Molecular Pairing in TBG Superconductivity

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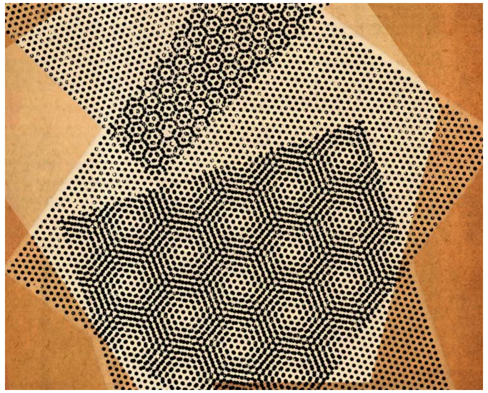

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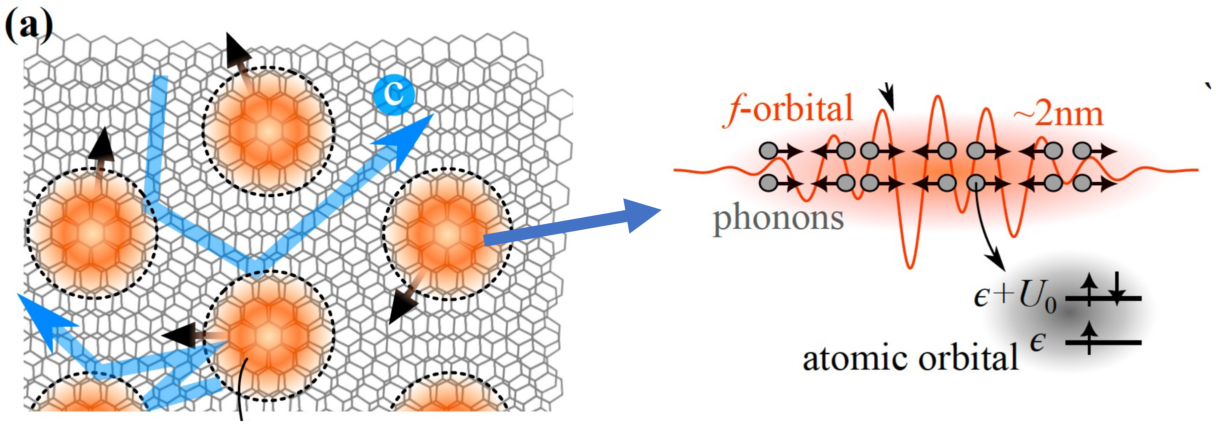

Refs:

[**Model**]: Z.-D. Song and B. A. Bernevig, Phys. Rev. Lett. **129**, 047601 (2022)
[**Kando Phase**]: G.-D. Zhou, Y.-J. Wang, N. Tong, and Z.-D. Song, *Kondo Phase in Twisted Bilayer Graphene*, Phys. Rev. B **109**, 045419 (2024).
[**Pairing mechanism**]: Y.-J. Wang, G.-D. Zhou, S.-Y. Peng, B. Lian, and Z.-D. Song,, arXiv:2402.00869 (2024)

arXiv:2402.00869 (2024)

Molecular Pairing in Twisted Bilayer Graphene Superconductivity

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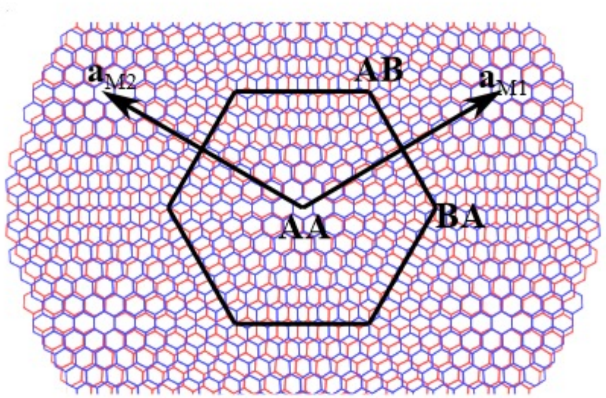
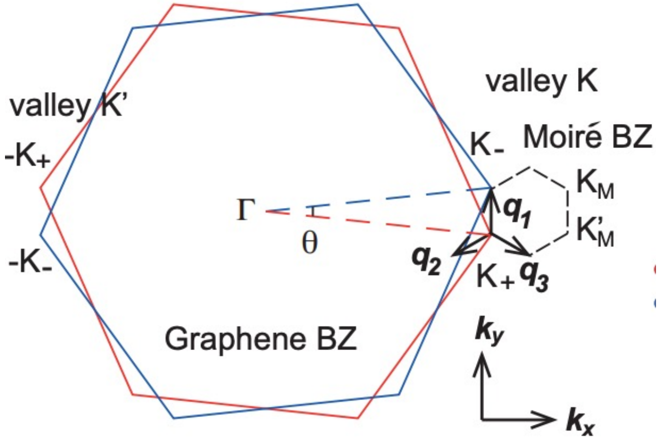
(Dated: February 2, 2024)

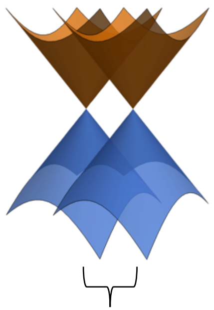
We propose a theory for how the weak phonon-mediated interaction ($J_A = 1 \sim 4$meV) wins over the prohibitive Coulomb repulsion ($U = 30 \sim 60$meV) and leads to a nematic superconductor in magic-angle twisted bilayer graphene (MATBG). We find the pairing mechanism akin to that in the A_3C_{60} family of molecular superconductors: Each AA stacking region of MATBG resembles a C_{60} molecule, in that optical phonons can

arXiv:2402.00869 (2024)

Single-particle bands







The Bistritzer-MacDonald (BM) continuum model (single valley):

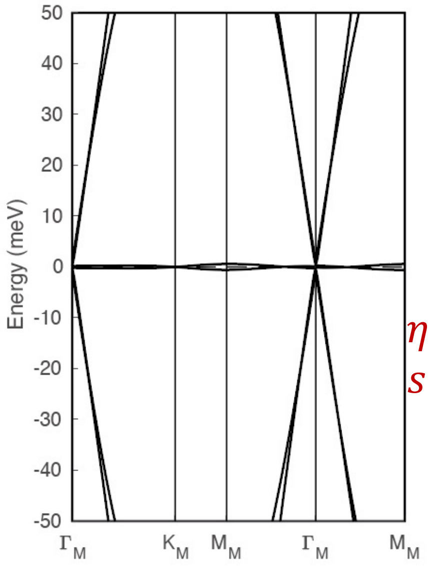
$$H^K(\boldsymbol{r}) = \begin{pmatrix} -iv_F\boldsymbol{\sigma}\cdot\nabla & T(\boldsymbol{r}) \\ T^\dagger(\boldsymbol{r}) & -iv_F\boldsymbol{\sigma}\cdot\nabla \end{pmatrix}$$

