Valley Fluctuations and SO(4) Symmetry in Twisted Bilayer Graphene

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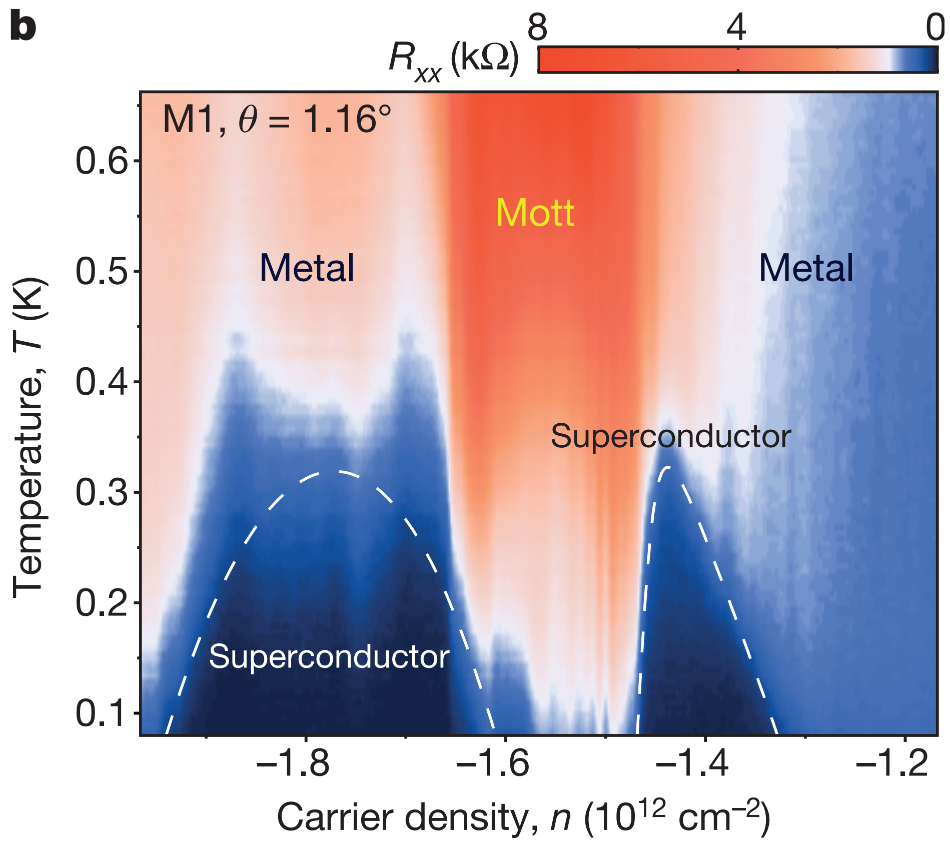
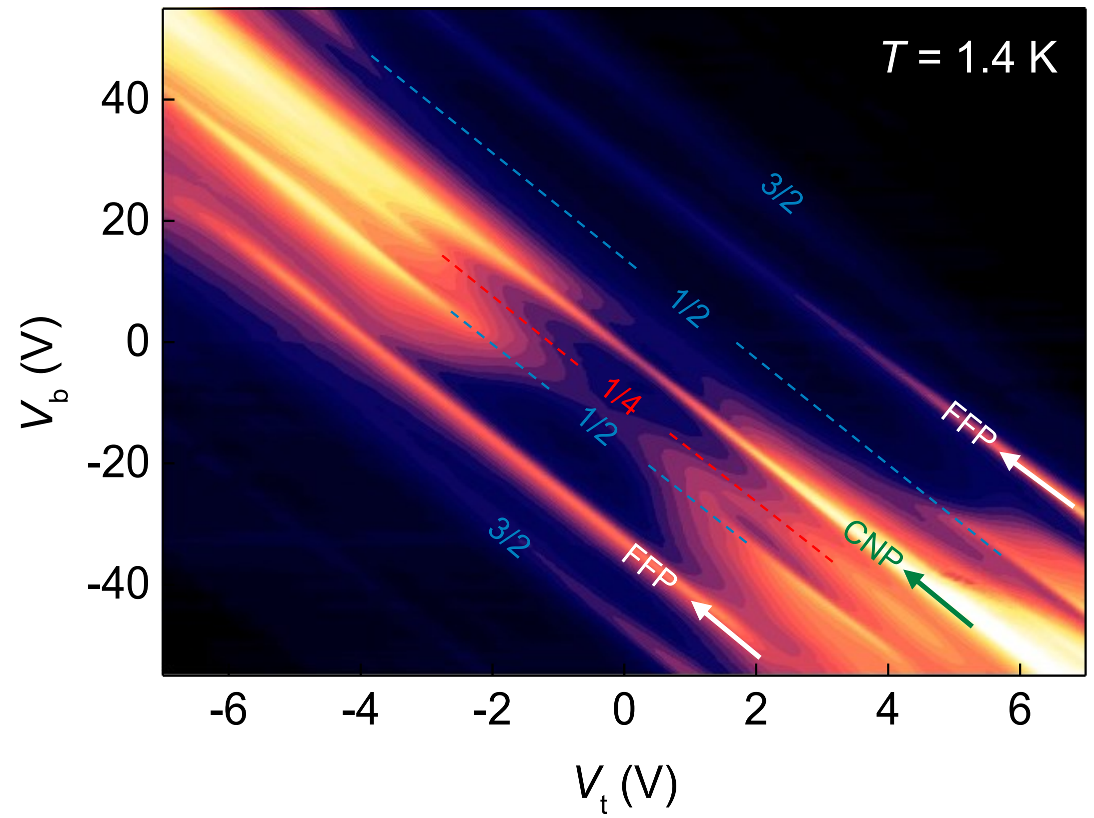
Y.-Z. You, A. Vishwanath, arXiv:1805.06867

KITS, July 2018

Background

- Mott insulator and superconductivity on Moire superlattice





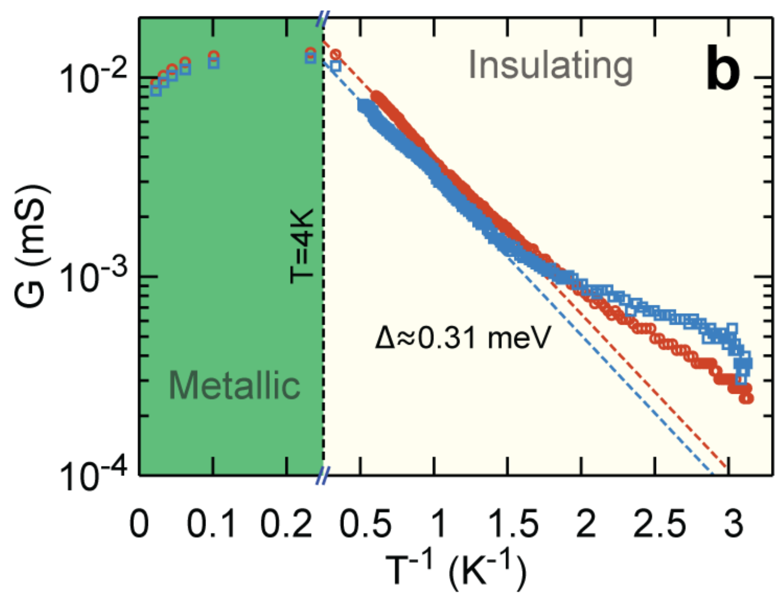
Cao, Fatemi et.al. Nature 2018

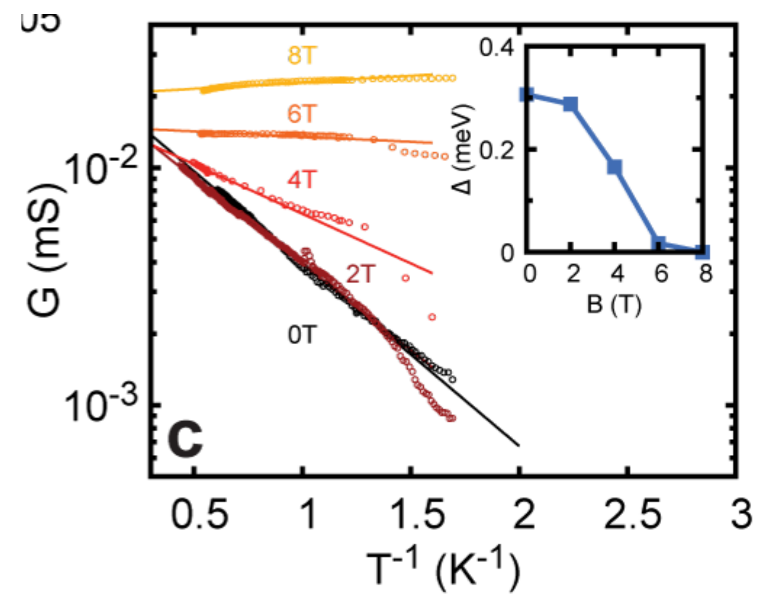
Chen et.al. 1803.01985

- Band width ~ interaction strength: correlated system
- Theoretical approaches
  - Strong coupling: starting from Mott limit
  - Weak coupling: starting from band limit

