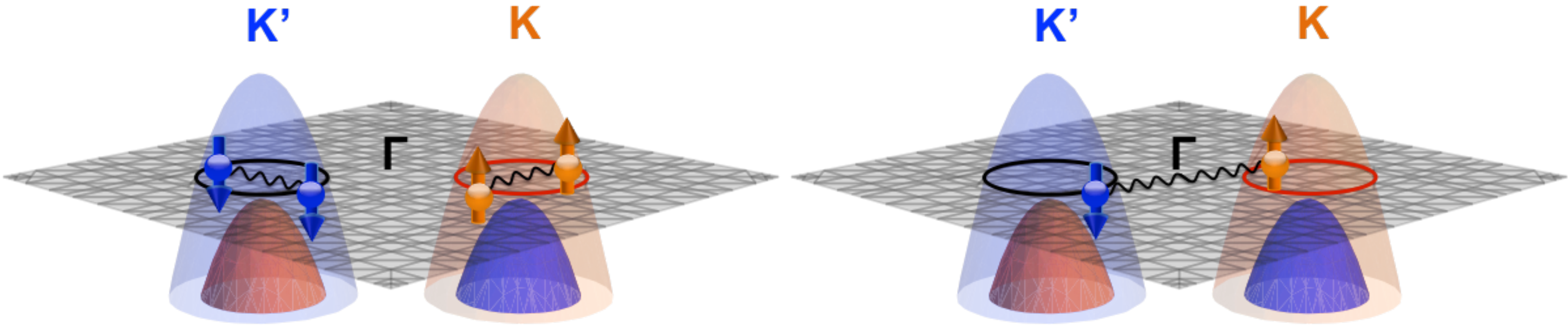
Exotic superconductivity in monolayer transition metal dichalcogenides



Yi-Ting Hsu

(Cornell/Maryland)

Discovery of superconductivity

The Nobel Prize in Physics 1913 was awarded to Heike Kamerlingh Onnes *"for his investigations on the properties of matter at low temperatures which led, inter alia, to the production of liquid helium"*.

Discovery of superfluidity

The Nobel Prize in Physics 1978 was divided, one half awarded to Pyotr Leonidovich Kapitsa *"for his basic inventions and discoveries in the area of low-temperature physics"*, the other half jointly to Arno Allan Penzias and Robert Woodrow Wilson *"for their discovery of cosmic microwave background radiation"*.

Discovery of He^3 superfluidity

The Nobel Prize in Physics 1996 was awarded jointly to David M. Lee, Douglas D. Osheroff and Robert C. Richardson *"for their discovery of superfluidity in helium-3"*.

Discovery of sc in cuprate

The Nobel Prize in Physics 1987 was awarded jointly to J. Georg Bednorz and K. Alexander Müller *"for their important break-through in the discovery of superconductivity in ceramic materials"*

Discovery of heavy fermion sc

E 52, NUMBER 8 PHYSICAL REVIEW LETTERS 20 FEBRUA

Possibility of Coexistence of Bulk Superconductivity and Spin Fluctuations in UPt_3

G. R. Stewart, Z. Fisk, J. O. Willis, and J. L. Smith
Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 24 October 1983)

Discovery of sc in Sr_2RuO_4

letters to nature

Nature **372**, 532 - 534 (08 December 1994); doi:10.1038/372532a0

Superconductivity in a layered perovskite without copper

Y. MAENO*, H. HASHIMOTO*, K. YOSHIDA*, S. NISHIZAKI*, T. FUJITA*, J. G. BEDNORZ† & F. LICHTENBERG†‡

Discovery of Fe-based sc

J. Am. Chem. Soc., **2008**, *130* (11), pp 3296–3297

Iron-Based Layered Superconductor $La[O_{1-x}F_x]FeAs$ ($x = 0.05–0.12$) with $T_c = 26$ K

Yoichi Kamihara ,*† Takumi Watanabe ,‡ Masahiro Hirano ,†§ and Hideo Hosono †‡§

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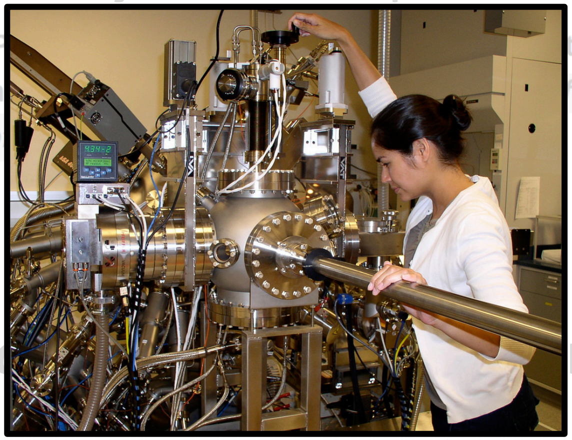
Experimental discoveries

Discovery of He^3 superfluidity

The Nobel P... to David M. Lee, Dougla... *for their discovery o...*



Disc... n sc

E 52, NUMBER 8 ... 20 FEBRUA...

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Theoretical predictions

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Theoretical puzzles & understandings

Dis... of sc in cuprate

The Nob... org Bednor... k- *through ... aterials"*

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Experimental confirmation

Far less examples

...very of Fe-based sc

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since making prediction for sc is challenging!

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Experimental discoveries

Theoretical puzzles

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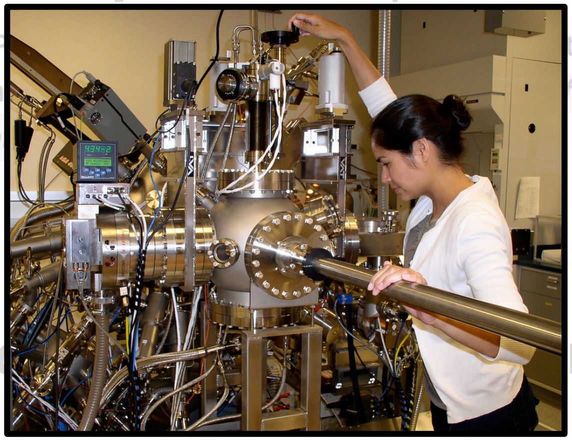

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Predict where to find exotic superconductivity

Realization of new exotic superconductors

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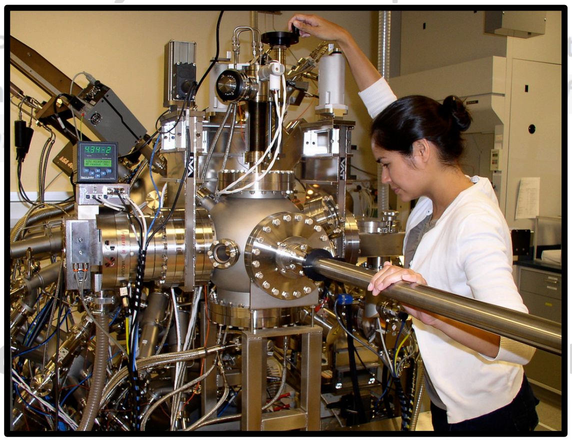

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...E 52, NUMBER 8 ... 20 FEBRUA...

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Predict where to find exotic superconductivity

↑

My goal here!

Discovery of superfluidity

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⇨

Theoretical puzzles

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Iron-Based Layered Superconductor La[$O_{1-x}F_x$]FeAs (x = 0.05–0.12) with ...

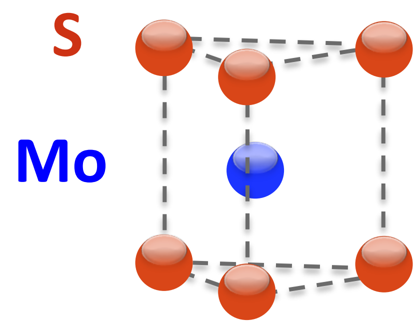
Yoichi Kamihara,*† Takumi Watanabe,‡ Masahiro Hirano,†§ and Hideo Hosono†‡§

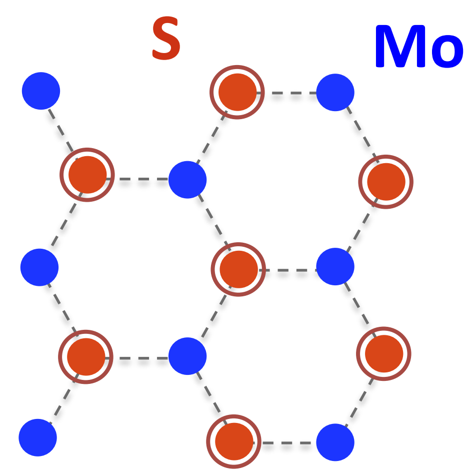
Monolayer transition metal dichalcogenides

- ❑ Group IV ***monolayer*** TMDs: MX_2 (M: Mo,W, X: S,Se)

  - ➢ 2D direct-gap semiconductors

  - ➢ Lattice ***breaks inversion symmetry***

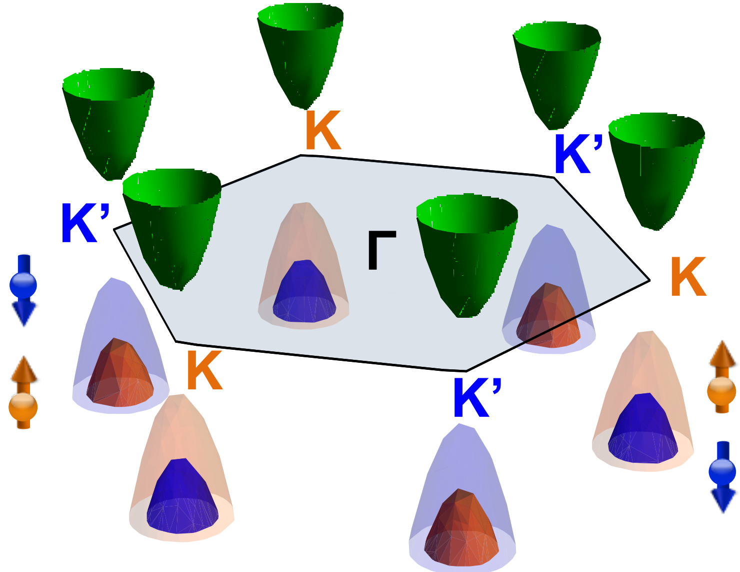




Group IV monolayer TMDs

- **Spin-orbit coupling**:
  - Align spins in z direction (Ising SOC)
  - **Orbital selective**: doesn't act on d_{z^2} (of transition metal)

=> Huge impact on low energy band structure



d_{z^2}

$d_{x^2-y^2}, d_{xy}$

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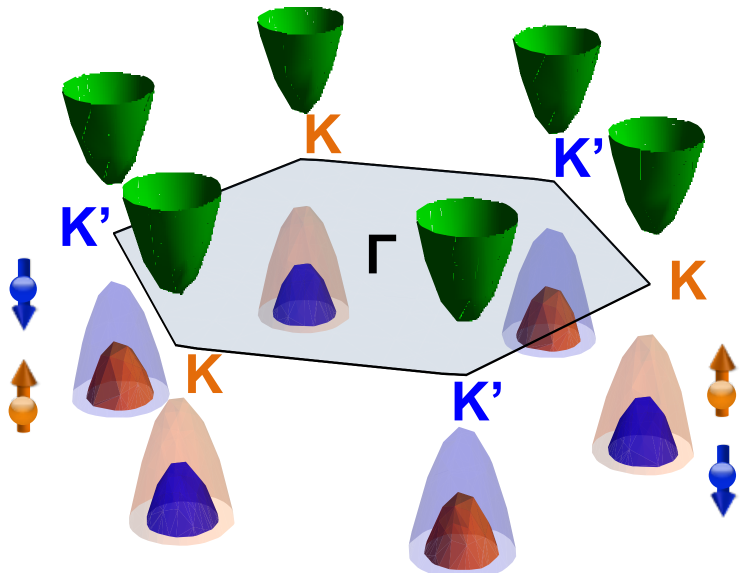


Nearly spin-degenerate

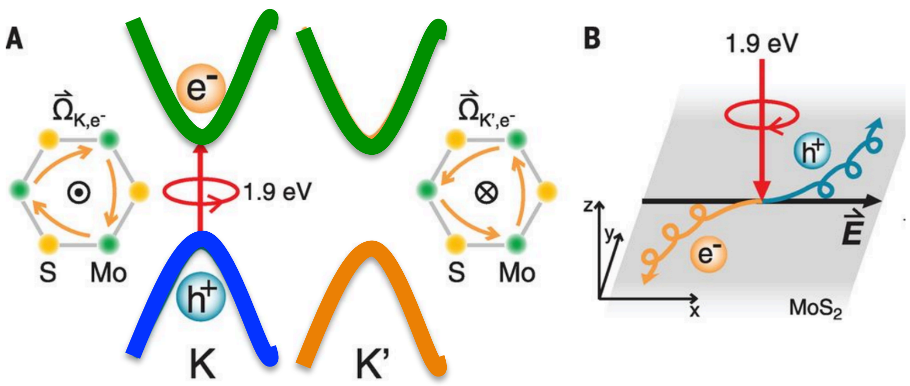
Large spin-split with time-reversal symmetry

TMDs: intriguing properties

◆ ***Transport, optical*** properties due to ***large spin-split***
(spin & valley DOFs coupled)