Interlayer hopping: $T(\boldsymbol{r}) = \sum_{j=1}^{3} T_j e^{i\boldsymbol{q}_j\cdot\boldsymbol{r}}$,

$$T_j = w_0\sigma_0 + w_1\left[\sigma_x \cos\frac{2\pi(j-1)}{3} + \sigma_y \sin\frac{2\pi(j-1)}{3}\right] .$$

w_0: AA hoping $\leq$ w_1: AB/BA hoping

$\theta = 1.05^\circ$



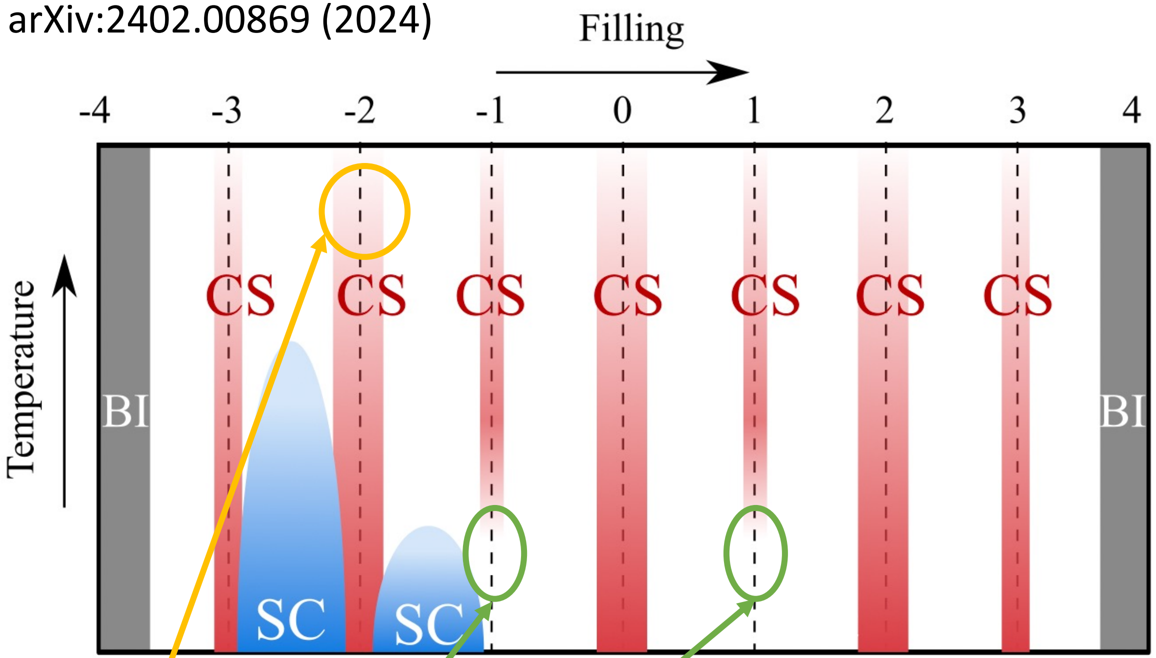
$\eta = \pm$: valley K, K'

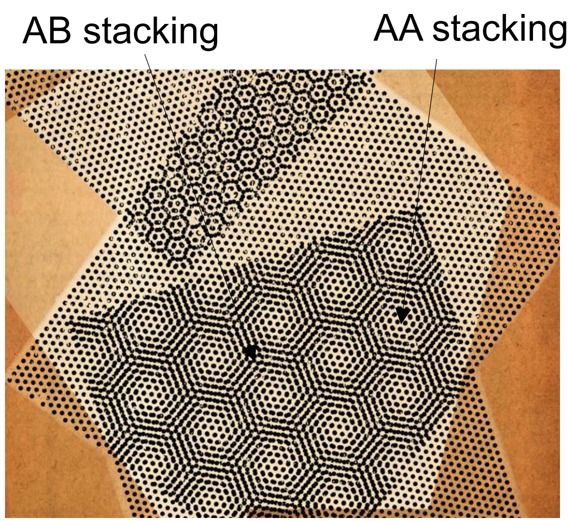
$s = \uparrow, \downarrow$: spin

Bistritzer, Macdonald (2011)

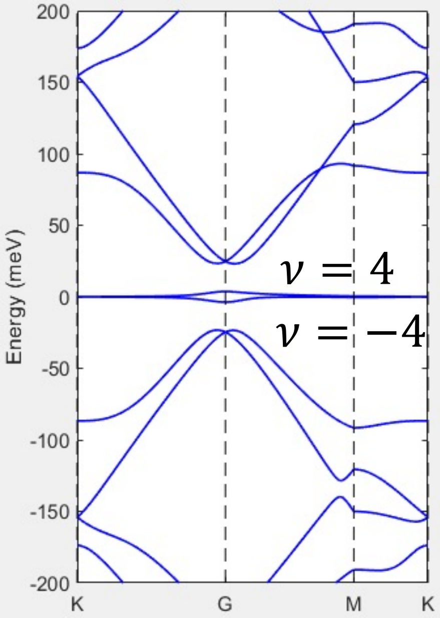
Experimental facts

arXiv:2402.00869 (2024)



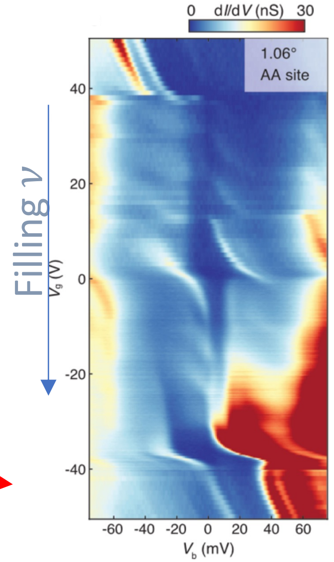


Magic angle $\boldsymbol{\theta = 1.05^\circ}$



Bistritzer, MacDonald 2011PNAS

1. Correlated insulator or correlated states (CS) — Cao et al. 2018, Lu et al. 2019, Sharpe et al. 2019, Saito et al. 2020, Stepanov et al. 2020, Wong et al. 2020, Choi et al. 2019, Kerelsky et al. 2019, Jiang et al. 2019
2. Chern insulator — Serlin et al. 2019, Nuckolls et al. 2020, Choi et al. 2020, Saito et al. 2021, Das et al. 2021, Park et al. 2021, Wu et al. 2021,
3. Superconductivity (CS) — Cao et al. 2018, Lu et al. 2019, Yankowitz et al. 2019, Saito et al. 2020, Stepanov et al. 2020
4. Strange metal — Cao et al. 2020, Polshyn et al. 2019
5. Pomeranchuk effect — Saito et al. 2021, Rozen et al. 2021
6. Dirac-like behavior — Zondiner et al. 2020, Saito et al. 2021, Rozen et al. 2021
7. Quantum-dot-like behavior — Wong et al. 2020, Xie et al. 2019, Choi et al. 2019, Kerelsky et al. 2019, Jiang et al. 2019
8. Zero-energy peak — Oh et al. 2021, Choi et al. 2021, Nuckolls et al. 2020,