Background

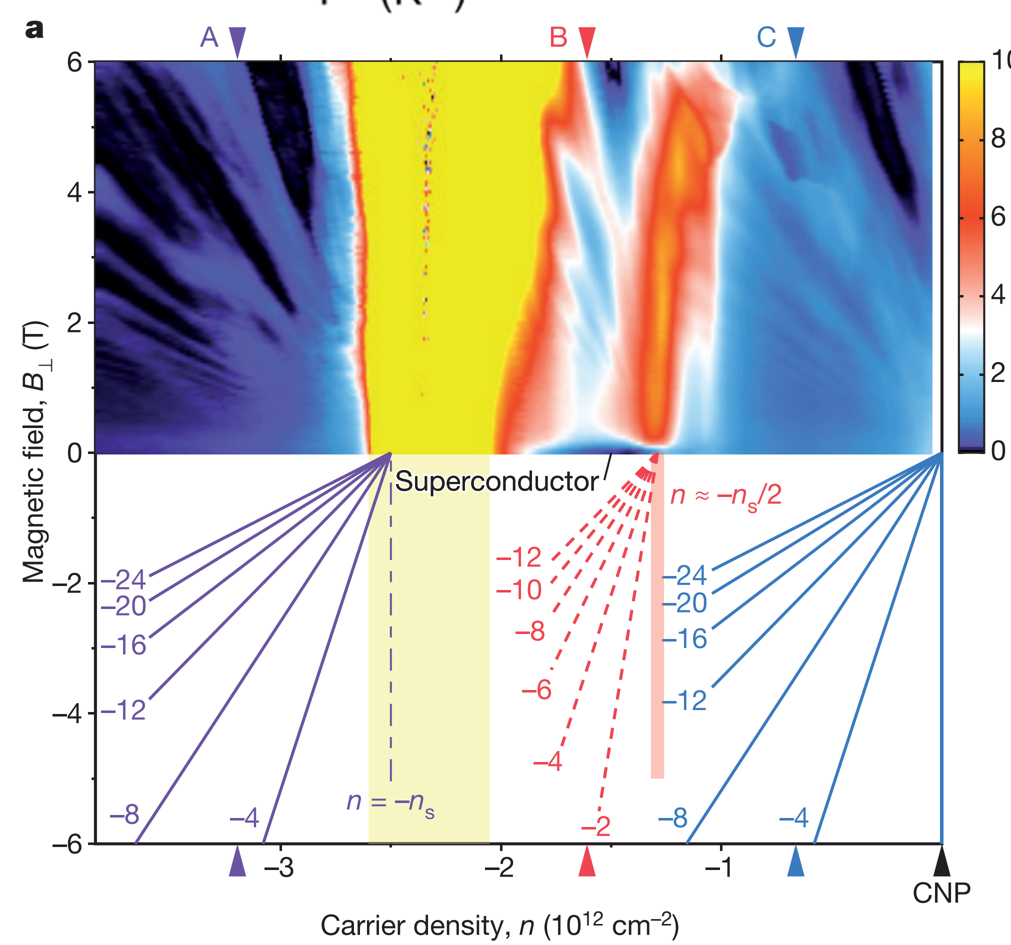
- Small Mott gap ~ 0.4meV compared to band width ~ 10 meV





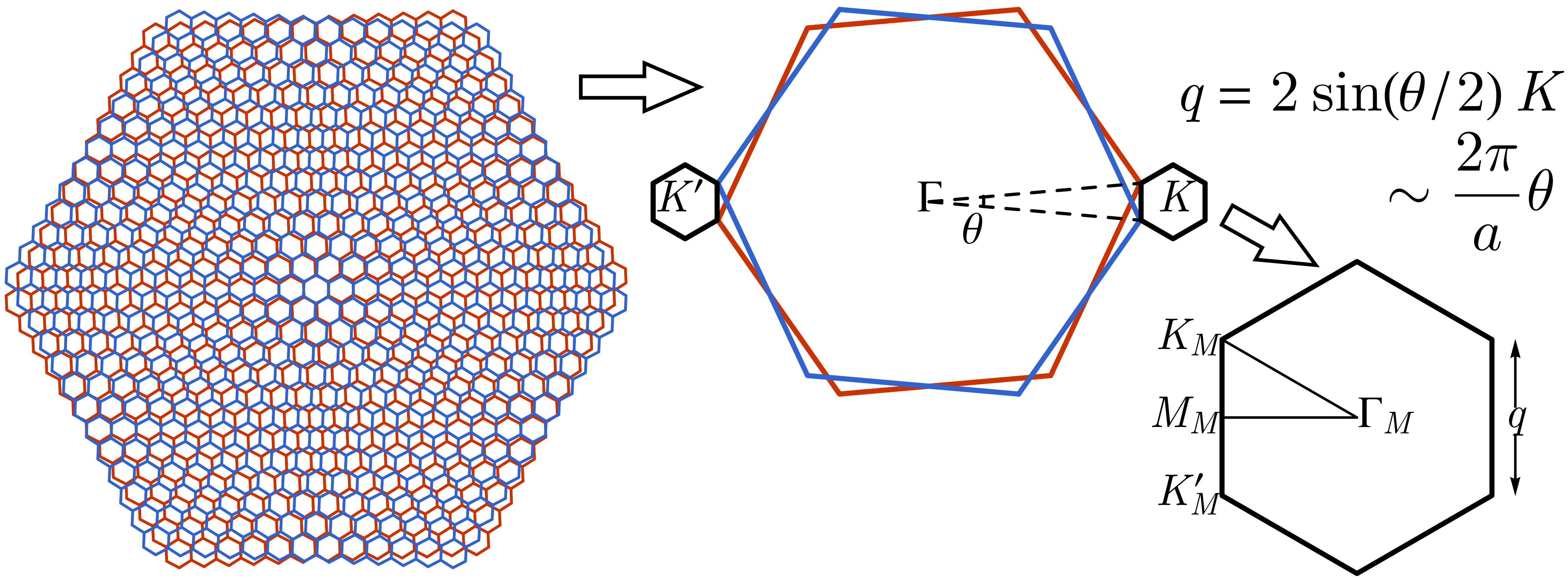
Cao, Fatemi et.al.
Nature 2018

- Different filling-factor sequences of Landau fans around the Mott insulator
  - 2,4,6,8 …
  - 4,8,12,16…



Band Structure

- We start with the weak coupling approach
- Twisted bilayer graphene



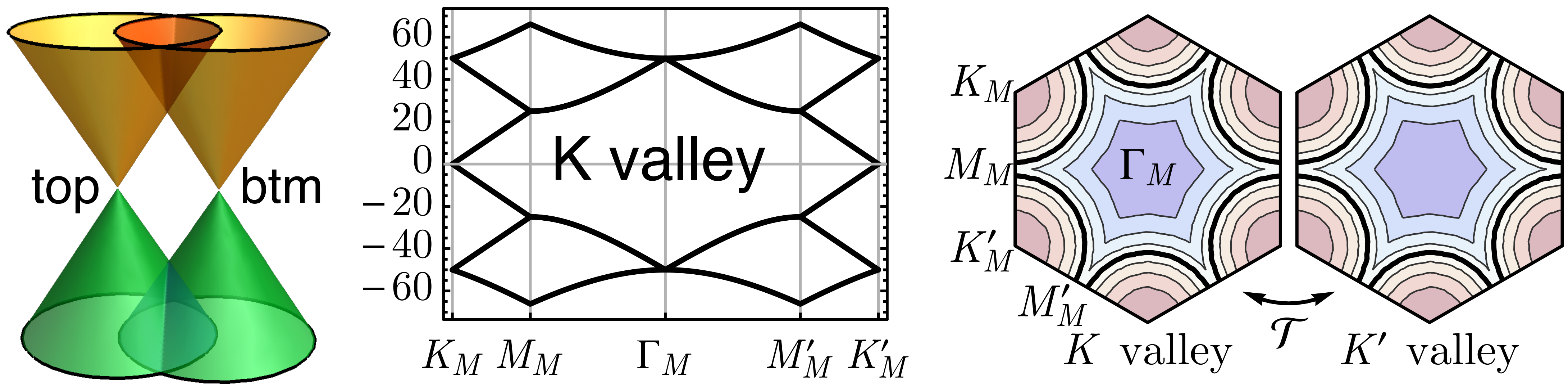
Moire superlattice

Moire Brillouin zone (MBZ)

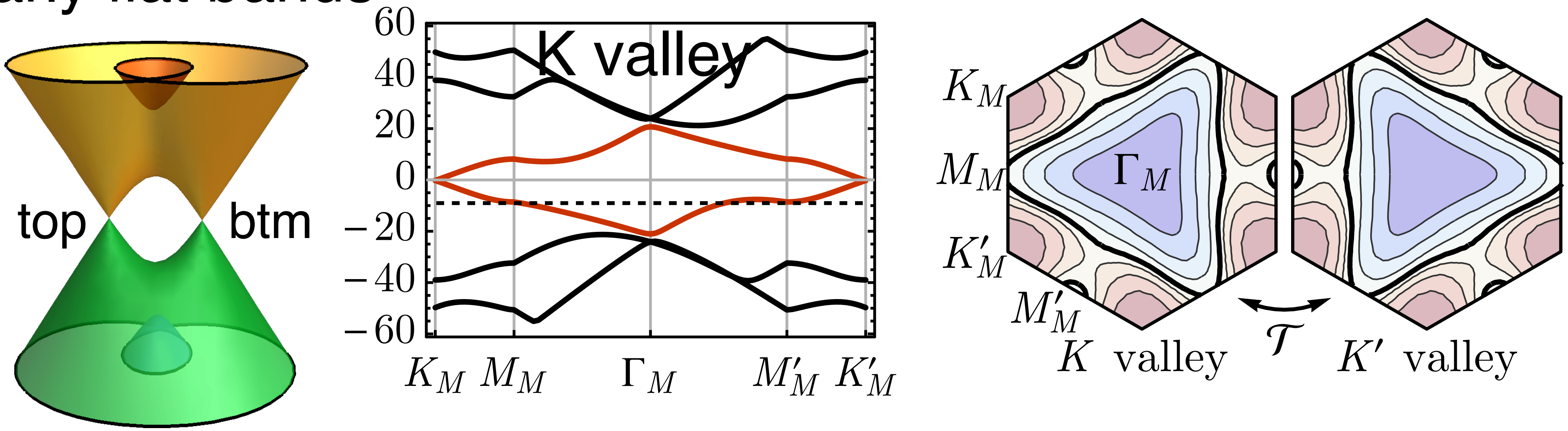
- Each super cell: 2 orbital (AB/BA) × 2 valley × 2 spin

Band Structure

- Without interlayer coupling, Dirac cones from top and bottom layers locate at conners of the MBZ