E.g. Spin & valley Hall effects

E.g. **Circular polarized light** => selectively control spin/valley DOFs

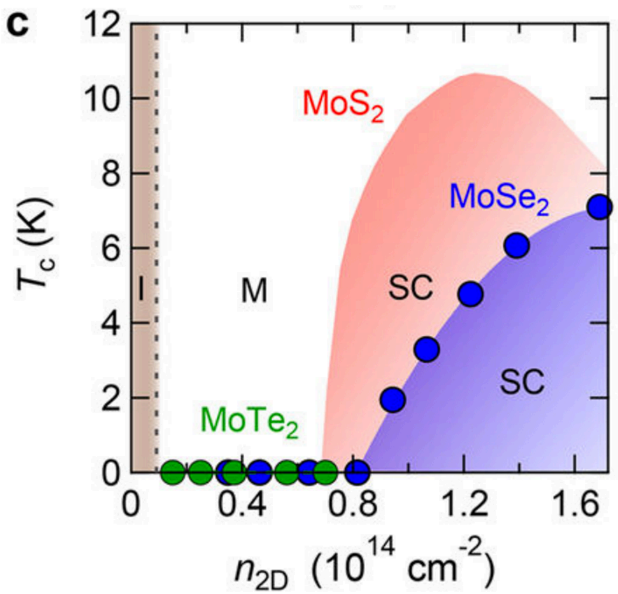


Thy: Xiao et al., PRL (2012)
Exp: Mak et al., Science (2014)

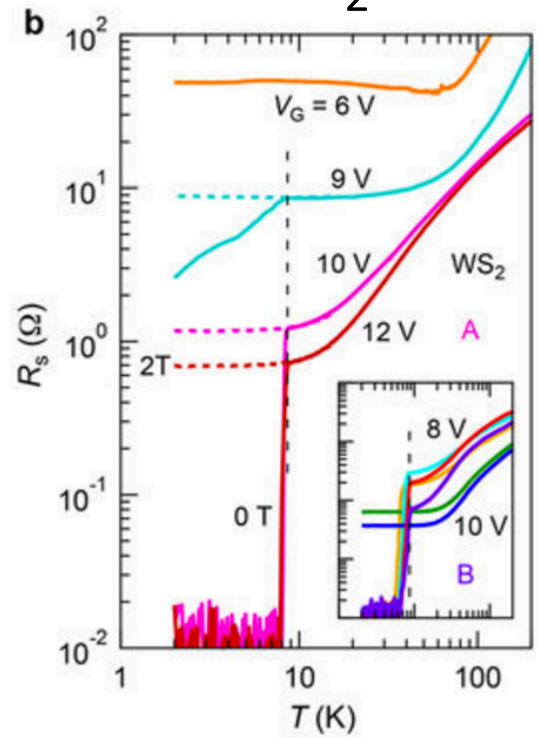
TMDs: superconductivity

- Superconducting upon electron doping:

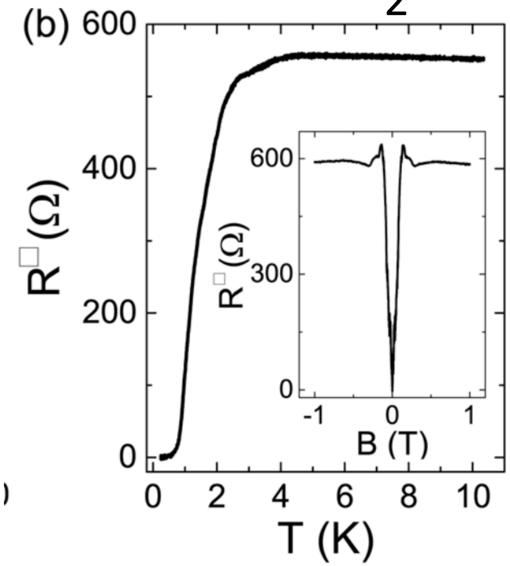
MoS_2[1], $MoSe_2$[2]



WS_2



WSe_2



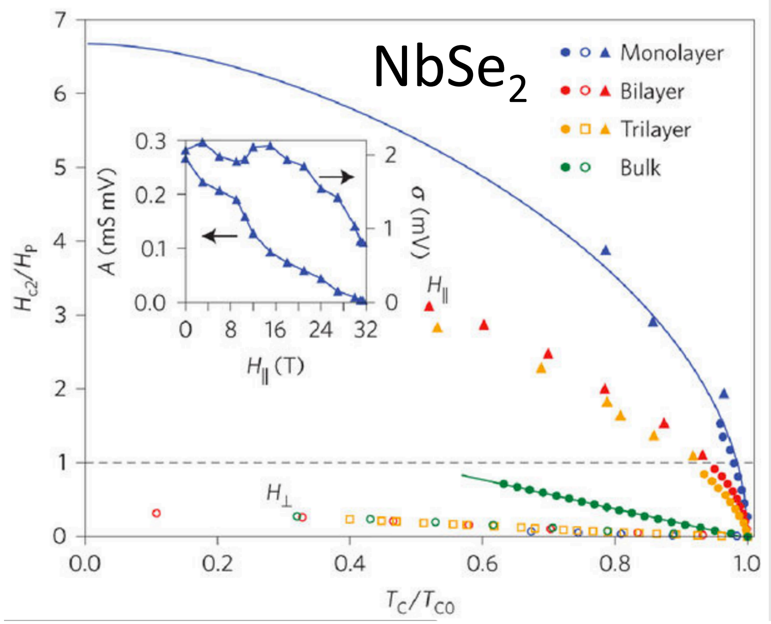
1: Ye et al., Science (2012)
2: Shi et al., Sci Rep(2015)

Shi et al., Sci Rep(2015)

Jo et al., Nano Lett (2015)

TMDs: superconductivity

- Superconductivity upon electron doping: What do we know?
  - Large in-plane H_{c2}: demonstration of Ising SOC



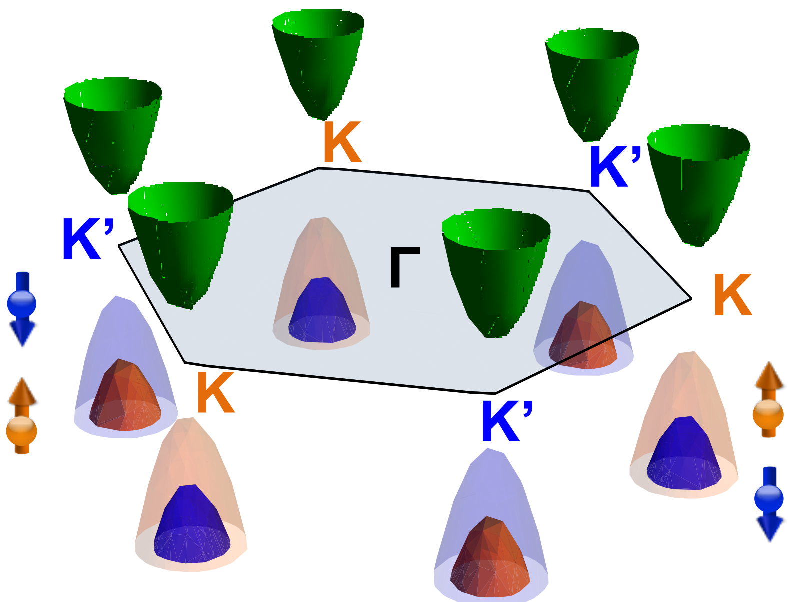
Xi et al., Nat Phys (2016)

TMDs: superconductivity

- Superconducting upon electron doping: what do we know?
  - Large in-plane H_{c2}: demonstration of Ising SOC
  - Pairing symmetry:
    Not a lot has been known
    Parity-mixing allowed

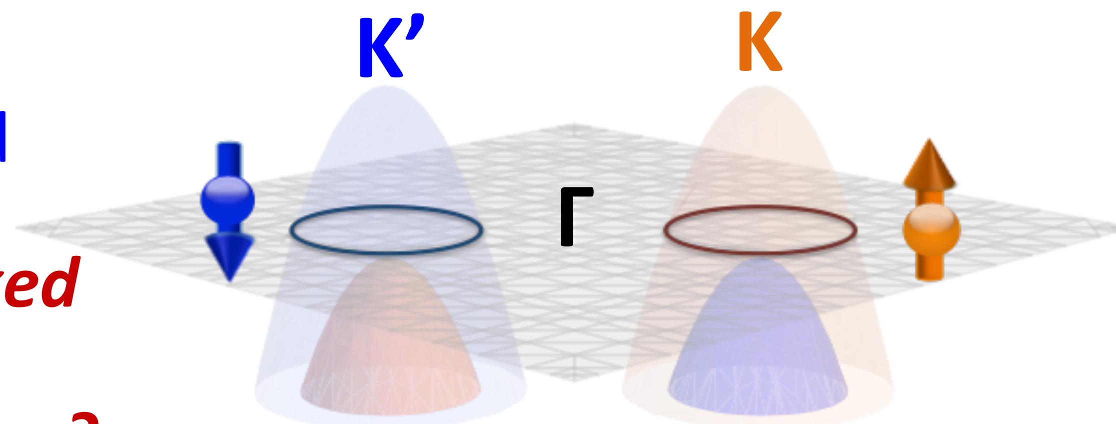
C_{3v}

Γ	Singlet	Triplet
A_1	s-wave	Nodeless f-wave
A_2		Nodal f-wave
E	(d_{x2-y2}, d_{xy})	(p_x, p_y)



So far observed sc:
all in the ***electron-doped side***

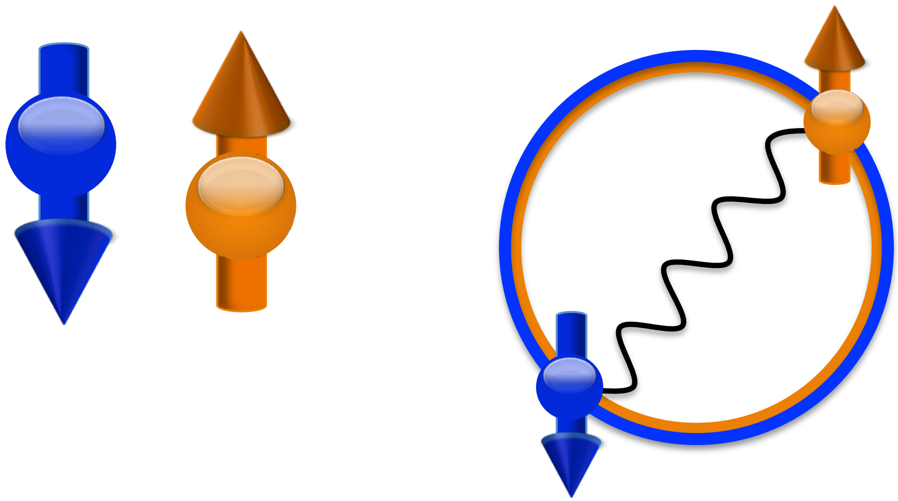
← μ within spin-split?



Lightly hole-doped

FS: Spin-valley locked

=> Good for exotic sc?