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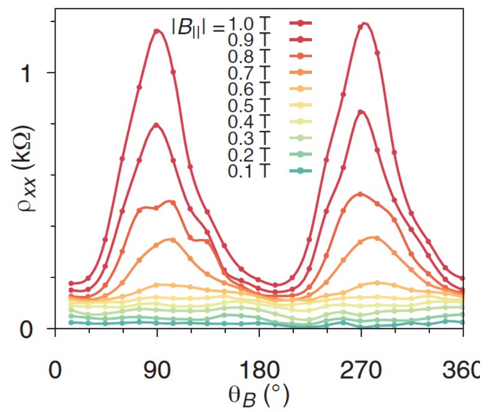
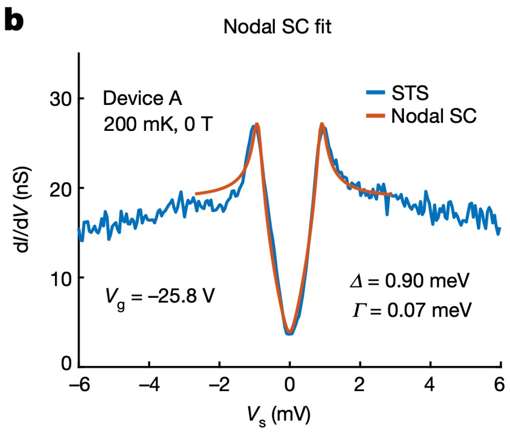
Experimental facts about the SC

- Nematicity



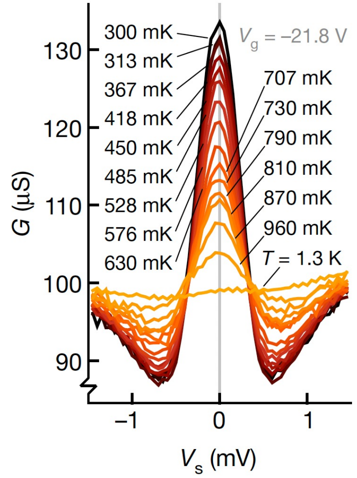
Cao et al. (2021) Science

- V-shaped gap



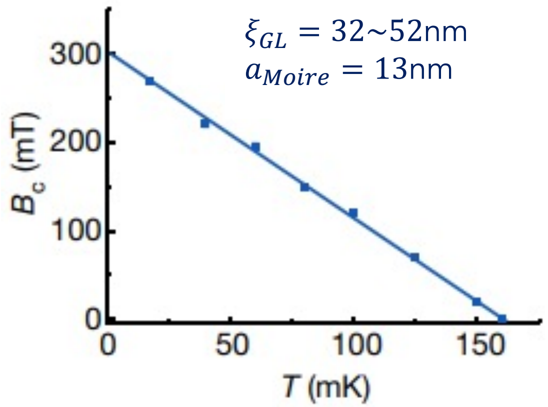
Oh et al. (2021) Nature

- SC Gap >> Tc



Oh et al. (2021) Nature

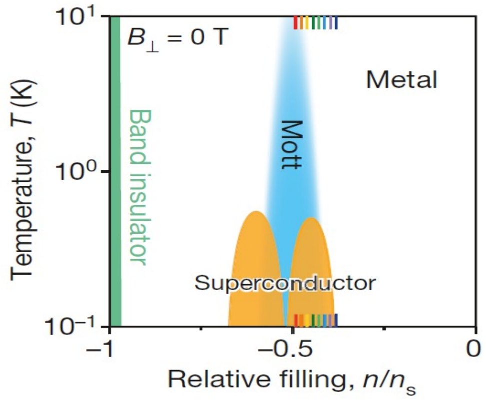
- Small coherence length



Cao et al. (2018) Nature

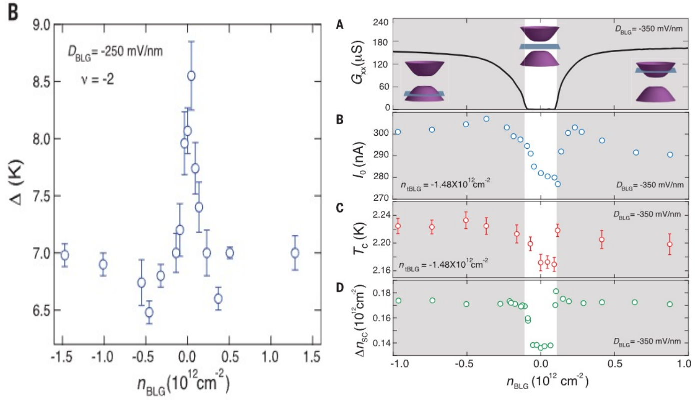
Lu et al. (2019) Nature

- Coexistence with strong correlation



Cao et al. (2018) Nature

- Enhanced by suppressing correlation



Liu et al. (2021) Science

Stepanov et al. (2018) Nature

Saito et al. (2020) Nature Physics

- Enhanced by SOC

Arora et al. (2020) Nature

arXiv:2402.00869 (2024)

Difficulties in understanding the SC

- Cuprates-like mechanism?
  - ✓ Coexistence with correlation
  - X No magnetism around SC

- BCS pairing?
  - ✓ Enhanced by suppressing U, by SOC
  - X Nematicity
  - X V-shaped gap
  - X Pairing (0.1-1meV) << U (~30-60meV)
  - X BEC-like feature

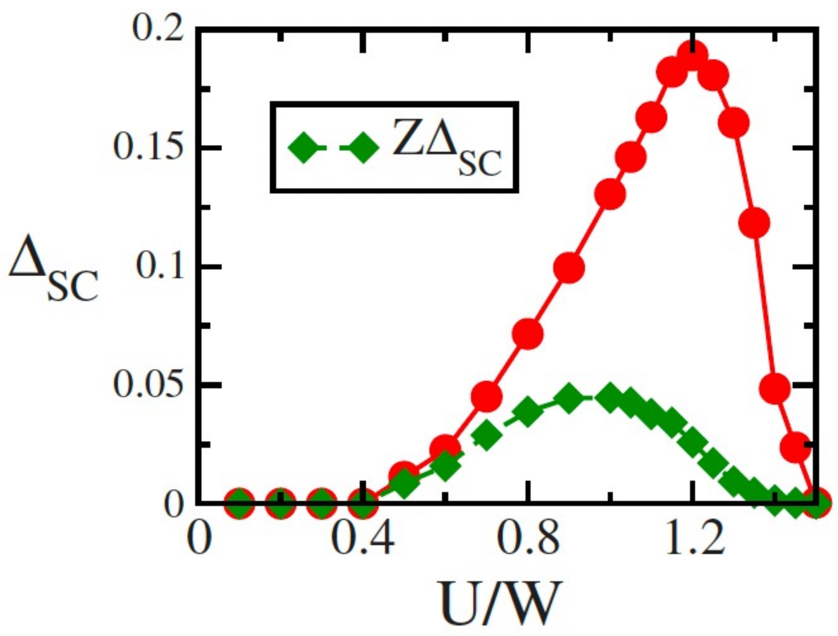
- Retardation effect?
  - Small bandwidth (D=1~10meV), comparable or higher ω_D
  - X Barely reduced pseudo potential $\mu^* = \frac{\mu}{1+\mu \ln D/\omega_D}$
  - X BEC-like feature …

arXiv:2402.00869 (2024)

