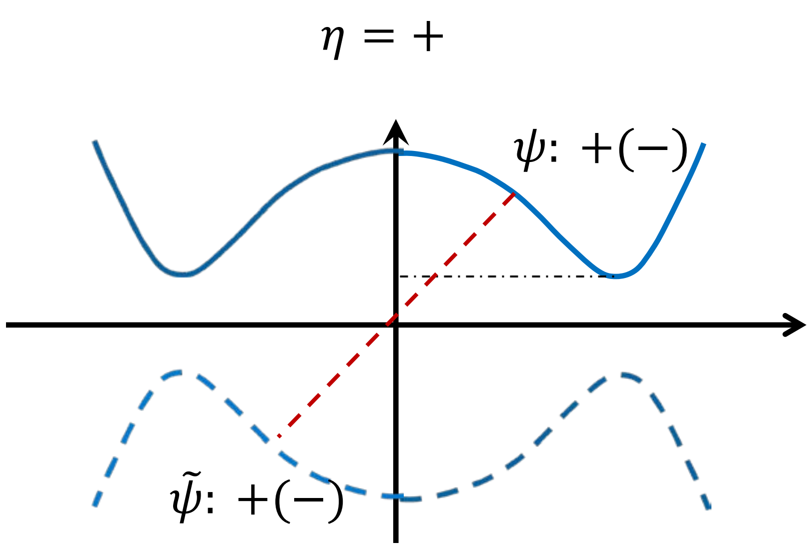
- The mirror parities of ψ and $\tilde{\psi}$ are determined by η.

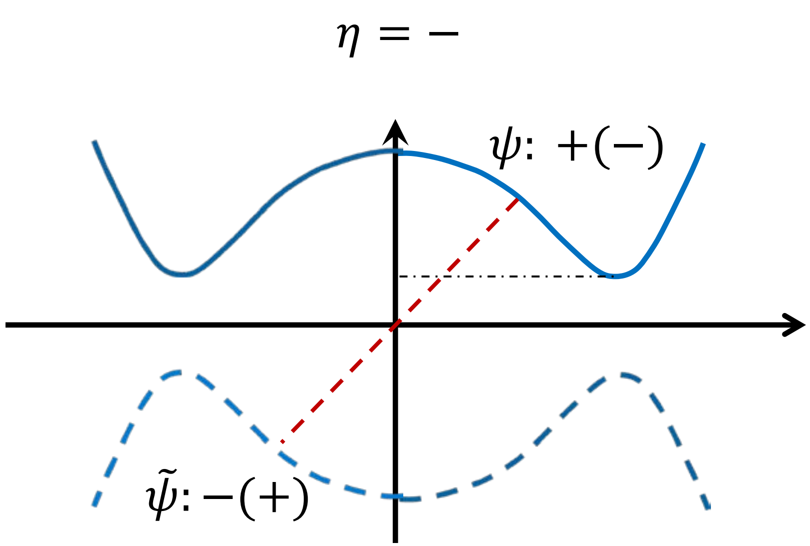
$$C\mathcal{D}(m)C^{-1} = \eta\mathcal{D}(m)$$

$$\tilde{\psi} = C\psi, \qquad H_{BdG}\tilde{\psi} = -E\tilde{\psi}, \qquad \mathcal{D}(m)\tilde{\psi} = \eta\delta_m\tilde{\psi}$$

Topological mirror Superconductors

- When $\eta = +$, ψ and $\tilde{\psi}$ have the same mirror parity, while $\eta = -$, ψ and $\tilde{\psi}$ have opposite mirror parities.





Topological non-symmorphic insulators

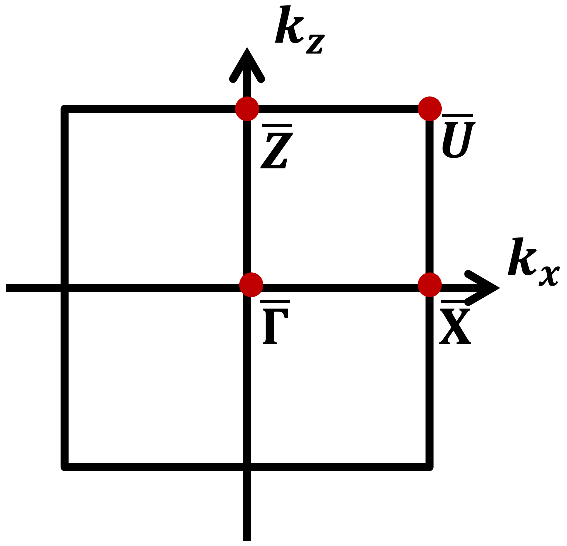
- Anti-commutation relation at $\bar{Z}$ and $\bar{U}$.

