Theoretic study on topological superconductors

Cheng-Cheng Liu
(ccliu@bit.edu.cn)
Beijing Institute of Technology, Beijing

Sep. 26 2023, Moscow

Outline

- Introduction (topological superconductors+ the higher-order ones)

- Interaction-driven conventional topological superconductivity in magic angle twisted bilayer graphene

- Proximity effect induced higher-order topological superconductors

Outline

- Introduction (topological superconductors+ the higher-order ones)

- Interaction-driven conventional topological superconductivity in magic angle twisted bilayer graphene

- Proximity effect induced higher-order topological superconductors

Dirac and Majorana Fermion

Dirac equation:

$$(i\gamma^\mu \partial_\mu - m)\psi = 0$$

- Dirac representation

$$\gamma^0 = \sigma \otimes \tau^3, \qquad \gamma^{\mu=1,2,3} = i\sigma^\mu \otimes \tau^2$$

$\psi \neq \psi^*$, Dirac Fermion

- Majorana representation

$$\tilde{\gamma}^0 = \sigma^2 \otimes \tau^1, \quad \tilde{\gamma}^1 = i\sigma^3 \otimes \tau^0,$$

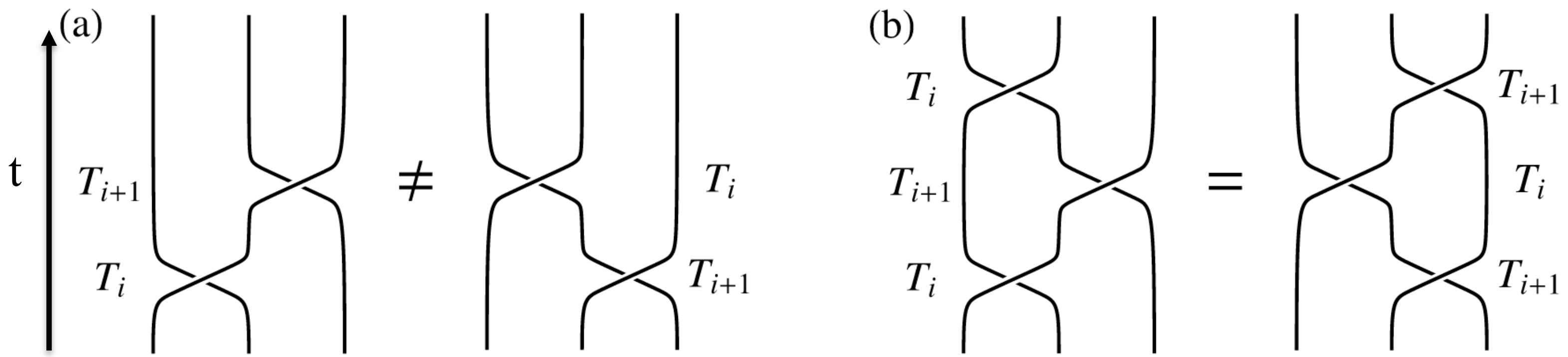
$$\tilde{\gamma}^2 = -i\sigma^2 \otimes \tau^2, \quad \tilde{\gamma}^3 = -i\sigma^1 \otimes \tau^0$$

$\psi = \psi^*$ Majorana Fermion !

Particle that is its own anti-particle

Majorana Fermion: Non-abelian statistics & Braiding

- Non-abelian statistics & Braiding

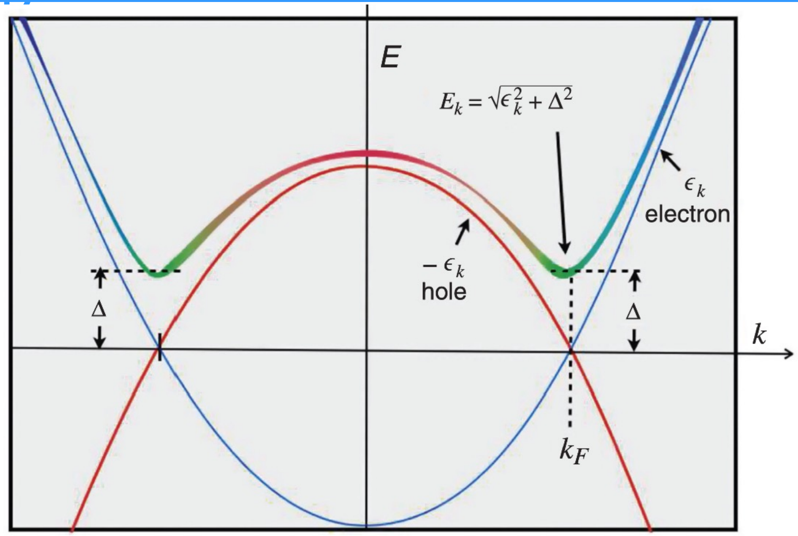


- Braiding Matrices

$$B_{\mathrm{boson}} = \begin{pmatrix} +1 & 0 & \cdots & 0 \\ 0 & +1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & +1 \end{pmatrix} \qquad B_{\mathrm{fermion}} = \begin{pmatrix} -1 & 0 & \cdots & 0 \\ 0 & -1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -1 \end{pmatrix} \qquad B_{\mathrm{non-Abelian}} = \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1N} \\ B_{21} & B_{22} & \cdots & B_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ B_{N1} & B_{N2} & \cdots & B_{NN} \end{pmatrix}$$

How to realize Majorana Fermion in condensed matter systems?

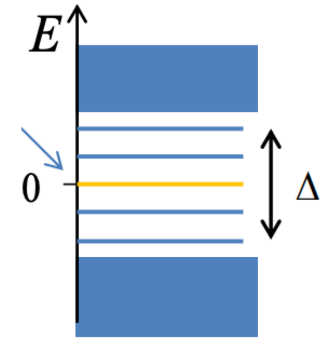
Superconductor BdG Hamiltonian



mean field: $c^\dagger c c^\dagger c \rightarrow < c^\dagger c^\dagger > cc = \Delta^* cc$

$$\mathcal{H}_{BdG}(\boldsymbol{k}) = \begin{pmatrix} \epsilon(\boldsymbol{k}) & 0 & 0 & \Delta \\ 0 & \epsilon(\boldsymbol{k}) & -\Delta & 0 \\ 0 & -\Delta^* & -\epsilon(-\boldsymbol{k}) & 0 \\ \Delta^* & 0 & 0 & -\epsilon(-\boldsymbol{k}) \end{pmatrix}$$

$$\Psi_{\boldsymbol{k}}^T = (c_{\boldsymbol{k}\uparrow}\ c_{\boldsymbol{k}\downarrow}\ c^\dagger_{-\boldsymbol{k}\uparrow}\ c^\dagger_{-\boldsymbol{k}\downarrow})$$



- Bogoliubov transformation

$$c_{\mathbf{k}\uparrow} = u_{\mathbf{k}}\gamma_{\mathbf{k}\uparrow} + v_{\mathbf{k}}\gamma^\dagger_{-\mathbf{k}\downarrow}$$
$$c^\dagger_{-\mathbf{k}\downarrow} = u_{\mathbf{k}}\gamma^\dagger_{-\mathbf{k}\downarrow} - v_{\mathbf{k}}\gamma_{\mathbf{k}\uparrow}$$

- Particle hole symmetry

Eigenvalues of H_{BdG} come in pairs $\pm\varepsilon$,with $\gamma^\dagger_{-\varepsilon} = \gamma_\varepsilon$

Eigenstates of H_{BdG} at $\varepsilon=0$: Majorana fermion, $\gamma_0^\dagger = \gamma_0$

Kitaev 1D Chain toy model

$$\mathcal{H} = \sum_{i=1}^{N-1} (-tc_i^\dagger c_{i+1} + \Delta c_i c_{i+1}) + h.c. - \mu \sum_{i=1}^{N} c_i^\dagger c_i,$$

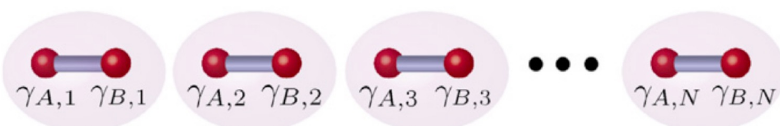
$$c_j = \frac{1}{2}(\gamma_{2j-1} + i\gamma_{2j}),$$

$$c_j^\dagger = \frac{1}{2}(\gamma_{2j-1} - i\gamma_{2j}).$$

$$\mathcal{H} = \frac{i}{2} \sum_{j=1}^{N-1} \left\{ (\Delta + t)\gamma_{2j}\gamma_{2j+1} + (\Delta - t)\gamma_{2j-1}\gamma_{2j+2} \right\} - \frac{i\mu}{2} \sum_{j=1}^{N} \gamma_{2j-1}\gamma_{2j}.$$

- $\Delta = t = 0$ and $\mu < 0$: For this case, the Hamiltonian reduces to

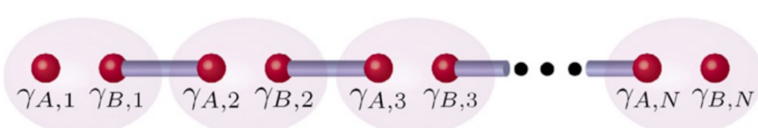
$$H_1 = -\frac{i\mu}{2} \sum_{j=1}^{N} \gamma_{2j-1}\gamma_{2j}.$$



dimer !

- $\Delta = t > 0$ and $\mu = 0$: For this case the Hamiltonian reduces to

$$H_2 = it \sum_{j=1}^{N-1} \gamma_{2j}\gamma_{2j+1}.$$



One isolated Majorana at each end!

Kitaev, 2001

Kitaev 1D p-wave Chain

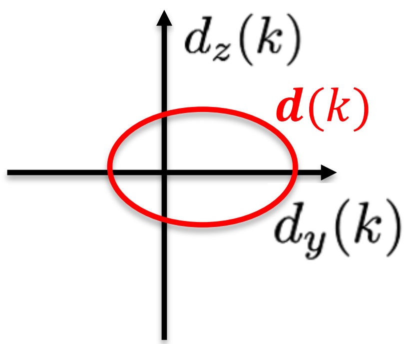
$$\mathcal{H} = \sum_k (-2t\cos k - \mu) c_k^\dagger c_k - \sum_k (i\Delta \sin k \; c_k^\dagger c_{-k}^\dagger + h.c.),$$

$$\mathcal{H} = \frac{1}{2}\sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} H(k) \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}$$

Nambu basis

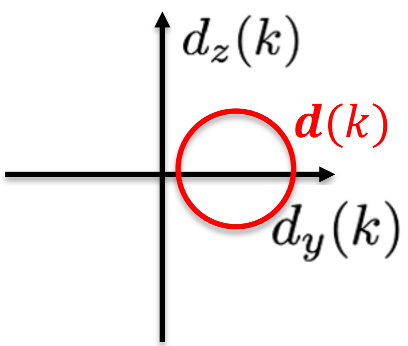
$$H(k) = d_y(k)\tau_y + d_z(k)\tau_z \qquad d_y(k) = 2\Delta \sin k, \qquad d_z(k) = -2t\cos k - \mu$$

$|\mu| < 2t$: weak pairing phase
Topological superconductor



Nontrivial

$|\mu| > 2t$: strong pairing phase
Trivial superconductor



Trivial

Kitaev 1D p-wave Chain

$$\mathcal{H} = \sum_k (-2t\cos k - \mu) c_k^\dagger c_k - \sum_k (i\Delta \sin k \, c_k^\dagger c_{-k}^\dagger + h.c.),$$

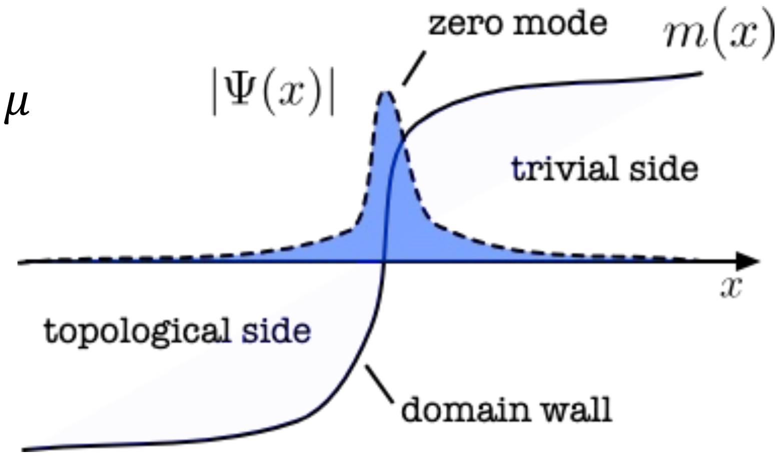
$$\mathcal{H} = \frac{1}{2}\sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} H(k) \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}$$

Nambu basis

$$H(k) = d_y(k)\tau_y + d_z(k)\tau_z \qquad d_y(k) = 2\Delta \sin k, \qquad d_z(k) = -2t\cos k - \mu$$

- Expanding the Hamiltonian around k=0

$$H_{\text{eff}} = -(2t+\mu)\tau_z + 2\Delta k \tau_y \qquad m = -2t - \mu$$



$$\boxed{\begin{gathered} \lim_{x\to\pm\infty} m(x) = \pm m, \\ m(x=0) = 0. \end{gathered}}$$

$$H(x) = m(x)\tau_z - 2i\Delta\tau_y\partial_x$$

$$H(x)\phi(x) = [m(x)\tau_z - 2i\Delta\tau_y\partial_x]\phi(x) = 0. \qquad \text{using } \tau_y\tau_z = i\tau_x \text{ and } \tau_y^2 = 1$$

$$\partial_x\phi(x) = \frac{m(x)}{2\Delta}\tau_x\phi(x)$$

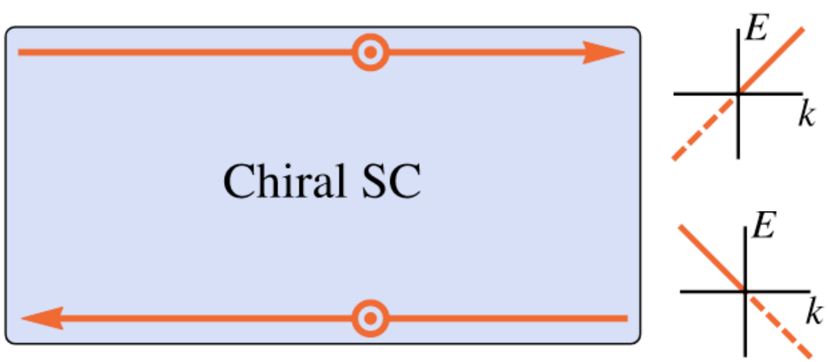
$$\boxed{\phi(x) = \exp\left(\pm\int_0^x \frac{m(x')}{2\Delta}dx'\right)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}}$$

Zero mode is real and localized.

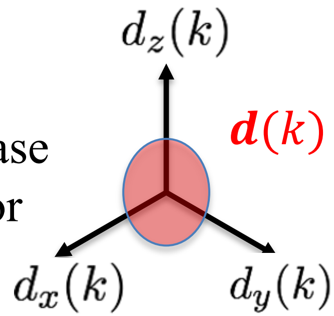
2D p+ip TSC (Read Green model)

$$\mathcal{H} = \frac{1}{2}\sum_{\boldsymbol{k}} \psi^{\dagger}_{\boldsymbol{k}} H(\boldsymbol{k}) \psi_{\boldsymbol{k}}, \quad \psi^{T}_{\boldsymbol{k}} = (c_{\boldsymbol{k}},\ c^{\dagger}_{-\boldsymbol{k}})$$

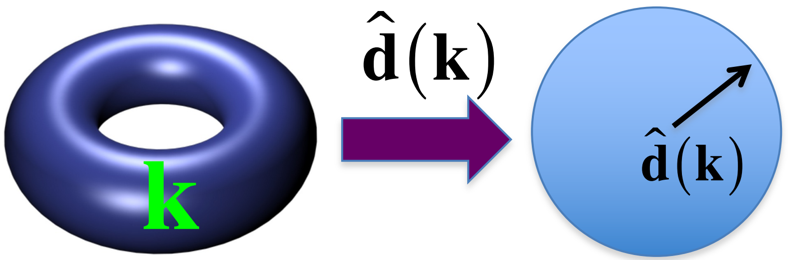
$$H(\boldsymbol{k}) = \sum_{i=x,y,z} d_i(k)\tau_i \qquad \begin{aligned} d_x(k) &= 2\Delta \sin k_x, \\ d_y(k) &= 2\Delta \sin k_y, \\ d_z(k) &= -2t(\cos k_x + \cos k_y) - \mu \end{aligned}$$



$|\mu| < 4t$: weak pairing phase
Topological superconductor



C≠0

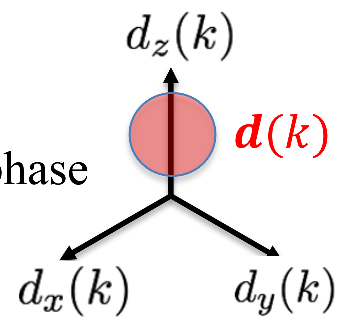


Must wrap around the sphere an integer C times

Homotopy $\pi_2(S^2) = C$ Chern number

$$C = \frac{1}{4\pi} \oiint_{BZ} \hat{\mathbf{d}} \cdot \left(\partial_{k_x} \hat{\mathbf{d}} \times \partial_{k_y} \hat{\mathbf{d}} \right)$$

$|\mu| > 4t$: strong pairing phase
Trivial superconductor



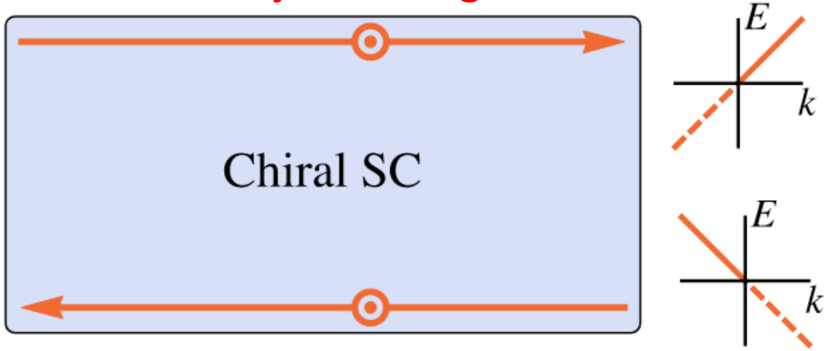
C=0

2D p+ip TSC: bulk-edge correspondence

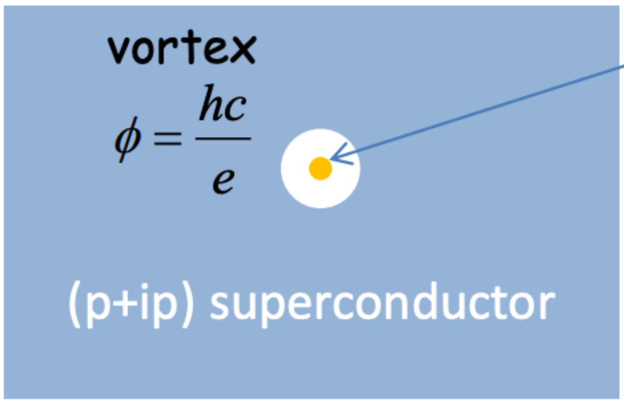
$$\mathcal{H} = \frac{1}{2}\sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k}} H(\boldsymbol{k}) \psi_{\boldsymbol{k}}, \quad \psi^T_{\boldsymbol{k}} = (c_{\boldsymbol{k}},\ c^\dagger_{-\boldsymbol{k}})$$

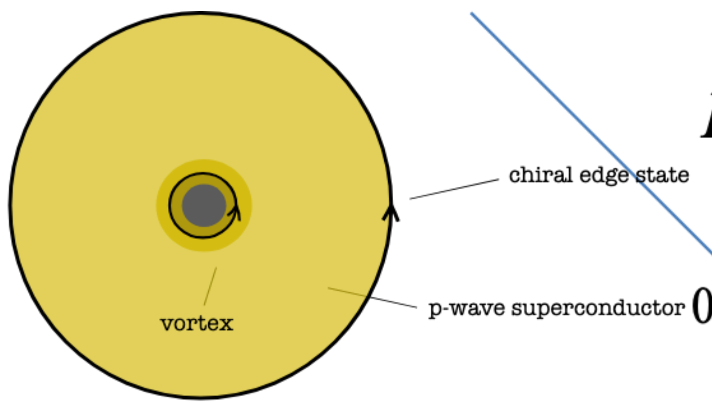
$$H(\boldsymbol{k}) = \sum_{i=x,y,z} d_i(k)\tau_i \qquad \begin{aligned} d_x(k) &= 2\Delta \sin k_x, \\ d_y(k) &= 2\Delta \sin k_y, \\ d_z(k) &= -2t(\cos k_x + \cos k_y) - \mu \end{aligned}$$