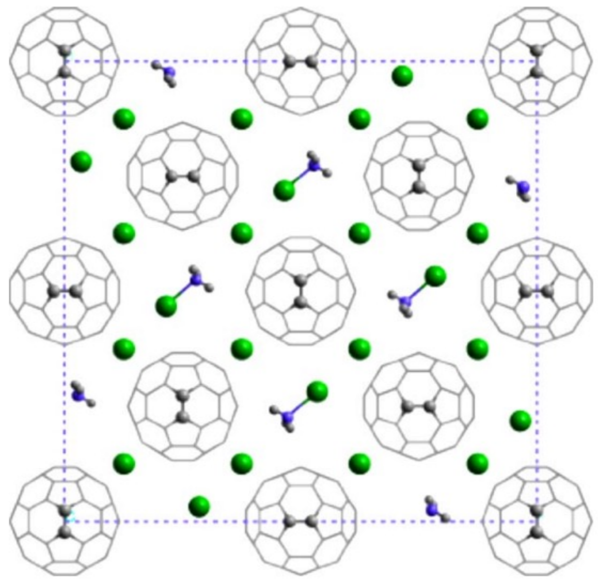
Difficulties in understanding the SC

*Dodaro, Kivelson et al., PRB **98**, 075154 (2018)*
*Angeli, Fabrizio et al., PRX **9**, 041010 (2019)*

- A3C60?
  - Jahn-Teller induced attractive: J ~ 0.1eV
  - Strong correlaton: U ~ 1eV
  - But J wins U due to Kondo screening!



*M. Capone, et al., Rev. Mod. Phys. **81**, 943 (2009).*



A molecule of 60 carbons

≈ a moire site?

Couples to numerous phonon modes

≈ a moire site also includes numerous phonon modes

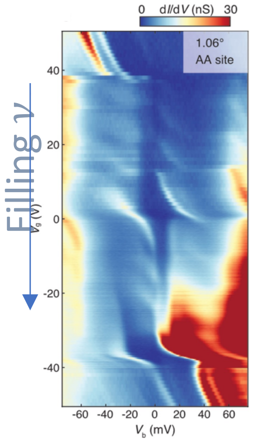
We find nematicity is also possible in this analogy.

arXiv:2402.00869 (2024)

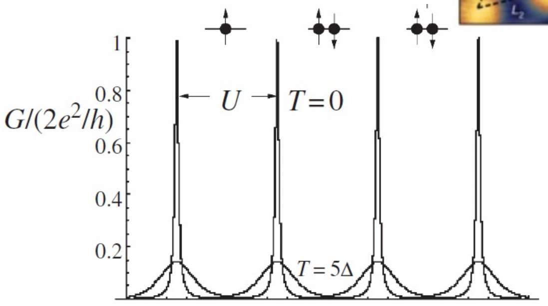
- ***Construction of Topological Heavy-Fermion Model***
- ***Summary of the correlation physics***
- ***Pairing mechanism***
- ***Superconductor phase***

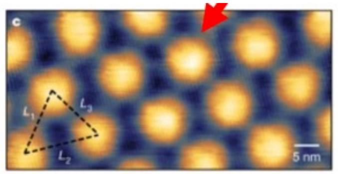
Experiments suggesting existence of *local moments*

Coulomb blockade seen in STM



→ large on-site repulsion



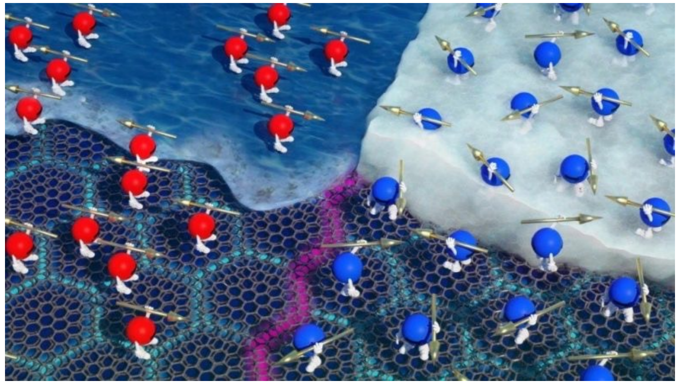


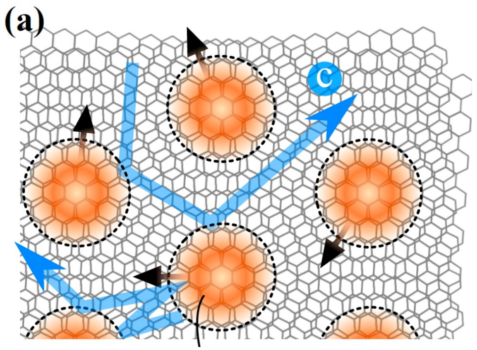
Wong et al. 2020, Xie et al. 2019, Choi et al. 2019, Kerelsky et al. 2019, Jiang et al. 2019,

Pomeranchuk effect

large entropy in the ordered phase,
which disappear under magnetic field
→ loosely coupled local moments