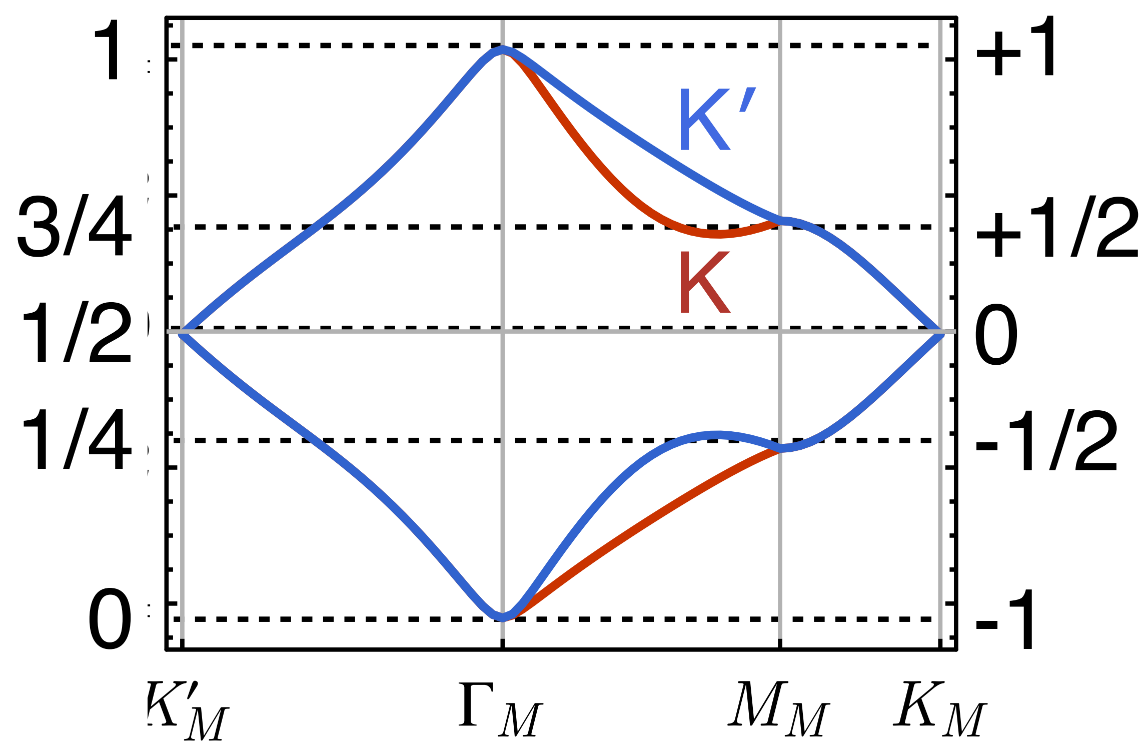
- With interlayer coupling, Dirac cones hybridize, leading to nearly flat bands



dos Santos et.al. 2007; Bistritzer, MacDonald, 2011

Band Structure

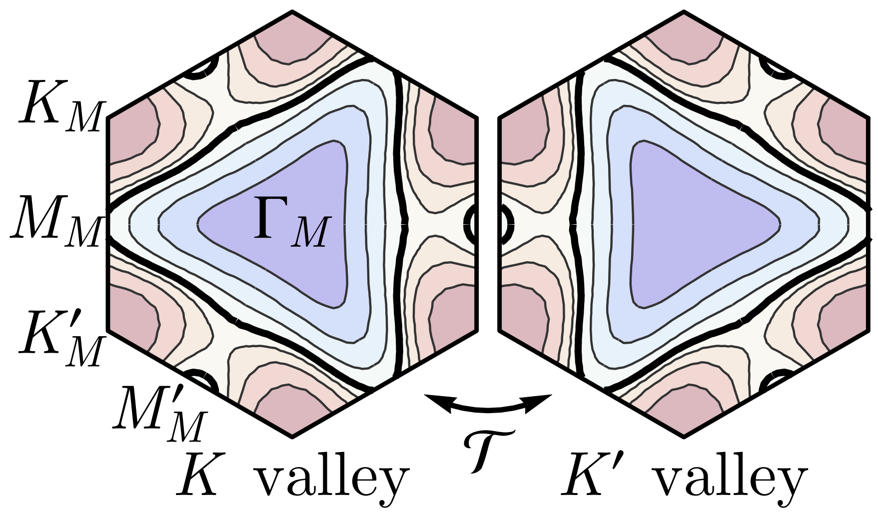
- Very close to the magic-angle, band structure is highly sensitive to parameters / lattice relaxation, hard to make universal statements.
- Stay away from magic (nominally θ ~ 2°)

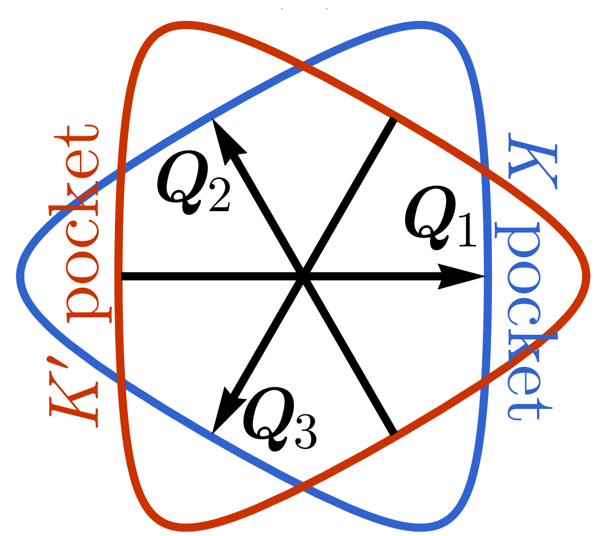


- Mott phases (and superconducting phases) found around ±1/2 filling.

Band Structure

- The triangular shape of Fermi surface is generic on symmetry ground (valley-preserving symmetries: $C_6 T$, M_y)





- Low-energy effective band theory: pocket model

$$H_0 = \sum_{\boldsymbol{k}} c^\dagger_{K\boldsymbol{k}} \epsilon_{\boldsymbol{k}} c_{K\boldsymbol{k}} + c^\dagger_{K'\boldsymbol{k}} \epsilon_{-\boldsymbol{k}} c_{K'\boldsymbol{k}},$$

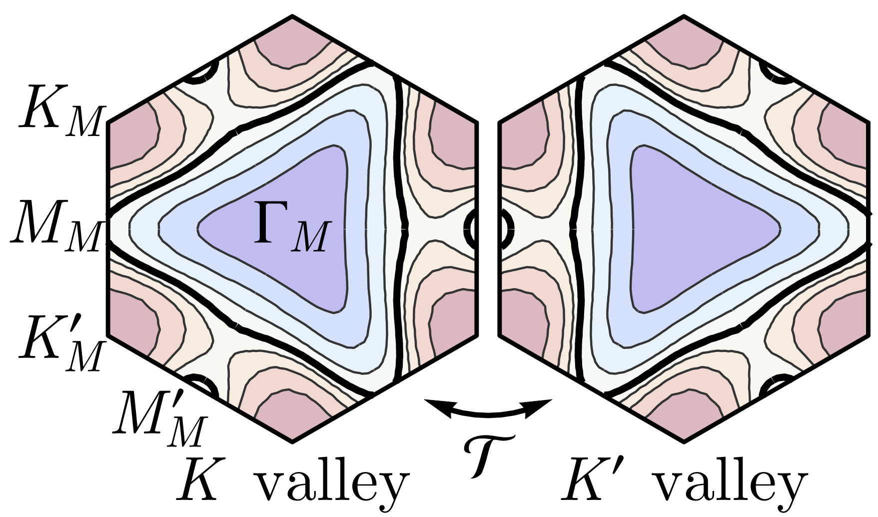
$\mathcal{T}$

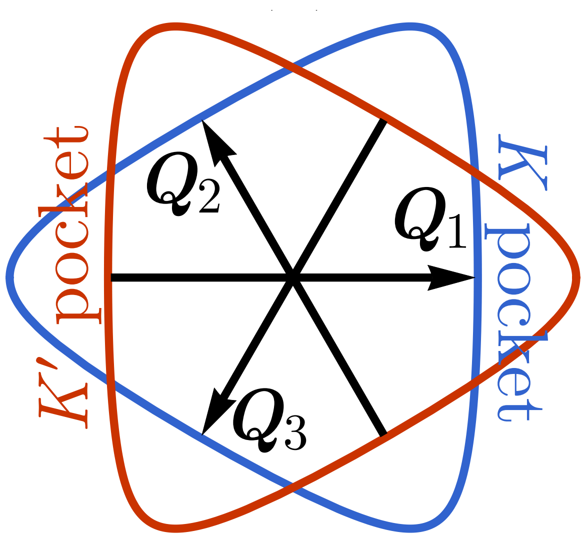
$$\epsilon_{\boldsymbol{k}} = \boldsymbol{k}^2 - \mu + \alpha \,\mathrm{Re}\, k_+^3, \qquad k_\pm \equiv k_x \pm \mathrm{i} k_y$$

- At each momentum: 2 valley × 2 spin (orbital frozen if we choose to focus on the lower branch)

Band Structure

- Working with pocket model in the momentum space circumvents the Wannier obstruction to construct valley-symmetric tight binding models. Po, Zou, Vishwanath, Senthil 1803.09742
- Parallel edges of the triangular Fermi surfaces are approximately nested





(at half-filling of the lower branch, or 1/4 filling of full band)

- Nesting vector close to M_M point momentum, but not exactly at that.

Zhu, Xiang, Zhang 1804.00302; Liu, Zhang, Chen, Yang 1804.10009

SO(4) Symmetry and Interaction

- 2 valley × 2 spin = 4 electron modes

$$(c_{K\uparrow}, c_{K\downarrow}, c_{K'\uparrow}, c_{K'\downarrow})$$

  - Emergent (approximate) $\mathrm{U}(4)$ symmetry?
  - Band structure breaks $\mathrm{U}(4)$ to $\mathrm{U}(1)_c \times \mathrm{U}(1)_v \times \mathrm{SO}(4)$ where $\mathrm{SO}(4) \sim \mathrm{SU}(2)_K \times \mathrm{SU}(2)_{K'}$ are two independent spin rotations in both valleys (approximate symmetry).