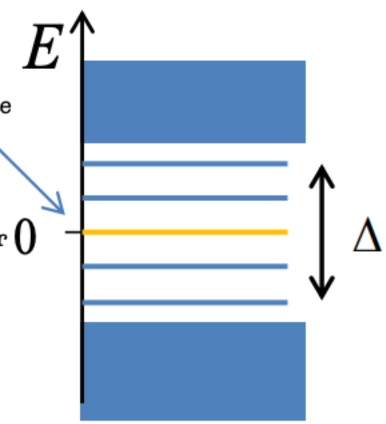
C=# Chiral Majorana edge states



Zero-energy Majorana bound state





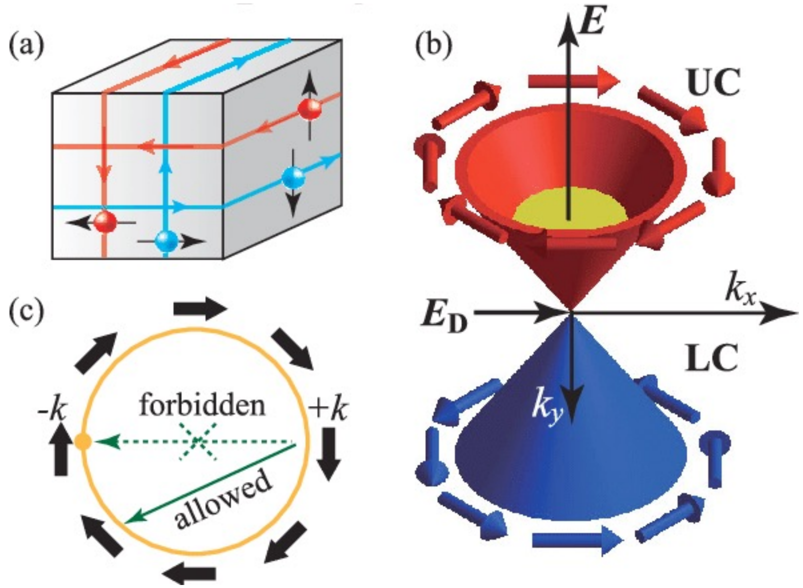


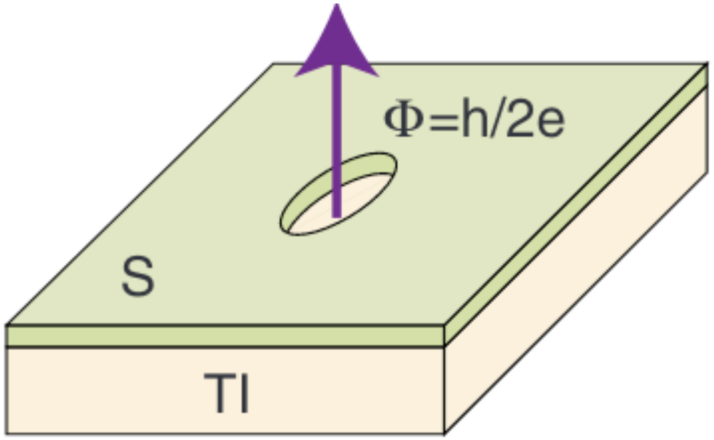
zero mode $\varepsilon_0 = 0$ $\gamma_0 = \gamma_0^+$

Majorana fermion

energy spectrum near a vortex

Engineering topological superconductors: TI+s-wave SC





- Similar to a spinless p+ip superconductor

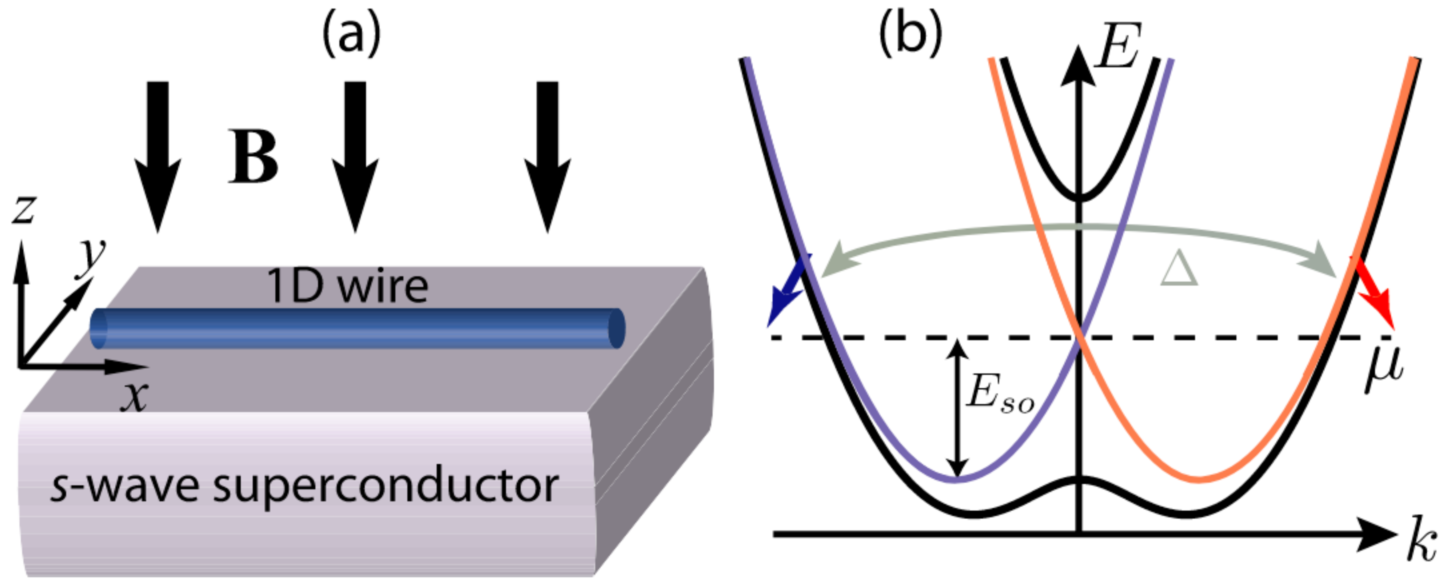
$$H_{surface} = H_0 + H_s$$
$$H_0 = \psi^\dagger(-iv\vec{\sigma}\cdot\nabla - \mu)\psi \qquad (\psi_\uparrow, \psi_\downarrow)^T$$
$$H_s = \Delta_0 \psi_\uparrow^\dagger \psi_\downarrow^\dagger + h.c.$$

$$c_{\mathbf{k}} = (\psi_{\uparrow\mathbf{k}} + e^{i\theta_{\mathbf{k}}}\psi_{\downarrow\mathbf{k}})/\sqrt{2}$$

$$H = \xi_k c_k^\dagger c_k + \Delta_0(k_x + ik_y)c_k^\dagger c_{-k}^\dagger + h.c.$$

Fu & Kane, 2008

Engineering topological superconductors: 1D wire+ s-wave SC



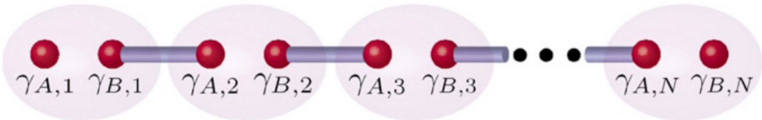
$$H = H_{\text{wire}} + H_{\Delta},$$

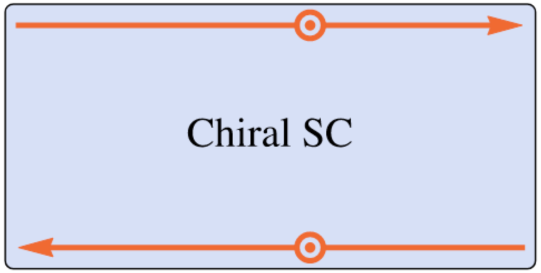
$$H_{\text{wire}} = \int \mathrm{d}x\, \psi^{\dagger} \left(-\frac{\partial_x^2}{2m} - \mu - \mathrm{i}\alpha\sigma^y \partial_x + h\sigma^z \right) \psi,$$

$$H_{\Delta} = \int \mathrm{d}x\, \Delta(\psi_{\uparrow}\psi_{\downarrow} + \mathrm{H.c.}).$$

Das Sarma et al, Alicea, von Oppen, Oreg, … Sato-Fujimoto-Takahashi, ….

Classification: Topological periodic table



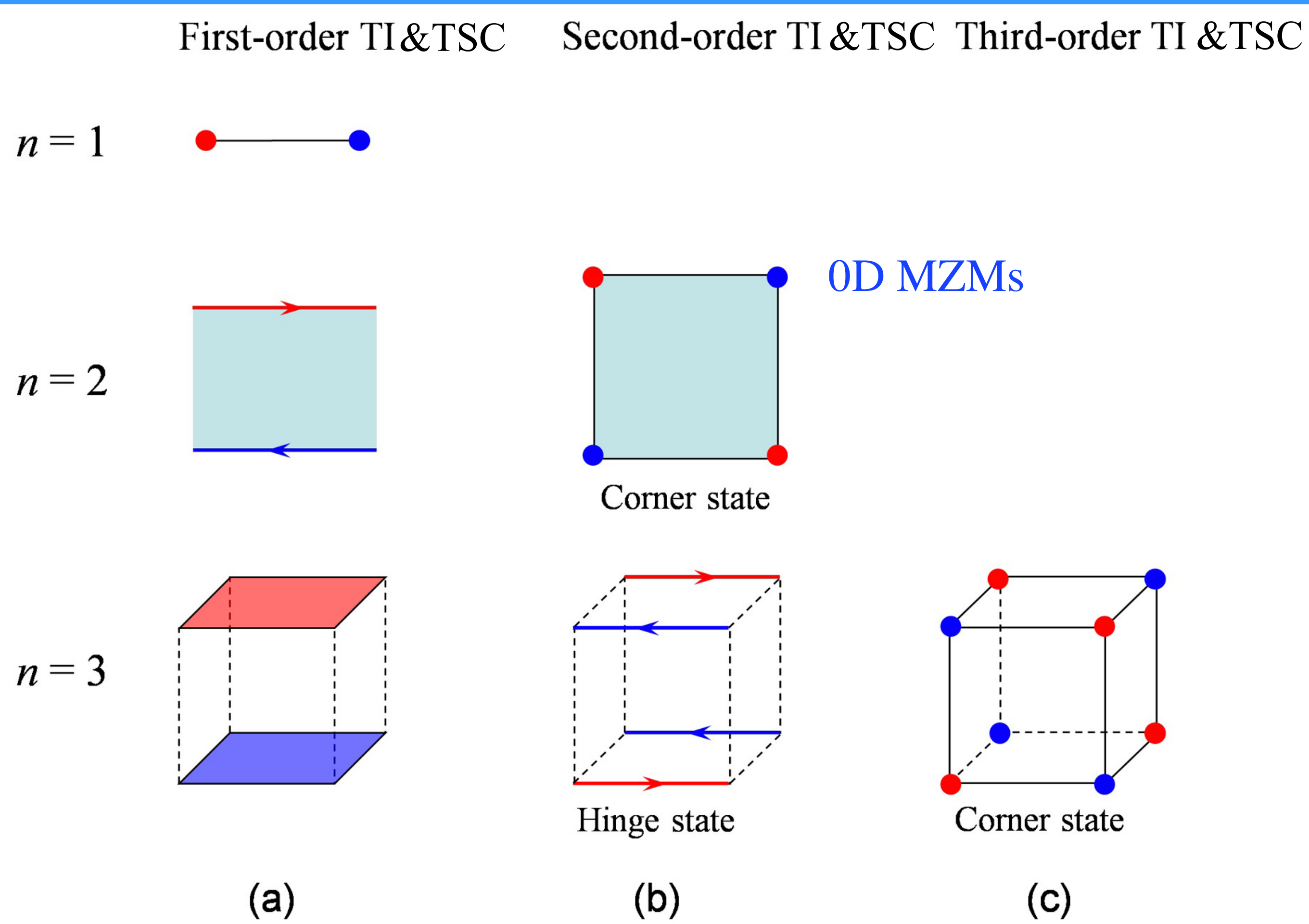


Altland-Zirnbauer RM classes

		$\mathcal{T}$	$\mathcal{P}$	$\mathcal{S}$	$d=1$	$d=2$	$d=3$
Standard (Wigner-Dyson)	A (unitary)	0	0	0	–	$\mathbb{Z}$	–
	AI (orthogonal)	+1	0	0	–	–	–
	AII (symplectic)	−1	0	0	–	$\mathbb{Z}_2$	$\mathbb{Z}_2$
Chiral (sublattice)	AIII (chiral unitary)	0	0	1	$\mathbb{Z}$	–	$\mathbb{Z}$
	BDI (chiral orthogonal)	+1	+1	1	$\mathbb{Z}$	–	–
	CII (chiral symplectic)	−1	−1	1	$\mathbb{Z}$	–	$\mathbb{Z}_2$
BdG	D	0	$\boxed{+1}$	0	$\boxed{\mathbb{Z}_2}$	$\boxed{\mathbb{Z}}$	–
	C	0	−1	0	–	$\mathbb{Z}$	–
	DIII	−1	+1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
	CI	+1	−1	1	–	–	$\mathbb{Z}$

Andreas P. Schnyder et al. 2008
Kitaev 2008

Higher-order topology & bulk-boundary correspondence



Conventional TSC with codimension dc=1，
HO-TSC with codimension dc>1

ZX Li et al. 2021

Outline

- Introduction

- Interaction-driven conventional topological superconductivity in magic angle twisted bilayer graphene

- Proximity effect induced higher-order topological superconductors

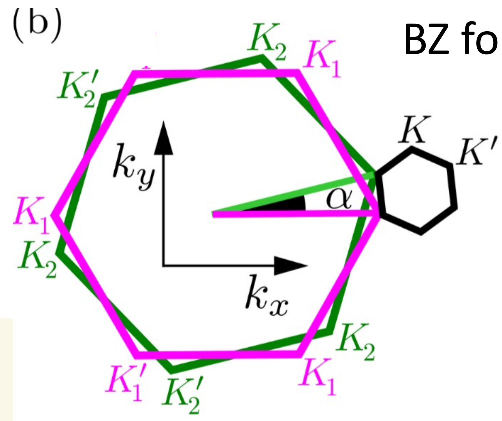
Interaction-driven topological superconductors

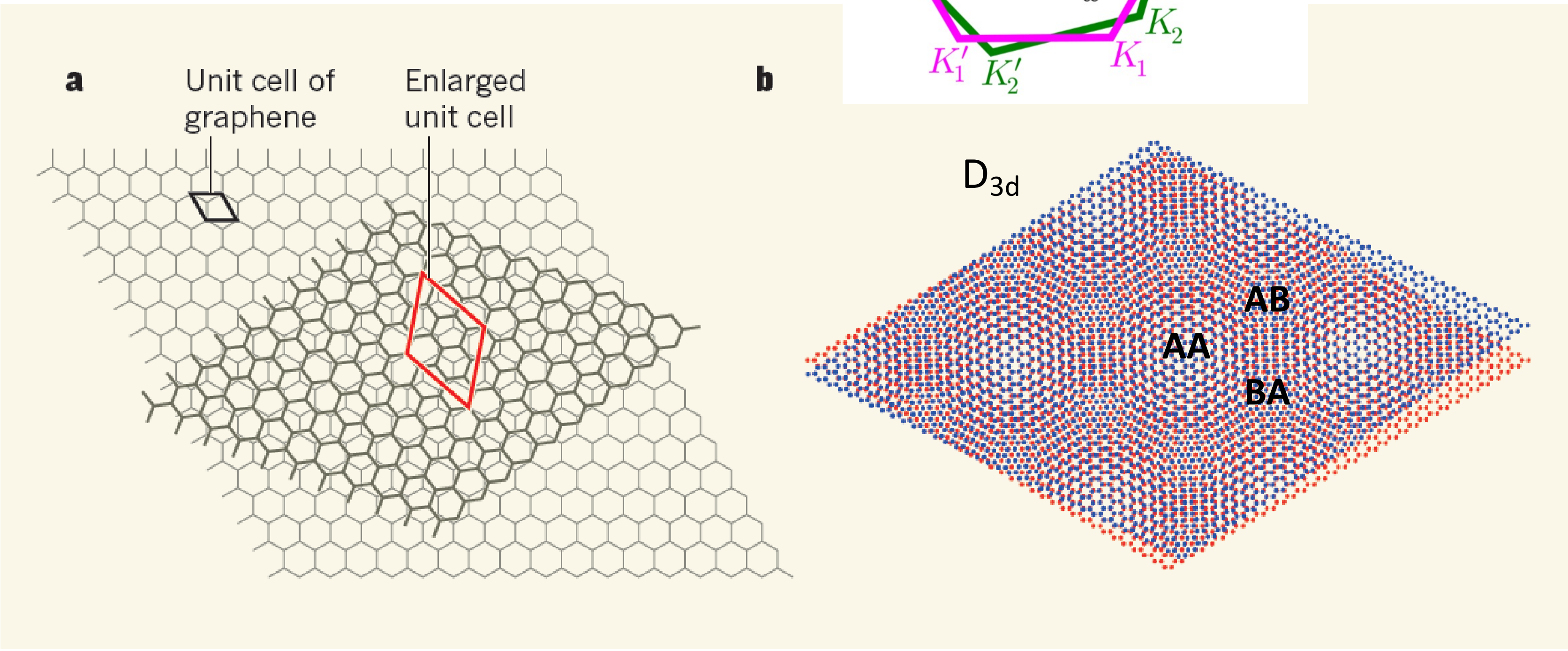
1. Chiral Spin Density Wave and d+id Superconductivity in the Magic-Angle-Twisted Bilayer Graphene,
CCL-Zhang-Chen-Yang, PRL 121, 217001 (2018).

Introduction : twisted bilayer graphene & some exciting experiments

- Twisted bilayer-graphene

BZ for Moiré pattern



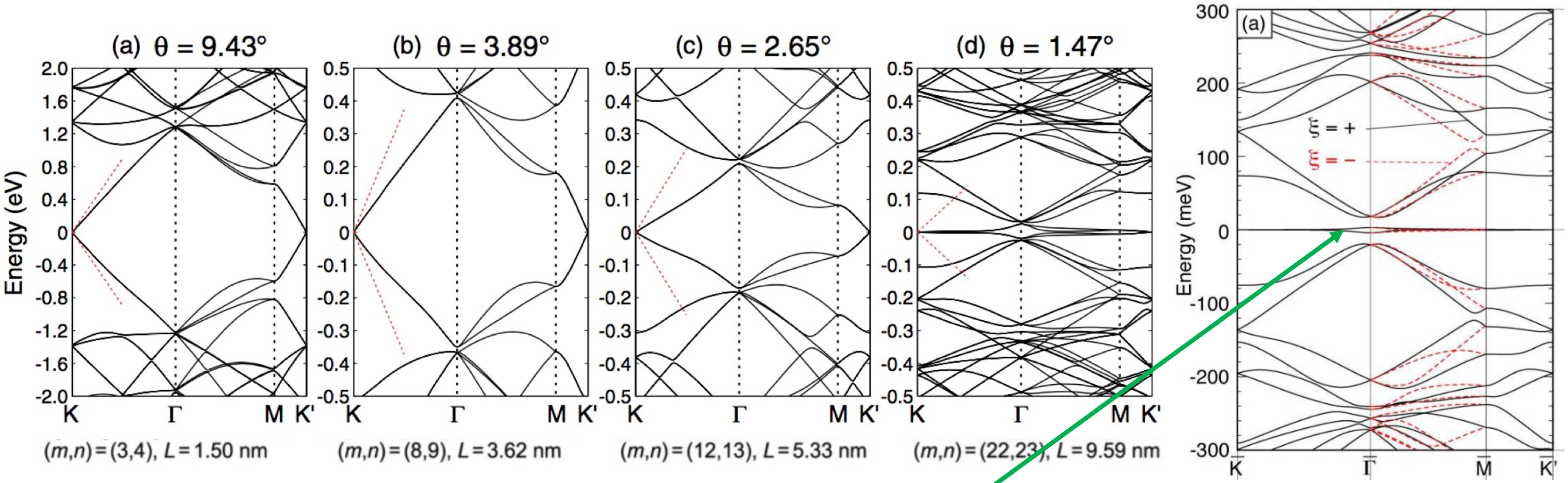


Two graphene layers stacked, relatively rotated for a small angle

The Moiré pattern generated for some certain angles (commensurate)

Twisted-angle depended band structure

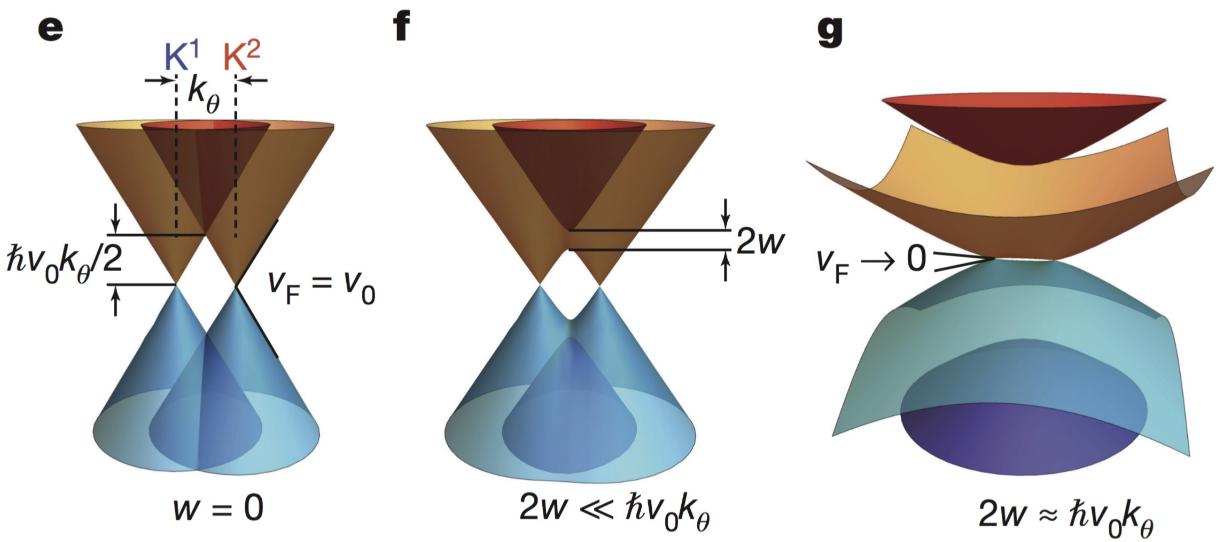
Moiré is different!