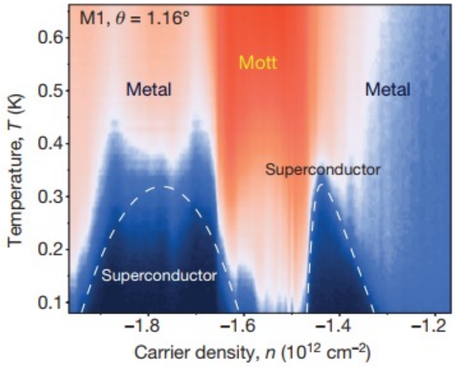
Saito et al. 2021, Rozen et al. 2021



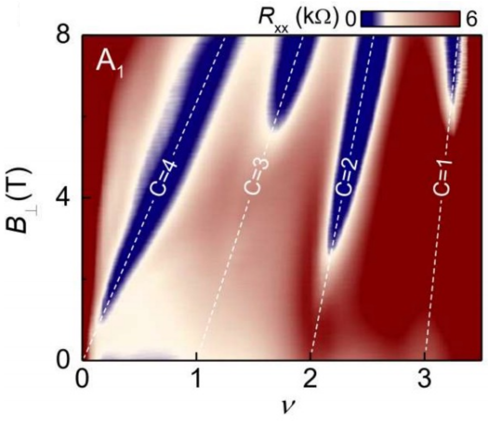


Experiments suggesting existence of *delocalized electron states*

Metallicity & Superconductivity



Landau fans



Transport & Hysteresis,
Efetov group 2020

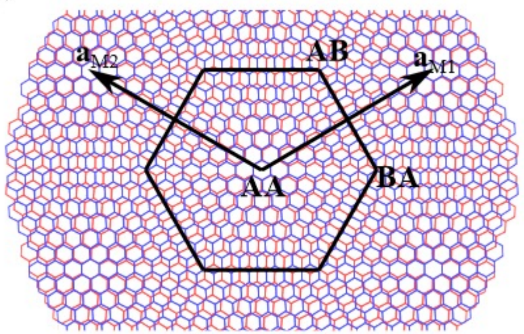
Dirac-like behaviors

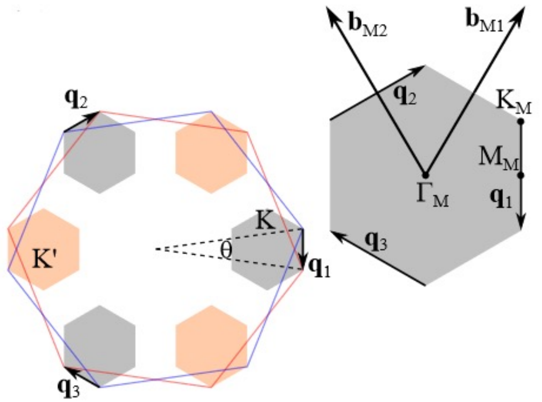
Zondiner et al. 2020

compressibility $\sim \sqrt{n}$

PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

Fragile and stable topology





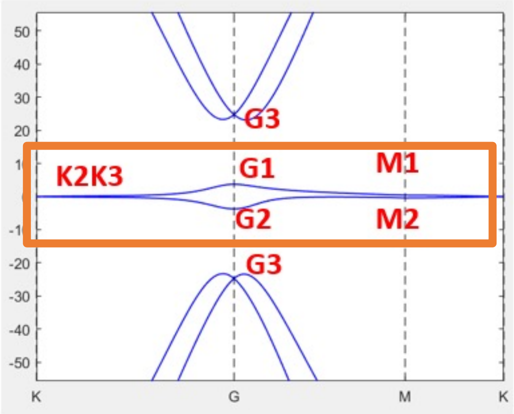
Crystalline symmetries in a single valley

- MSG 177.151 P6’2’2 ← C3z, C2zT, C2x
- Valley-U(1)
- Time-reversal

Bistritzer, MacDonald 2011PNAS

Fragile topology

Song et al. 2019PRL, Po et al. 2019PRB, Liu, Dai et al. 2019PRB



Bistritzer, MacDonald 2011PNAS

	Γ_1	Γ_2	Γ_3		M_1	M_2		K_1	K_2K_3
E	1	1	2	E	1	1	E	1	2
$2C_3$	1	1	-1	C_2'	1	-1	C_3	1	-1
$3C_2'$	1	-1	0				C_3^{-1}	1	-1

Bradlyn et al. 2017Nature, Po et al. 2017NC

Elcoro et al. 2021NC: we derive all magnetic BRs & topological indices

Band representations (local orbitals)

Wyckoff pos.	$1a$ (000)			$2c$ $(\frac{1}{3}\frac{2}{3}0)$, $(\frac{2}{3}\frac{1}{3}0)$		
Site sym.	$6'22'$, 32			32, 32		
EBR	$[A_1]_a \uparrow G$	$[A_2]_a \uparrow G$	$[E]_a \uparrow G$	$[A_1]_c \uparrow G$	$[A_2]_c \uparrow G$	$[E]_c \uparrow G$
Orbitals	s	p_z	p_x, p_y	s	p_z	p_x, p_y
Γ (000)	Γ_1	Γ_2	Γ_3	$2\Gamma_1$	$2\Gamma_2$	$2\Gamma_3$
K $(\frac{1}{3}\frac{1}{3}0)$	K_1	K_1	K_2K_3	K_2K_3	K_2K_3	$2K_1 \oplus K_2K_3$
M $(\frac{1}{2}00)$	M_1	M_2	$M_1 \oplus M_2$	$2M_1$	$2M_2$	$2M_1 \oplus 2M_2$

→ Obstruction to two-band symmetric & local lattice models

Two-band models where C2zT becomes nonlocal *Kang et al. 2018PRX, Kang et al. 2019PRL, Koshino et al. 2018PRX, Yuan et al. 2018PRB*

(Fragile) topology *Po et al. 2019PRB, Ahn 2019 PRX, Song et al. 2019PRL*

PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

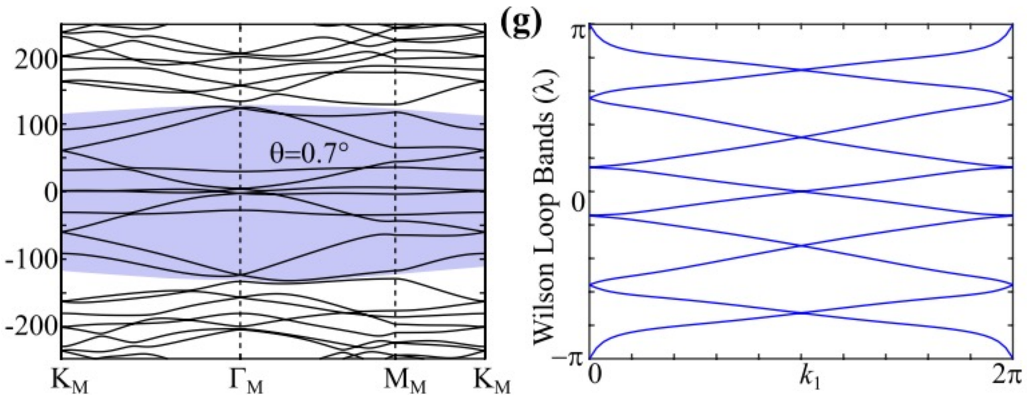
Fragile and stable topology

Stable topology

P ($E_k = -E_{-k}$) is an emergent particle-hole symmetry of the BM continuous model

Reflected as charge-conjugation symmetry in experiments

Song2021PRB TBG-II

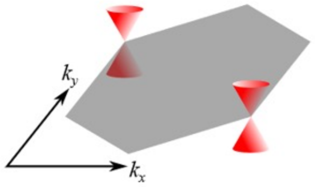


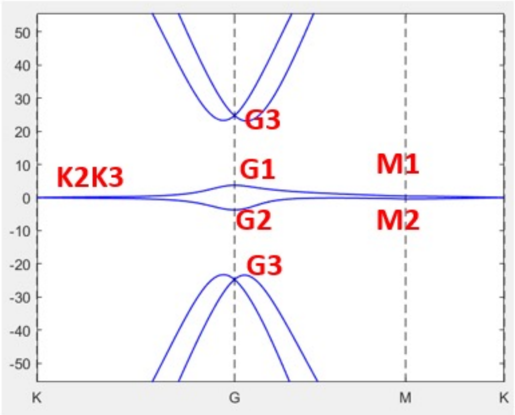
Wilson loop

Non-abelian berry's connection

$$W(k_x) = T\exp\left(i\int dk_y \cdot A(k_y)\right)$$

We further prove that 4n+2 ($n \in \mathbb{N}$) Dirac points ←→ Topology





Symmetry Anomaly

→ forbids symmetric & short-range lattice models with any finite number of bands

Two-band models where C2zT becomes nonlocal *Kang et al. 2018PRX, Kang et al. 2019PRL, Koshino et al. 2018PRX, Yuan et al. 2018PRB*