- Fermion bilinears can be classified by symmetry

<table>
<tr><td rowspan="4">$\mathrm{U}(4)$</td><td colspan="2">$\mathrm{U}(1)_c$</td><td colspan="4">$q_c = 0$</td><td colspan="2">$q_c = 2$</td></tr>
<tr><td colspan="2">$\mathrm{SU}(4)$</td><td>1</td><td colspan="3">15</td><td colspan="2">$6 \oplus 6'$</td></tr>
<tr><td>$\simeq$</td><td>$\mathrm{U}(1)_v$</td><td colspan="3">$q_v = 0$</td><td>$q_v = 2$</td><td>$q_v = 0$</td><td>$q_v = 2$</td></tr>
<tr><td>$\mathrm{SO}(6)$</td><td>$\mathrm{SO}(4)$</td><td>1</td><td>$1'$</td><td>6</td><td>$4 \oplus 4'$</td><td>$4 \oplus 4'$</td><td>$2(1 \oplus 1')$</td></tr>
<tr><td></td><td></td><td></td><td>n_c</td><td>n_v</td><td>$\boldsymbol{S}_v$</td><td>I^μ</td><td>Δ^μ</td><td>Δ_v</td></tr>
</table>

  - Their instabilities can be analyzed one by one

SO(4) Symmetry and Interaction

- SO(4) is not exact, but without further knowledge of how it is broken, we first ignore SO(4) breaking terms
- SO(4) Symmetric Interaction (in momentum space)

$$H_{\rm int} = \sum_{\boldsymbol{q}} U_0 n_{K-\boldsymbol{q}} n_{K'\boldsymbol{q}} + \frac{U_1}{2}(n_{K-\boldsymbol{q}} n_{K\boldsymbol{q}} + n_{K'-\boldsymbol{q}} n_{K'\boldsymbol{q}})$$

inter-valley density-density

intra-valley density-density

where density operator: $n_{v\boldsymbol{q}} \equiv \sum_{\boldsymbol{k},\sigma} c^\dagger_{v\sigma\boldsymbol{k}+\boldsymbol{q}} c_{v\sigma\boldsymbol{k}}$

- Full Hamiltonian

$$H = H_0 + H_{\rm int}$$

$$H_0 = \sum_{\boldsymbol{k}} c^\dagger_{K\boldsymbol{k}} \epsilon_{\boldsymbol{k}} c_{K\boldsymbol{k}} + c^\dagger_{K'\boldsymbol{k}} \epsilon_{-\boldsymbol{k}} c_{K'\boldsymbol{k}}$$

$$H_{\rm int} = \sum_{\boldsymbol{q}} U_0 n_{K-\boldsymbol{q}} n_{K'\boldsymbol{q}} + \frac{U_1}{2}(n_{K-\boldsymbol{q}} n_{K\boldsymbol{q}} + n_{K'-\boldsymbol{q}} n_{K'\boldsymbol{q}})$$

Random Phase Approximation

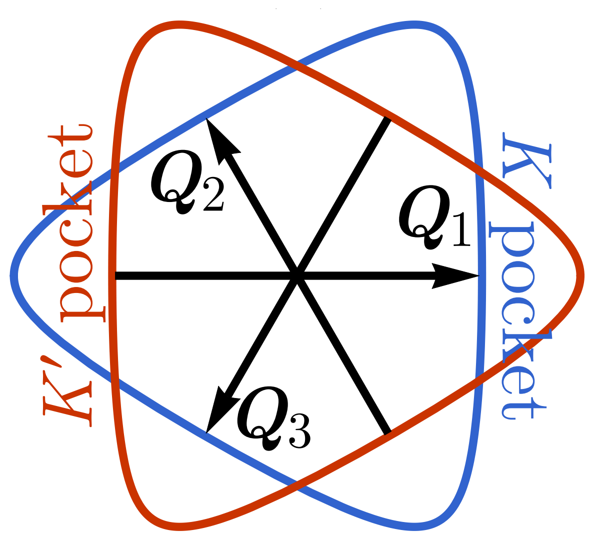
- Decouple the interaction in fermion bilinear channels

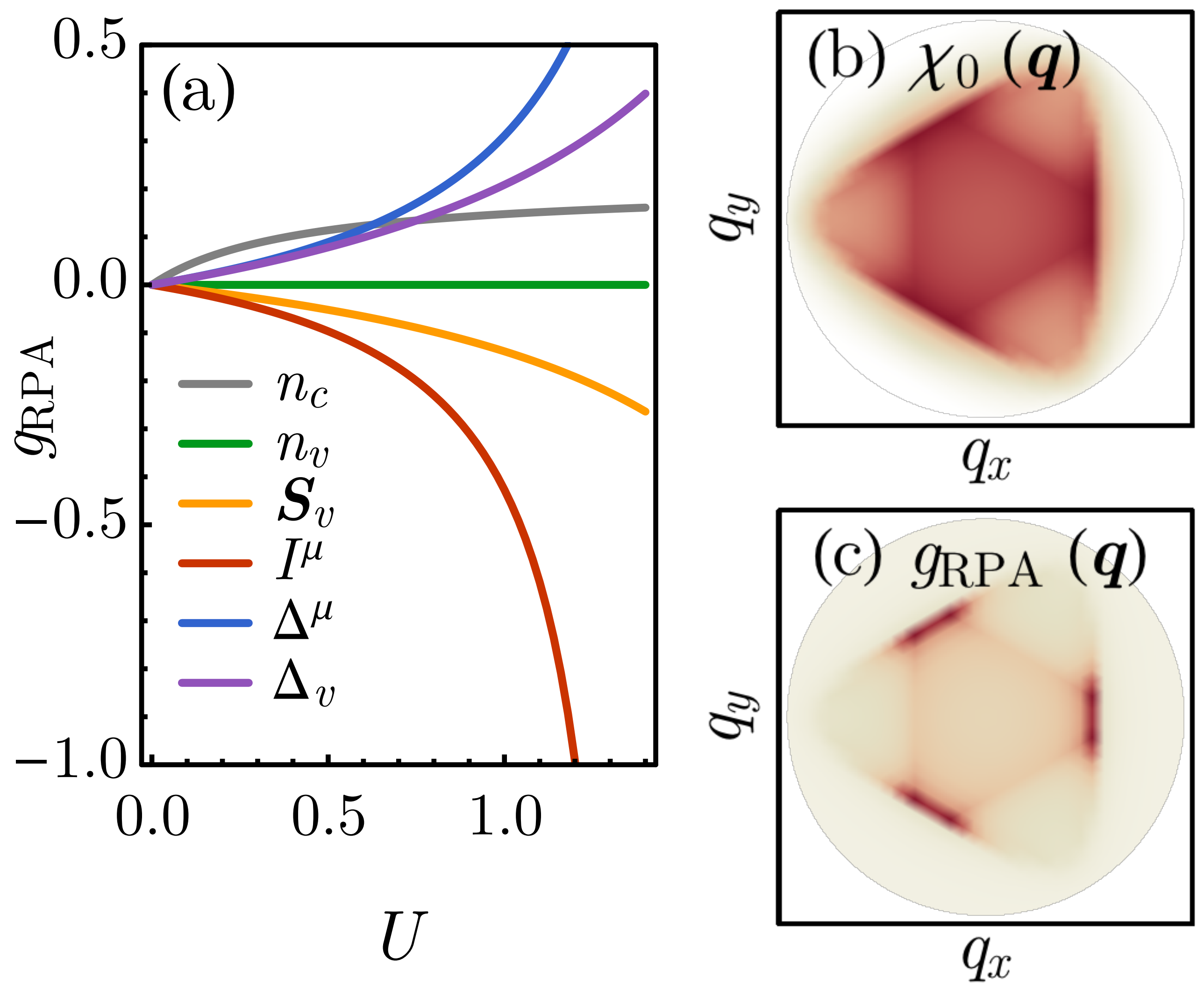
$$H_{\text{int}} = g_0 \sum_{\boldsymbol{q}} A_{\boldsymbol{q}}^{\dagger} A_{\boldsymbol{q}} + \cdots$$

- RPA corrected coupling $g_{\text{RPA}}(\boldsymbol{q}) = g_0(1 + g_0\chi_0(\boldsymbol{q}))^{-1}$
- Strongest instability appears in the inter-valley coherence (IVC) channel

$$I_{\boldsymbol{q}}^{\mu} = \sum_{\boldsymbol{k}} c_{K\boldsymbol{k}+\boldsymbol{q}}^{\dagger} \sigma^{\mu} c_{K'\boldsymbol{k}}$$

[O(4) vector] $\mu = 0, 1, 2, 3$





Superconductivity

- If the valley fluctuation does not condense, it could serves as a pairing glue.

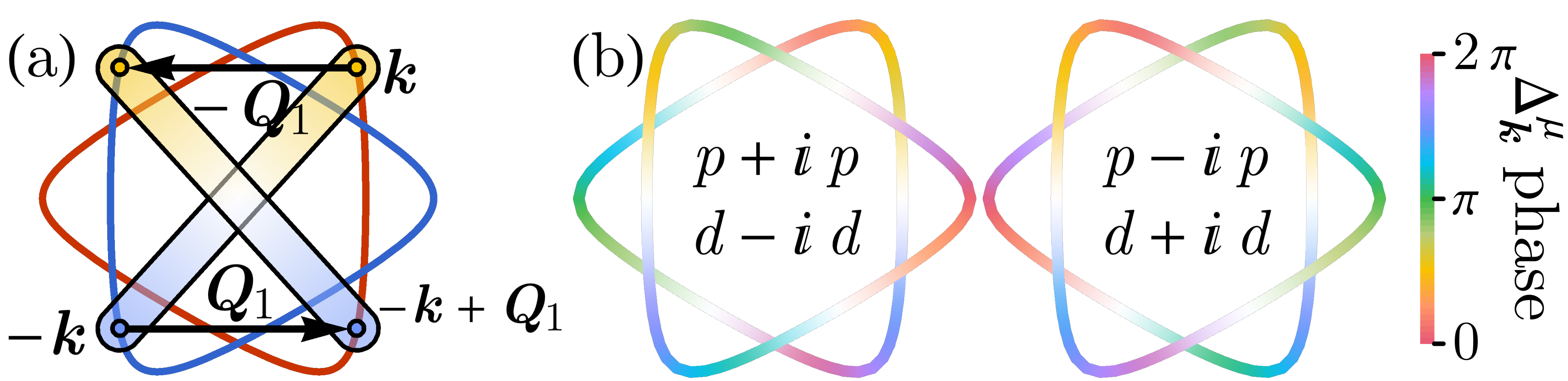
$$\sum_{\boldsymbol{q},\mu} g_{\text{RPA}}(\boldsymbol{q}) I_{\boldsymbol{q}}^{\mu\dagger} I_{\boldsymbol{q}}^{\mu} \simeq -\sum_{\boldsymbol{q},\boldsymbol{k},\mu} g_{\text{RPA}}(\boldsymbol{q}) \Delta_{-\boldsymbol{k}+\boldsymbol{q}}^{\mu\dagger} \Delta_{\boldsymbol{k}}^{\mu} \quad (g_{\text{RPA}} < 0)$$