- Spin-degenerate Fermi Surfaces

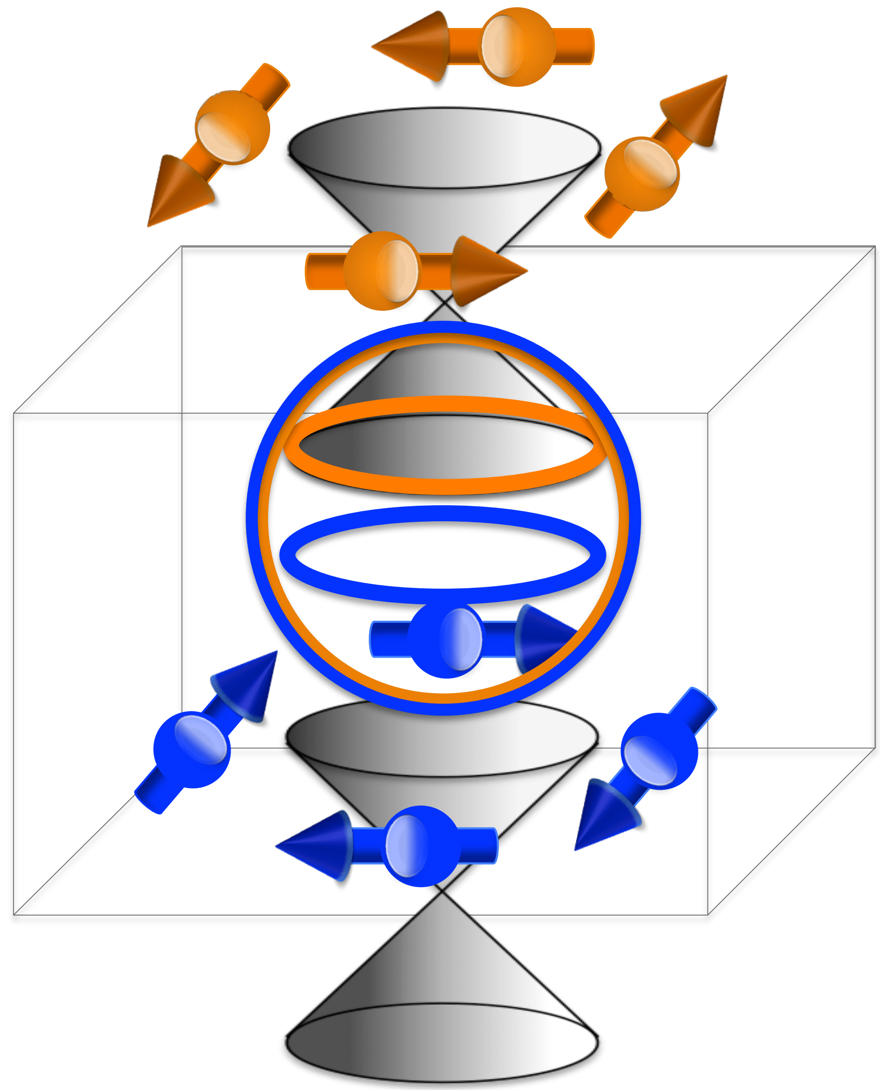
=> Likely singlet superconductivity

Fu-Kane proposal

Split FS spin-degeneracy in
real space

e.g. TI surface states

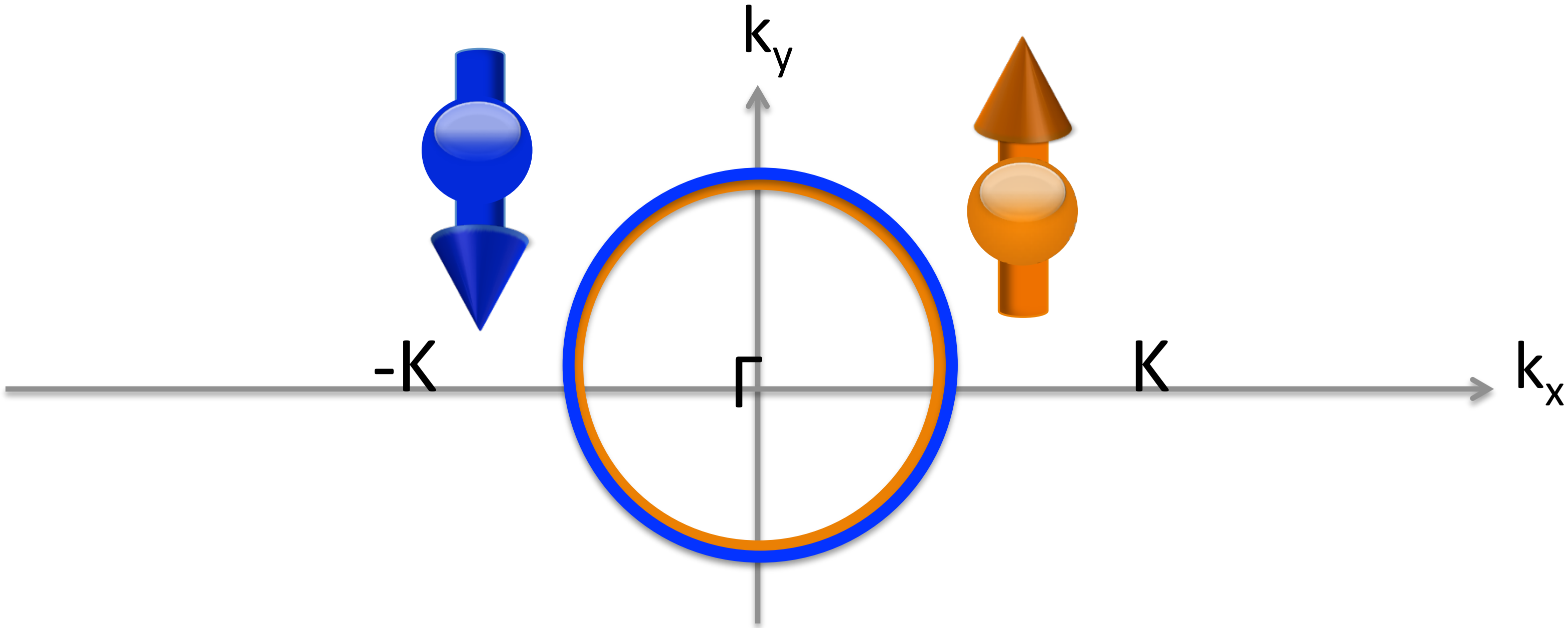
⇨ Real-space-separated
'spinless' femions



Fu & Kane:
One surface of TI + s-wave sc => ***Topological sc***

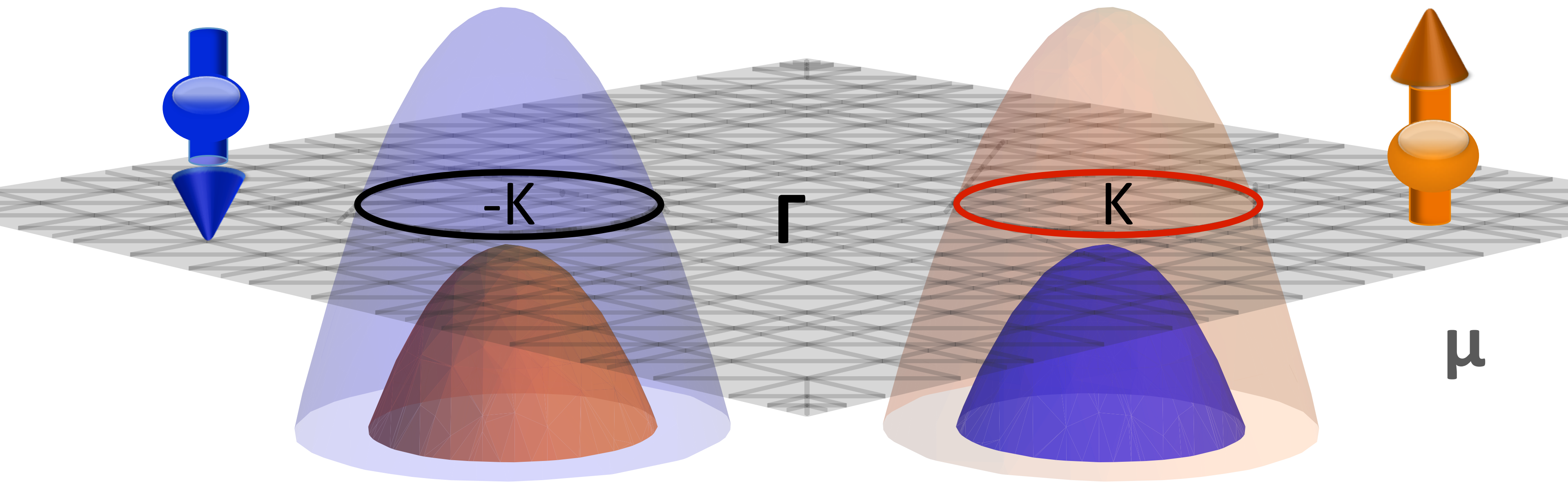
Fu, Kane (PRL 2008)

Our proposal



Split spin-degeneracy in momentum space

Lightly hole-doped monolayer TMDs

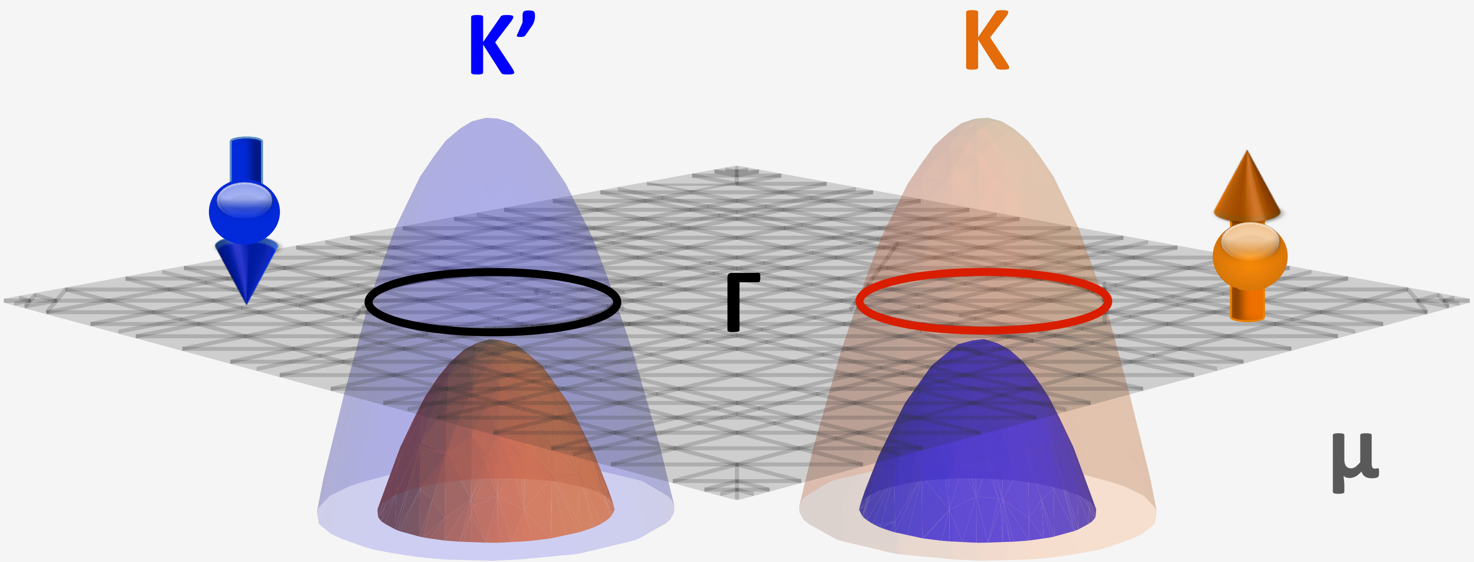


⇨ *Momentum-separated **spinless** fermions*

⇨ **Topo** sc?

Finite-momentum pairs => **Modulated** sc?

Exotic pairing in lightly hole-doped TMDs



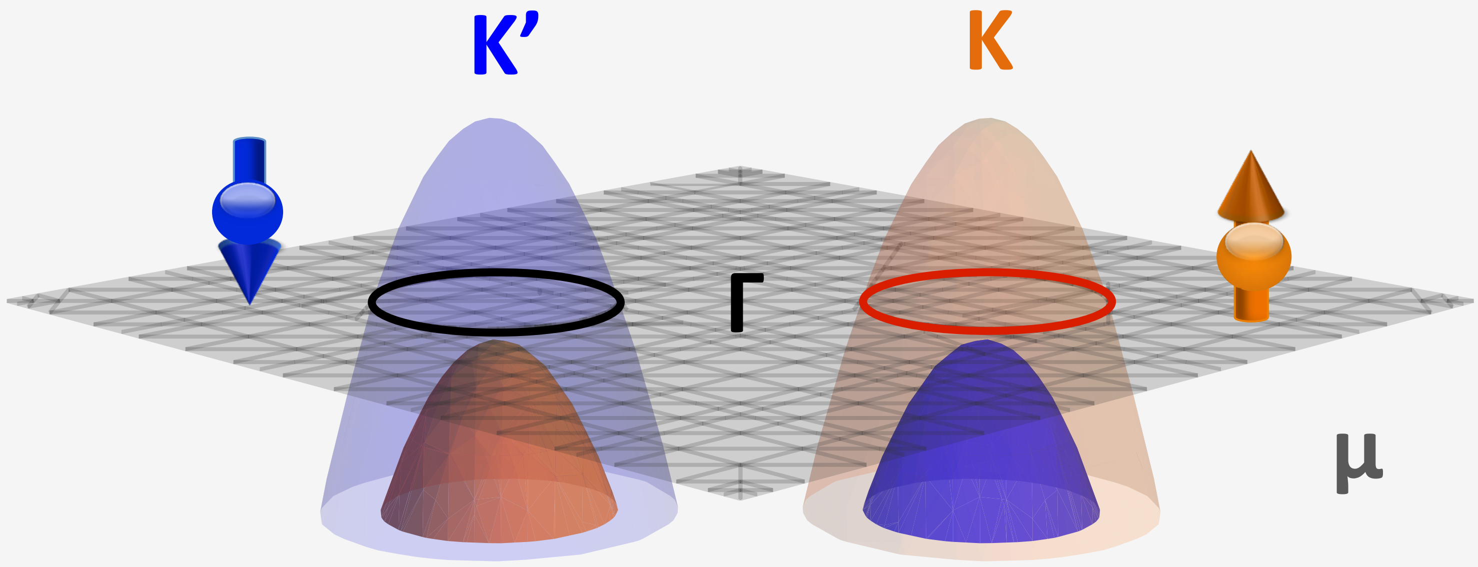
- ❑ Intrinsic pairing

  YTH et al., Nat Comm (2017)

- ❑ Proximity-induced pairing

  In preparation

Exotic pairing in lightly hole-doped TMDs



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YTH et al., Nat Comm (2017)

- ❑ Proximity-induced pairing

In preparation

Abolhassan Vaezi
Stanford University

Mark Fischer
Weizmann Institute

Eun-Ah Kim
Cornell University

Want to predict:

The pairing symmetry of intrinsic superconductivity

Pairing mechanism

- d-electrons: moderate electronic repulsion

  => could be the dominant source for sc

  Roldan, Cappelluti, Guinea, PRB (2013)

- Kohn-Luttinger mechanism => Unconventional sc

- Theoretical tool:

  Two-step weak-coupling RG

  Raghu, Kivelson, Scalapino, PRB (2010)

  (Had been recently applied on ruthenates[1,2,3])

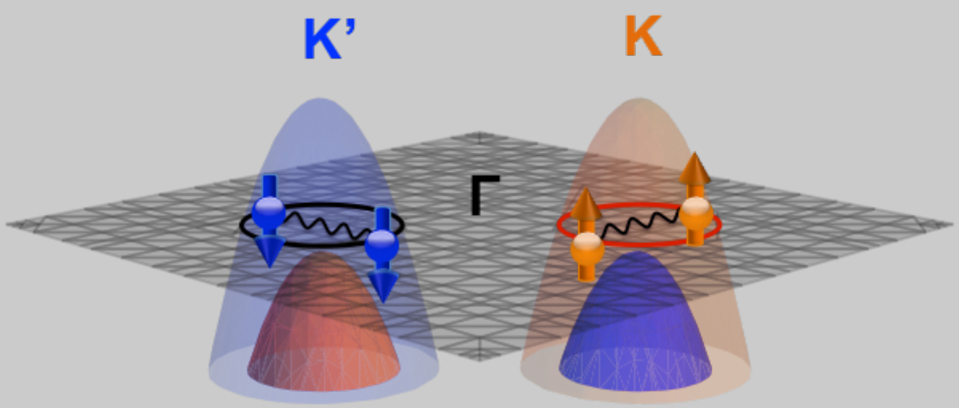
1: Raghu et al, PRL (2010)