Ten-band model where P becomes nonlocal *Po et al. 2019PRB*

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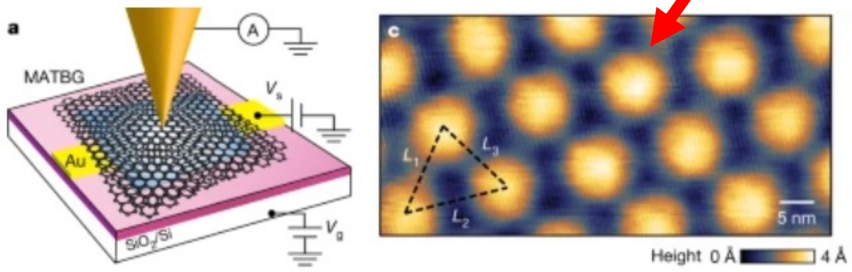
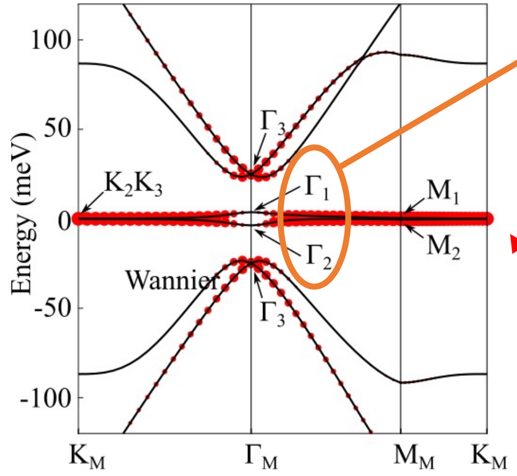
Construction of the heavy fermion model

Our strategy: Step I. Where does the local states come from?



Wong et al. 2020, Xie et al. 2019, Choi et al. 2019, Kerelsky et al. 2019, Jiang et al. 2019,



Suppose we can replace $\Gamma_1+\Gamma_2$ by Γ_3, then flat bands match px,py orbitals at triangular lattice

Wyckoff pos.	$1a$ (000)		
Site sym.	$6'22'$, 32		
EBR	$[A_1]_a \uparrow G$	$[A_2]_a \uparrow G$	$[E]_a \uparrow G$
Orbitals	s	p_z	p_x, p_y
Γ (000)	Γ_1	Γ_2	Γ_3
K $(\frac{1}{3}\frac{1}{3}0)$	K_1	K_1	K_2K_3
M $(\frac{1}{2}00)$	M_1	M_2	$M_1 \oplus M_2$

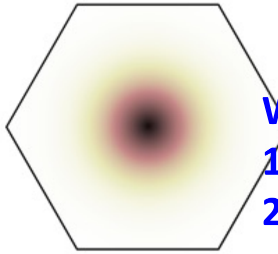
1a is AA-stacking region

We hence introduce trial Guassian-type WFs, $|W'_{\alpha=1,2}\rangle \sim |p_x\rangle \pm i|p_y\rangle$ and computed $\sum_\alpha |\langle W'_\alpha|\psi_n(k)\rangle|^2$ for each band

Large overlap ➔ **The flat bands at $k \neq 0$ are almost the trial WFs**

Wannier90

$\langle W'_\alpha|\psi_n(k)\rangle$



Maximally localized WFs

WFs are extremely localized:
1. Spread ~ 0.2a_M
2. Hopping between NN ~ 0.1meV

96% of the flat bands are contributed by the WFs

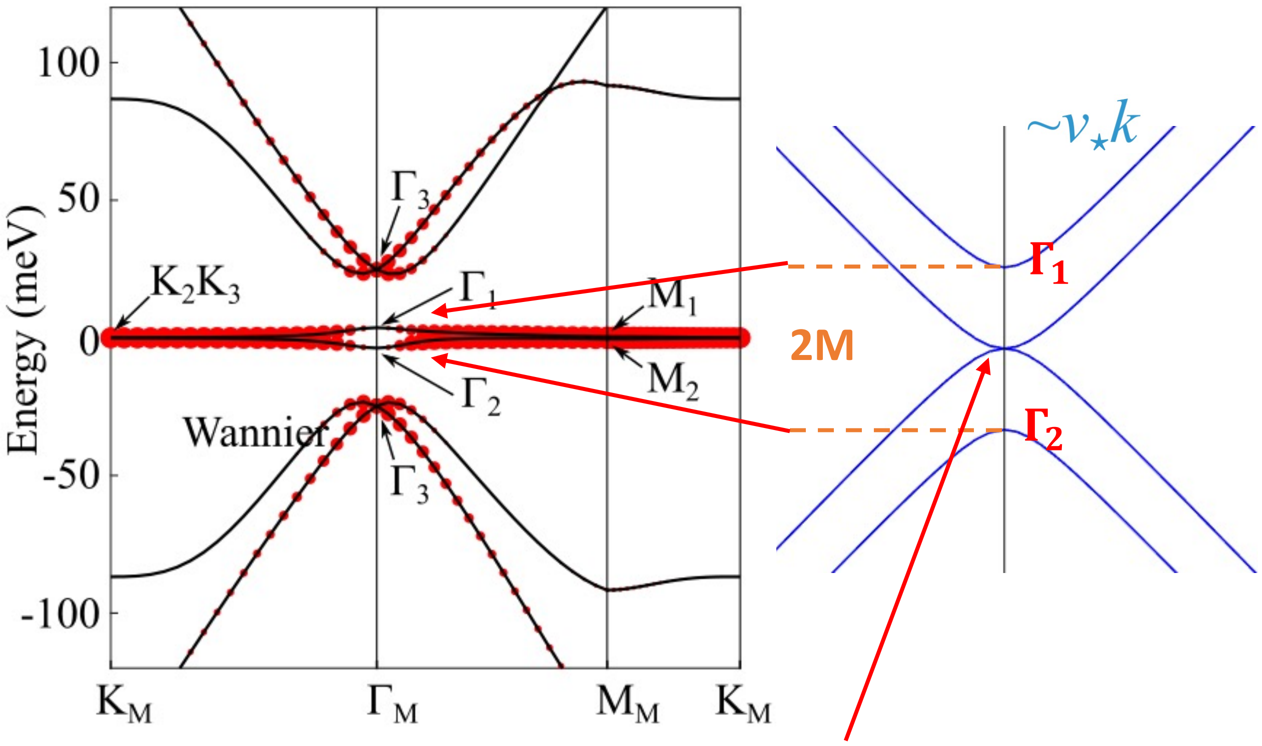
$$\frac{1}{2N}\sum_{kn}\sum_{R\alpha}|\langle W_{R\alpha}|\psi_n(k)\rangle|^2 = 96\%$$

The correlation physics of flat bands must mainly come from these WFs!

PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

Construction of the heavy fermion model

Our strategy: Step II. Model the remaining 4% states



The quadratic touching.