- Inter-valley pairing $\Delta_{\boldsymbol{k}}^{\mu} = c_{K\boldsymbol{k}}^{\intercal} \mathrm{i}\sigma^2 \sigma^{\mu} c_{K'-\boldsymbol{k}}$ [O(4) vector]
  - Spin-singlet $\Delta_{\boldsymbol{k}}^{0}$
  - Spin-triplet $\boldsymbol{\Delta}_{\boldsymbol{k}} = (\Delta_{\boldsymbol{k}}^{1}, \Delta_{\boldsymbol{k}}^{2}, \Delta_{\boldsymbol{k}}^{3})$

(Valley sym. will adjust)

- Linearized gap equation $\sum_{\boldsymbol{k}' \in \text{FS}} v_F^{-1}(\boldsymbol{k}') g_{\text{RPA}}(\boldsymbol{k}+\boldsymbol{k}') \Delta_{\boldsymbol{k}'}^{\mu} = \lambda \Delta_{\boldsymbol{k}}^{\mu}$

$$\Delta_{\boldsymbol{k}}^{\mu} = -\Delta_{-\boldsymbol{k}+\boldsymbol{Q}_a}^{\mu}$$



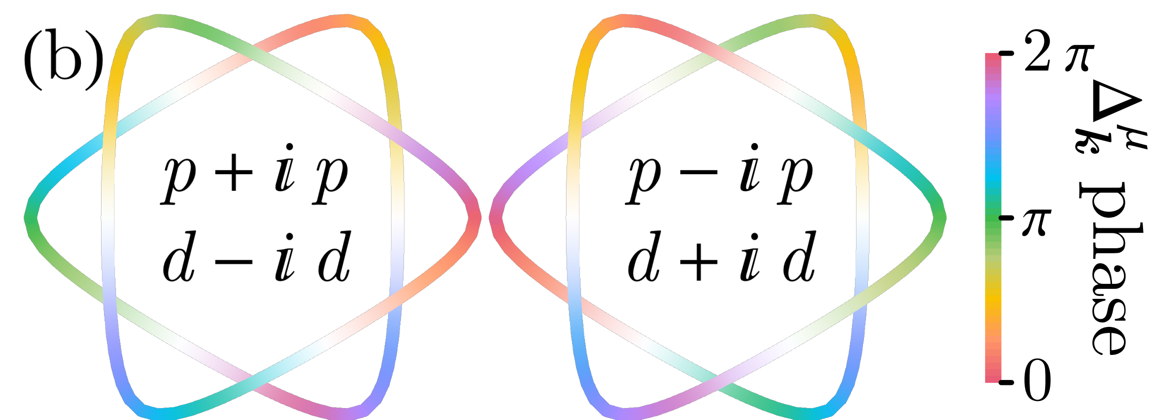
Superconductivity

- Leading gap function

$$\Delta^{\mu}_{\boldsymbol{k}} = u^{\mu} w_{\boldsymbol{k}} + v^{\mu} w^{*}_{\boldsymbol{k}}$$

$$w_{\boldsymbol{k}} = w_d k_+^2 + w_p k_-$$

$(d + \mathrm{i}d) \quad (p - \mathrm{i}p)$



degenerated

- Band structure only C_3 symmetric → d+id and p-ip must mix on symmetry ground

- Landau-Ginzburg theory (beyond linearized gap equation)

$$F = \sum_{\boldsymbol{k}} r \Delta^{\mu *}_{\boldsymbol{k}} \Delta^{\mu}_{\boldsymbol{k}} + \kappa (2 (\Delta^{\mu *}_{\boldsymbol{k}} \Delta^{\mu}_{\boldsymbol{k}})^2 - |\Delta^{\mu}_{\boldsymbol{k}} \Delta^{\mu}_{\boldsymbol{k}}|^2) + \cdots$$

$$\text{chiral}: \begin{cases} u^{\mu} = e^{\mathrm{i}\phi} n^{\mu}, \\ v^{\mu} = 0, \end{cases} \quad \text{helical}: \begin{cases} u^{\mu} = e^{\mathrm{i}\phi_1} (n_1^{\mu} + \mathrm{i} n_2^{\mu}), \\ v^{\mu} = e^{\mathrm{i}\phi_2} (n_1^{\mu} - \mathrm{i} n_2^{\mu}), \end{cases}$$

(Type A) (Type B)

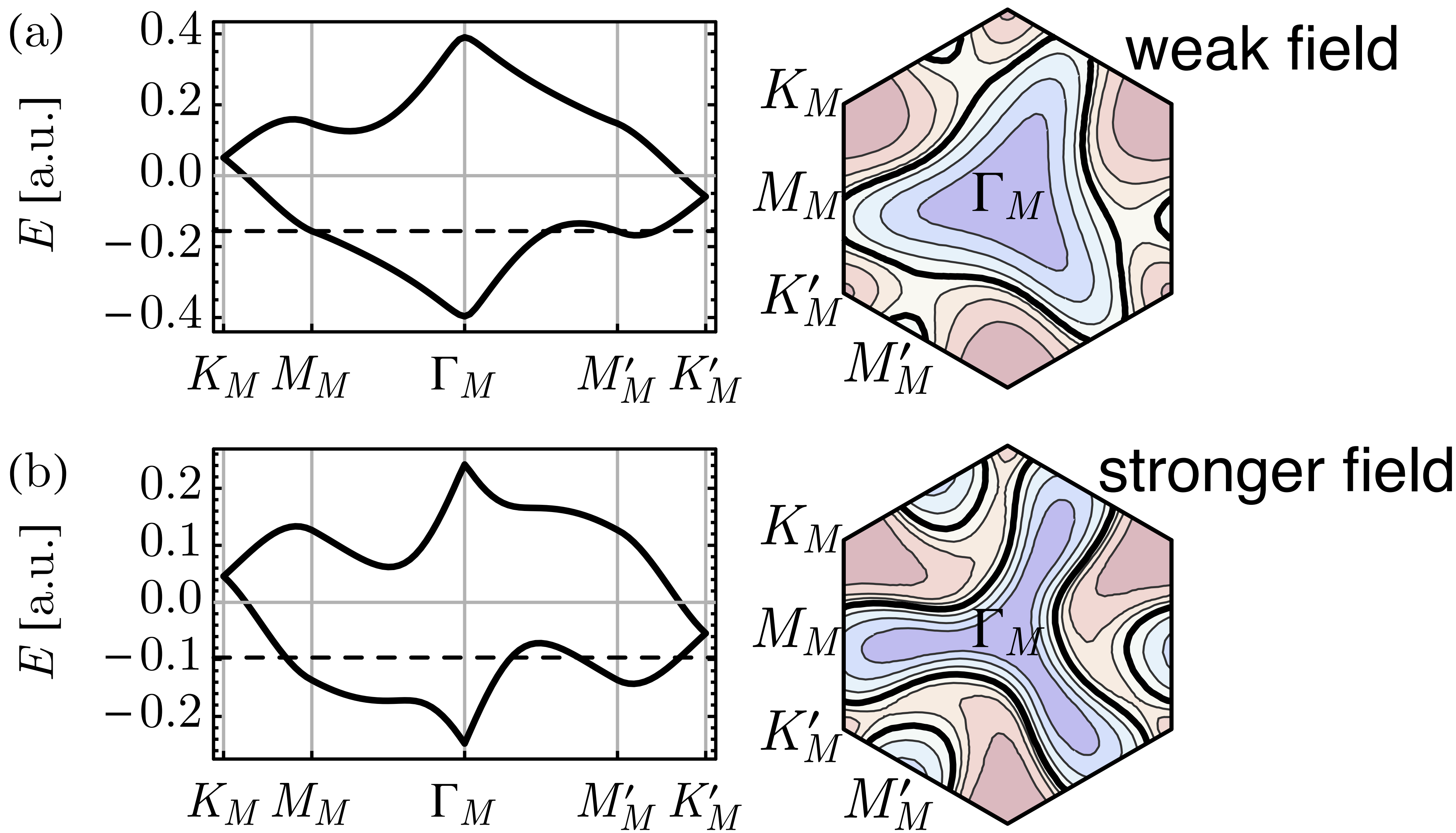
Xu, Balents 1803.08057

Superconductivity

- Topological Superconductor $\Delta_{\boldsymbol{k}}^{\mu} = c_{K\boldsymbol{k}}^{\intercal} \mathrm{i}\sigma^2 \sigma^{\mu} c_{K'-\boldsymbol{k}}$
  - Chiral $\Delta_{\boldsymbol{k}}^{\mu} = e^{\mathrm{i}\phi} n^{\mu} w_{\boldsymbol{k}}$
    - 4 copies of d+id or p-ip (2 valley × 2 spin)
    - $\mathrm{U}(1)_c \times \mathrm{U}(1)_v \times \mathrm{SO}(4) \times \mathbb{Z}_2^{\mathcal{T}} \to \mathbb{Z}_2^F \times \mathrm{U}(1)_v \times \mathrm{SO}(3)$
  - Helical $\Delta_{\boldsymbol{k}}^{\mu} = e^{\mathrm{i}\phi}(n_1^{\mu} \,\mathrm{Re}\, w_{\boldsymbol{k}} + n_2^{\mu} \,\mathrm{Im}\, w_{\boldsymbol{k}}) \qquad n_1^{\mu} n_2^{\mu} = 0$
    - 2 copies of d±id or p∓ip (2 "valley")
    - $\mathrm{U}(1)_c \times \mathrm{U}(1)_v \times \mathrm{SO}(4) \times \mathbb{Z}_2^{\mathcal{T}} \to \mathbb{Z}_2^F \times \mathrm{U}(1)_v \times \mathrm{SO}(2) \times \mathbb{Z}_2^{\mathcal{T}}$
- Topological transition between d/p-wave: 12 Majorana cones
- Consider SO(4) explicitly broken to SO(3)
  - spin-singlet pairing: can only be chiral
  - spin-triplet pairing: can be both chiral and helical