2: **YTH** et al, PRB (2016)

3. Scaffidi et al, PRB (2014)

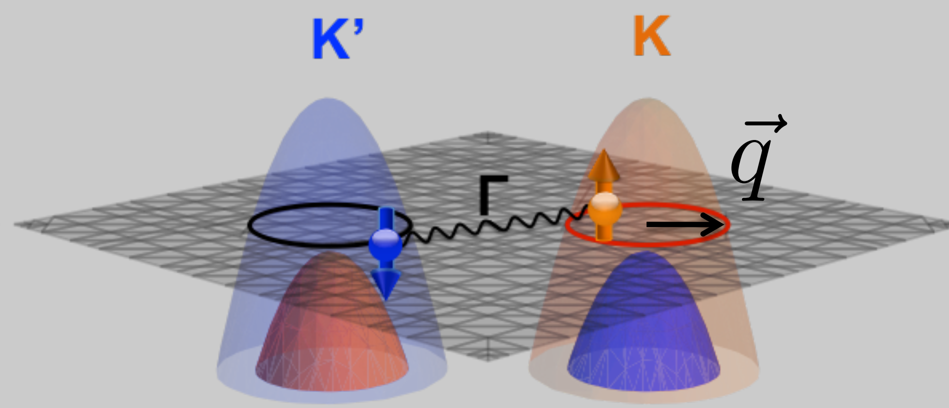
Effective interactions in Cooper channel

- Near the Fermi surface:



$$g^{(0)}_{\mathrm{intra}}(\vec{q}, \vec{q}')$$

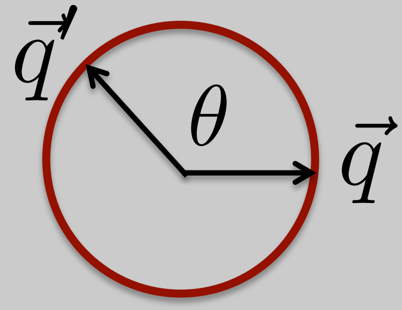
incoming outgoing

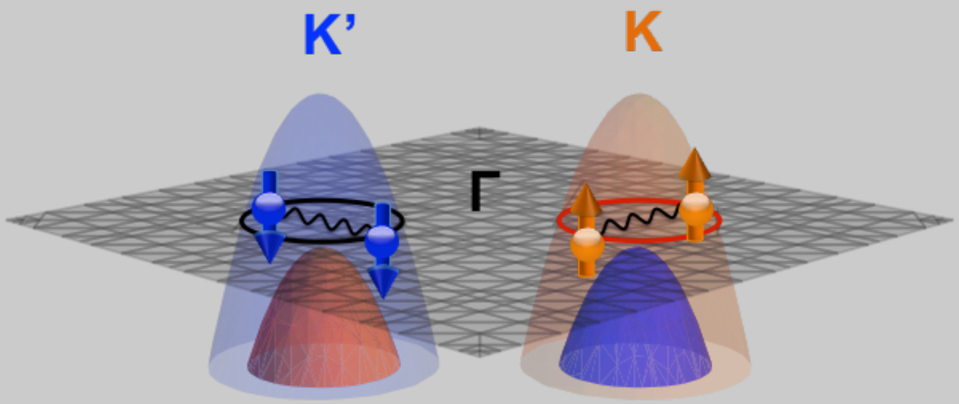


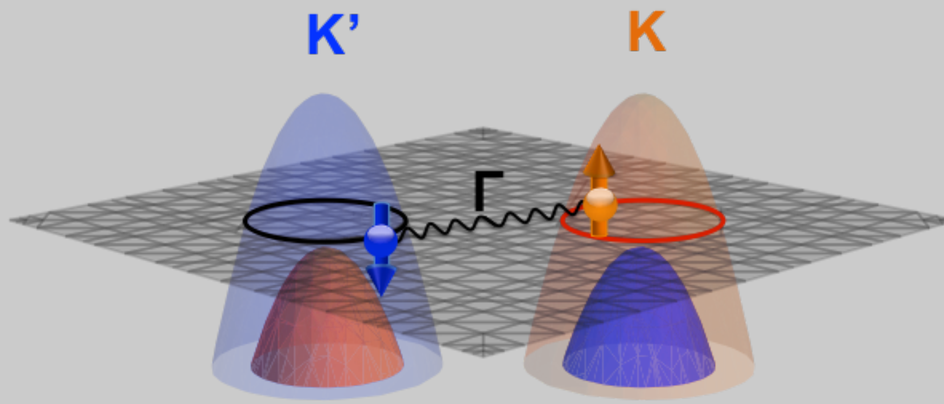
$$g^{(0)}_{\mathrm{inter}}(\vec{q}, \vec{q}')$$

Effective interactions in Cooper channel

Light doping:
Circular pockets







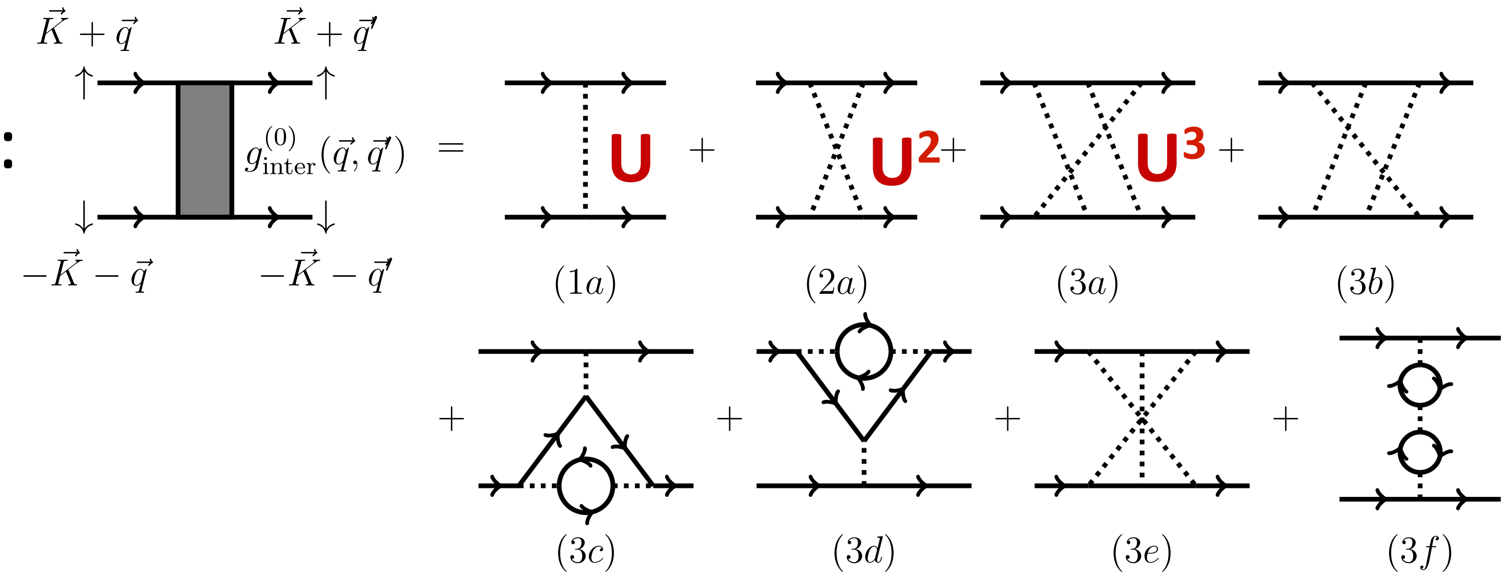
$$g_i^{(0)}(\vec{q},\vec{q}') \longrightarrow g_i^{(0)}(\theta) = \sum_{\tilde{l}} \lambda_i^{\tilde{l},(0)} \cos(\tilde{l}\theta)$$

i = inter,intra

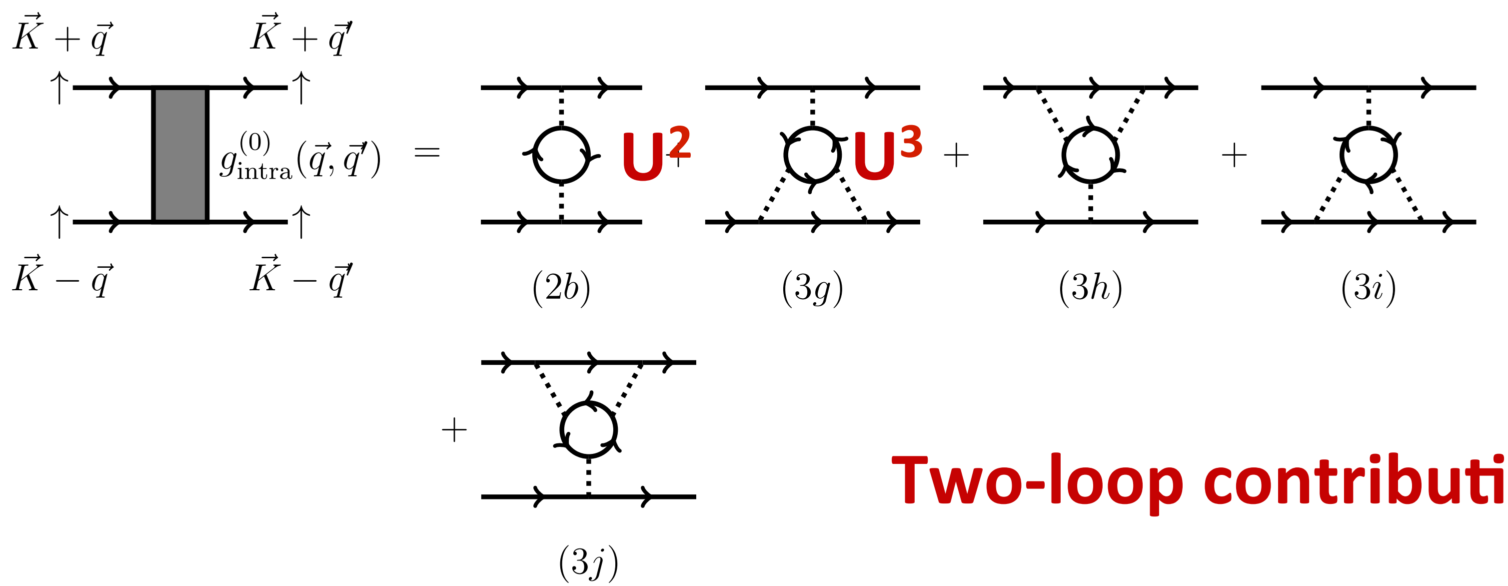
Interaction in partial-wave channel $\tilde{l}$

Derive effective interactions $\lambda_i^{\tilde{l},(0)}$

Inter:



Intra:



Two-loop contributions

Result: Dominant pairing symmetry

$$\lambda_{\text{inter}}^{|\tilde{l}|=1,(0)} = \lambda_{\text{intra}}^{|\tilde{l}|=1,(0)} < 0$$ are the largest attractions!

↓

- Dominant pairing channels:
  inter- & intra-pocket $|\tilde{l}| = 1$ paired states

Result: Dominant pairing symmetry

$\lambda_{\text{inter}}^{|\tilde{l}|=1,(0)} = \lambda_{\text{intra}}^{|\tilde{l}|=1,(0)} < 0$ are the largest attractions!

- Dominant pairing channels:
  inter- & intra-pocket $|\tilde{l}| = 1$ paired states

  (degenerate: artifact due to the circular pockets)

- Inter $|\tilde{l}| = 1$: p/d-wave (2-dim irrep)
  Intra $|\tilde{l}| = 1$: p-wave

chiral

(energetics)

Result: Dominant pairing symmetry

$\lambda_{\text{inter}}^{|\tilde{l}|=1,(0)} = \lambda_{\text{intra}}^{|\tilde{l}|=1,(0)} < 0$ are the largest attractions!