$$g_x m_z = m_z g_x + 2\vec{\tau}$$

When $\vec{k} = \left(0, k_y, \frac{\pi}{c}\right) = \left(\frac{\pi}{a}, k_y, \frac{\pi}{c}\right)$,

$$g_x m_z |\phi_{\vec{k}}\rangle = e^{2i\vec{k}\cdot\vec{\tau}} m_z g_x |\phi_{\vec{k}}\rangle$$
$$= -m_z g_x |\phi_{\vec{k}}\rangle$$

$\{m_z, g_x\} = 0$ at $\bar{Z}$ and $\bar{U}$

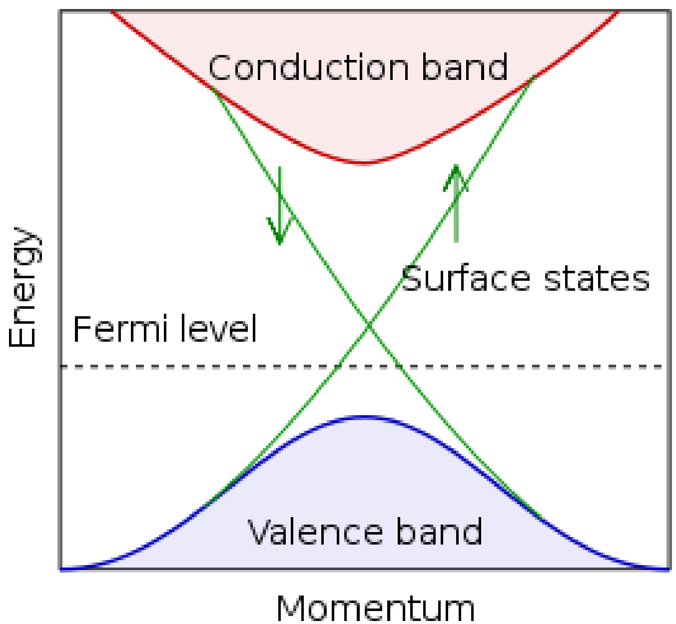


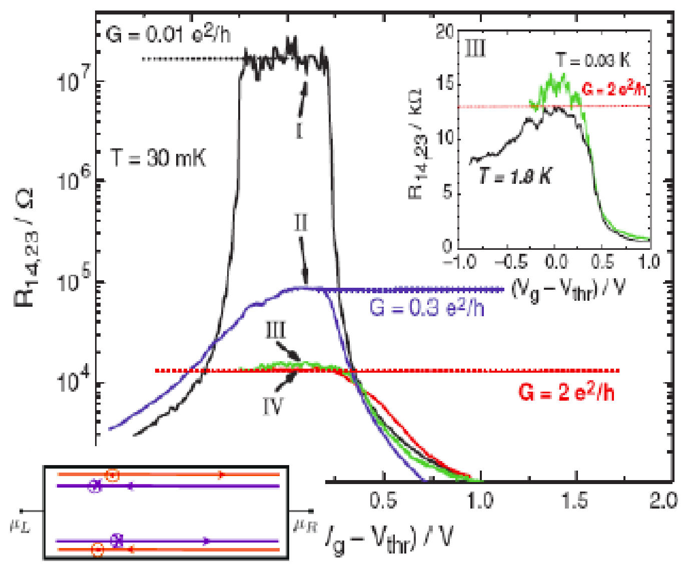
Liu's group (2014)

PENNSTATE
1855

Symmetry and topological states of matter

- Topological insulators and time reversal symmetry
  - Insulating bulk gap and helical edge states which are protected by time reversal symmetry.





Molenkamp's group, Science (2007)

Qi and Zhang, RMP (2011), Hasan and Kane, RMP (2010).