Electric Field Effect

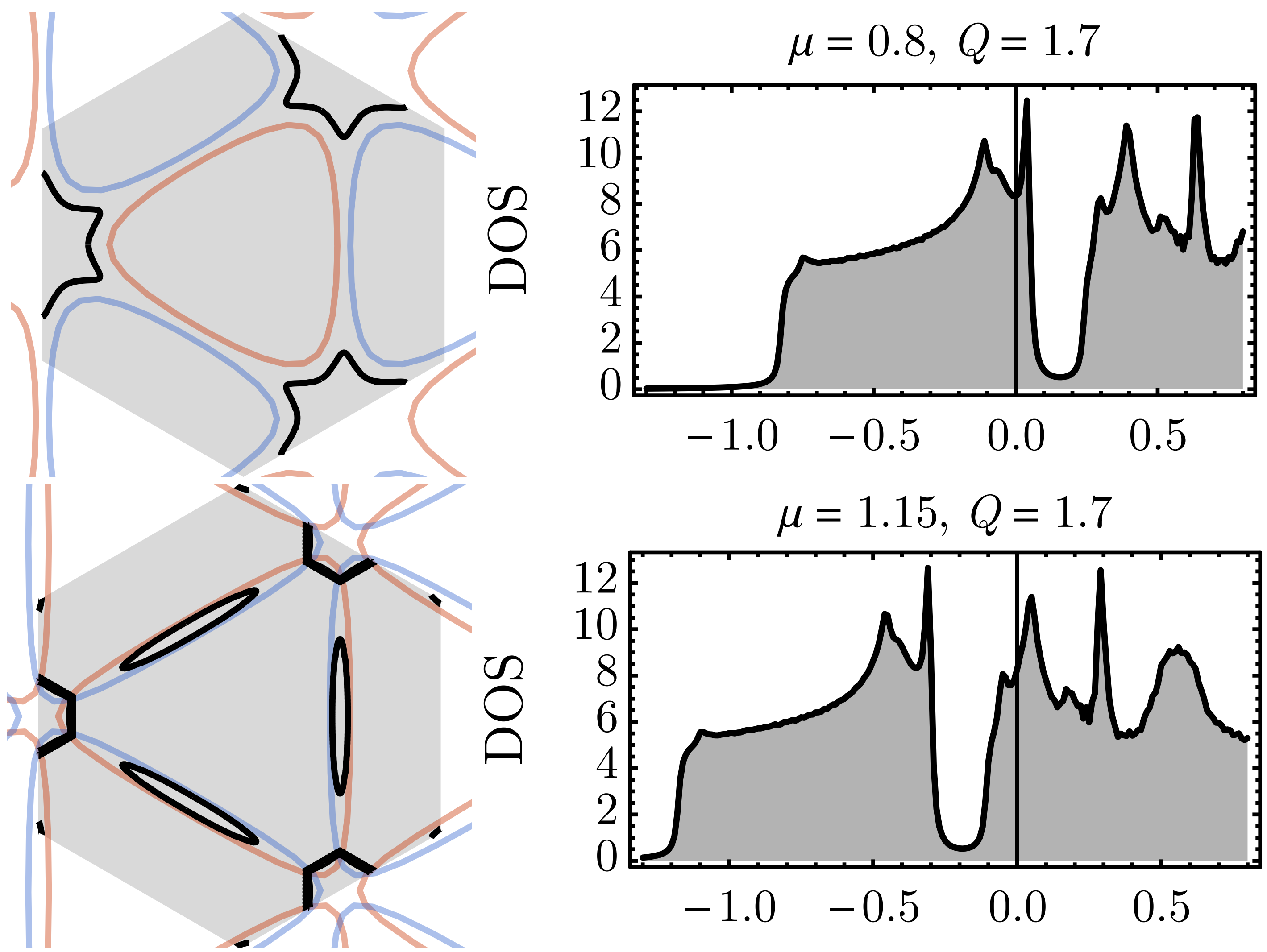
- Applying vertical electric field: destroy nesting → suppress valley fluctuations and superconductivity



Valley Order and Slater Insulator

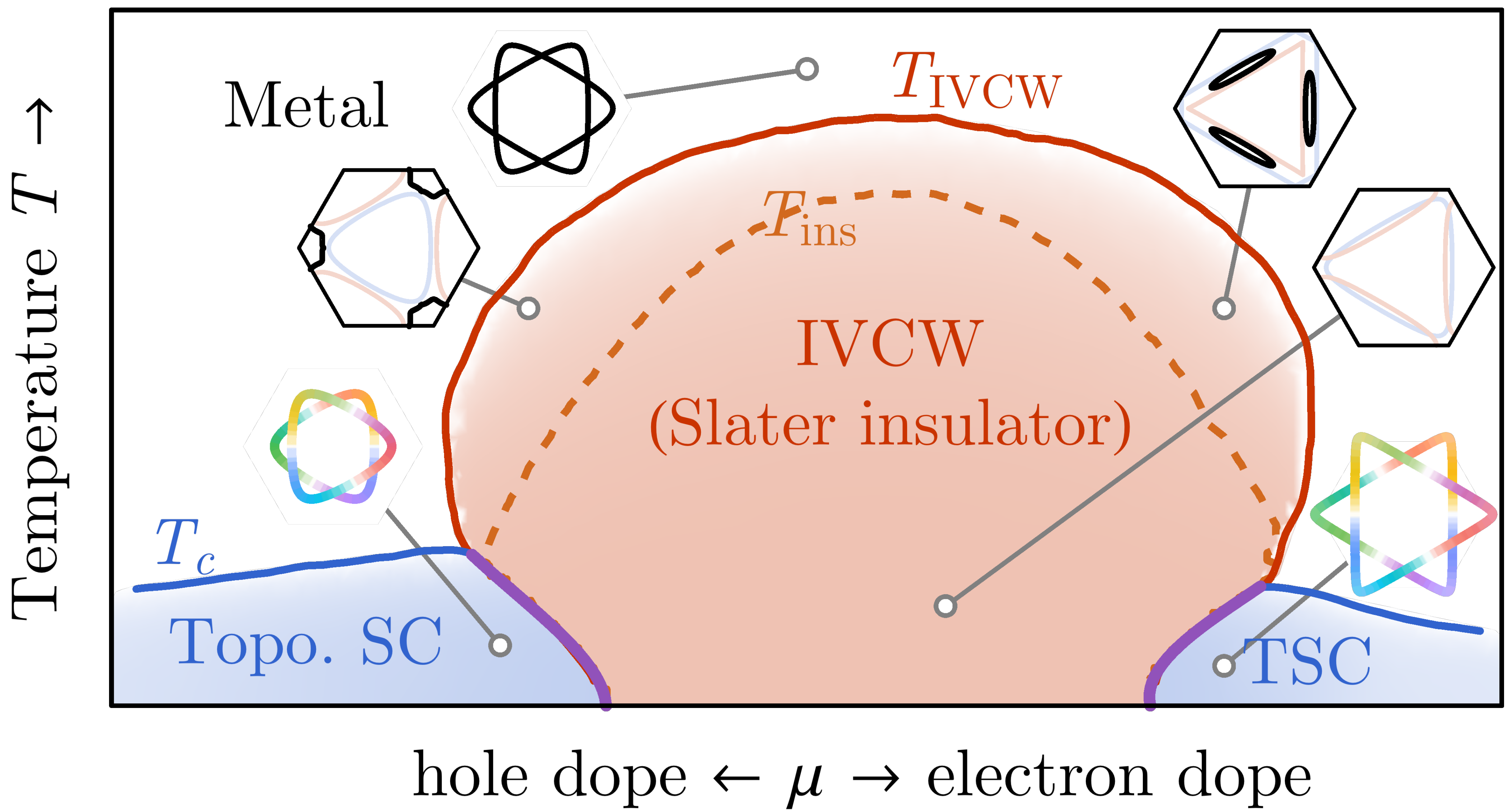
- If the valley fluctuation condenses → IVC wave order
- Will it open a full gap?
  - Typically not. If away from optimal nesting, small Fermi pockets remains.

(pocket model)



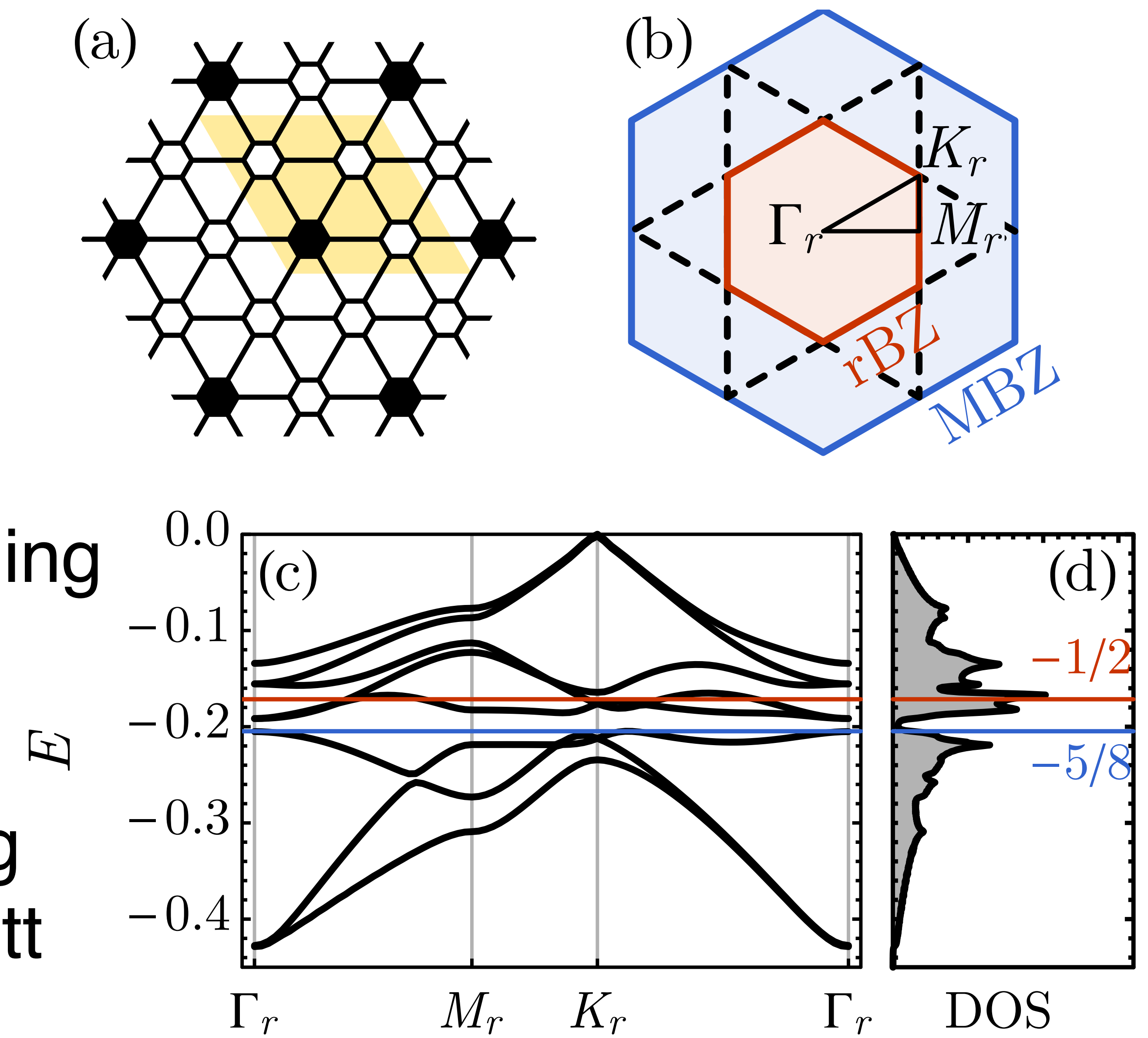
Valley Order and Slater Insulator

- If the valley fluctuation condenses → IVC wave order
- Will it open a full gap?
  - Mean field phase diagram (pocket model)