1. Fermi velocity is significantly **renormalized**.
2. The **four isolated flat bands** are relevant.
3. e-e interaction will plays a role in MA-BLG

Y. Cao1 et al Nature (2018)
Y. Cao2 et al Nature (2018)
J. M. B. Lopes dos Santos et al. PRL (2007)
R. Bistritzer and A. H. MacDonald PNAS (2011)
E. J. Mele PRB (2010)
P. Moon and M. Koshino (2012)
Nguyen N. T. Nam and M. Koshino PRB (2017)
M. Koshino et al., Arxiv:1805.06819

Twist → "Magic"



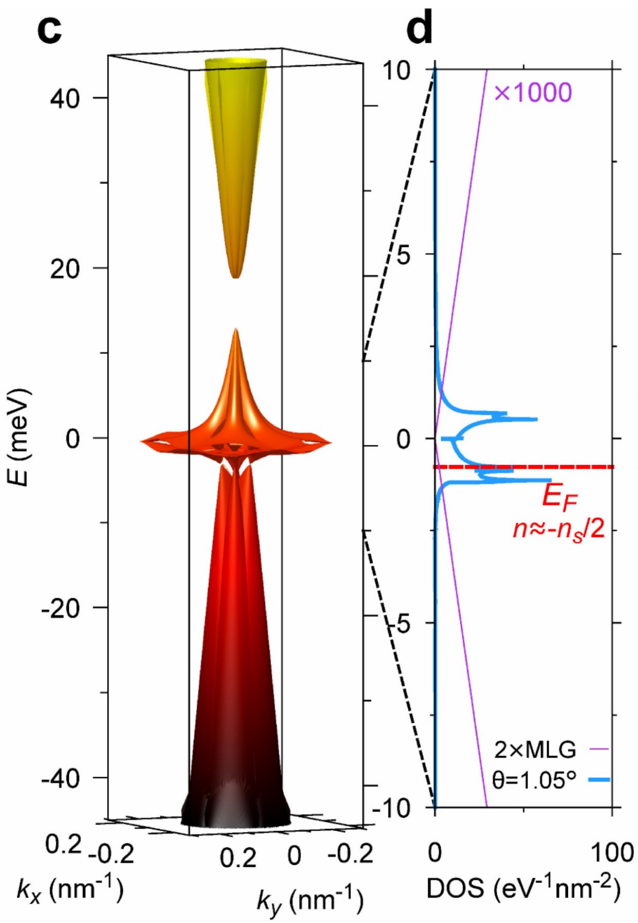
w≈110meV

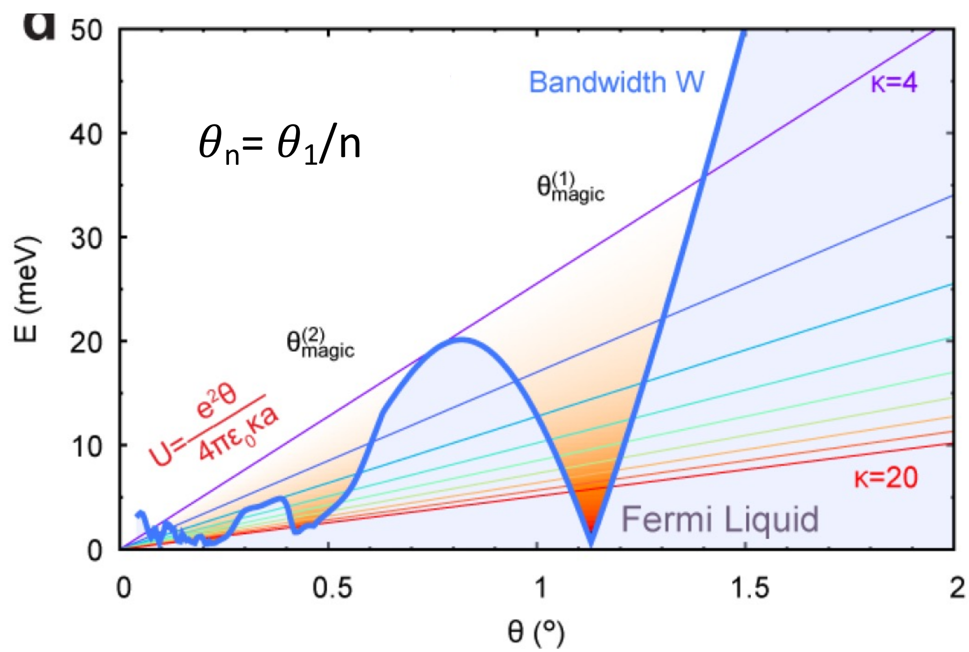
Lowering the twisted angle

$$\frac{v^\star}{v} = \frac{1-3\alpha^2}{1+6\alpha^2}$$

$\alpha = w/vk_\theta \qquad k_\theta = 2k_D \sin(\theta/2)$ R. Bistritzer and A. H. MacDonald PNAS (2011)

e-e interaction plays important role in flat bands



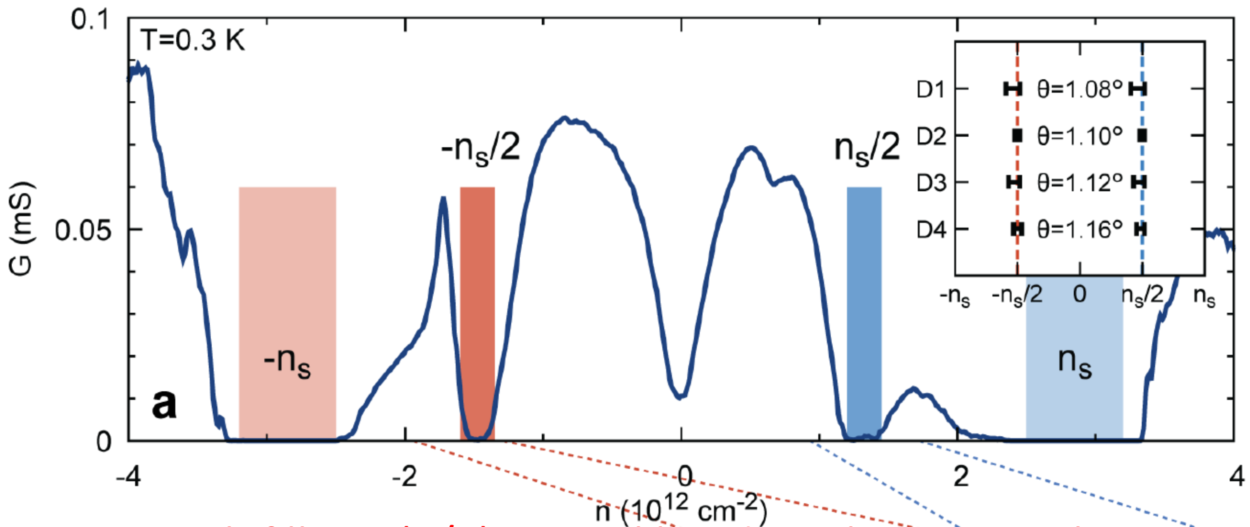


strong correlation $U > W$

Y. Cao et al, Nature 2018

What's found in experiment?

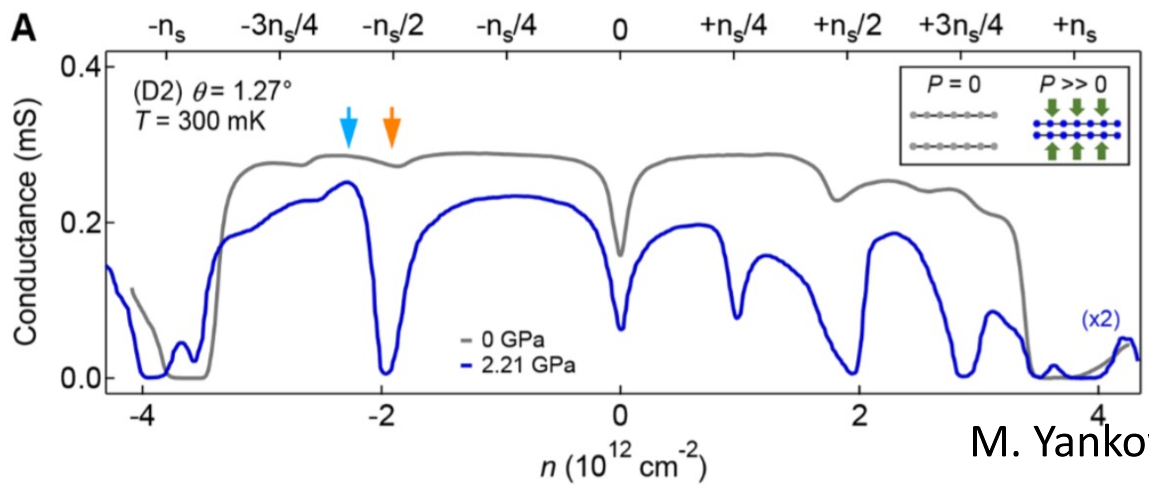
- Correlated-insulating state at half-filled flat band



Y. Cao et al Nature 2018.

At such fillings (1/2) normal band insulator in single-e picture is forbidden!

- Pressure-induced correlated behavior

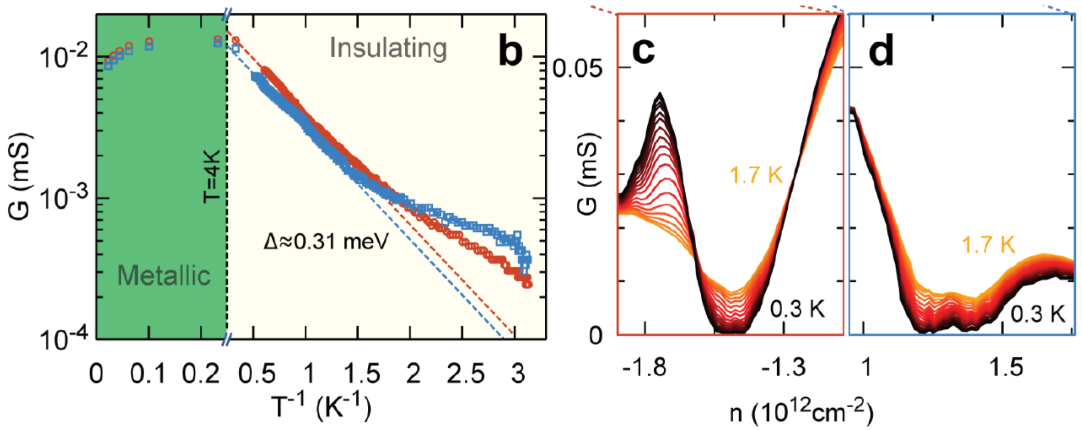


2.21 GPa

M. Yankowitz et al., Science 2019.

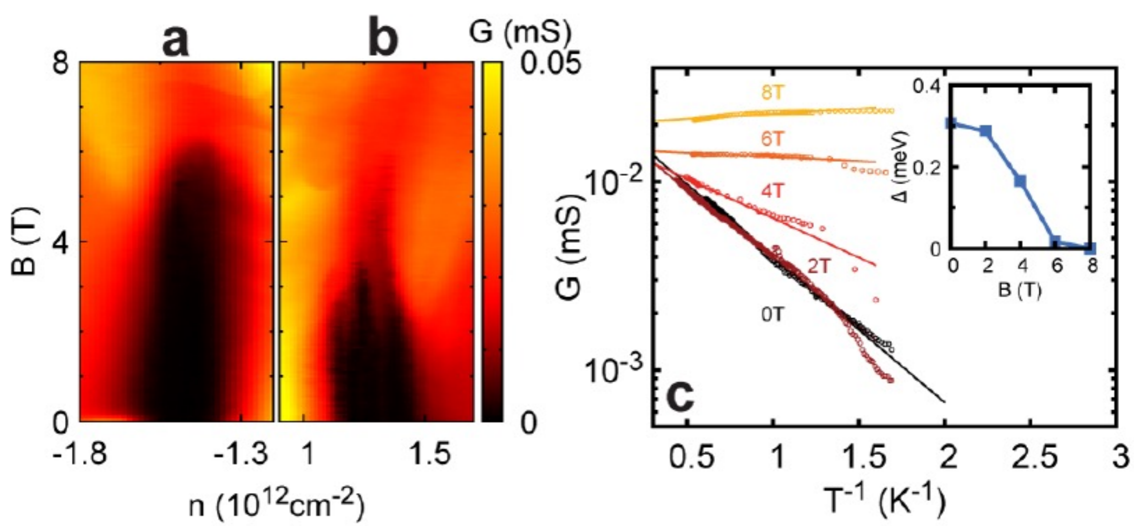
Correlated-insulator at half-filling

- Temperature-dependence



Temperature (>4 K) kills the insulating state !

- Magnetic-field dependence

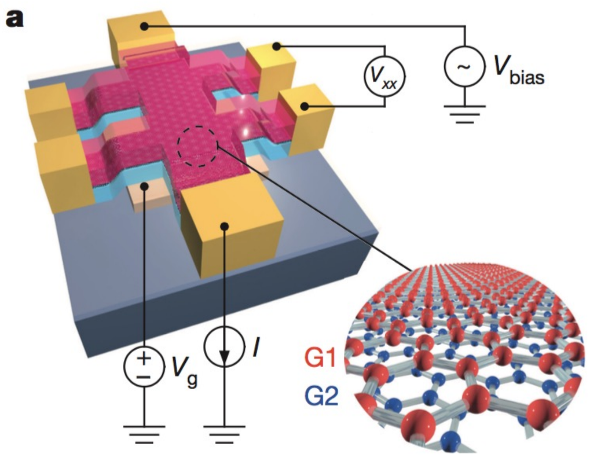


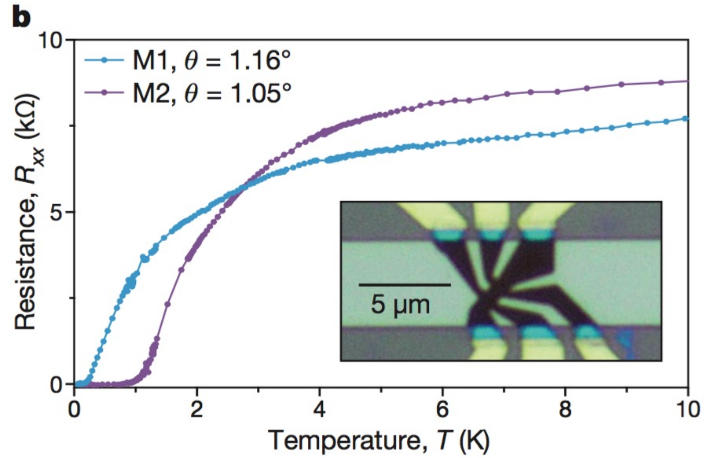
Magnetic-field (>8 T) kills the insulating state !

Y. Cao1 et al Nature 2018.

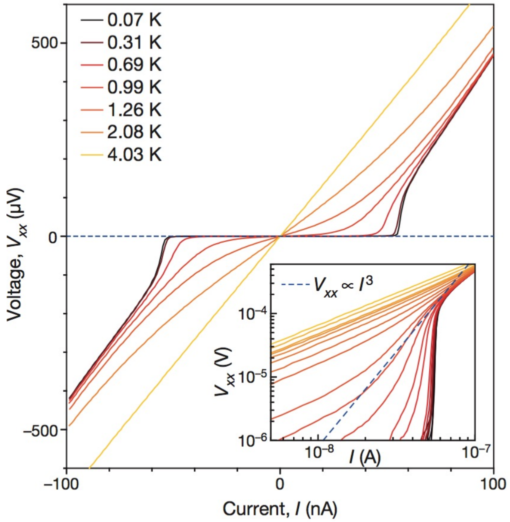
SC upon electrostatic doping

- Superconductivity (T_c=1.7 K) found





- The V-I relation: 2D BKT SC

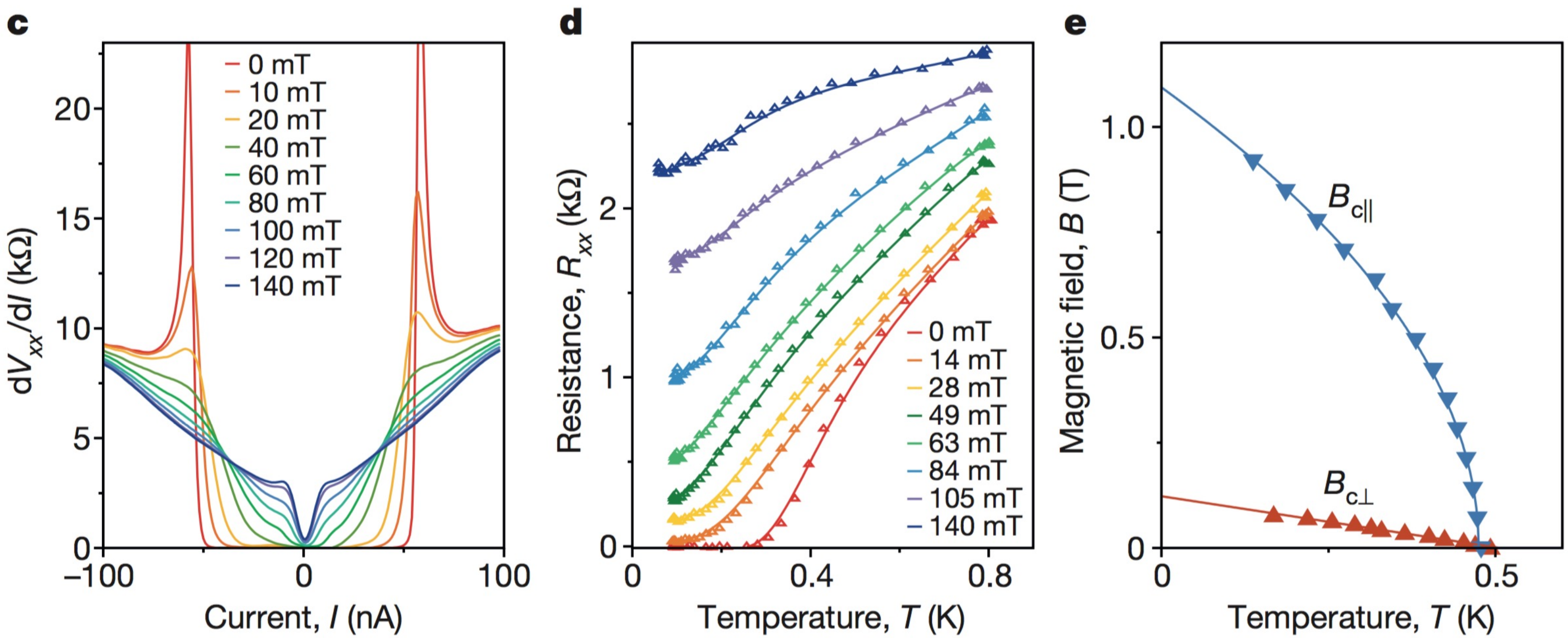


a critical current of 50 nA

Y. Cao2 et al Nature 2018.

SC upon doping

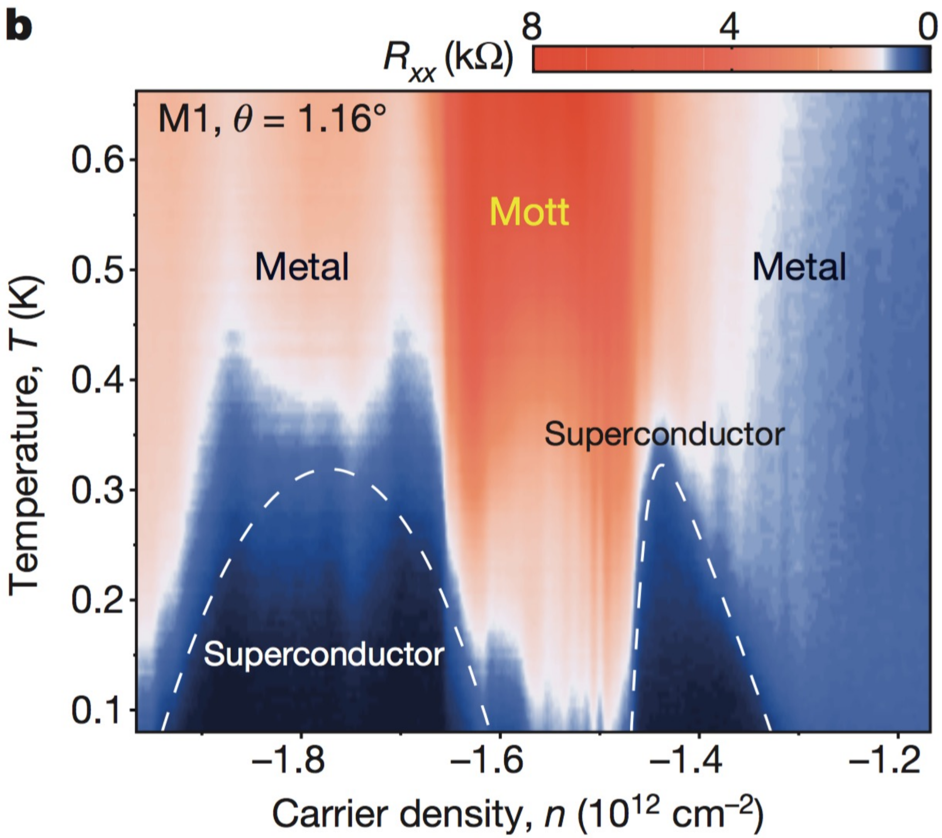
- Magnetic-field suppresses SC



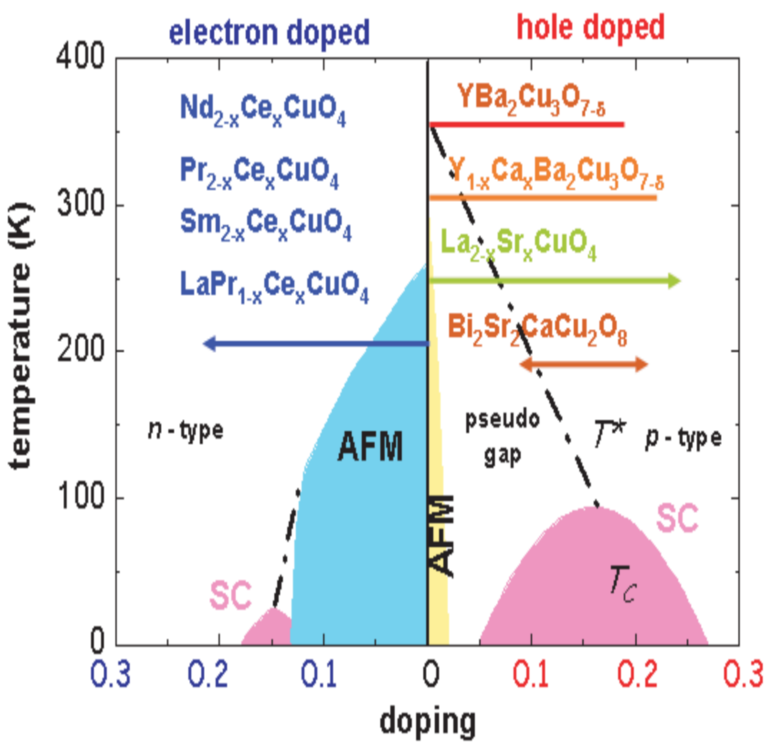
Consistent with Messner-effect and Ginzberg-Landau theory

Similar to the cuprates

MA-BLG



Cuprates



Hole doping electron doping

Asymmetric about half-filling

Y. Cao2 et al Nature 2018.

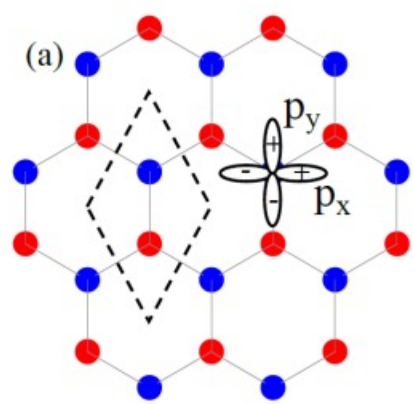
Several issues

- Is the correlated insulator identified at half-filling really Mott-insulator ?
- How to characterize it if not?
- What's the pairing mechanism of SC upon doping?
- What's the pairing symmetry?