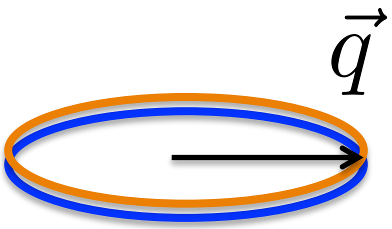
- Dominant pairing channels:
  inter- & intra-pocket $|\tilde{l}| = 1$ paired states

- *Both are chiral*

=> Both are topological!

p-wave pairing in ordinary 2D Fermi liquid

- Single spin-degenerate pocket + repulsive Hubbard U[1]

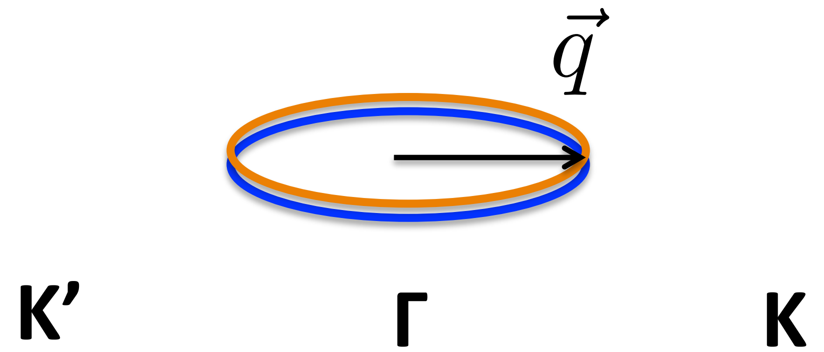


⇨ *Largest attraction appears in p-wave channel ($l=1$)*[1]

1: Chubukov, PRB (1993)

Pairings in p-doped TMDs

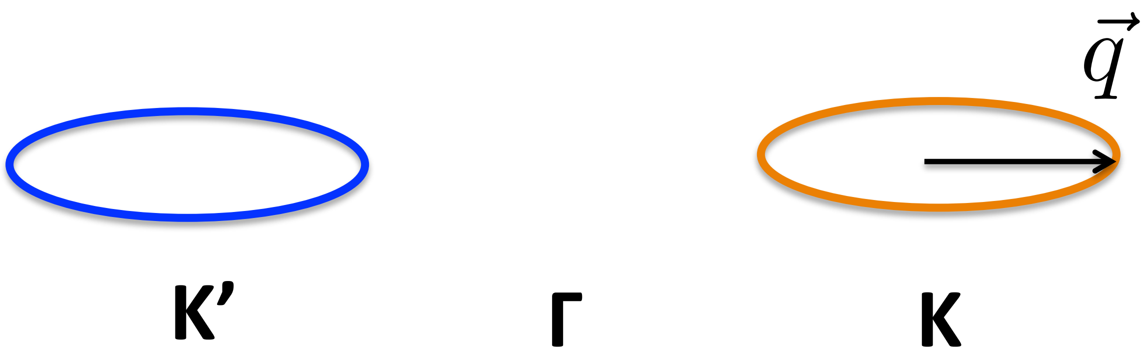
- Two spinless pockets centered at K and K’ + repulsive Hubbard U



⇨ 1-1 correspondence for each possible pairing channel

Pairings in p-doped TMDs

- Two spinless pockets centered at K and K’
  + repulsive Hubbard U

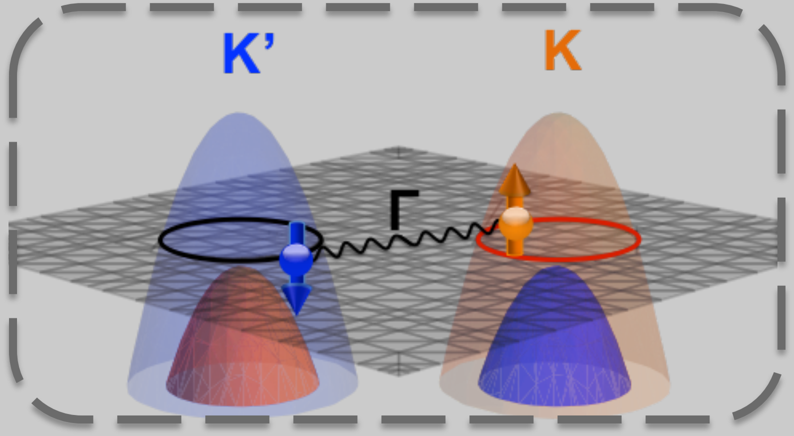


⇨ *Largest attraction appears in*

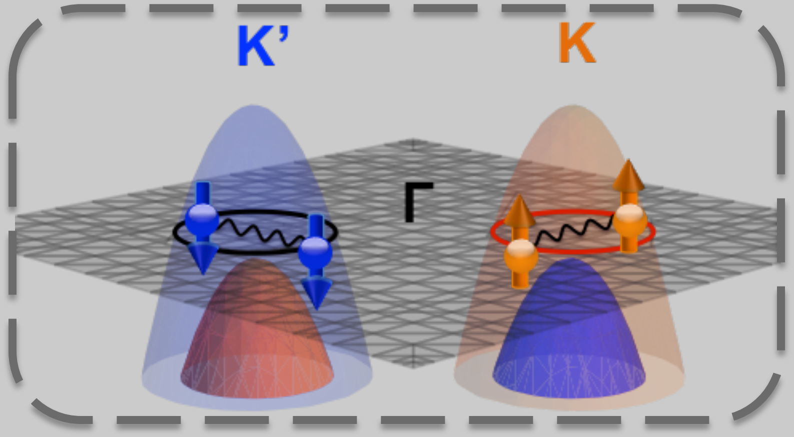
Inter- & intra-pocket $\tilde{l} = 1$ channel

Dominant topological paired states

Inter-pocket $|\tilde{l}| = 1$ pair



Intra-pocket $|\tilde{l}| = 1$ pair

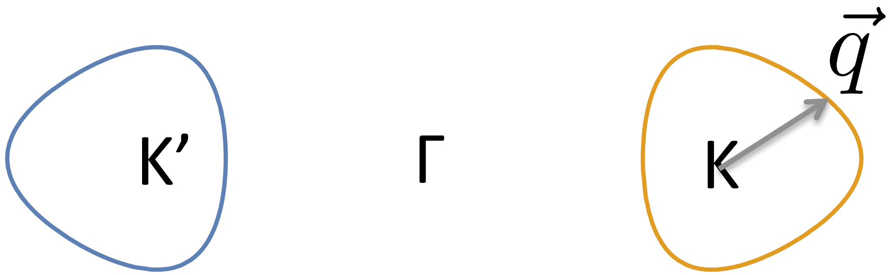


- Mixture of singlet and triplet
- Chiral (p/d)-wave
- Topo: C=2

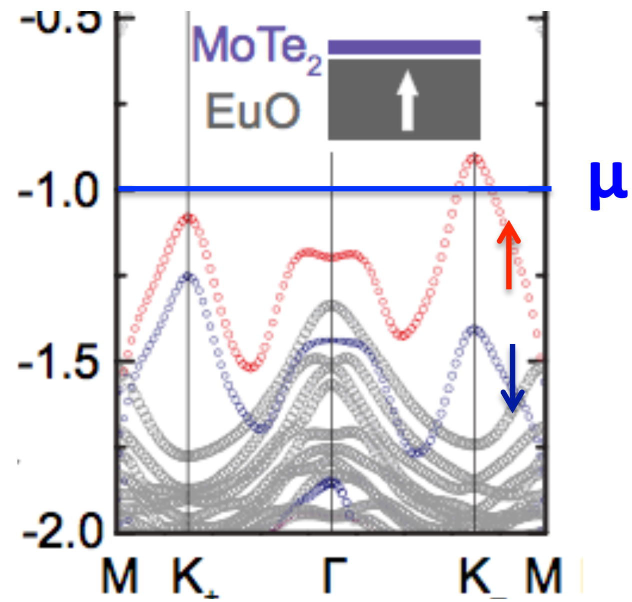
- Spin-triplet
- Chiral p-wave
- Topo: C=±1 per pocket
- Phase modulated at ±2K

Balance between Inter- and Intra-

- Trigonal warping prefers inter-pocket pairing

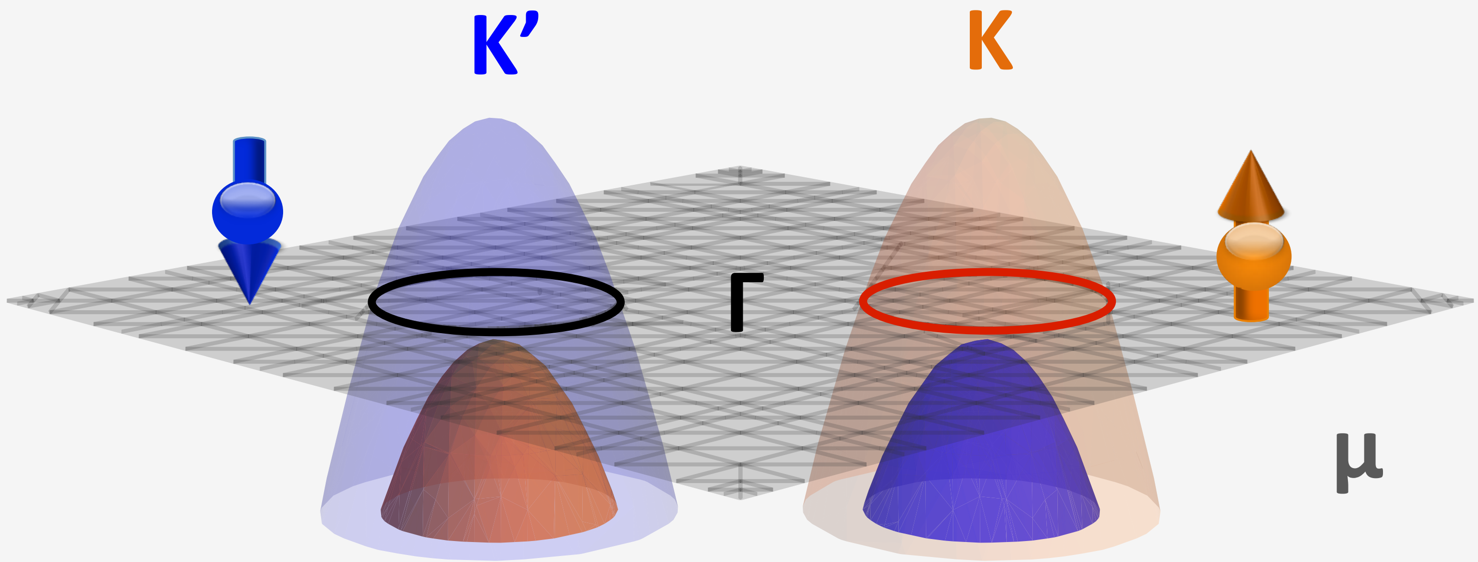


- Ferromagnetic substrate prefers intra-pocket pairing



Qi, PRB(2015)

Induced pairing in lightly hole-doped TMDs



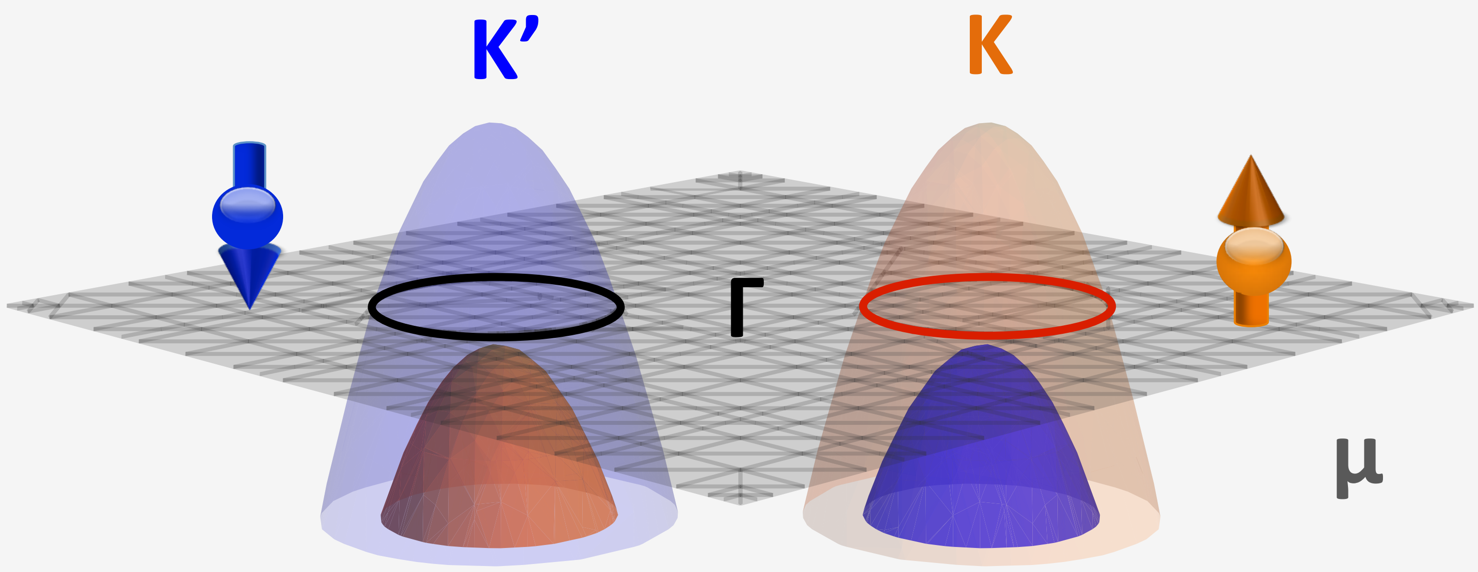
- ❑ Intrinsic pairing: topological

Nature Communication **8**, 14985

- ❑ Proximity-induced pairing

In preparation

Induced pairing in lightly hole-doped TMDs



❑ Intrinsic pairing

Nature Communication 8, 14985

❑ Proximity-induced pairing

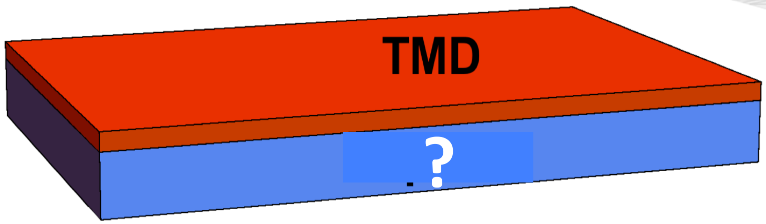
In preparation

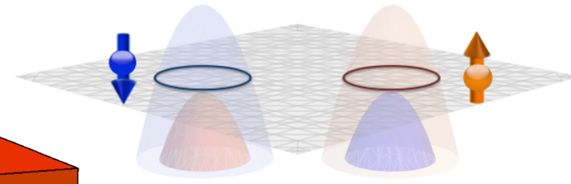
Kyungmin Lee
Ohio State University

Eun-Ah Kim
Cornell University

Choose the superconductor

- Lightly hole-doped TMD with ? sc



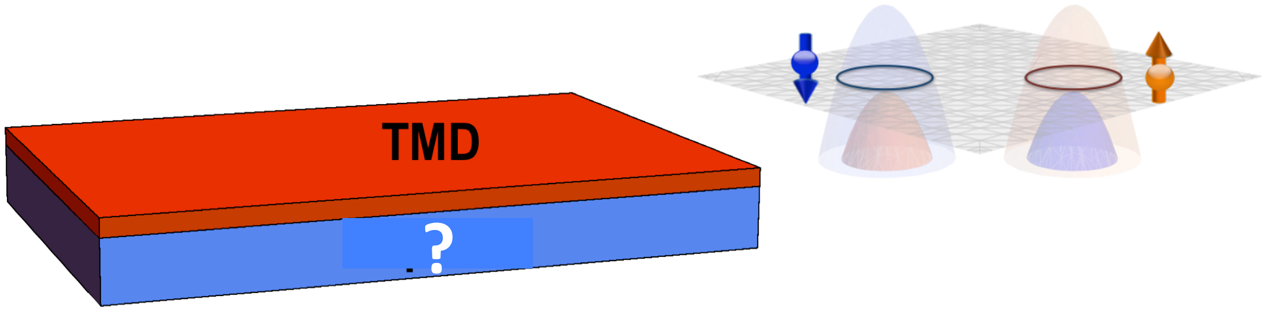


C_{3v}

Γ	Singlet	Triplet
A_1	s-wave	Nodeless f-wave
A_2		Nodal f-wave
E	$(d_{x2\text{-}y2}, d_{xy})$	(p_x, p_y)