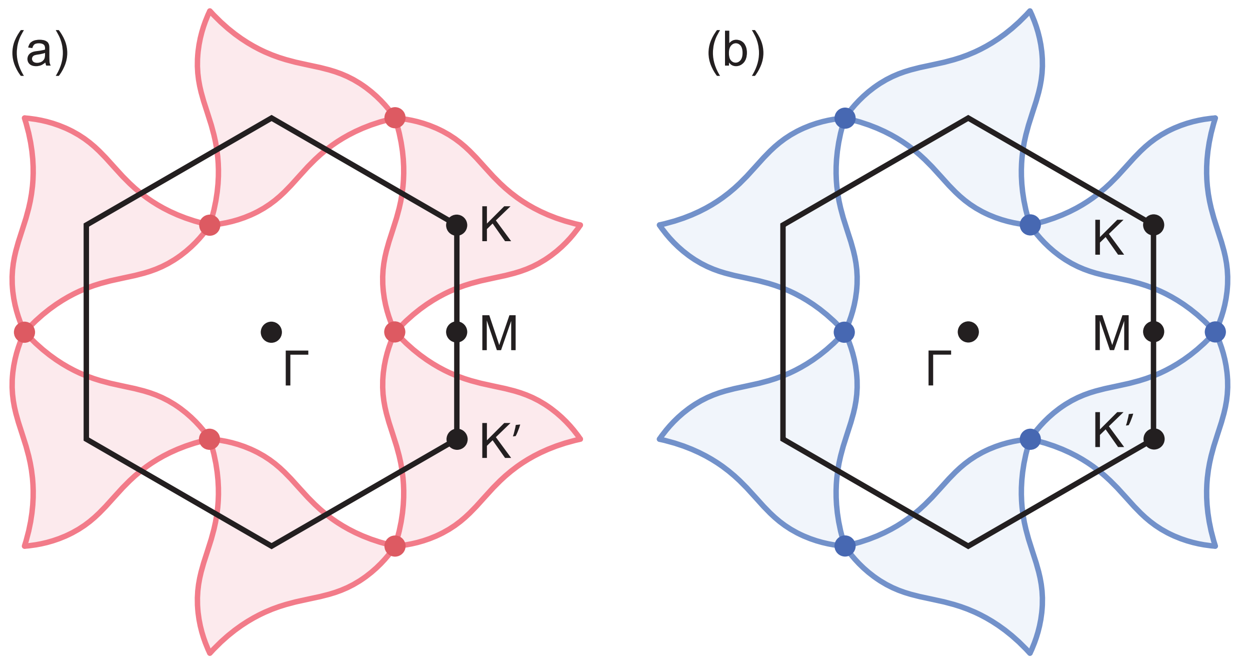
Valley Order and Slater Insulator

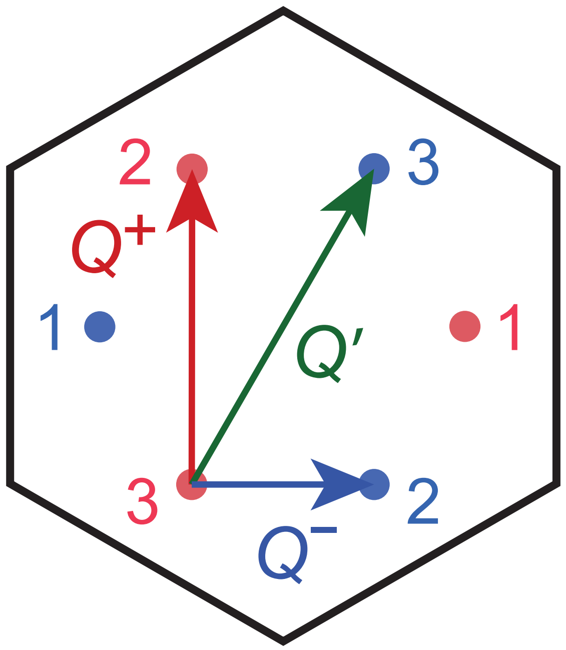
- If the valley fluctuation condenses → IVC wave order
- Will it open a full gap?
  - Consider a commensurate IVC wave order
  - Ordering momentum = Moire *M*-point (2×2 modulation)
  - 2 valley × 4 sublattice = 8 bands
  - Full gap opens at -5/8 filling from charge neutrality (not at -1/2 filling)
- Conclusion: Valley ordering not sufficient to explain Mott

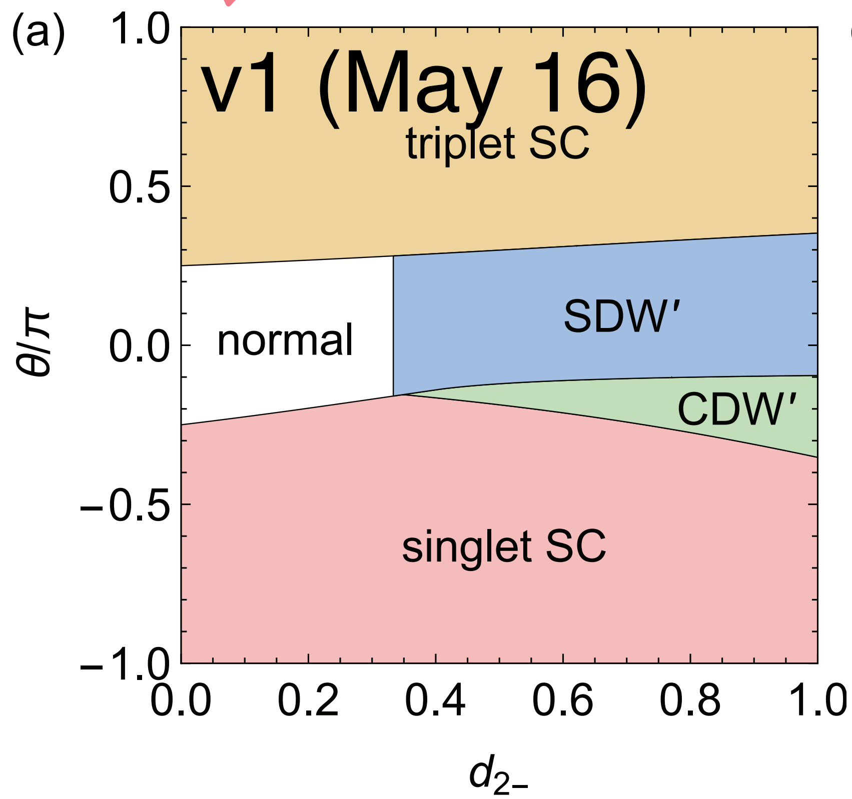


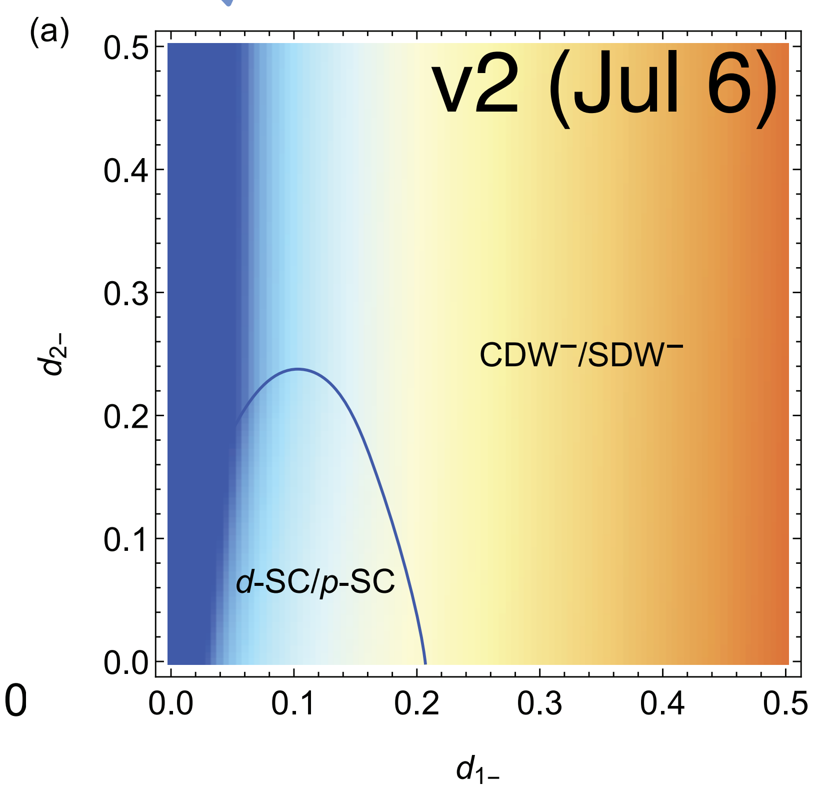
Valley Order and Slater Insulator

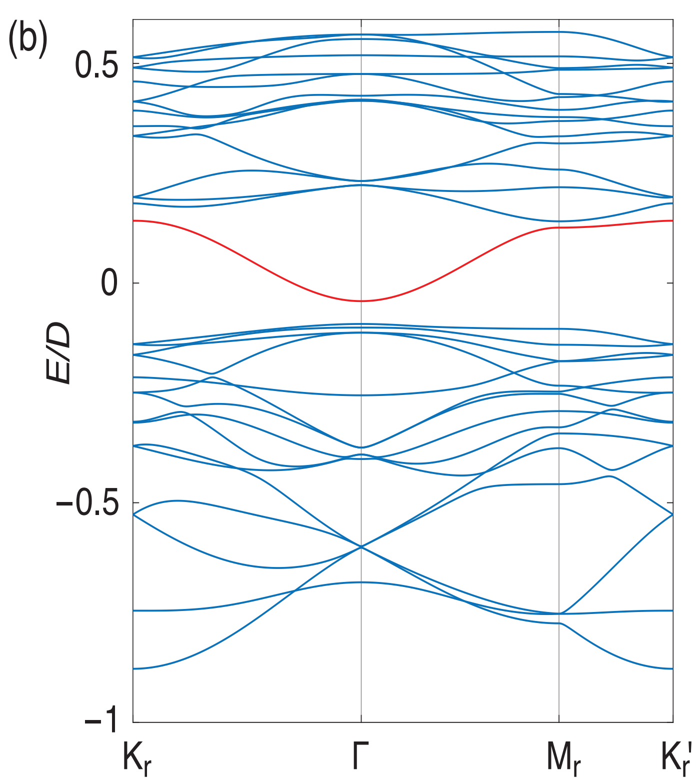
- Hot spot RG [Isobe, Yuan, Fu 1805.06449]