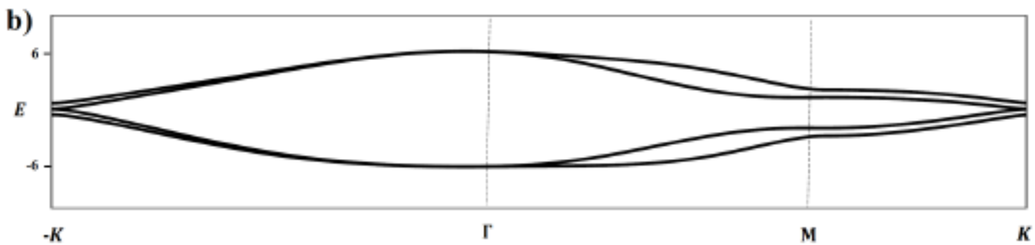
Model: p_x, p_y like Wannier orbitals on Honeycomb

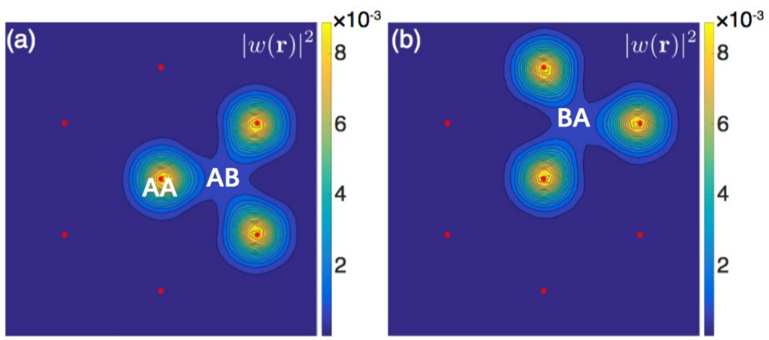
- By symmetry argument and group theory Yuan and Fu proposed a p_x, p_y - like Wannier orbitals Hubbard model on the emergent Honeycomb lattice for the MA-BLG.

	Γ	K	M
Group	D_3	D_3	C_2
Reps	$\{E, E\}$	$\{A_1, A_2, E\}$	$\{A, A, B, B\}$
C_{3z}	$\{\pm 1, \pm 1\}$	$\{0, 0, \pm 1\}$	NA
C_{2y}	NA	$\{+1, -1, \text{NA}\}$	$\{+1, +1, -1, -1\}$



N. F. Q. Yuan and L. Fu, PRB 98, 045103 (2018)





The Wannier orbital center and maximum

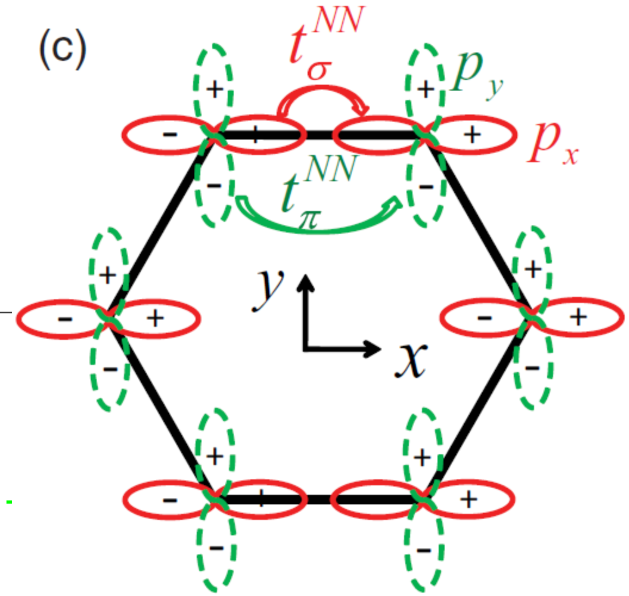
H. C. Po, et al, Phys. Rev.X 8, 031089 (2018)

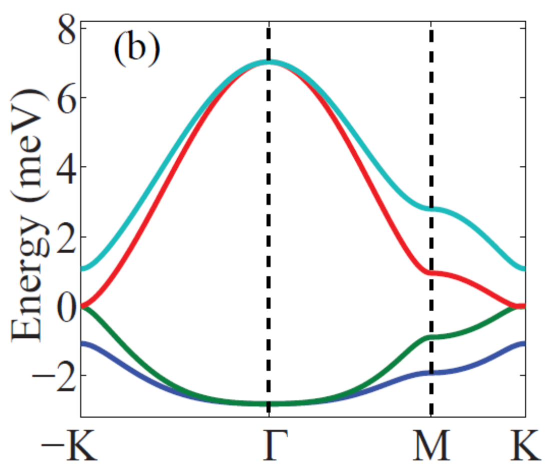
Model: p_x,p_y like Wannier orbitals on Honeycomb

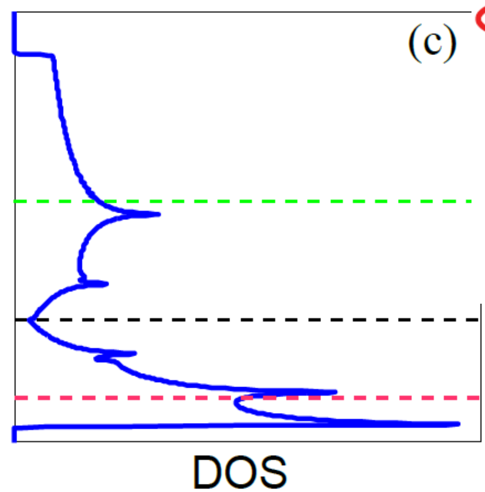
- The Slater-Koster formulism for the px,py- Honeycomb

$$H_{tb} = \sum_{i\mu,j\nu,\sigma} t_{i\mu,j\nu} c^{\dagger}_{i\mu\sigma} c_{j\nu\sigma} - \mu_c \sum_{i\mu\sigma} c^{\dagger}_{i\mu\sigma} c_{i\mu\sigma}.$$

$$t_{i\mu,j\nu} = t^{ij}_{\sigma} \cos\theta_{\mu,ij} \cos\theta_{\nu,ij} + t^{ij}_{\pi} \sin\theta_{\mu,ij} \sin\theta_{\nu,ij}$$







Degeneracy-pattern consistent with the irrep. on high symmetry points

VHS at $\delta_V \approx \pm 0.425$

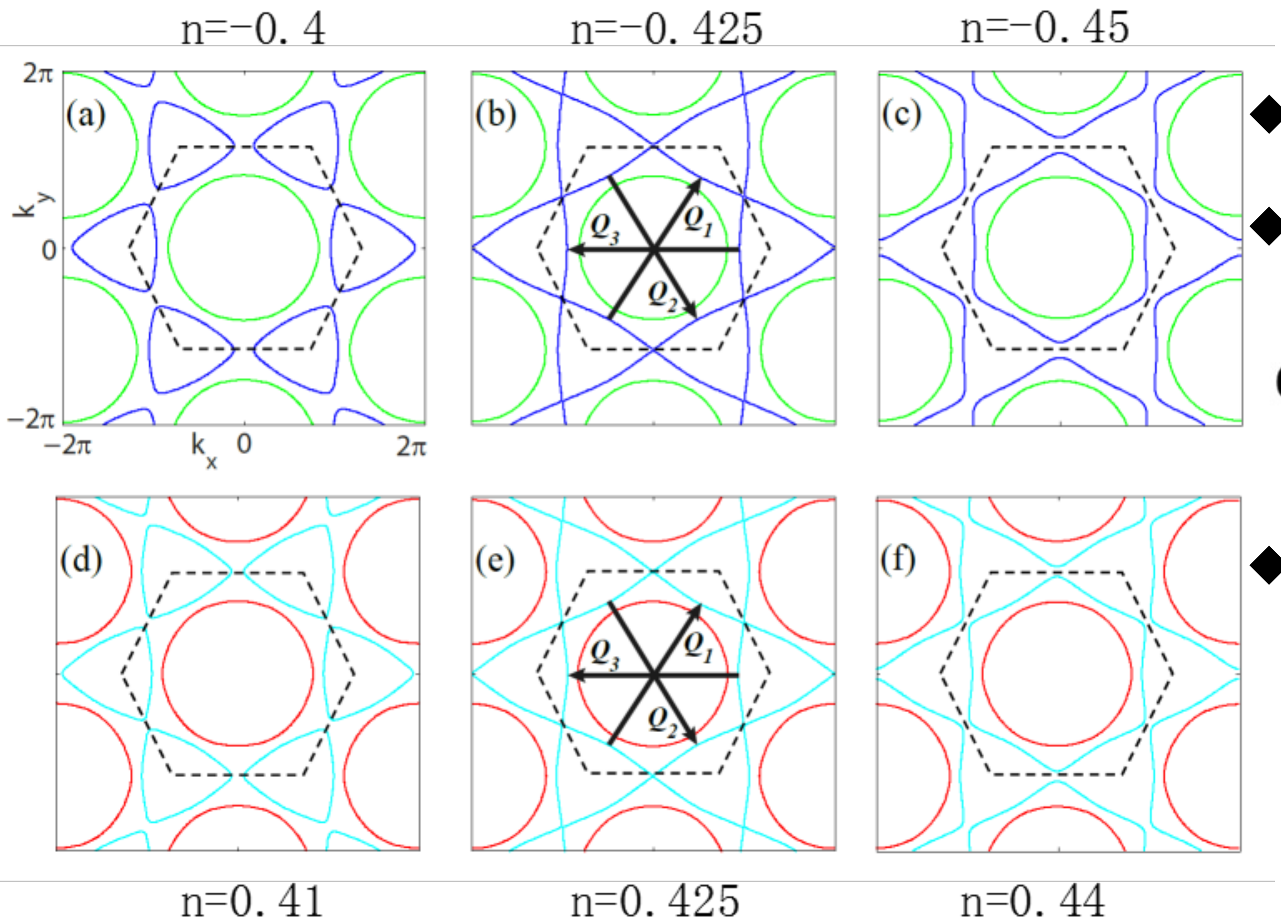
C. Wu PRL 2008
G.-F. Zhang et al. PRB 2014
CCL et al. PRB 2014
F. Yang, et al. PRB 2015

CCL-Zhang-Chen-Yang, PRL 121, 217001 (2018)

Fermi surface

- Evolution of the FS with doping:

VHS and FS-nesting are found!



- Lifshitz transition at δ_V
- VHS at three M points with Good FS nesting

$\mathbf{Q}_i$ –the nesting vectors.

- FS nesting is asymmetric, FS nesting with higher doping is much better than the one with lower doping

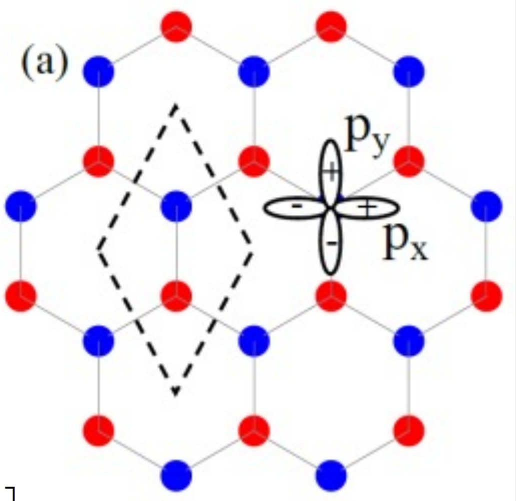
Full model and approach

- The $p_{x,\bar{y}}$ orbital Honeycomb lattice Hubbard-model

$$H = H_{tb} + H_{int}$$

$$H_{tb} = \sum_{i\mu,j\nu,\sigma} t_{i\mu,j\nu} c^{\dagger}_{i\mu\sigma} c_{j\nu\sigma} - \mu_c \sum_{i\mu\sigma} c^{\dagger}_{i\mu\sigma} c_{i\mu\sigma}.$$

$$H_{int} = U \sum_{i\mu} n_{i\mu\uparrow} n_{i\mu\downarrow} + V \sum_{i} n_{ix} n_{iy} + J_H \sum_{i} \Big[\sum_{\sigma\sigma'} c^{\dagger}_{ix\sigma} c^{\dagger}_{iy\sigma'} c_{ix\sigma'} c_{iy\sigma} + (c^{\dagger}_{ix\uparrow} c^{\dagger}_{ix\downarrow} c_{iy\downarrow} c_{iy\uparrow} + h.c.) \Big]$$



- The weak-coupling multi-orbital RPA approach

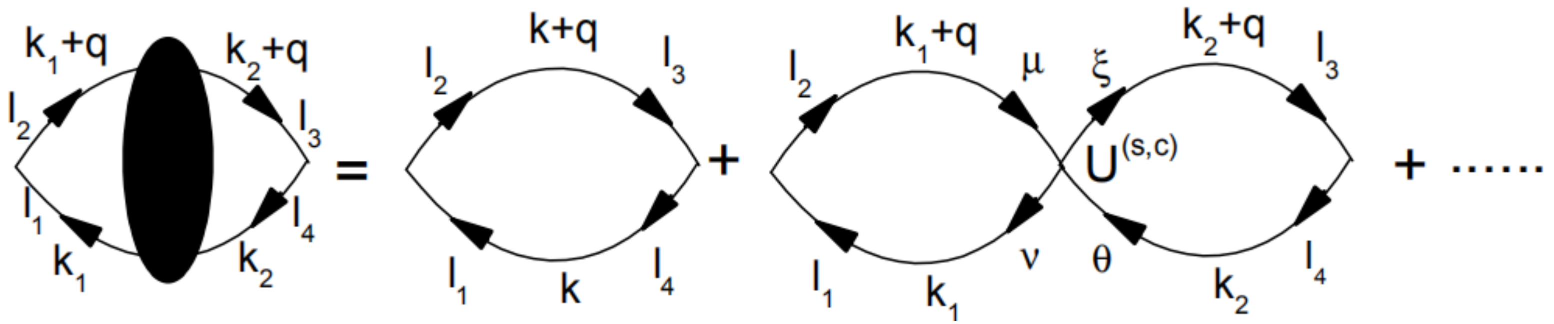
CCL-Zhang-Chen-Yang, PRL 121, 217001 (2018)

The multi-orbital RPA approach

- The bare and renormalized susceptibility

$$\chi^{(0)l_1,l_2}_{l_3,l_4}(\boldsymbol{q},\tau) \equiv \frac{1}{N}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\left\langle T_\tau c^\dagger_{l_1}(\boldsymbol{k}_1,\tau)c_{l_2}(\boldsymbol{k}_1+\boldsymbol{q},\tau)c^\dagger_{l_3}(\boldsymbol{k}_2+\boldsymbol{q},0)c_{l_4}(\boldsymbol{k}_2,0)\right\rangle_0,$$

$$= \frac{1}{N}\sum_{\boldsymbol{k},\alpha,\beta}\xi^{\alpha}_{l_4}(\boldsymbol{k})\xi^{\alpha,*}_{l_1}(\boldsymbol{k})\xi^{\beta}_{l_2}(\boldsymbol{k}+\boldsymbol{q})\xi^{\beta,*}_{l_3}(\boldsymbol{k}+\boldsymbol{q})\frac{n_F(\varepsilon^{\beta}_{\boldsymbol{k}+\boldsymbol{q}})-n_F(\varepsilon^{\alpha}_{\boldsymbol{k}})}{i\omega_n+\varepsilon^{\alpha}_{\boldsymbol{k}}-\varepsilon^{\beta}_{\boldsymbol{k}+\boldsymbol{q}}}$$



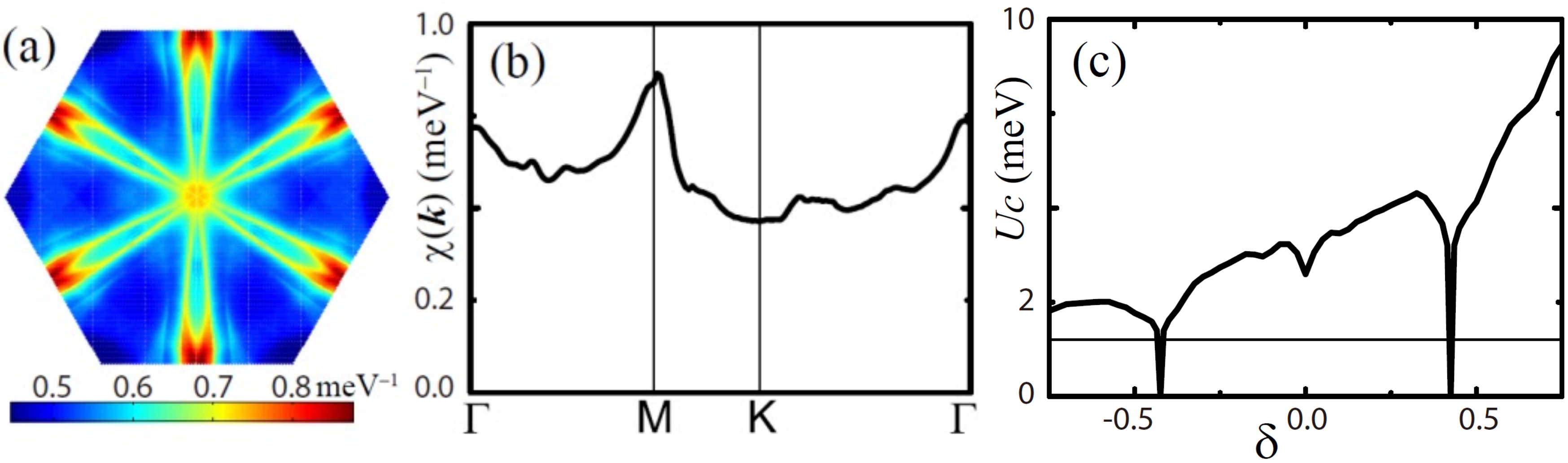
$$\chi^{(s)}(\boldsymbol{q},i\nu) = \left[I-\chi^{(0)}(\boldsymbol{q},i\nu)U^{(s)}\right]^{-1}\chi^{(0)}(\boldsymbol{q},i\nu),$$

$$\chi^{(c)}(\boldsymbol{q},i\nu) = \left[I+\chi^{(0)}(\boldsymbol{q},i\nu)U^{(c)}\right]^{-1}\chi^{(0)}(\boldsymbol{q},i\nu),$$

S. Graser et al, NJP 11, 025016 (2009)

The multi-orbital RPA and SDW instability

- Bare susceptibility at δ_V : peaks at the 3 M-points



$$\chi(\vec{q}, iw_n = 0)$$

$$U_c^{SDW}(\delta_V) = 0$$

Noncoplanar SDW

- Divergent $\chi^{(s)}\left(\vec{Q}_\alpha\right)$ requires SDW instability with

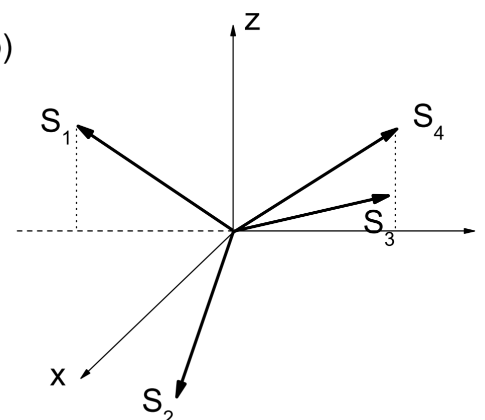
$$\left\langle \hat{\vec{s}}_i \right\rangle \propto e^{i\vec{Q}_\alpha \bullet \vec{R}_i}$$

- Now we have three nesting vectors $\vec{Q}_\alpha, (\alpha = 1,2,3)$, perfectly fitting into the three components of $s_{i\alpha}, \left(\alpha = x, y, z\right)$, so

$$\left(\left\langle \hat{s}_{ix} \right\rangle, \left\langle \hat{s}_{iy} \right\rangle, \left\langle \hat{s}_{iz} \right\rangle\right) \propto \left(e^{i\vec{Q}_1 \bullet \vec{R}_i}, e^{i\vec{Q}_2 \bullet \vec{R}_i}, e^{i\vec{Q}_3 \bullet \vec{R}_i}\right)$$

- Noncoplanar SDW with spin-chirality (4-spin)

(b)

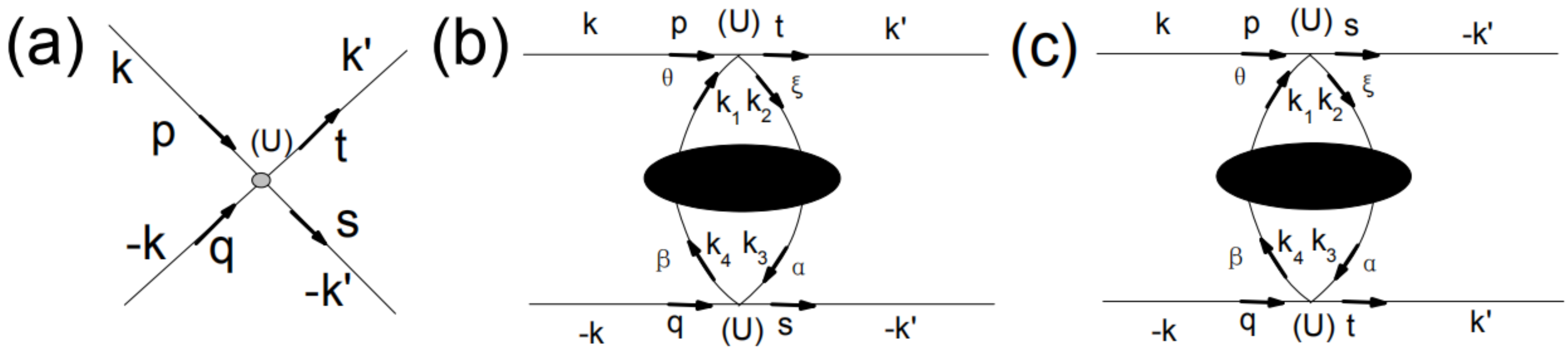


Nontrivial Chern-number in the ordered band structure
Spontaneous quantum Hall (QAH).