Choose the superconductor

- Lightly hole-doped TMD with ? sc



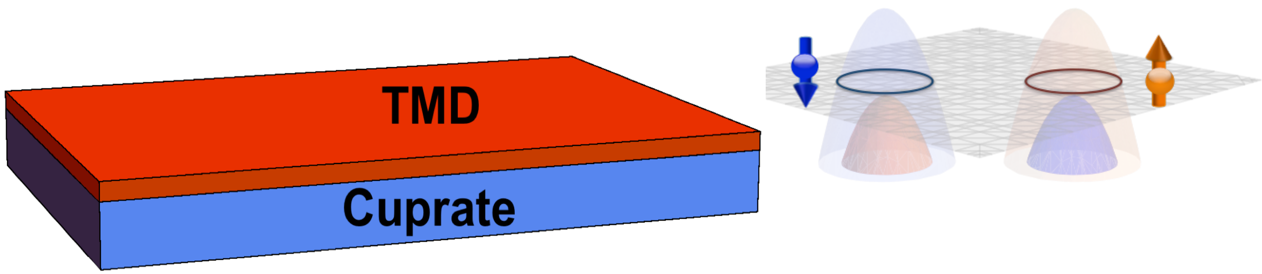
C$_{3v}$

Γ	Singlet	Triplet
A_1	s-wave	Nodeless f-wave
A_2		Nodal f-wave
E	(**d_{x2-y2}**, d_{xy})	(**p_x**, p_y)

=> Use cuprate!

Our proposal

◆ Lightly hole-doped TMD with cuprate



❖ Induce p-wave component?

❖ Possible high Tc

Recent exp: High-Tc sc induced by cuprate in

Graphene[1], TaS_2[2]

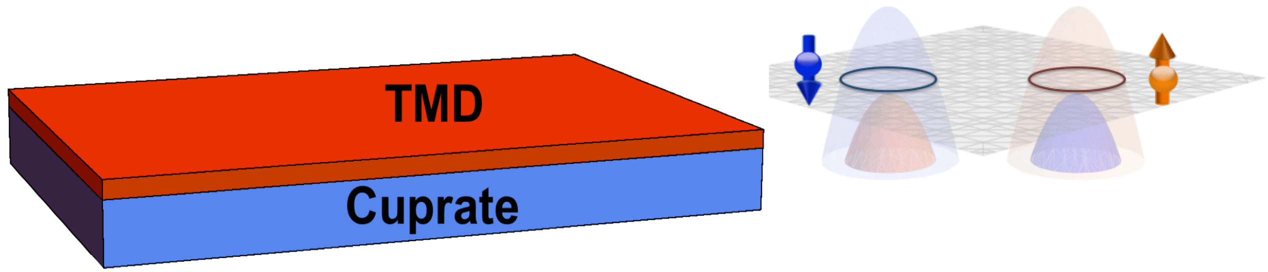
=> High-Tc odd-parity pairing?

1: Bernardo et al, Ncomms (2017)

2: Li et al, arxiv:1703.00867 (2017)

Our proposal

◆ Lightly hole-doped TMD with cuprate

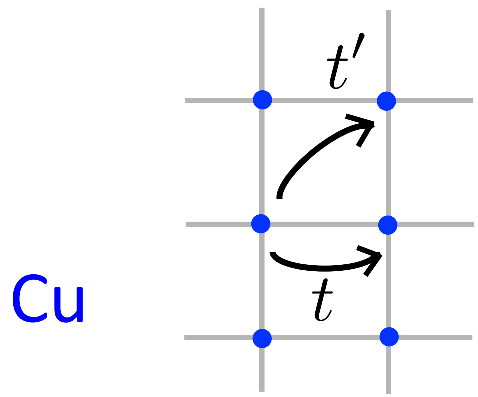


❖ Induce p-wave component?

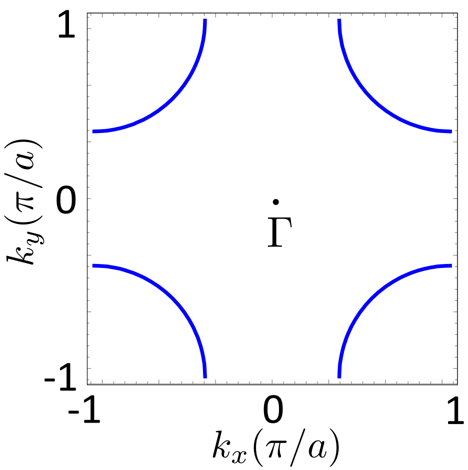
Confirm the guess: do a self-consistent calculation

Model: kinetic terms

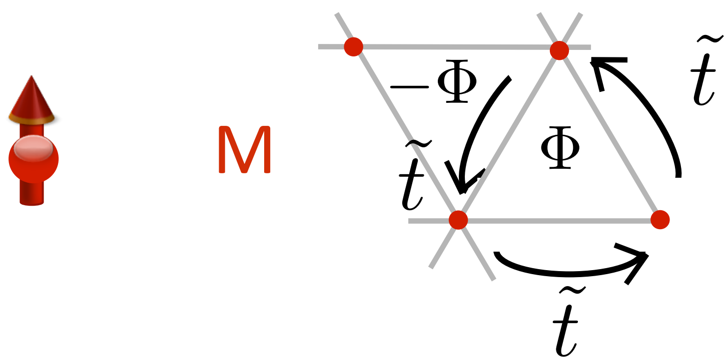
- Cuprate layer



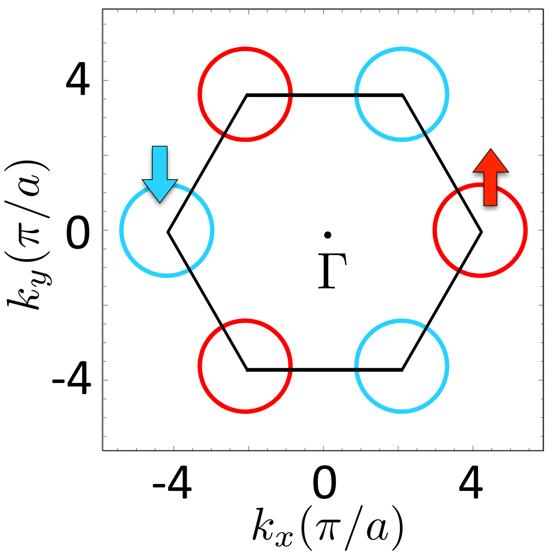
Spin-degenerate



- monolayer TMD: two band



Spin-valley locked



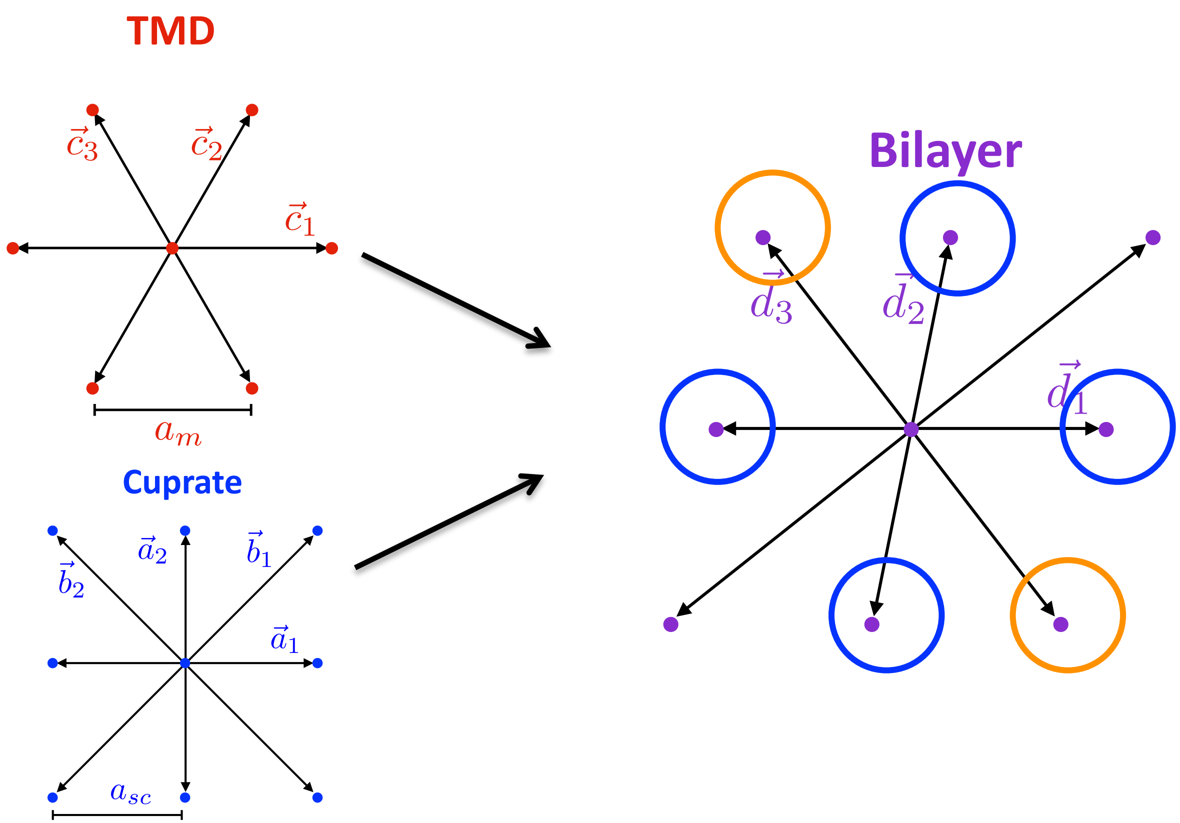
$\Phi = 0.9\pi$ $H_\downarrow = H_\uparrow^*$ => TRS

Mutual lattice straining

- Inter-layer tunneling: onsite, nn, nnn

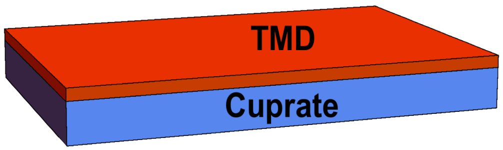
Assume

$a_{sc} \sim a_m$



Mean-field Hamiltonian

- Mean-field Hamiltonian for the bilayer:



ψ : cuprate

ϕ : TMD

$$H_{\mathrm{BdG}} = \sum_{\mathbf{x},\mathbf{y}} \begin{pmatrix} \psi^\dagger_{\uparrow\mathbf{x}} & \phi^\dagger_{\uparrow\mathbf{x}} & \psi_{\downarrow\mathbf{x}} & \phi_{\downarrow\mathbf{x}} \end{pmatrix} \begin{pmatrix} t^{sc}_{\mathbf{xy}} & \lambda_{\mathbf{xy}} & \Delta^{sc}_{\mathbf{xy}} & 0 \\ \lambda^*_{\mathbf{yx}} & t^m_{\mathbf{xy}} & 0 & \Delta^m_{\mathbf{xy}} \\ \Delta^{sc*}_{\mathbf{yx}} & 0 & -t^{sc}_{\mathbf{yx}} & -\lambda^*_{\mathbf{xy}} \\ 0 & \Delta^{m*}_{\mathbf{yx}} & -\lambda_{\mathbf{yx}} & -t^{m*}_{\mathbf{yx}} \end{pmatrix} \begin{pmatrix} \psi_{\uparrow\mathbf{y}} \\ \phi_{\uparrow\mathbf{y}} \\ \psi^\dagger_{\downarrow\mathbf{y}} \\ \phi^\dagger_{\downarrow\mathbf{y}} \end{pmatrix}$$

Mean-field Hamiltonian

- Mean-field Hamiltonian for the bilayer:

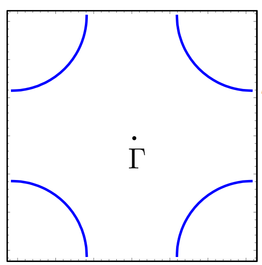
ψ : cuprate

ϕ : TMD

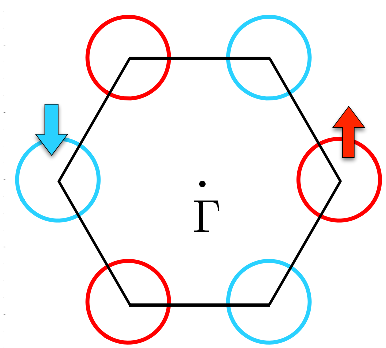
Normal

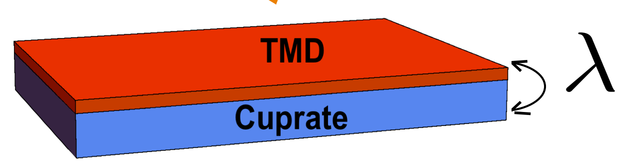
$$H_{\rm BdG} = \sum_{\mathbf{x},\mathbf{y}} \begin{pmatrix} \psi^\dagger_{\uparrow\mathbf{x}} & \phi^\dagger_{\uparrow\mathbf{x}} & \psi_{\downarrow\mathbf{x}} & \phi_{\downarrow\mathbf{x}} \end{pmatrix} \begin{pmatrix} t^{sc}_{\mathbf{xy}} & \lambda_{\mathbf{xy}} & \Delta^{sc}_{\mathbf{xy}} & 0 \\ \lambda^*_{\mathbf{yx}} & t^m_{\mathbf{xy}} & 0 & \Delta^m_{\mathbf{xy}} \\ \Delta^{sc*}_{\mathbf{yx}} & 0 & -t^{sc}_{\mathbf{yx}} & -\lambda^*_{\mathbf{xy}} \\ 0 & \Delta^{m*}_{\mathbf{yx}} & -\lambda_{\mathbf{yx}} & -t^{m*}_{\mathbf{yx}} \end{pmatrix} \begin{pmatrix} \psi_{\uparrow\mathbf{y}} \\ \phi_{\uparrow\mathbf{y}} \\ \psi^\dagger_{\downarrow\mathbf{y}} \\ \phi^\dagger_{\downarrow\mathbf{y}} \end{pmatrix}$$

Cuprate



TMD





Mean-field Hamiltonian

- Mean-field Hamiltonian for the bilayer:

ψ : cuprate

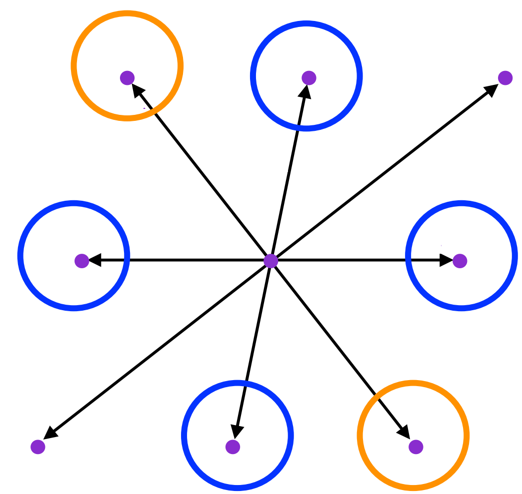
ϕ : TMD

Pairing

$$H_{\mathrm{BdG}} = \sum_{\mathbf{x},\mathbf{y}} \begin{pmatrix} \psi^{\dagger}_{\uparrow\mathbf{x}} & \phi^{\dagger}_{\uparrow\mathbf{x}} & \psi_{\downarrow\mathbf{x}} & \phi_{\downarrow\mathbf{x}} \end{pmatrix} \begin{pmatrix} t^{sc}_{\mathbf{xy}} & \lambda_{\mathbf{xy}} & \Delta^{sc}_{\mathbf{xy}} & 0 \\ \lambda^{*}_{\mathbf{yx}} & t^{m}_{\mathbf{xy}} & 0 & 0 \\ \Delta^{sc*}_{\mathbf{yx}} & 0 & -t^{sc}_{\mathbf{yx}} & -\lambda^{*}_{\mathbf{xy}} \\ 0 & 0 & -\lambda_{\mathbf{yx}} & -t^{m*}_{\mathbf{yx}} \end{pmatrix} \begin{pmatrix} \psi_{\uparrow\mathbf{y}} \\ \phi_{\uparrow\mathbf{y}} \\ \psi^{\dagger}_{\downarrow\mathbf{y}} \\ \phi^{\dagger}_{\downarrow\mathbf{y}} \end{pmatrix}$$

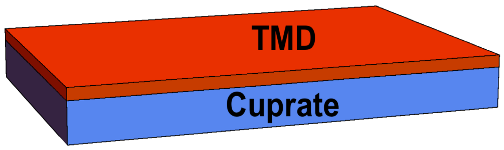
Cuprate

$\Delta^{sc}_{\mathbf{xy}}$: nn & nnn pairing



Calculation

- Mean-field Hamiltonian for the bilayer:



ψ : cuprate

ϕ : TMD

$$H_{\rm BdG} = \sum_{\mathbf{x},\mathbf{y}} \begin{pmatrix} \psi^\dagger_{\uparrow\mathbf{x}} & \phi^\dagger_{\uparrow\mathbf{x}} & \psi_{\downarrow\mathbf{x}} & \phi_{\downarrow\mathbf{x}} \end{pmatrix} \begin{pmatrix} t^{sc}_{\mathbf{xy}} & \lambda_{\mathbf{xy}} & \Delta^{sc}_{\mathbf{xy}} & 0 \\ \lambda^*_{\mathbf{yx}} & t^m_{\mathbf{xy}} & 0 & \Delta^m_{\mathbf{xy}} \\ \Delta^{sc*}_{\mathbf{yx}} & 0 & -t^{sc}_{\mathbf{yx}} & -\lambda^*_{\mathbf{xy}} \\ 0 & \Delta^{m*}_{\mathbf{yx}} & -\lambda_{\mathbf{yx}} & -t^{m*}_{\mathbf{yx}} \end{pmatrix} \begin{pmatrix} \psi_{\uparrow\mathbf{y}} \\ \phi_{\uparrow\mathbf{y}} \\ \psi^\dagger_{\downarrow\mathbf{y}} \\ \phi^\dagger_{\downarrow\mathbf{y}} \end{pmatrix}$$

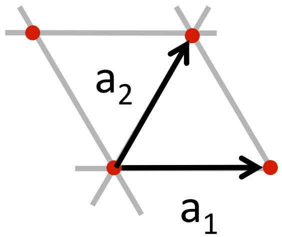
- Self-consistently solve gap equation

Cuprate: $\Delta^{sc}_{\mathbf{xy}} = U \langle \psi_{\downarrow\mathbf{y}} \psi_{\uparrow\mathbf{x}} \rangle$ $\quad U < 0$

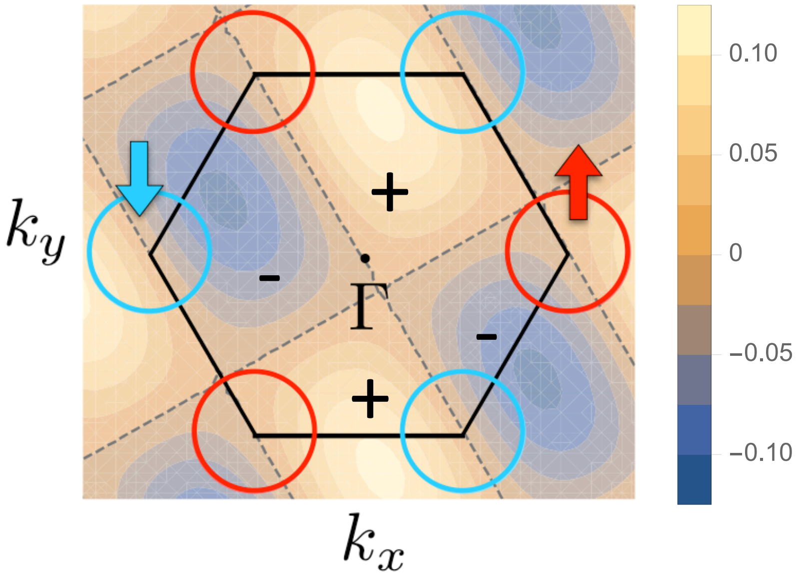
=> Obtain finite TMD pair amplitude from Andreev reflection

Result

◆ The induced pairing amplitude in TMD:



$$F(\mathbf{k}) = 2\eta_s(\cos k_1 - \cos k_2) - 2\eta_t(\sin k_1 + \sin k_2) \qquad k_i = \mathbf{k}\cdot\mathbf{a}_i$$



Coloring: pairing amplitude

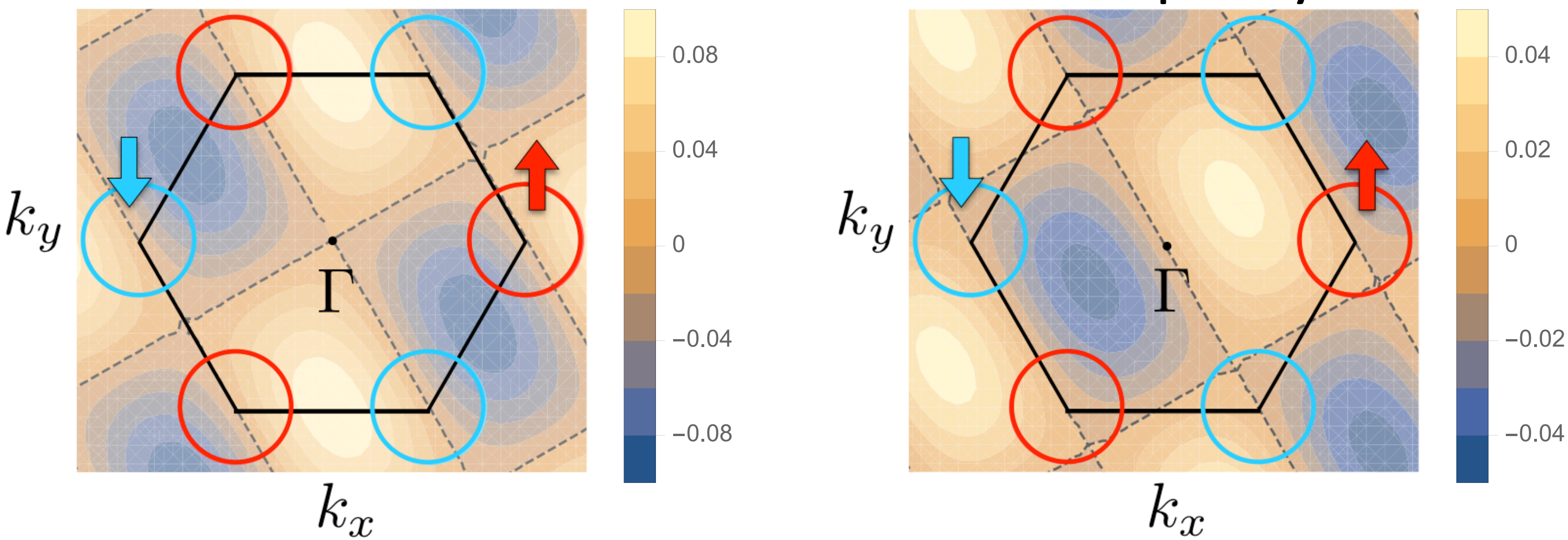
- Exists finite odd-parity component (η_s~$3\eta_t$)
- Nodal: partial-wave $|\tilde{l}| = 1$ about K and K’

Induced pairing symmetry

◆ The induced pairing in TMD: **Nematic (p+d)-wave**

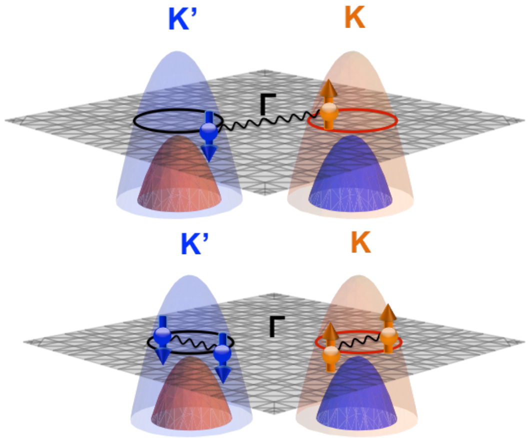
- Even: d-wave Odd: p-wave
- Nematic: single component

Even-parity Odd-parity

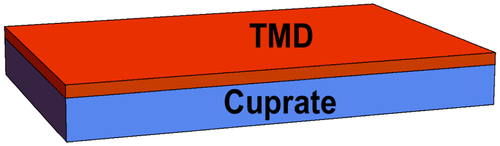


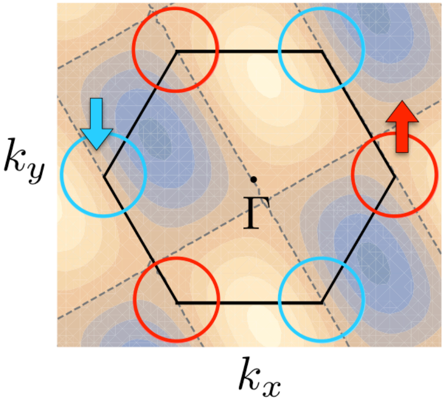
Summary: Lightly p-doped monolayer TMDs

- Two types of intrinsic topological superconductivity:
  (Nat Comm **8**, 14985)
  - Inter: Chiral (p+d)-wave
    Favored by trigonal warping
  - Intra: Chiral p-wave & Modulated
    Favored by ferro substrate



- Proximity-induced pairing by cuprate: (In preparation)
  - Sizable p-wave component with possibly higher-Tc
  - Nematic
  - Nodal

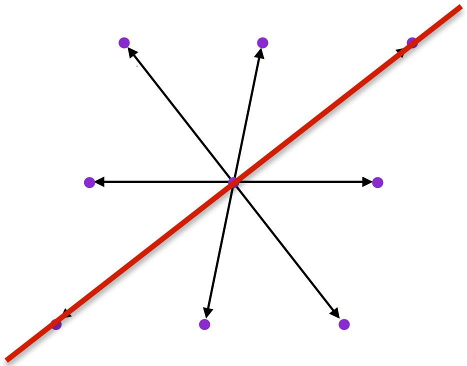




Induced pairing symmetry

- The point group symmetry of the bilayer Hamiltonian: **C_s**

Mirror (x+y)



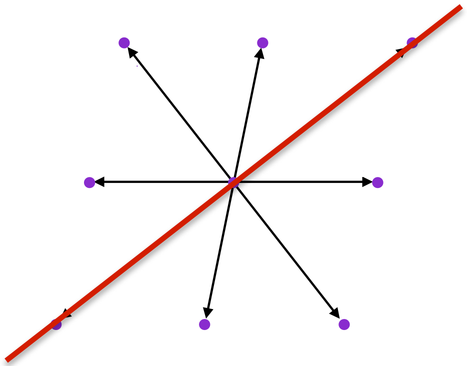
C_s

Γ	Singlet	Triplet
A_1	s-wave etc.	f-wave etc.
A_1'	d_{x2-y2}, d_{xy} etc.	$p_{x,}$ p_y etc.