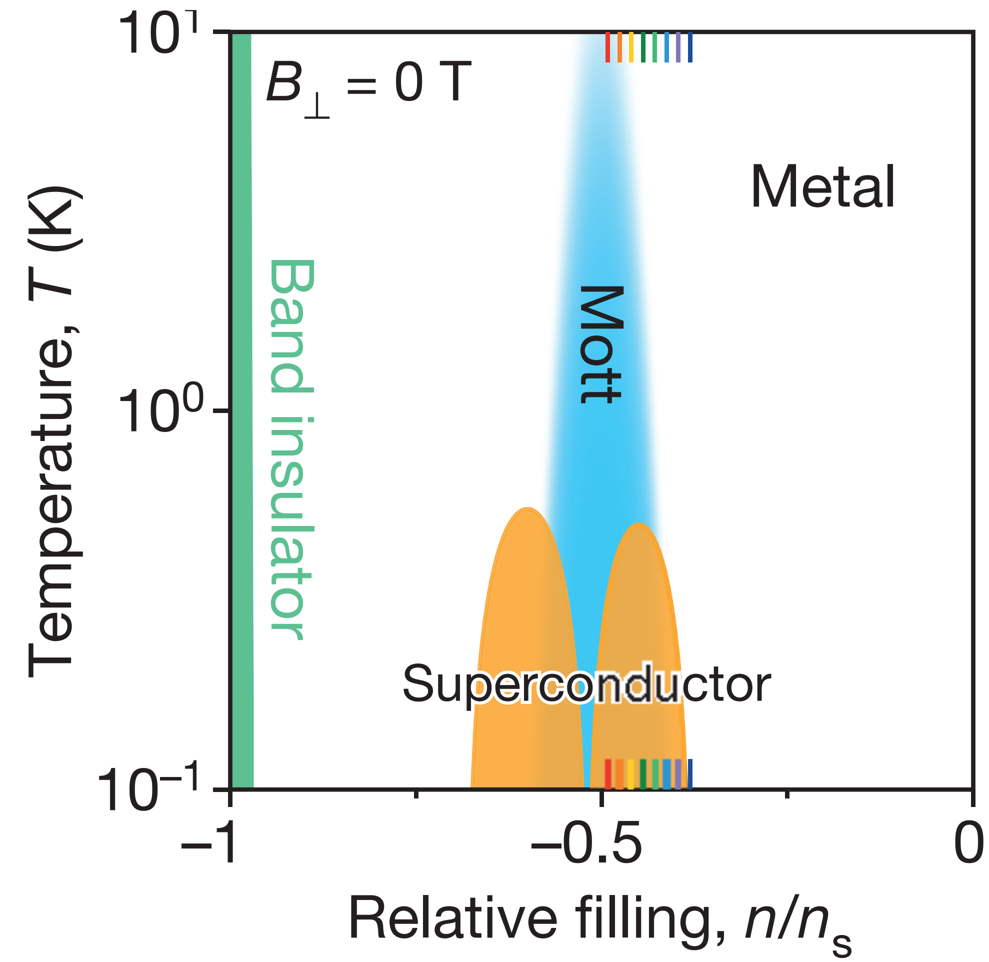






Topological Order and Mott Insulator

- Mott phase is adjacent to superconducting phases
- Strong Coupling Approach
  - Starting from the SC phase
  - Suppress charge fluctuations by proliferating double vortices of SC order parameter
  - Single vortex becomes anyonic excitation → topological order



Cao et.al. Nature 2018

  - The topological order will be determined by the type of the superconducting order in the adjacent phase.
- This approach circumvents the explicit lattice realization.

Topological Order and Mott Insulator

- Field theory formulation
  - Fractionalization of electron $c_{v\sigma} = b f_{v\sigma}$
  - Assign $\mathrm{U}(1)_c$ quantum number to bosonic parton, and $\mathrm{U}(1)_v \times \mathrm{SO}(4)$ quantum number to fermionic parton.
  - Place the fermionic parton in the SC mean-field state, gap out bosonic parton → valley-spin liquid (VSL)

SC phase		Mott phase	
type	pairing	state	symmetry
chiral	$d+\mathrm{i}d$	$\mathrm{SO}(8)_1$ VSL	$\mathrm{U}(1)_c \times \mathrm{U}(1)_v$ $\times \mathrm{SO}(3)$
	$p-\mathrm{i}p$	$\mathrm{SO}(4)_{-1}$ VSL	
helical	$d \pm \mathrm{i}d$	$\mathbb{Z}_2$ VSL + BSPT	$\mathrm{U}(1)_c \times \mathrm{U}(1)_v$ $\times \mathrm{U}(1)_s \times \mathbb{Z}_2^{\mathcal{T}}$
	$p \mp \mathrm{i}p$	$\mathbb{Z}_2$ VSL (SET)	

Topological Order and Mott Insulator

- These topological order all have four anyon sectors, labeled by {1, e, m, f}
- Chiral Valley-Spin Liquid (VSL) $\mathrm{U}(1)_c \times \mathrm{U}(1)_v \times \mathrm{SO}(3)$
  - $\mathrm{SO}(4)_{-1}$ VSL (from $p - \mathrm{i}p$ TSC) $c = -2$
    - e and m are semions: one carries spin-1/2, the other carries valley charge.
    - They fuse to fermion f, that carries both spin and valley quantum numbers.
  - $\mathrm{SO}(8)_1$ VSL (from $d + \mathrm{i}d$ TSC) $c = 4$
    - e, m, f are fermions: m carries no symmetry charge; e and f carries both spin and valley.
- Chiral central charge → thermal Hall conductance

$$\kappa_{\mathrm{H}} = c\pi k_B^2 T/(6\hbar)$$

Topological Order and Mott Insulator

- Helical Valley-Spin Liquid $\mathrm{U}(1)_c \times \mathrm{U}(1)_v \times \mathrm{U}(1)_s \times \mathbb{Z}_2^{\mathcal{T}}$
  - $\mathbb{Z}_2$ topological order (toric code) with {1, e, m, f}
  - Topological response between valley and spin

$$\mathcal{L}[A_v, A_s] = \frac{\sigma_{\mathrm{vsH}}}{2\pi} A_v \wedge \mathrm{d}A_s$$

  - Symmetry enriched topological (SET) state (from $p \mp \mathrm{i}p$)
    - Symmetry fractionalization: e and m separately carry valley and spin
    - Fractionalized valley-spin Hall $\sigma_{\mathrm{vsH}} = -1/2$
  - Symmetry protected topological (SPT) state (from $d \pm \mathrm{i}d$)
    - m is neutral and Kramers singlet → can condense …
    - Integer valley-spin Hall $\sigma_{\mathrm{vsH}} = 1$

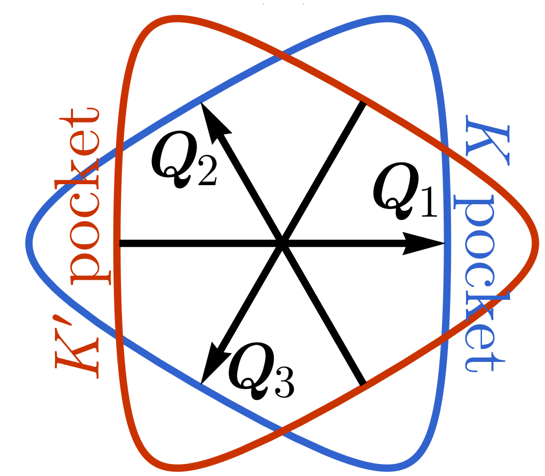
Explicit SO(4) Symmetry Breaking

- SO(4) is not exact. There are always small SO(4) breaking terms.
  - Inter-valley AFM spin-spin interaction (anti-Hund's)
  $$H_J = \sum_{\boldsymbol{q}} J(\boldsymbol{q}) \boldsymbol{S}_{K\boldsymbol{q}} \cdot \boldsymbol{S}_{K'-\boldsymbol{q}}$$
  - Spin locking $\mathrm{SO}(4) \sim \mathrm{SU}(2)_K \times \mathrm{SU}(2)_{K'} \to \mathrm{SO}(3)$
  - Favors both spin-singlet IVC wave and spin-singlet pairing, which is consistent with the fact that Zeeman field kills both Mott and SC gaps.
  - But the microscopic origin (and the generality) of anti-Hund's is not clear yet …

Dodaro, Kivelson et.al. 1804.03163

Summary

- Pocket model with SO(4) symmetry is analyzed by weak coupling approach
  - Inter-valley coherence wave (IVCW)
  - Valley fluctuation driven topological SC



- In our model,
  - d+id always mixed with p-ip due to triangular distortion
  - Nesting typically do not happen at half-filling
  - Small Fermi surface may appear on both sides of doping
  - Proliferating double-vortex from topological SC leads to exotic Mott phase with topological order (SET/SPT)
  - Anti-Hund's coupling is needed to break SO(4) and to select spin-singlet IVCW and SC.