I. Martin et al. (2008), Tao Li (2012)

The multi-orbital RPA approach

- Effective interaction vertex generated from exchanging susceptibility



singlet
$$\Gamma^{pq(s)}_{st}(\boldsymbol{k},\boldsymbol{k}') = \left(\frac{U^{(c)}+3U^{(s)}}{4}\right)^{pt}_{qs} + \frac{1}{4}\left[3U^{(s)}\chi^{(s)}\left(\boldsymbol{k}-\boldsymbol{k}'\right)U^{(s)} - U^{(c)}\chi^{(c)}\left(\boldsymbol{k}-\boldsymbol{k}'\right)U^{(c)}\right]^{pt}_{qs} + \frac{1}{4}\left[3U^{(s)}\chi^{(s)}\left(\boldsymbol{k}+\boldsymbol{k}'\right)U^{(s)} - U^{(c)}\chi^{(c)}\left(\boldsymbol{k}+\boldsymbol{k}'\right)U^{(c)}\right]^{ps}_{qt},$$

triplet
$$\Gamma^{pq(t)}_{st}(\boldsymbol{k},\boldsymbol{k}') = \left(\frac{U^{(c)}-U^{(s)}}{4}\right)^{pt}_{qs} - \frac{1}{4}\left[U^{(s)}\chi^{(s)}\left(\boldsymbol{k}-\boldsymbol{k}'\right)U^{(s)} + U^{(c)}\chi^{(c)}\left(\boldsymbol{k}-\boldsymbol{k}'\right)U^{(c)}\right]^{pt}_{qs} + \frac{1}{4}\left[U^{(s)}\chi^{(s)}\left(\boldsymbol{k}+\boldsymbol{k}'\right)U^{(s)} + U^{(c)}\chi^{(c)}\left(\boldsymbol{k}+\boldsymbol{k}'\right)U^{(c)}\right]^{ps}_{qt},$$

The multi-orbital RPA approach

- The linearized gap equation and classification of symmetry

$$V_{eff} = \frac{1}{N}\sum_{\alpha\beta,\boldsymbol{k}\boldsymbol{k}'} V^{\alpha\beta}(\boldsymbol{k},\boldsymbol{k}')c^{\dagger}_{\alpha}(\boldsymbol{k})c^{\dagger}_{\alpha}(-\boldsymbol{k})c_{\beta}(-\boldsymbol{k}')c_{\beta}(\boldsymbol{k}'),$$

$$V^{\alpha\beta}(\boldsymbol{k},\boldsymbol{k}') = \sum_{pqst,\boldsymbol{k}\boldsymbol{k}'} \Gamma^{pq}_{st}(\boldsymbol{k},\boldsymbol{k}',0)\xi^{\alpha,*}_{p}(\boldsymbol{k})\xi^{\alpha,*}_{q}(-\boldsymbol{k})\xi^{\beta}_{s}(-\boldsymbol{k}')\xi^{\beta}_{t}(\boldsymbol{k}').$$

$$-\frac{1}{(2\pi)^2}\sum_{\beta}\oint_{FS} dk'_{\parallel}\frac{V^{\alpha\beta}(\boldsymbol{k},\boldsymbol{k}')}{v^{\beta}_{F}(\boldsymbol{k}')}\Delta_{\beta}(\boldsymbol{k}') = \lambda\Delta_{\alpha}(\boldsymbol{k})$$

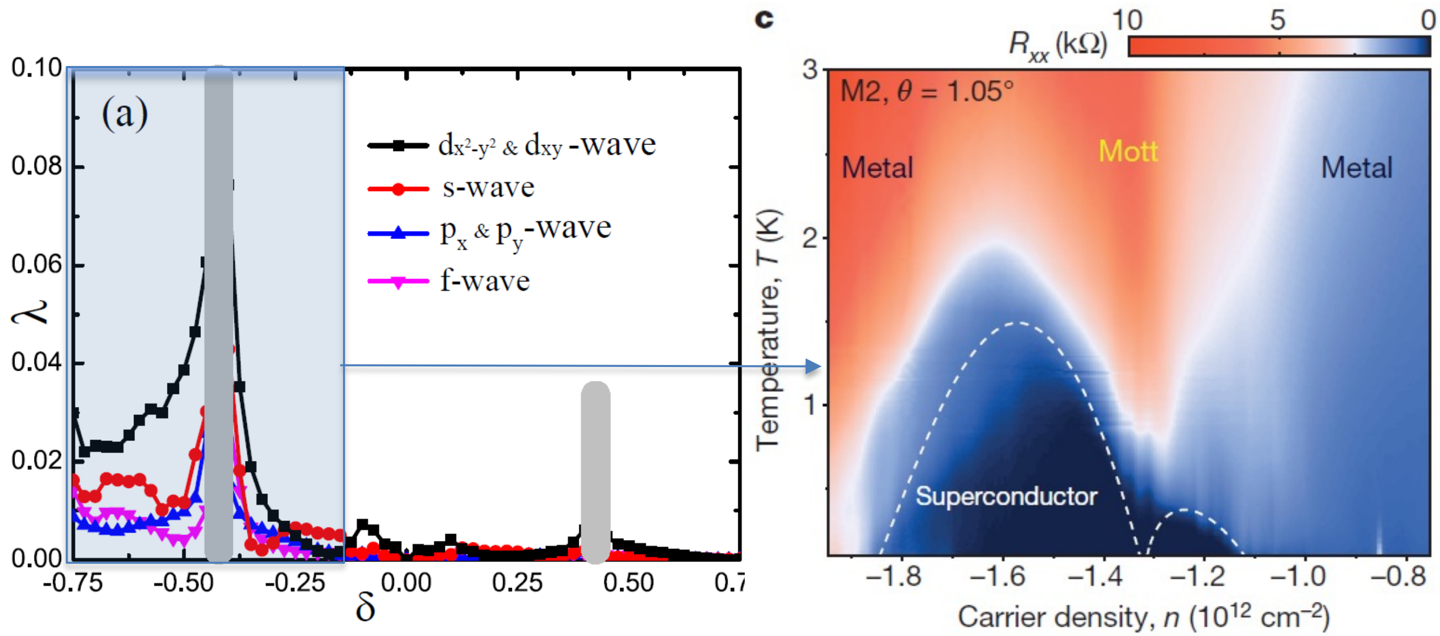
TABLE II. Character table for point group D_3 and possible superconductivity pairing symmetry.

D_3	E	$2C_3(z)$	$3C_2'$	odd funcitons	even funcutons
A_1	$+1$	$+1$	$+1$	$x(x^2-3y^2)$ f-wave	(x^2+y^2) s-wave
A_2	$+1$	$+1$	-1	$y(3x^2-y^2)$ f'-wave	—
E	$+2$	-1	0	(x,y) p-wave	(x^2-y^2,xy) d-wave

d+id superconductivity

- The phase-diagram: calculation & experiment

Through exchanging short-ranged spin fluctuations between a Cooper pair.



$$T_c \propto e^{-1/\lambda}$$

our results

experiment

CCL-Zhang-Chen-Yang, PRL 121, 217001 (2018)

Y. Cao2 et al Nature 2018.

Summary

- The correlated-insulator found is noncoplanar chiral SDW, spontaneous QH (QAH), driven by FS-nesting , so easily killed by magnetic field (8T)
- The pairing symmetry is gapped d+id SC driven by the antiferromagnetic spin-fluctuations
- The SC is d+id topological SC.

Outline

- Introduction
- Interaction-driven conventional topological superconductivity in magic angle twisted bilayer graphene
- Proximity effect induced higher-order topological superconductors

Proximity effect induced higher-order topological superconductors

1. High-Temperature Majorana Corner States,
Wang-**CCL**-Lu-Zhang, PRL 121, 186801 (2018).

2. High-temperature Majorana corner modes in a d+id‘ superconductor heterostructure: Application to twisted bilayer cuprate superconductors,
Li-**CCL**, PRB 107, 235125 (2023).

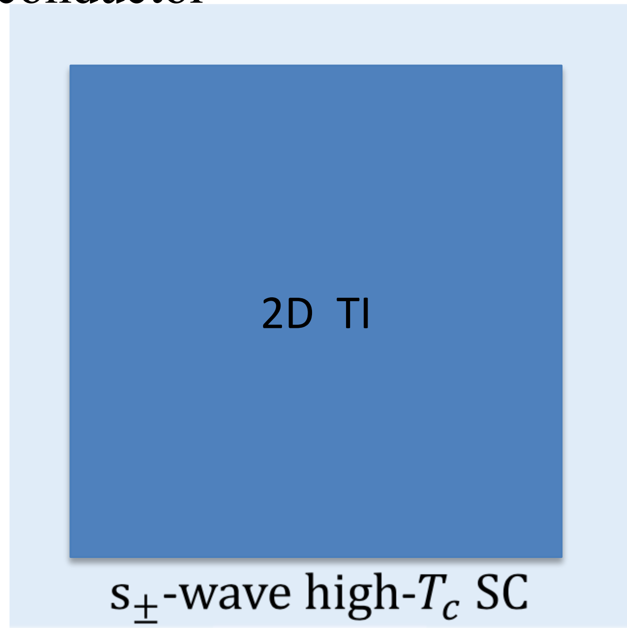
Model

a 2D TI proximitized by a Fe-based s+- wave superconductor

$$\mathcal{H}_{\boldsymbol{k}}^{\mathrm{BdG}} = (h_{\boldsymbol{k}}^{\mathrm{TI}} - \mu)\tau_z + \Delta_{\boldsymbol{k}}\tau_x,$$

$$h_{\boldsymbol{k}}^{\mathrm{TI}} = [2t(\cos k_x - \cos k_y) + 4t_1 \cos k_x \cos k_y]\sigma_z + 2\lambda(\sin k_x s_y - \sin k_y s_x)\sigma_x,$$

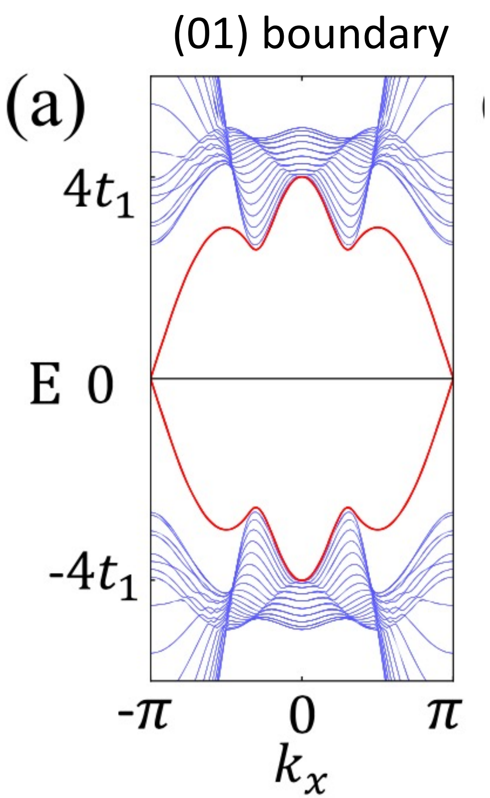
$$\Delta_{\boldsymbol{k}} = \Delta_0 + 2\Delta_1(\cos k_x + \cos k_y),$$



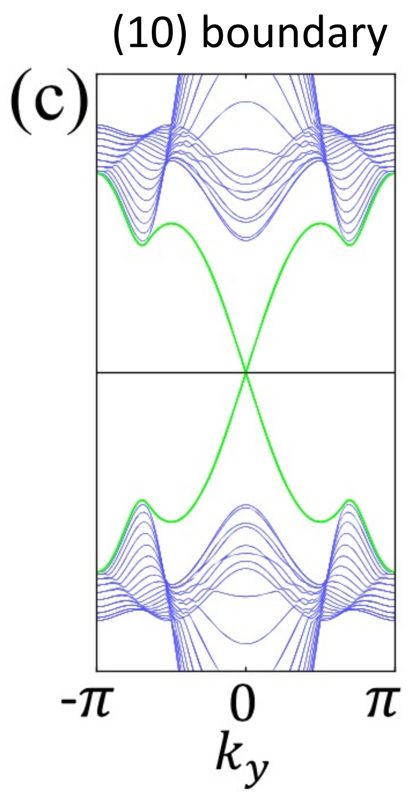
Wang-**CCL**-Lu-Zhang, PRL 121, 186801 (2018)

Gapless helical edge states of the 2D TI

$$h_{\boldsymbol{k}}^{\mathrm{TI}} = [2t(\cos k_x - \cos k_y) + 4t_1 \cos k_x \cos k_y]\sigma_z$$
$$+ 2\lambda(\sin k_x s_y - \sin k_y s_x)\sigma_x,$$



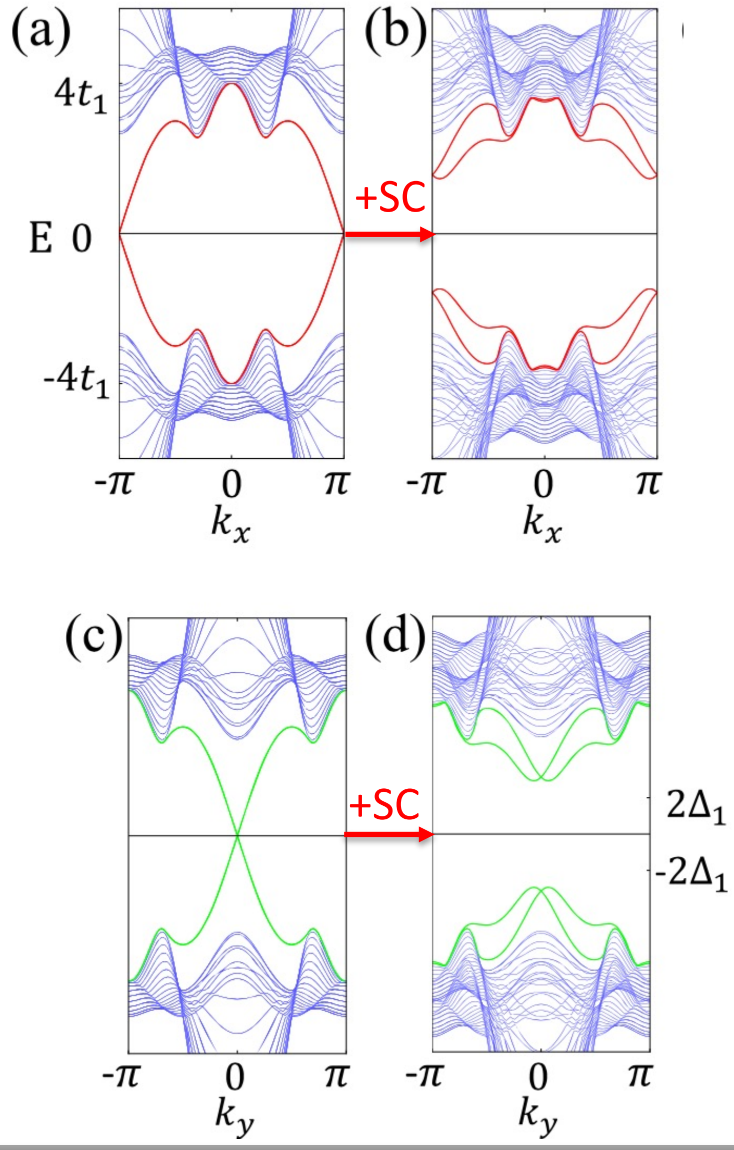
The cone is at kx=0

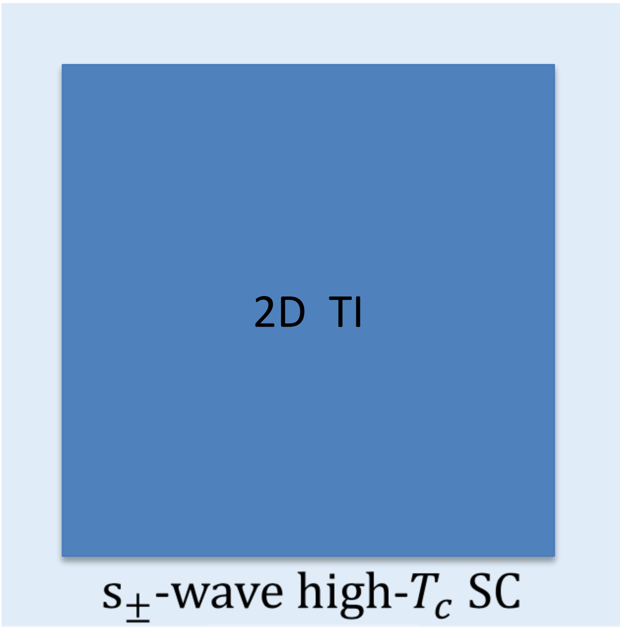


The cone is at ky=π

The Gapless helical edge states protected by TRS and U(1)

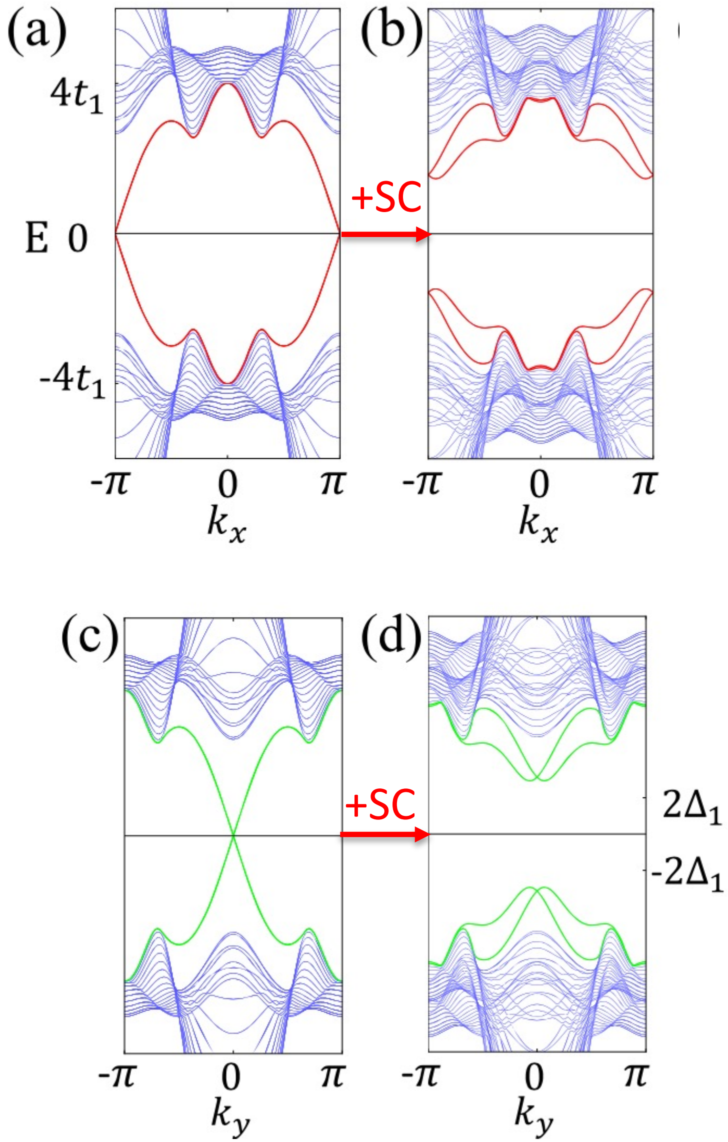
Gap the gapless helical edges by SC

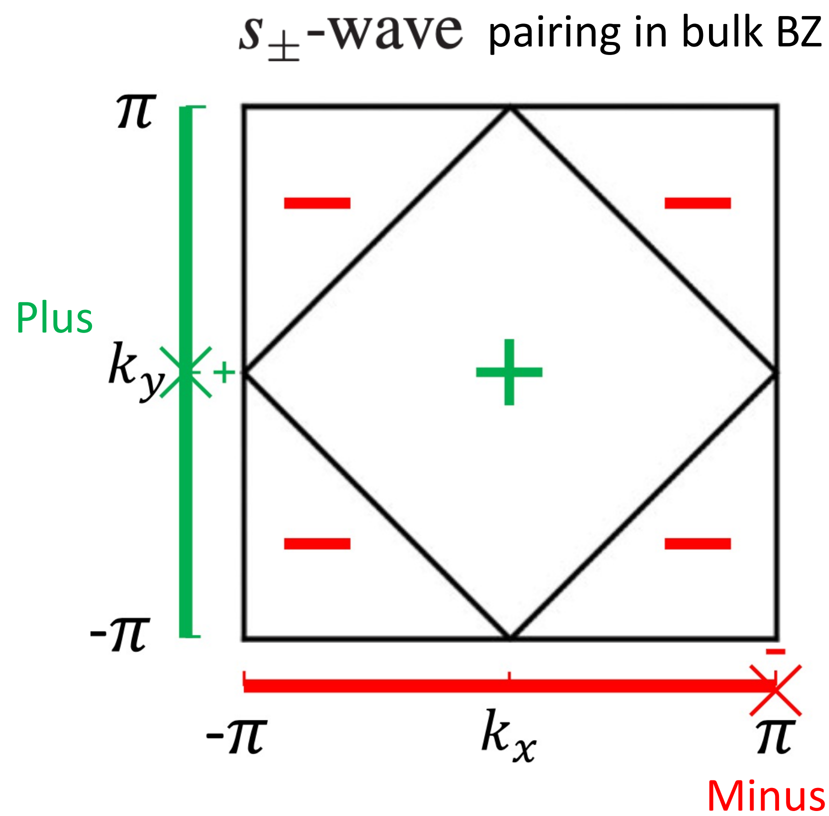




The SC pairing term gaps the helical states can be considered as mass term.