Hc has to be gapless: Since the WFs are trivial, H^c must have 4n+2 ($n \in \mathbb{N}$) Dirac points due to the ***symmetry anomaly****.*

The quadratic touching is equivalent to two DPs.

$$H^c = P_c H^{BM} P_c, \quad P_c = 1 - P_f$$

We consider the lowest six bands

P_f contains Γ_3 at k=0

➔ P_c contains $\Gamma_3 + \Gamma_1 + \Gamma_2$

Γ_3 (L=±1) | $\Gamma_1 + \Gamma_2$ (L=0)

$$H^{(c,\eta)} = \left(\begin{array}{c|c} 0_{2\times2} & v_\star(\eta k_x\sigma_0 + i k_y\sigma_z) \\ \hline v_\star(\eta k_x\sigma_0 - i k_y\sigma_z) & M\sigma_x \end{array}\right)$$

$\eta = \pm$ is the valley index

Determine the parameters:

$$H_{ab}^{(c,\eta)}(k) = \langle u_a^\eta(0) | H_{BM}^\eta(k) | u_b^\eta(0) \rangle \quad \text{a,b=1 ... 4}$$

BM model, linear in k ➔ $H^{(c,\eta)}$ is linear in k

M=3.7meV
$v_\star = -4.3\text{eV}\cdot\text{Å}$

PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

Construction of the heavy fermion model

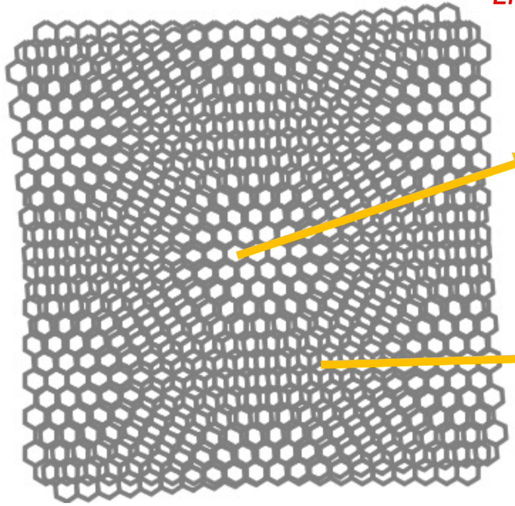
Our strategy: Step III. Couple the two parts

$$\hat{H}_0 = \sum_{|\mathbf{k}|<\Lambda_c} \sum_{aa'\eta s} H^{(c,\eta)}_{aa'}(\mathbf{k}) c^\dagger_{\mathbf{k}a\eta s} c_{\mathbf{k}a'\eta s} + \frac{1}{\sqrt{N}} \sum_{\substack{|\mathbf{k}|<\Lambda_c \\ \mathbf{R}}} \sum_{\alpha a \eta s} \left(e^{i\mathbf{k}\cdot\mathbf{R} - \frac{|\mathbf{k}|^2\lambda^2}{2}} H^{(fc,\eta)}_{\alpha a}(\mathbf{k}) f^\dagger_{\mathbf{R}\alpha\eta s} c_{\mathbf{k}a\eta s} + h.c. \right)$$

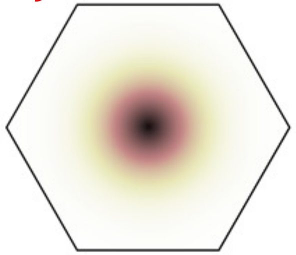
Λ_c: cutoff for the conduction band

Large enough k → decoupled
Only coupling around Gamma is relevant

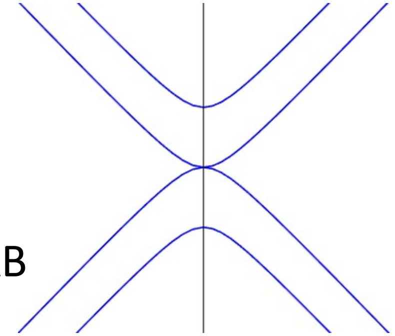
Liu, Dai et al. 2019PRB



f-electron



c-electron



	Reps	L
a=1,2 c-electrons	Γ_3	± 1
a=3,4 c-electrons	$\Gamma_1 + \Gamma_2$	0
α=1,2 f-electrons	Γ_3	± 1

$$H^{(c,\eta)} = \begin{pmatrix} 0_{2\times 2} & v_\star(\eta k_x\sigma_0 + i k_y\sigma_z) \\ v_\star(\eta k_x\sigma_0 - i k_y\sigma_z) & M\sigma_x \end{pmatrix}$$

$$H^{(cf,\eta)}_{a\,\alpha}(k) = \langle u^\eta_a(0)|H_{BM}(k)|v^\eta_\alpha(0)\rangle = \begin{pmatrix} \gamma + v'_\star(\eta k_x\sigma_x + k_y\sigma_y) \\ 0_{2\times 2} \end{pmatrix}$$