Induced pairing symmetry

- The bilayer Hamiltonian has point group symmetry **C_s**

Mirror (x+y)



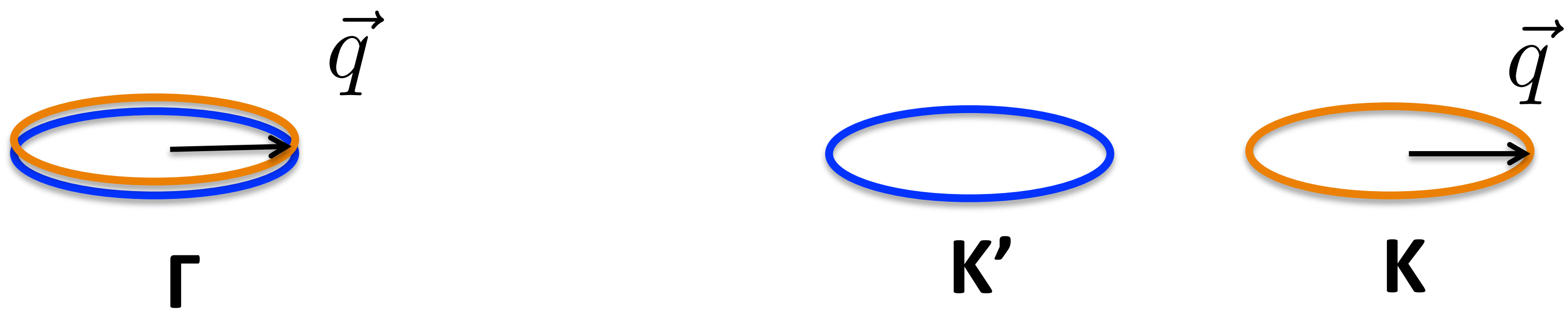
- The **'nematic (p+d)-wave'** pairing belongs to **nontrivial irrep A1'**

C_s

Γ	Singlet	Triplet
A_1	s-wave etc.	f-wave etc.
A_1'	**d_{x2-y2}**, d_{xy} etc.	**$p_{x+}p_y$**, p_x-p_y etc.

Result: Pairings in p-doped TMDs

- Two spinless pockets centered at K and K'
  + repulsive Hubbard U



- l even, spin-singlet ⟷ Inter, $\tilde{l}$ even
- l odd, spin-triplet $s_z=\pm1$ ⟷ Intra, $\tilde{l}$ odd
  $s_z=0$ ⟷ Inter, $\tilde{l}$ odd

  (Intra, $\tilde{l}$ odd and Inter, $\tilde{l}$ odd: degenerate)

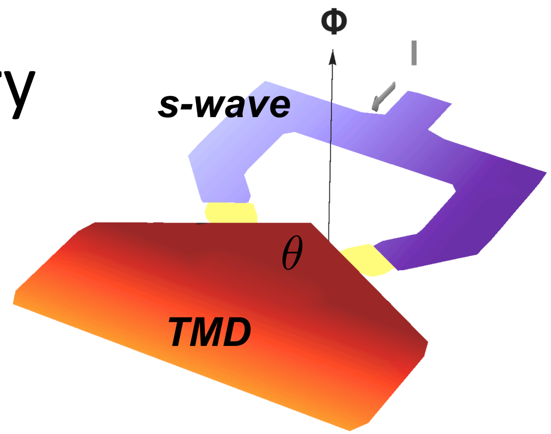
Experimental Detection

Intrinsic : inter-pocket $\tilde{l} = 1$ pairing

- Inter-pocket pairing

  - Existence of triplet component:
    in-plane field dependence (?)

  - Anisotropy: SQUID interferometry
    Ic(Φ) is θ-dependent



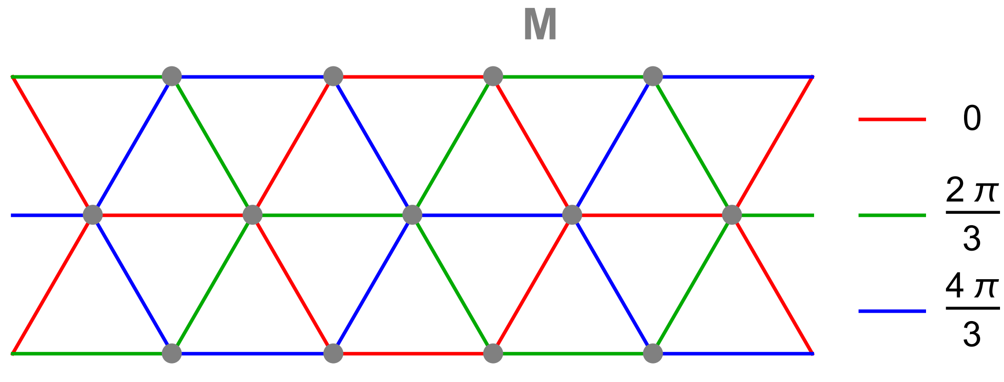
  - Topological with C=2:
    - Quantized thermal Hall conductivity
    - Two chiral Majorana edge states

  - Chiral: Polar Kerr effect

Intrinsic : intra-pocket $\tilde{l} = 1$ pairing

❑ Intra-pocket pairing

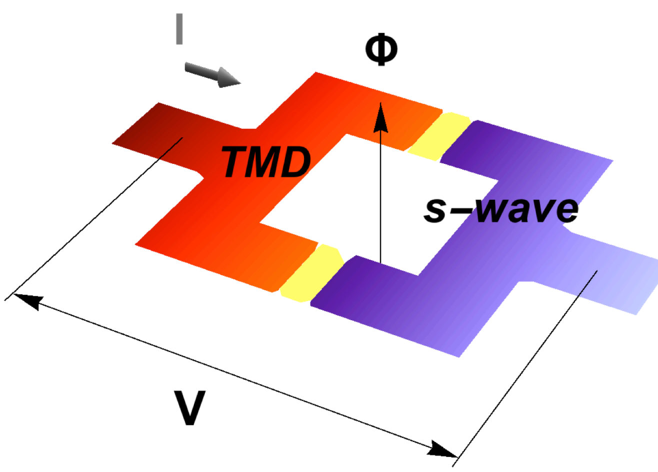
◆ Phase modulation



◆ SQUID loop in resistive mode:

- If pairing in TMD were uniform

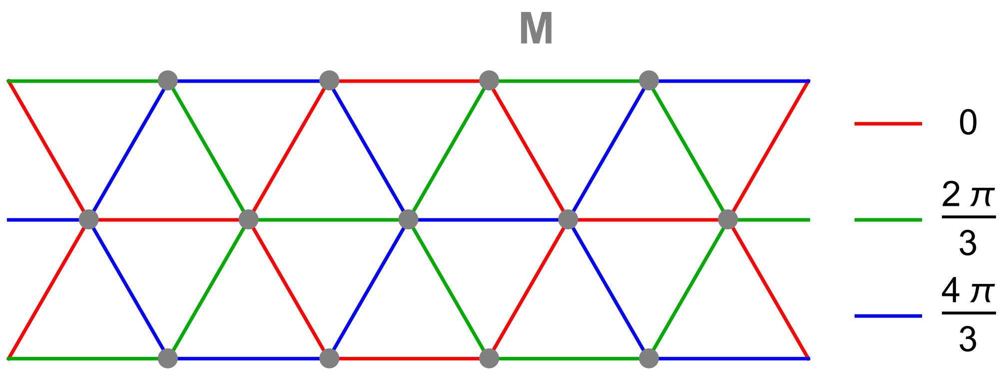
=> V oscillates in Φ with a period hc/(2e)



Intrinsic : intra-pocket $\tilde{l} = 1$ pairing

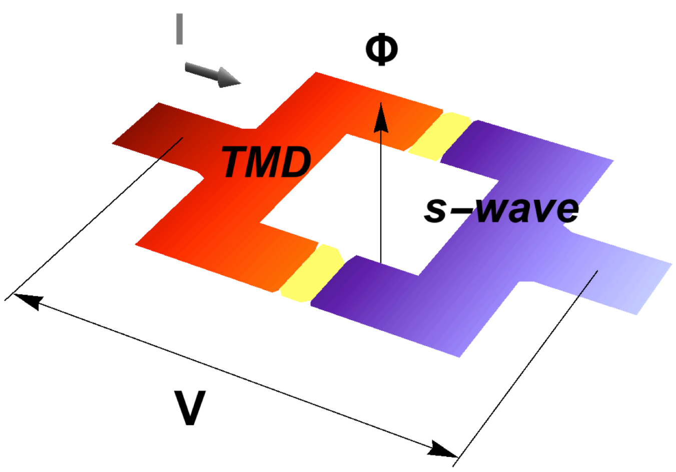
❑ Intra-pocket pairing

◆ Phase modulation



◆ SQUID loop in resistive mode:

- If TMD has modulated pairing
  ↑↑: pair momentum = 2K
  ↓↓: pair momentum = -2K

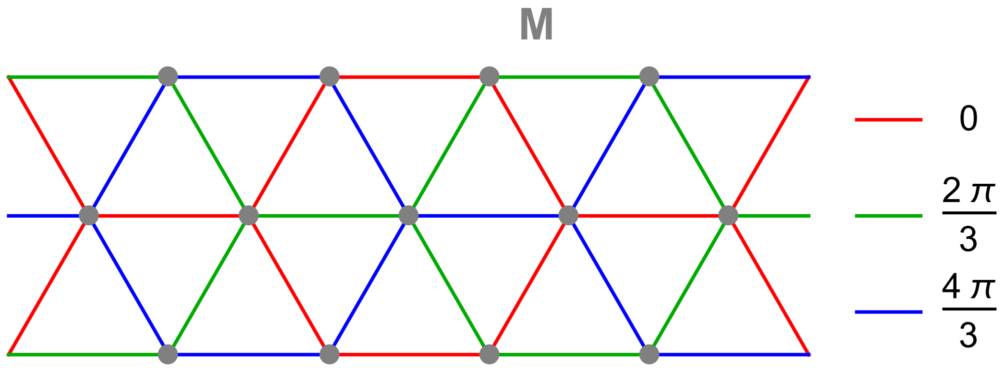


Match two sides' momenta
=> Two pairs tunnel together

Intrinsic : intra-pocket $\tilde{l} = 1$ pairing

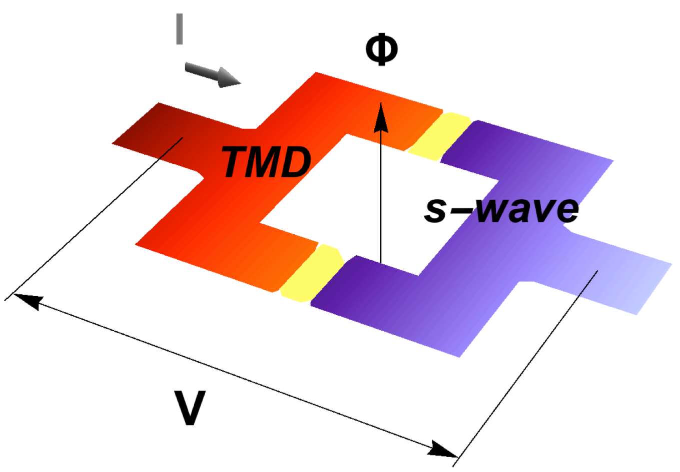
❑ Intra-pocket pairing

- Phase modulation



- SQUID loop in resistive mode:
  - If TMD has modulated pairing
    ↑↑: pair momentum = 2K
    ↓↓: pair momentum = -2K

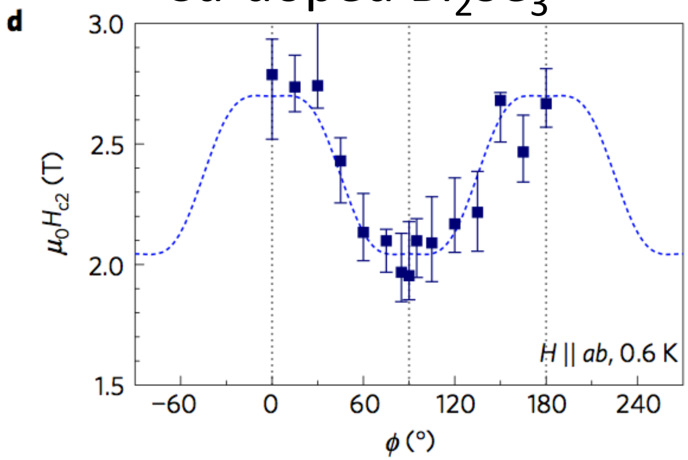
Period becomes hc/(4e) !



Proximity-induced pairing

- Nematic: angular dependence of the in-plane Hc_2 should be two-fold despite trigonal lattice

Cu-doped Bi_2Se_3



Yonezawa et al, Nphys (2016)

- Existence of triplet component:

  in-plane field dependence (?)