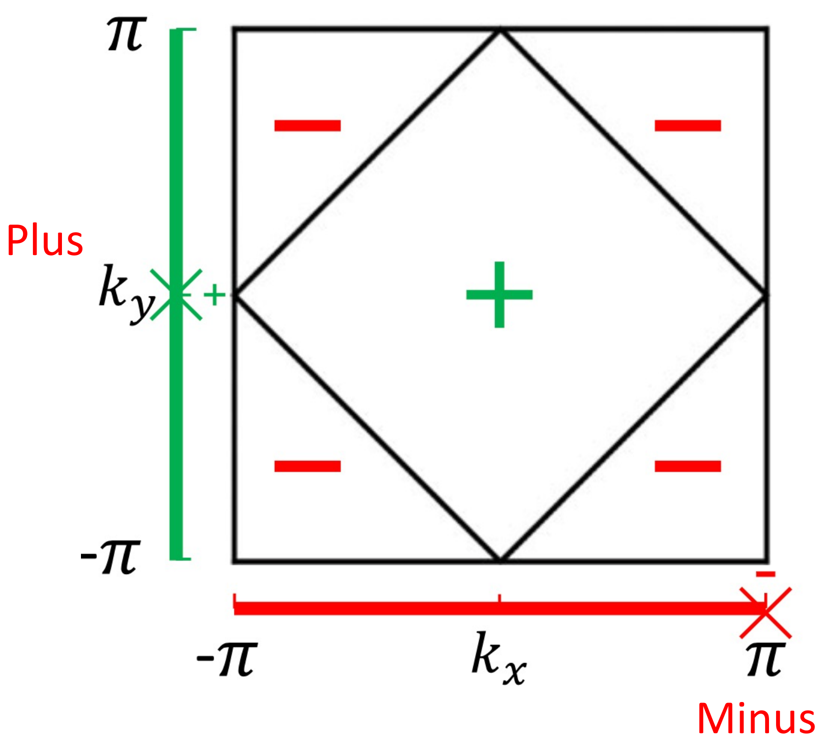
Mass domain wall

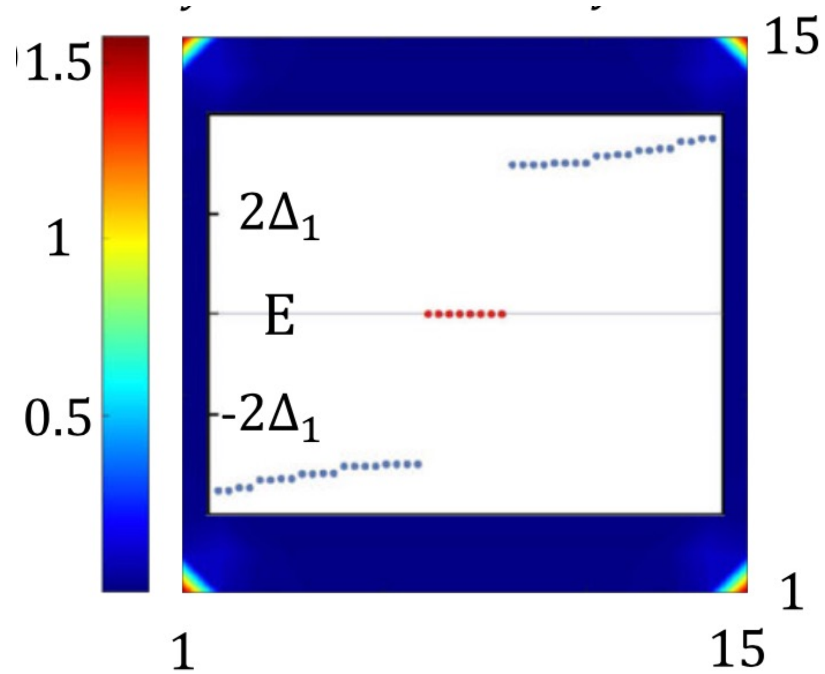




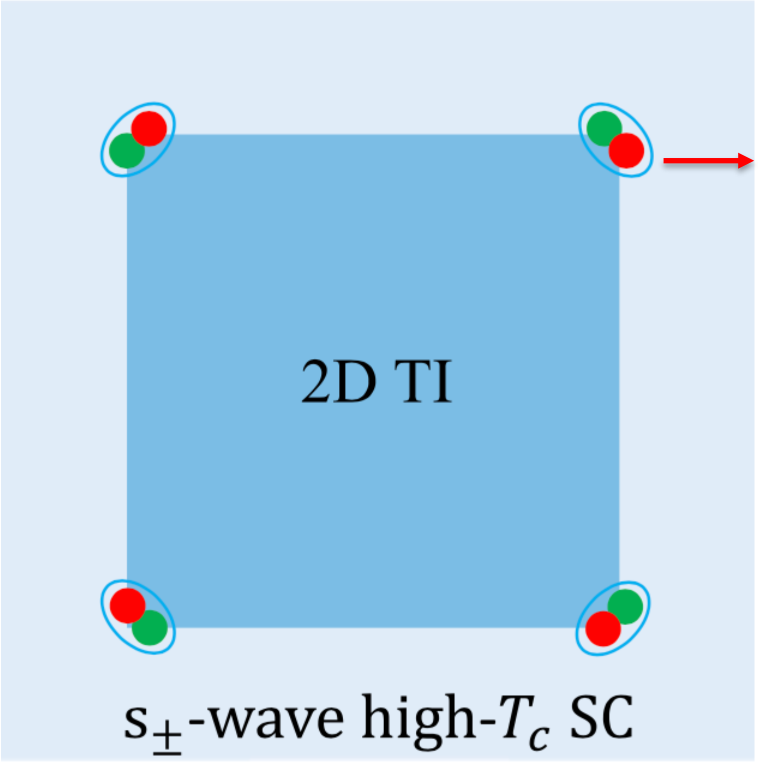
Wang-**CCL**-Lu-Zhang, PRL 121, 186801 (2018)

Mass domain wall => Majorana corner states





Higher-order topological superconductors

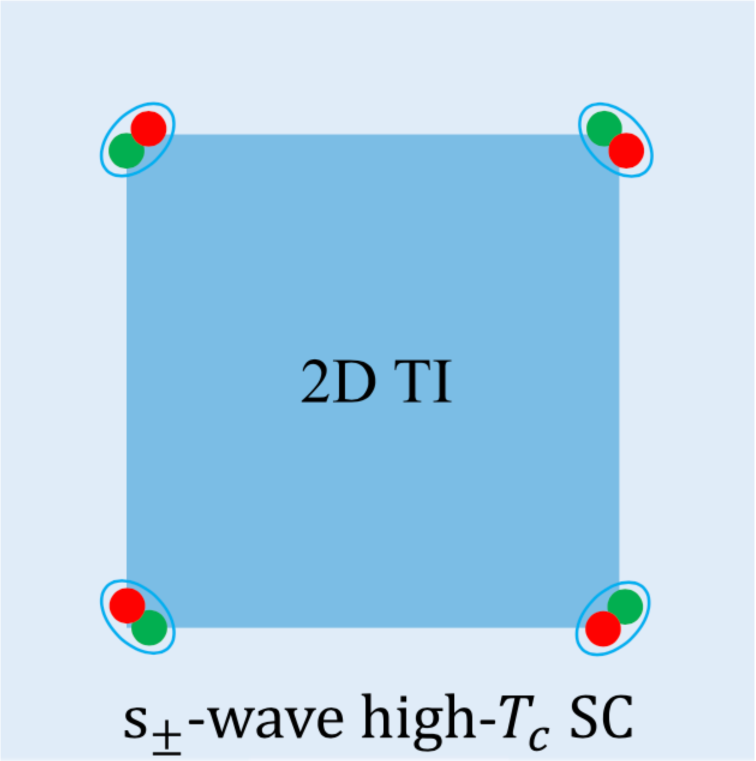


One Majorana Kramers pair at each corner.

A candidate material for experimental realizations

A tunable 2D TI PbS with independently controllable band inversions at X or Y
+
an iron pnictide with s+- SC pairing.

The monolayer PbS has a square lattice constant of 4.03 Å , comparable to 3.95–4.05 Å of iron pnictides.

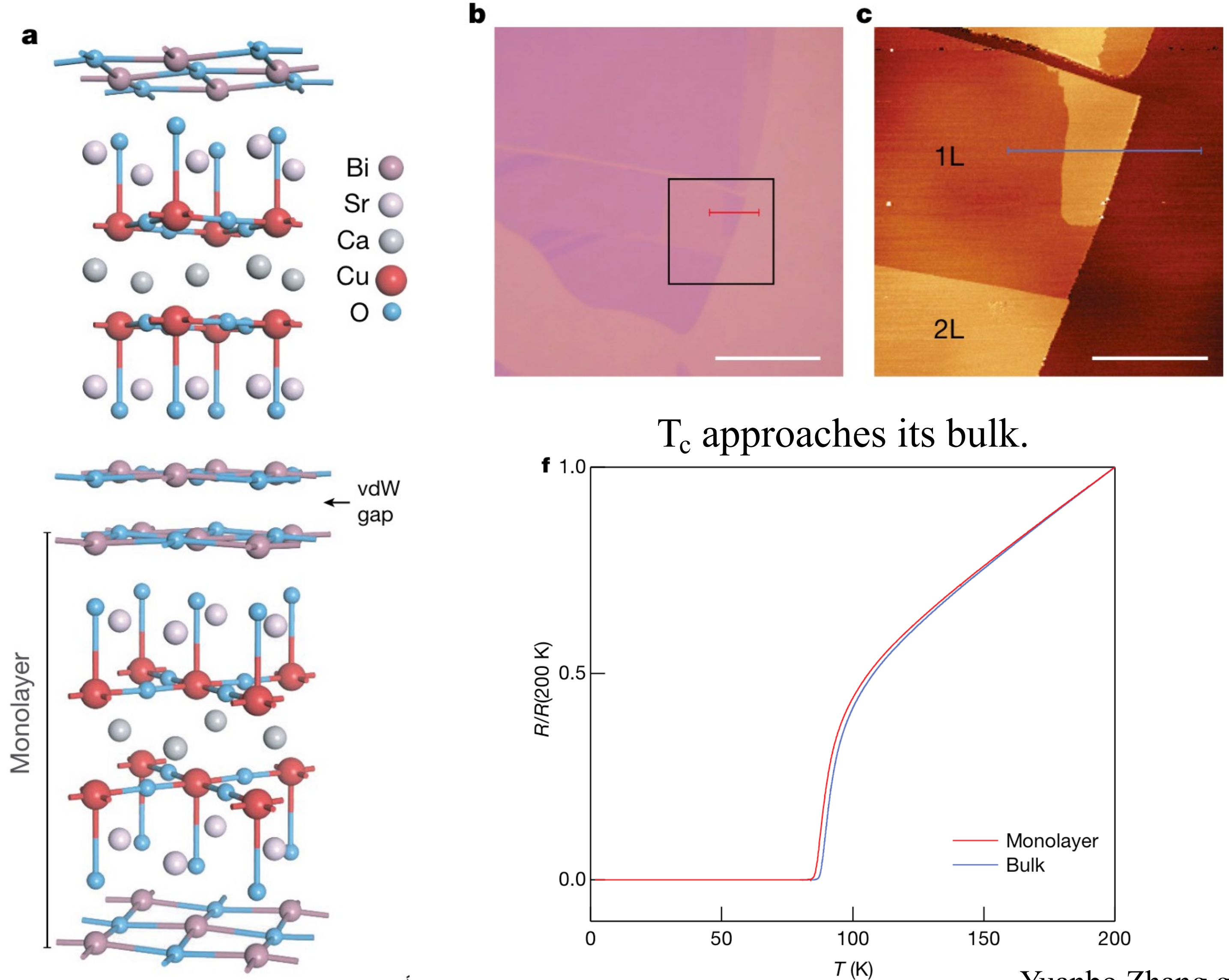


Proximity effect induced higher-order topological superconductors

1. High-Temperature Majorana Corner States,
Wang-**CCL**-Lu-Zhang, PRL 121, 186801 (2018).

2. High-temperature Majorana corner modes in a d+id’ superconductor heterostructure: Application to twisted bilayer cuprate superconductors,
Li-**CCL**, PRB 107, 235125 (2023).

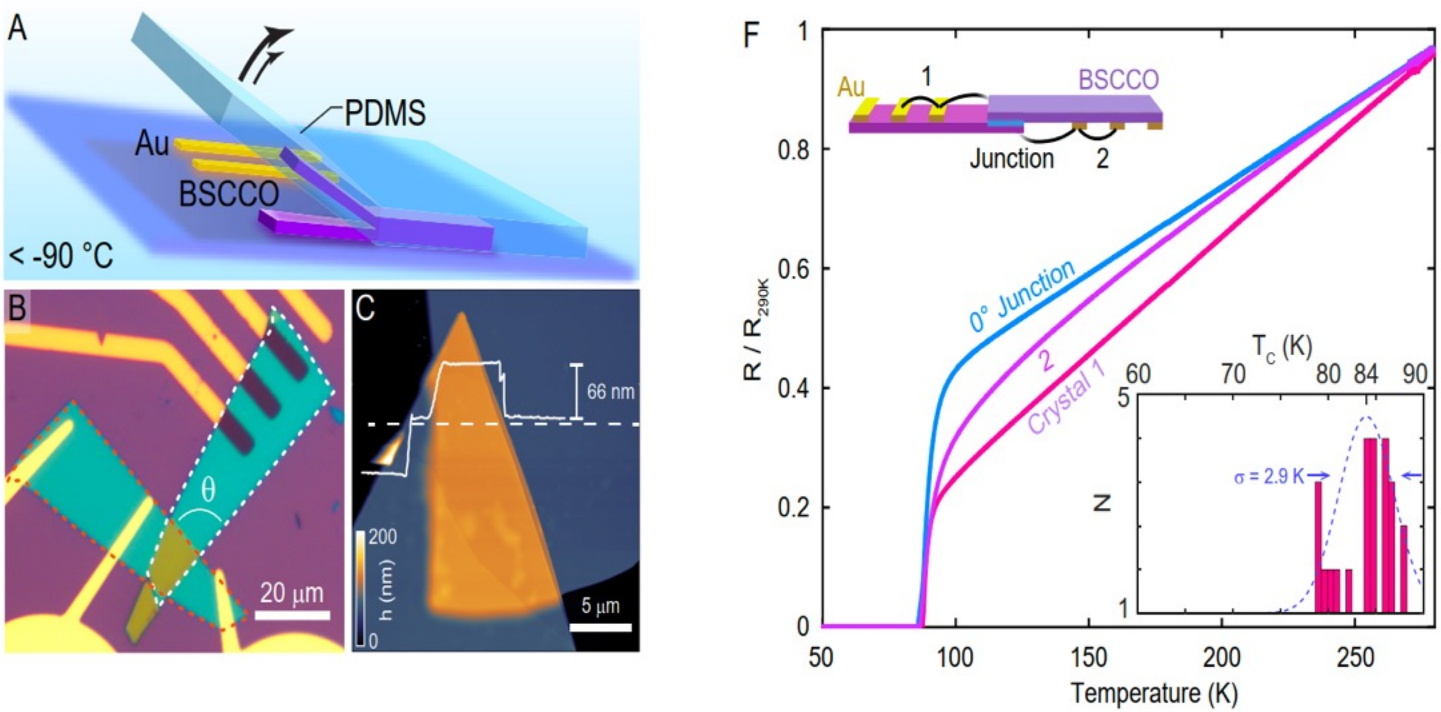
Monolayer Cu-based superconductor



T_c approaches its bulk.

Yuanbo Zhang group, Nature (2019)

Twisted bilayer cuprate

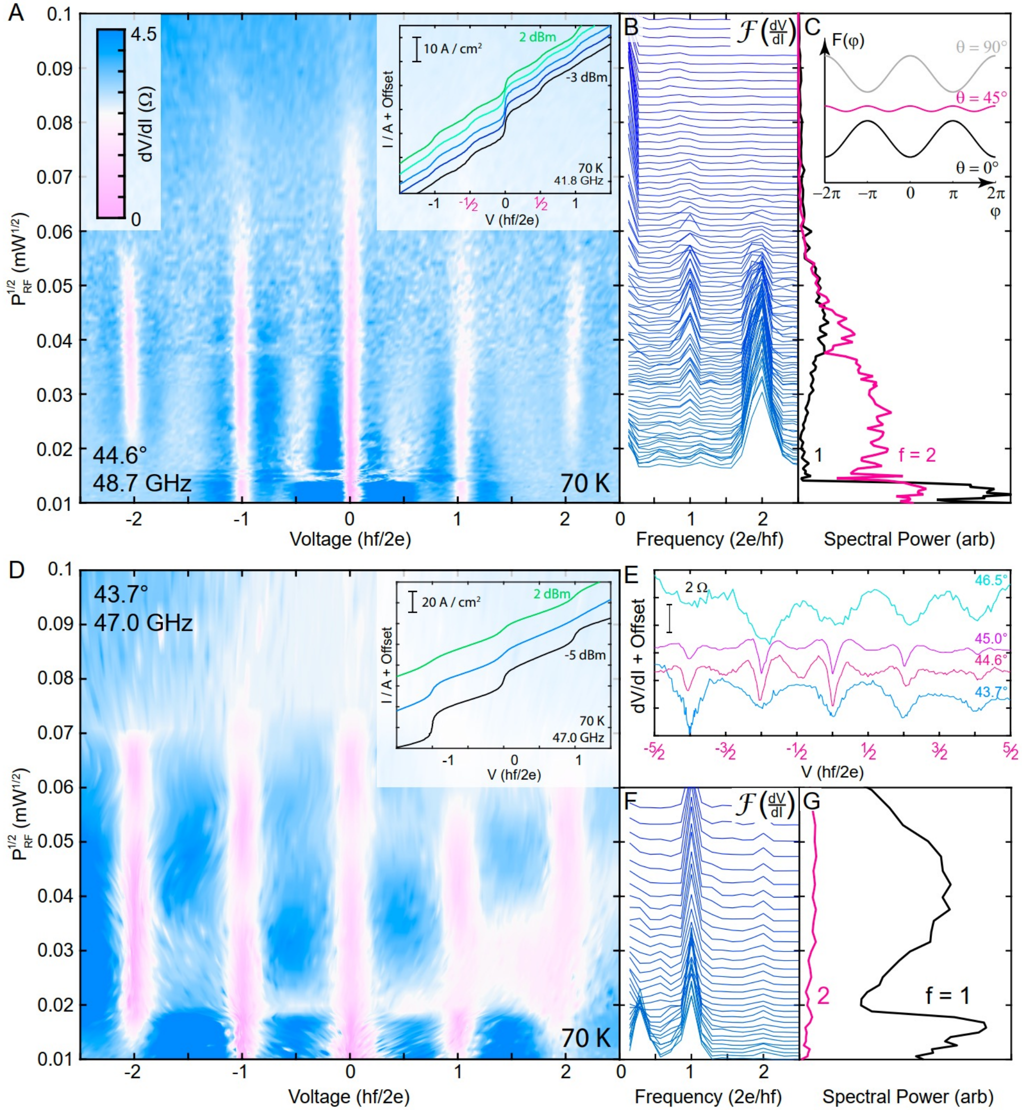


- They fabricated 24 devices with different twist angle θ between 0◦ to 180◦ with $T_C \geq 79$ K, and average T_C of 84 K

- Normalizing to junction area, they obtain a critical current density $J_C \approx$ 1.2 kA/cm2 for this junction, similar to J_C of intrinsic junctions

Kim Philip Group, arxiv:2108.13455

Twisted bilayer cuprate with cotunneling of Cooper pairs

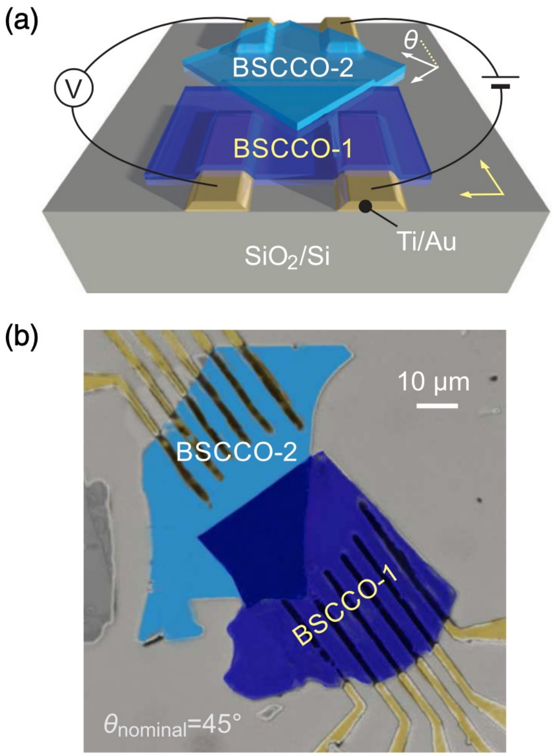


$$I(t) = I_0 \sin(\omega_0 t + \gamma_0) \quad (\omega_0 = 2eV_0/\hbar)$$

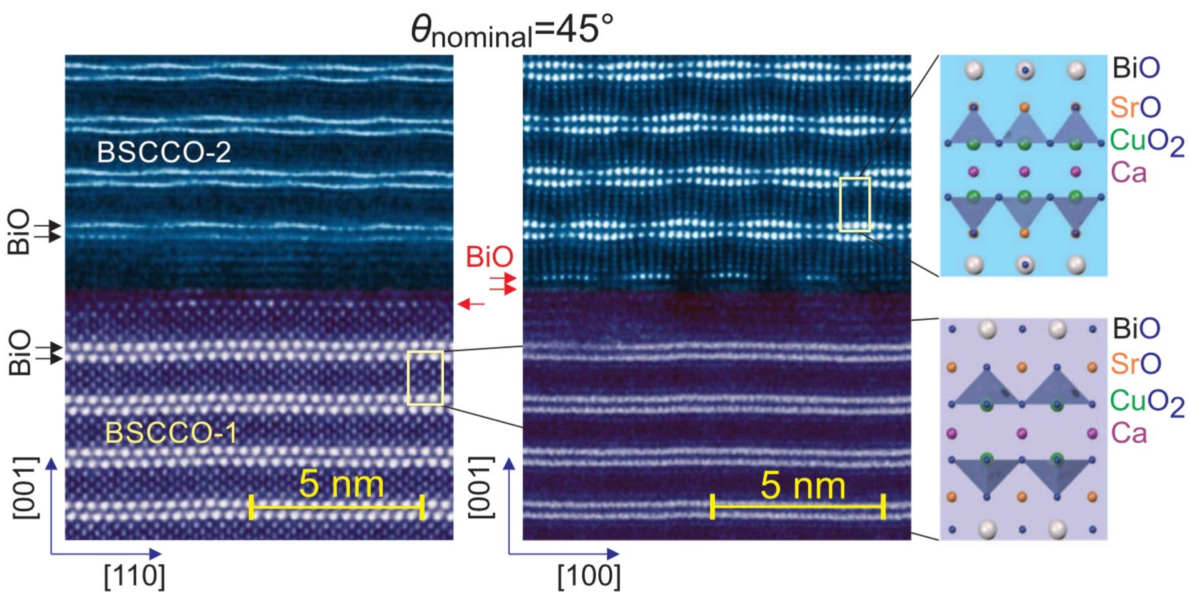
The corresponding dV/dI shows dips of similar strength at half integer and integer steps, indicating that the cotunneling of Cooper pairs dominates over the conventional Josephson coupling close to 45∘

Kim Philip Group, arxiv:2108.13455

Twisted ultrathin cuprates with atomically flat junction interfaces

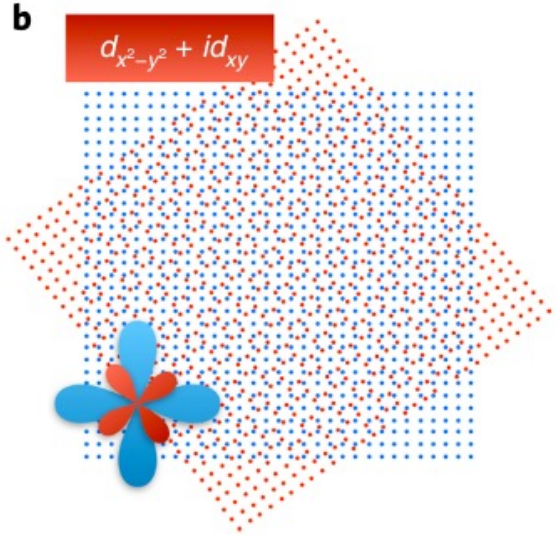


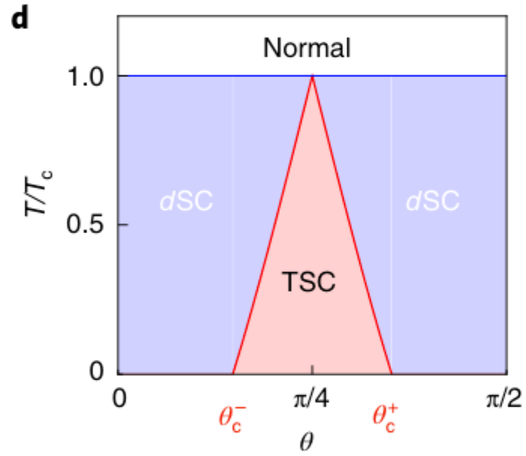
Atomically resolved TEM images of sections

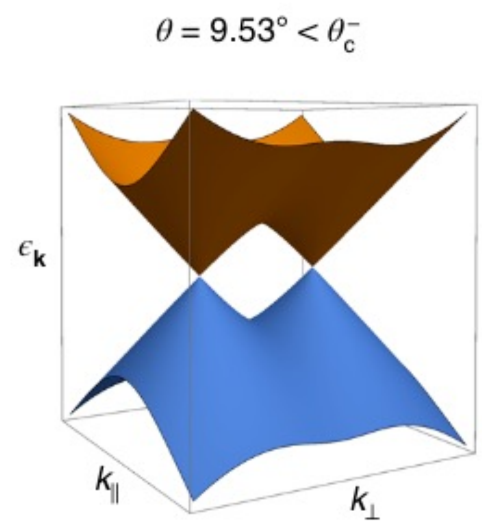


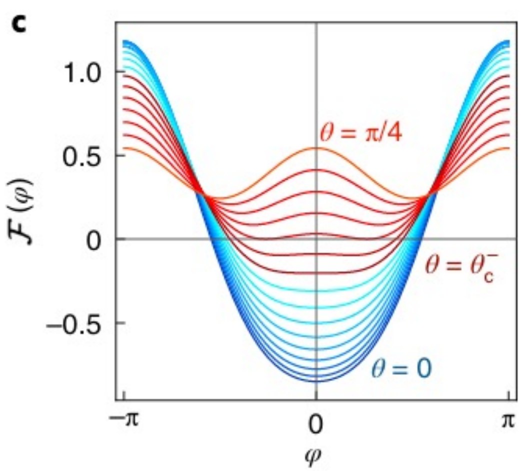
Zhang & Xue Group, PRX 11, 031011 (2021)

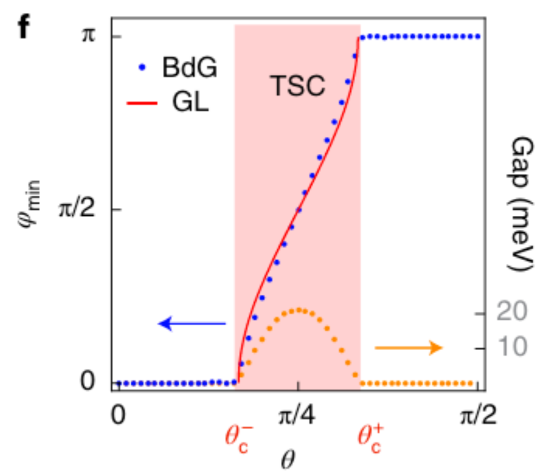
Twisted bilayer cuprate predicted to be a d+id TSC

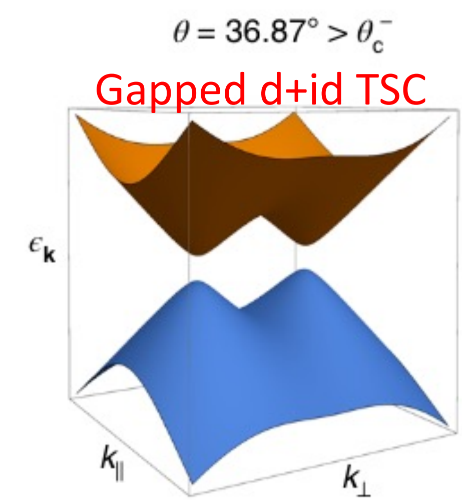










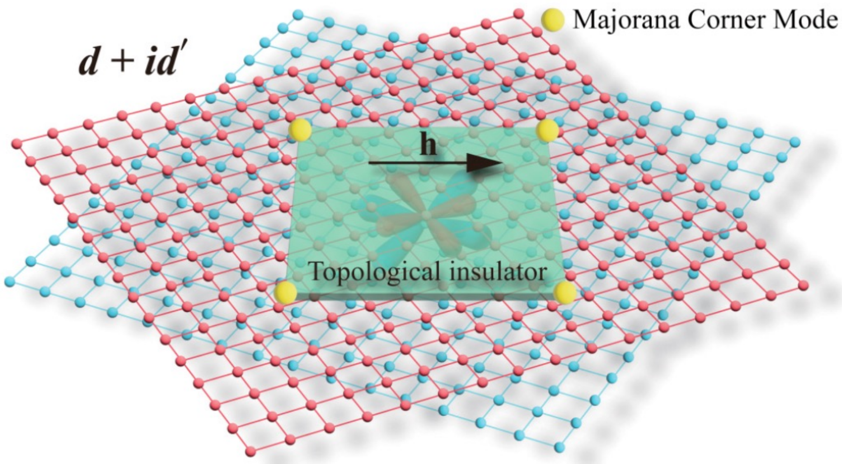


Franz Marcel group, NP(2021)
Yang et al, PRB (2018)

Motivation

- Recently, some schemes for realizing HOTSC with MCMs have been proposed, in which the key component is the utilization of various superconductors, such as unconventional d-wave, s±, as well as p-wave superconductors, and conventional s-wave superconductors. However, the bulk nodes in unconventional superconductors and the low Tc of s-wave superconductors hinder the experimental detection of zero-energy MCMs.

High T_c gapped SC platform to realize MCMs

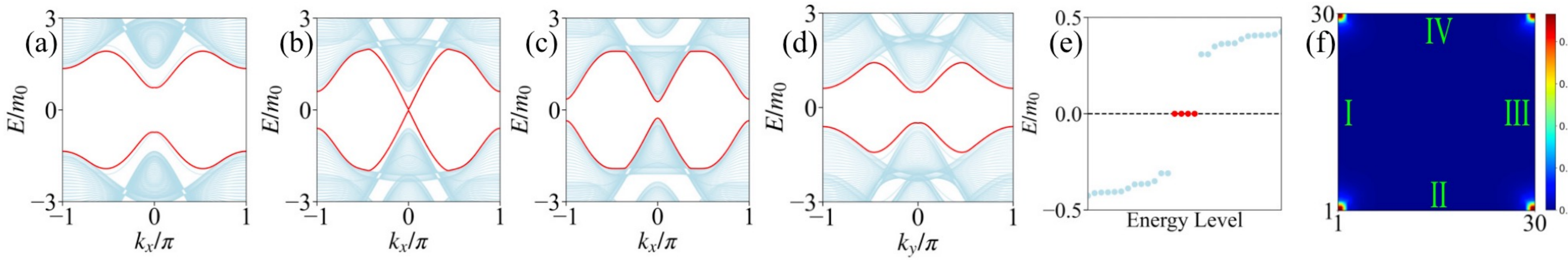


$$H^{\mathrm{BdG}}(\mathbf{k}) = \begin{pmatrix} H(\mathbf{k}) & \Delta(\mathbf{k}) \\ -\Delta^*(-\mathbf{k}) & -H^*(-\mathbf{k}) \end{pmatrix}.$$

$$H(\mathbf{k}) = (m_0 - t_x \cos k_x - t_y \cos k_y)\sigma_z + (\lambda_x \sin k_x s_y + \lambda_y \sin k_y s_x)\sigma_x + \mathbf{h}\cdot\mathbf{s} - \mu,$$

$$\Delta(\mathbf{k}) = [\Delta_1(\cos k_x - \cos k_y) + i\Delta_2 \sin k_x \sin k_y](-is_y).$$

- $h_y = h_z = 0,\ h_x$ changes: topo. phase transition along edge

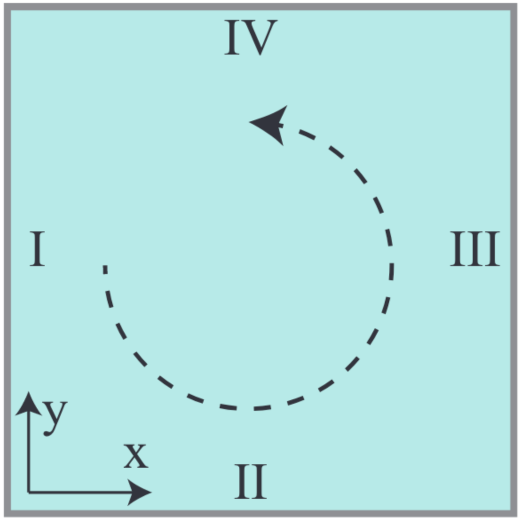


Li-**CCL**, PRB 107, 235125 (2023)

Edge theory

$$H^{\mathrm{BdG}}(\mathbf{k}) = \begin{pmatrix} H(\mathbf{k}) & \Delta(\mathbf{k}) \\ -\Delta^*(-\mathbf{k}) & -H^*(-\mathbf{k}) \end{pmatrix}.$$

Expanding Hamiltonian around k=(0,0) to second order



$$H_{\mathrm{eff}}(\mathbf{k}) = \left(m + \frac{t_x}{2}k_x^2 + \frac{t_y}{2}k_y^2\right)\sigma_z\tau_z + \lambda_x k_x \sigma_x s_y \tau_z$$
$$+ \lambda_y k_y \sigma_x s_x - \frac{\Delta_1}{2}(k_x^2 - k_y^2) s_y \tau_y + \Delta_2 k_x k_y s_y \tau_x$$
$$+ h_x s_x \tau_z,$$

- For the Edge I, we can replace $k_x \to -i\partial_x$

$$H_0(-i\partial_x, k_y) = (m - t_x\partial_x^2/2)\tau_z\sigma_z - i\lambda_x\tau_z s_y\sigma_x\partial_x,$$
$$H_p(-i\partial_x, k_y) = \lambda_y k_y s_x\sigma_x + \Delta_1/2\tau_y s_y\partial_x^2 - i\Delta_2 k_y\tau_x s_y\partial_x + h_x\tau_z s_x,$$

Solving $H_0\psi_\alpha(x) = E_\alpha\psi_\alpha(x)$ $\quad \boxed{\psi_\alpha(0) = \psi_\alpha(+\infty) = 0}$

One can obtain that $\psi_\alpha(x) = \mathcal{N}_x \sin(\kappa_1 x)\boxed{e^{-\kappa_2 x}}e^{ik_y y}\xi_\alpha,$ $\quad s_y\sigma_y\xi_\alpha = -\xi_\alpha$

Edge theory

The eigenvectors ξ_α satisfy $s_y\sigma_y\xi_\alpha = -\xi_\alpha$. Here we choose

$$\begin{aligned}
\xi_1 &= |\tau_z = +1\rangle \otimes |\sigma_y = +1\rangle \otimes |s_y = -1\rangle, \\
\xi_2 &= |\tau_z = +1\rangle \otimes |\sigma_y = -1\rangle \otimes |s_y = +1\rangle, \\
\xi_3 &= |\tau_z = -1\rangle \otimes |\sigma_y = +1\rangle \otimes |s_y = -1\rangle, \\
\xi_4 &= |\tau_z = -1\rangle \otimes |\sigma_y = -1\rangle \otimes |s_y = +1\rangle.
\end{aligned}$$

In this basis set, the matrix elements of H_p are

$$H_{\mathrm{I},\alpha\beta} = \int_0^\infty dx \psi_\alpha^*(x) H_p(-i\partial_x, k_y)\psi_\beta(x).$$

After some algebraic calculation, we obtain

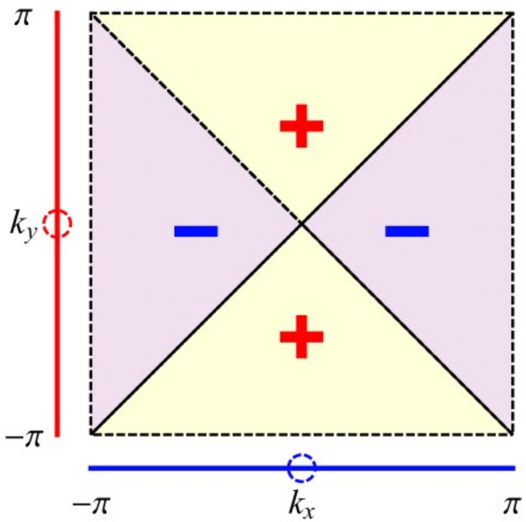
$$H_\mathrm{I} = \lambda_y k_y \eta_x - M_\mathrm{I}\tau_y\eta_z - M'_\mathrm{I} k_y \tau_x \eta_z,$$

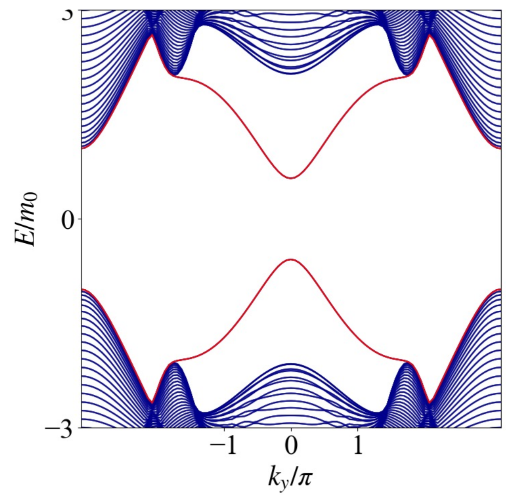
$$M_\mathrm{I} = \frac{\Delta_1}{2}\int_0^\infty dx \psi_\alpha^*(x)(\partial_x^2)\psi_\alpha(x) = -\frac{\Delta_1|m|}{t_x}, \qquad M'_\mathrm{I} = \Delta_2 \int_0^\infty dx \psi_\alpha^*(x)(\partial_x)\psi_\alpha(x) = 0.$$

$$\boxed{H_\mathrm{I} = \lambda_y k_y \eta_x - M_\mathrm{I}\tau_y\eta_z.}$$

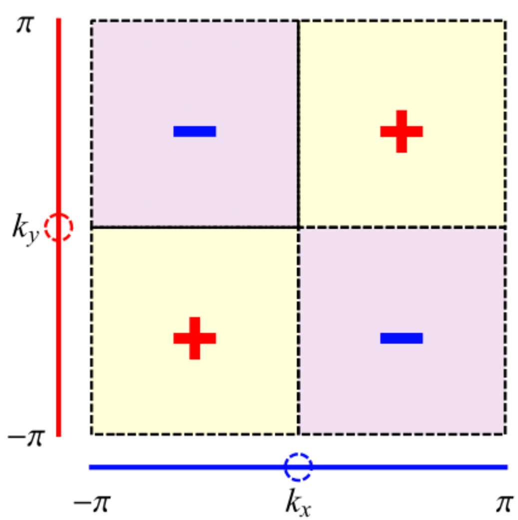
Edge theory

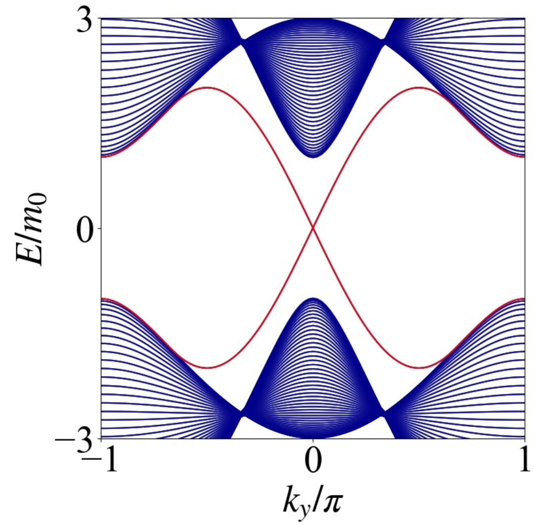
$$\Delta(\mathbf{k}) = [\Delta_1(\cos k_x - \cos k_y) + i\Delta_2 \sin k_x \sin k_y](-is_y).$$





$$M_{\mathrm{I}} = -\frac{\Delta_1|m|}{t_x},$$





$$M'_{\mathrm{I}} = 0.$$

Edge theory

- For the Edge II, we can replace $k_x \to -i\partial_x$

$$H_0(k_x,-i\partial_y) = (m - t_y\partial_y^2/2)\tau_z\sigma_z - i\lambda_y s_x\sigma_x\partial_y,$$

$$H_p(k_x,-i\partial_y) = \lambda_x k_x\tau_z s_y\sigma_x - \frac{\Delta_1}{2}\tau_y s_y\partial_y^2 - i\Delta_2 k_x\tau_x s_y\partial_y + h_x s_x\tau_z.$$

$$H_0\psi_\alpha(y) = E_\alpha\psi_\alpha(y) \quad \psi_\alpha(0) = \psi_\alpha(+\infty) = 0$$

$$\boxed{H_{\mathrm{II}}(k_x) = -\lambda_x k_x\eta_x + M_{\mathrm{II}}\tau_x\eta_z - h_x\eta_z.}$$

- For the Edge III, we can replace $k_x \to -i\partial_x$

$$H_0(-i\partial_x,k_y) = (m - t_x\partial_x^2/2)\tau_z\sigma_z - i\lambda_x\tau_z s_y\sigma_x\partial_x,$$
$$H_p(-i\partial_x,k_y) = \lambda_y k_y s_x\sigma_x + \Delta_1/2\tau_y s_y\partial_x^2 - i\Delta_2 k_y\tau_x s_y\partial_x + h_x\tau_z s_x,$$

$$H_0\psi_\alpha(x) = E_\alpha\psi_\alpha(x) \quad \psi_\alpha(0) = \psi_\alpha(-\infty) = 0$$

$$\boxed{H_{\mathrm{III}} = -\lambda_y k_y\eta_x - M_{\mathrm{III}}\tau_y\eta_z,}$$

Edge theory

- For the Edge II, we can replace $k_x \to -i\partial_x$

$$H_0(k_x, -i\partial_y) = (m - t_y\partial_y^2/2)\tau_z\sigma_z - i\lambda_y s_x\sigma_x\partial_y,$$

$$H_p(k_x, -i\partial_y) = \lambda_x k_x\tau_z s_y\sigma_x - \frac{\Delta_1}{2}\tau_y s_y\partial_y^2 - i\Delta_2 k_x\tau_x s_y\partial_y + h_x s_x\tau_z.$$

$$H_0\psi_\alpha(y) = E_\alpha\psi_\alpha(y) \qquad \psi_\alpha(0) = \psi_\alpha(-\infty) = 0$$

$$\boxed{H_{\mathrm{IV}}(k_x) = \lambda_x k_x\eta_x + M_{\mathrm{IV}}\tau_x\eta_z - h_x\eta_z,}$$

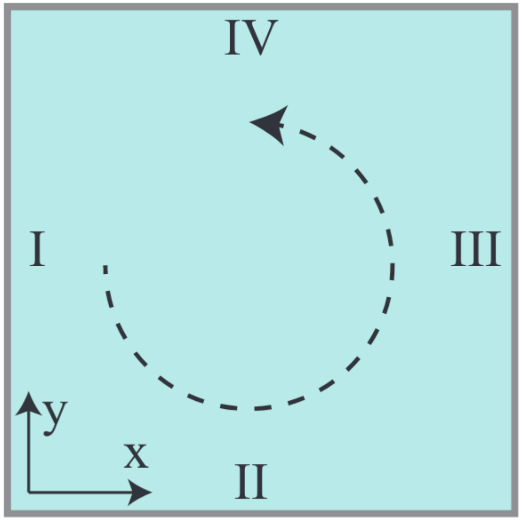
- Applying the unitary transformation for Edge II and Edge IV

$$U = e^{i\frac{\pi}{4}\tau_z} \otimes \mathbf{I}_{2\times 2},$$

- Edge effective Hamiltonian

$$\begin{aligned}
H_{\mathrm{I}}(k_y) &= \lambda_y k_y\eta_x - M_{\mathrm{I}}\tau_y\eta_z,\\
H_{\mathrm{II}}(k_x) &= -\lambda_x k_x\eta_x - M_{\mathrm{II}}\tau_y\eta_z - h_x\eta_z,\\
H_{\mathrm{III}}(k_y) &= -\lambda_y k_y\eta_x - M_{\mathrm{III}}\tau_y\eta_z,\\
H_{\mathrm{IV}}(k_x) &= \lambda_x k_x\eta_x - M_{\mathrm{IV}}\tau_y\eta_z - h_x\eta_z,
\end{aligned}$$

Edge theory



$$H_{\text{edge},l} = i\lambda(l)\eta_x\partial_l - M(l)\tau_y\eta_z - h(l)\eta_z,$$

For $\tau_y = -1$ we obtain

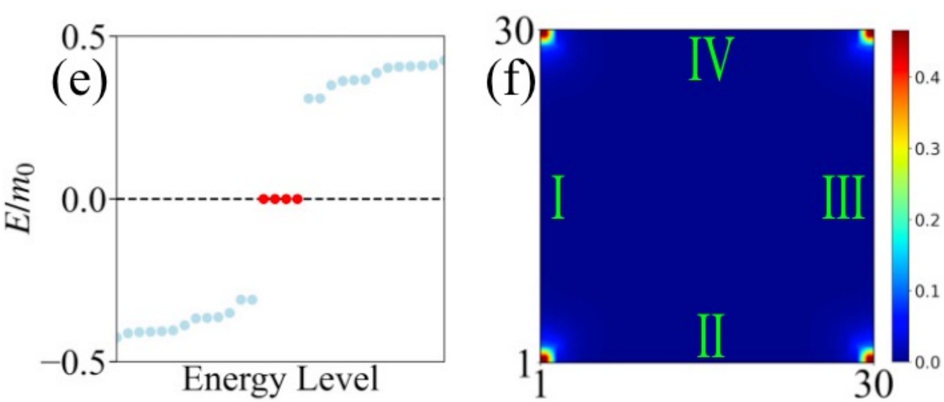
$$H^{-}_{\text{edge},l} = i\lambda(l)\eta_x\partial_l + \tilde{\tilde{M}}(l)\eta_z,$$

For $\tau_y = +1$ we obtain

$$H^{+}_{\text{edge},l} = i\lambda(l)\eta_x\partial_l + \tilde{M}(l)\eta_z,$$

$$\tilde{M}(l = \text{I-IV}) = -M(l) - h(l) = \{\Delta_1|m|/t_x, -\Delta_1|m|/t_y - h_x, \Delta_1|m|/t_x, -\Delta_1|m|/t_y - h_x\}.$$

$$\tilde{\tilde{M}}(l = \text{I-IV}) = M(l) - h(l) = \{-\Delta_1|m|/t_x, \Delta_1|m|/t_y - h_x, -\Delta_1|m|/t_x, \Delta_1|m|/t_y - h_x\}$$

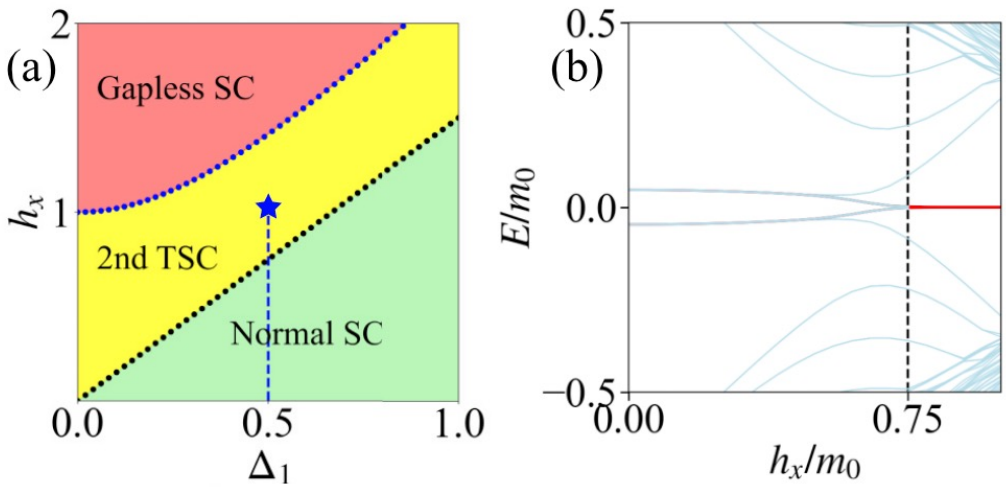


$h_x > M_{\text{II}} \equiv \Delta_1|m|/t_y.$

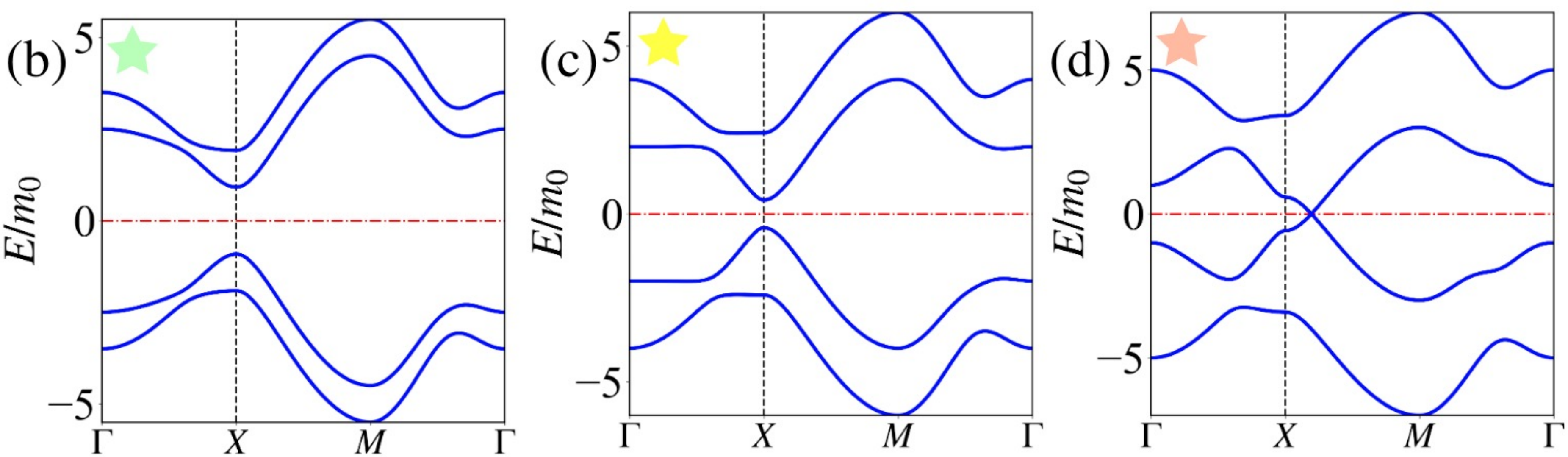
opposite masses of adjacent edges

$$\tilde{M}(l)\tilde{M}(l \pm 1) < 0,$$

Phase diagram



$$
\begin{aligned}
0 < h_x < M_{\mathrm{II}}, &\quad \text{normal SC}, \\
M_{\mathrm{II}} < h_x < h_x^{\mathbf{X}}, &\quad \text{second TSC}, \\
h_x > h_x^{\mathbf{X}} &\quad \text{gapless SC}.
\end{aligned}
$$

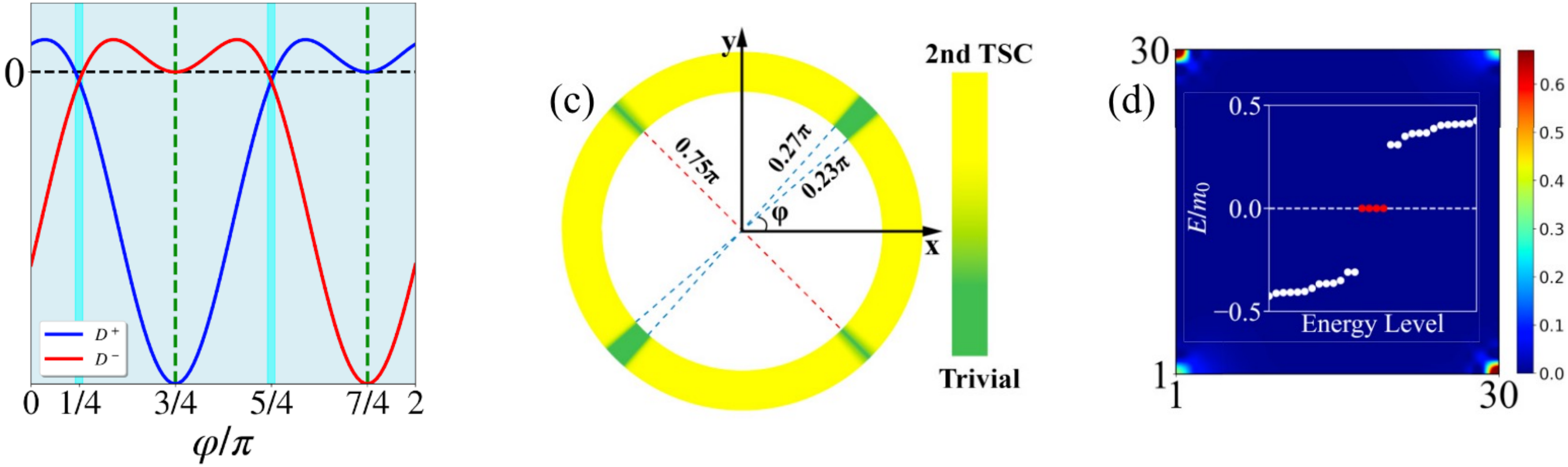


In-plane rotation

$$H(\mathbf{k}) = (m_0 - t_x \cos k_x - t_y \cos k_y)\sigma_z + (\lambda_x \sin k_x s_y + \lambda_y \sin k_y s_x)\sigma_x + \mathbf{h}\cdot\mathbf{s} - \mu,$$

$\boxed{\text{in-plane } h_{\parallel} = |\mathbf{h}| \sin\theta(\cos\varphi, \sin\varphi)}$ out-of-plane $h_{\perp} = |\mathbf{h}|\cos\theta$

$$H_{\mathrm{I}}(k_y) = \lambda_y k_y \eta_x - M_{\mathrm{I}}\tau_y\eta_z - h_{\parallel}\sin\varphi\eta_z,$$
$$H_{\mathrm{II}}(k_x) = -\lambda_x k_x \eta_x - M_{\mathrm{II}}\tau_y\eta_z - h_{\parallel}\cos\varphi\eta_z,$$
$$H_{\mathrm{III}}(k_y) = -\lambda_y k_y \eta_x - M_{\mathrm{III}}\tau_y\eta_z - h_{\parallel}\sin\varphi\eta_z,$$
$$H_{\mathrm{IV}}(k_x) = \lambda_x k_x \eta_x - M_{\mathrm{IV}}\tau_y\eta_z - h_{\parallel}\cos\varphi\eta_z,$$



Out-of-plane component

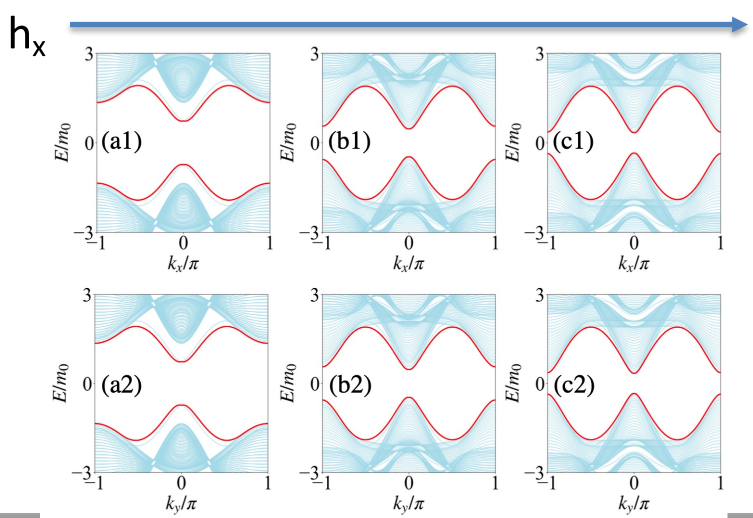
$$H(\mathbf{k}) = (m_0 - t_x \cos k_x - t_y \cos k_y)\sigma_z$$
$$+ (\lambda_x \sin k_x s_y + \lambda_y \sin k_y s_x)\sigma_x + \mathbf{h}\cdot\mathbf{s} - \mu,$$

in-plane $h_{||} = |\mathbf{h}| \sin\theta(\cos\varphi, \sin\varphi)$

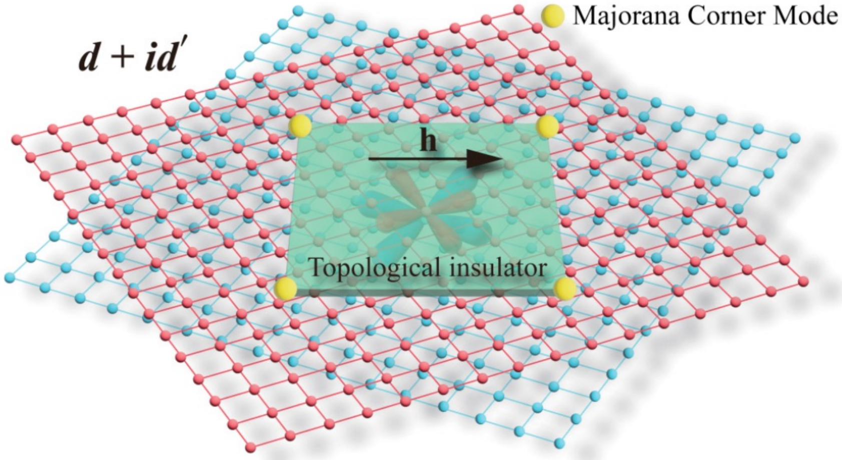
$\boxed{\text{out-of-plane } h_{\perp} = |\mathbf{h}| \cos\theta}$

$$H_{\mathrm{I}}(k_y) = \lambda_y k_y \eta_x - M_{\mathrm{I}} \tau_y \eta_z,$$
$$H_{\mathrm{II}}(k_x) = -\lambda_x k_x \eta_x - M_{\mathrm{II}} \tau_y \eta_z,$$
$$H_{\mathrm{III}}(k_y) = -\lambda_y k_y \eta_x - M_{\mathrm{III}} \tau_y \eta_z,$$
$$H_{\mathrm{IV}}(k_x) = \lambda_x k_x \eta_x - M_{\mathrm{IV}} \tau_y \eta_z,$$

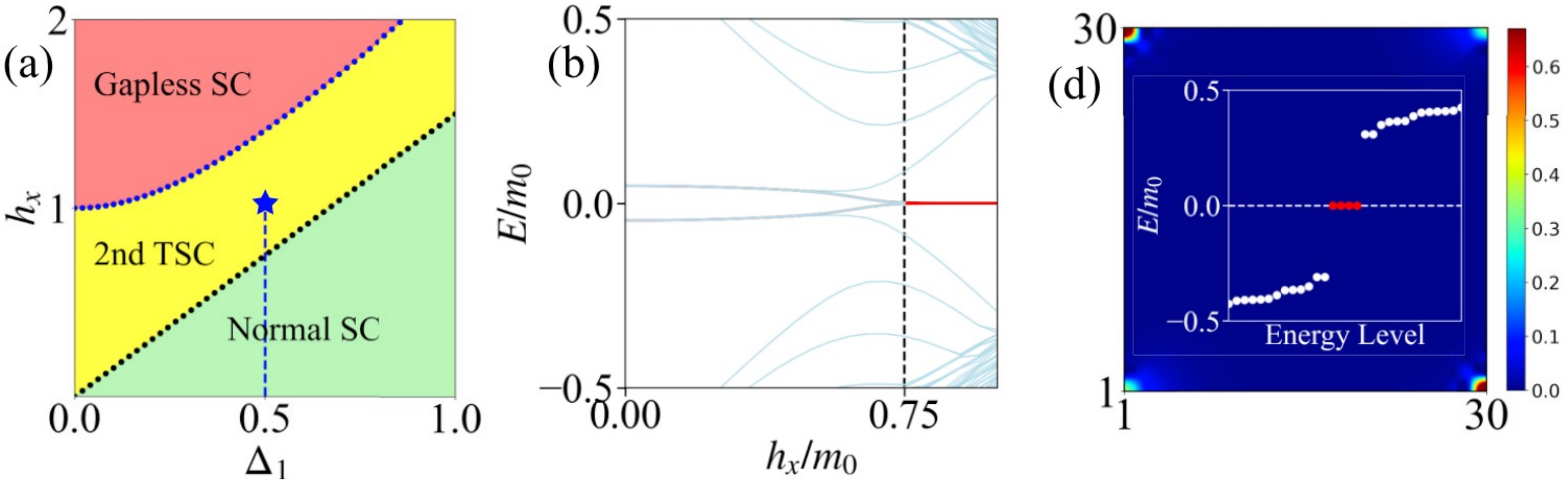
Out-of-plane component has no influence on edge states



Summary



$$\Delta(\mathbf{k}) = [\Delta_1(\cos k_x - \cos k_y) + i\Delta_2 \sin k_x \sin k_y](-is_y).$$



See more details in Poster Session on Thurs.

Acknowledgement

My collaborators：

- ➢BIT: Fan Yang, Li-Da Zhang, Yugui Yao
  Yu-Xuan Li
- ➢Wei-Qiang Chen (SUST), Qiyue Wang (UTD), Yuan-Ming Lu (Ohio State U), Fan Zhang (UTD)

Thank you for your attention!