a=1…4 $\qquad \alpha = 1,2$

γ=-24.8meV $v'_\star$ =1.6eV· Å

PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

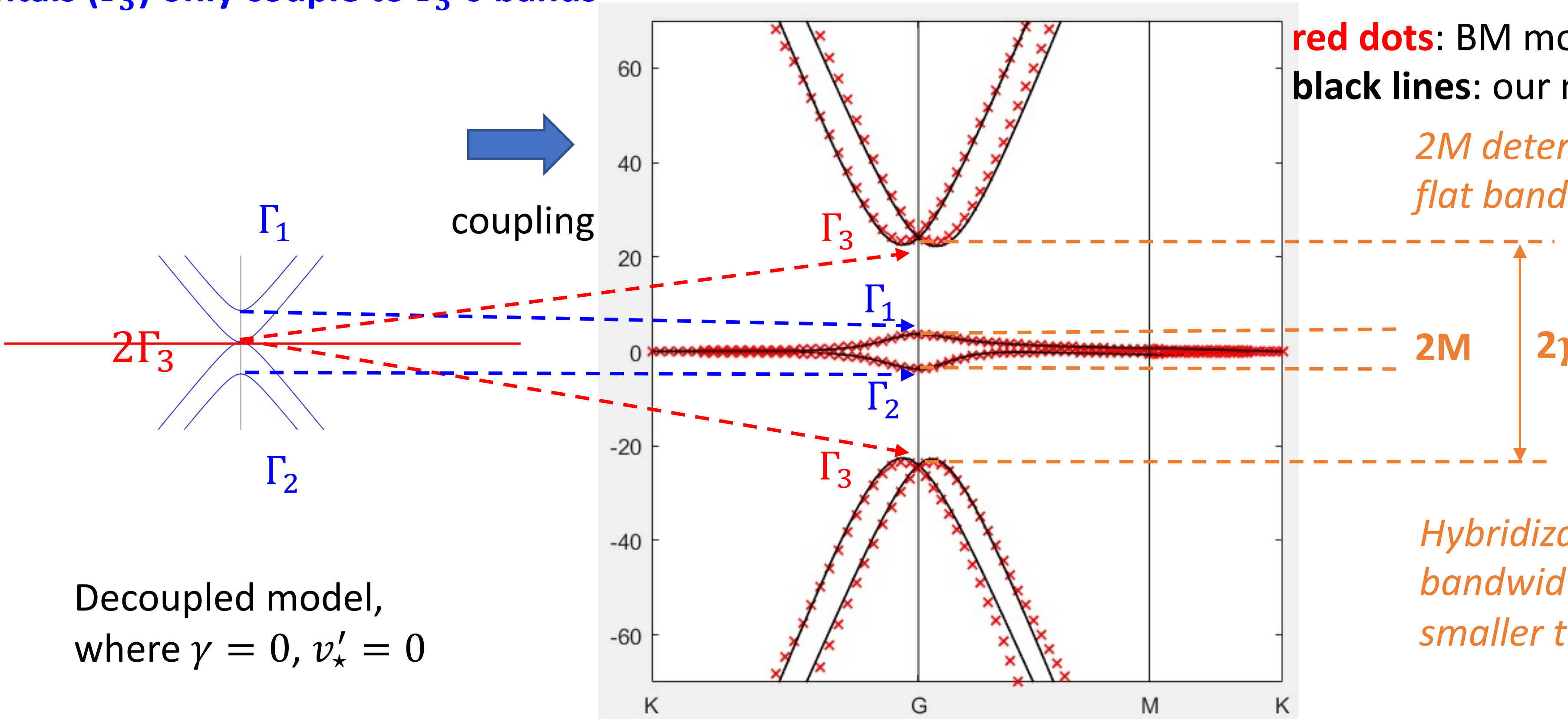
Construction of the heavy fermion model

Recover the BM model bands

For small k

$$H^{\eta}(k) = \begin{pmatrix} 0_{2\times2} & v_\star(k_x\eta\sigma_0 + ik_y\sigma_z) & \gamma + v_\star'(k_x\sigma_x + k_y\sigma_y) \\ v_\star(k_x\eta\sigma_0 - ik_y\sigma_z) & M\sigma_x & 0_{2\times2} \\ \gamma + v_\star'(k_x\eta\sigma_x + k_y\sigma_y) & 0_{2\times2} & 0_{2\times2} \end{pmatrix}$$

f-orbitals (Γ_3) only couple to Γ_3 c-bands



Decoupled model, where $\gamma = 0$, $v_\star' = 0$

red dots: BM model
black lines: our model

2M determines the bandwidth of the flat bands

γ=-24.8meV
M =3.7meV

Hybridization γ is larger than bandwidth, but, as shown below, smaller than on-site repulsion

PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

Interaction Hamiltonian

$U_1 \approx 60\text{meV}$, J=16.38meV

H_U

$$\hat{H}_I = \frac{U_1}{2}\sum_{\mathbf{R}} :\rho^f_{\mathbf{R}} :: \rho^f_{\mathbf{R}}: - \frac{J}{2N}\sum_{\mathbf{R}}\sum_{\substack{\alpha_1\eta_1 s_1\\ \alpha_2\eta_2 s_2}}\sum_{|\mathbf{k}_1|,|\mathbf{k}_2|<\Lambda_c} e^{i(\mathbf{k}_1-\mathbf{k}_2)\cdot\mathbf{R}}(\eta_1\eta_2+(-1)^{\alpha_1+\alpha_2}) : f^\dagger_{\mathbf{R}\alpha_1\eta_1 s_1} f_{\mathbf{R}\alpha_2\eta_2 s_2} :: c^\dagger_{\mathbf{k}_2,\alpha_2+2,\eta_2 s_2} c_{\mathbf{k}_1,\alpha_1+2,\eta_1 s_1} :$$

H_J

$$+Vc^+cc^+c \;+\; Wc^+cf^+f$$

U4 symmetry

$$\hat{H}_J = -J\sum_{\mu\nu\xi} e^{-i\mathbf{q}\cdot\mathbf{R}} : \hat{\Sigma}^{(f,\xi)}_{\mu\nu}(\mathbf{R}) :: \hat{\Sigma}^{(c\prime\prime,\xi)}_{\mu\nu}(\mathbf{q}) :$$

U1: the main source of symmetry breaking

(> hybridization $\gamma = -24.75\text{meV}$)

(>>bandwidth $2M = 7.4\text{meV}$)

→ tend to freeze the charge fluctuation of f-electrons

→ leading to a local flat-U(4) moment

J: Ferromagnetic coupling between U(4)-moments (defined later)

Density-density between f- and c-

→ Only change relative energy between f- and c-

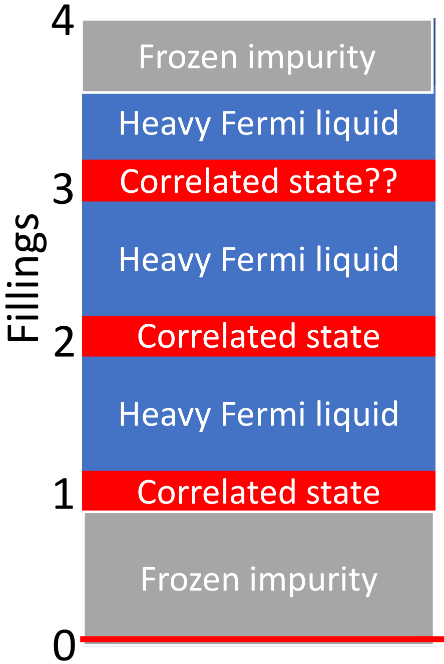
PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

- ***Construction of Topological Heavy-Fermion Model***
- ***Summary of the correlation physics***
- ***Pairing mechanism***
- ***Superconductor phase***

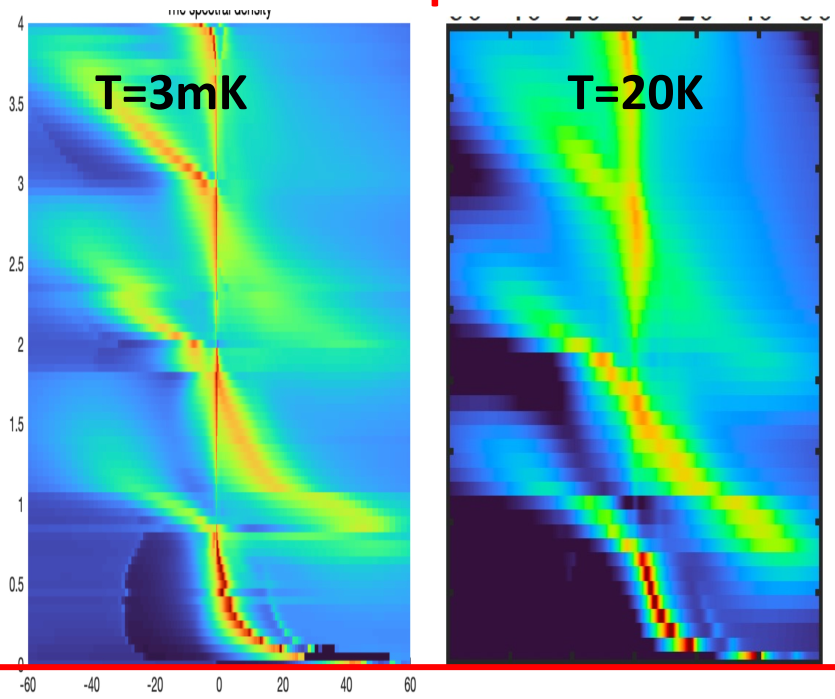
PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

Results from NRG+DMFT

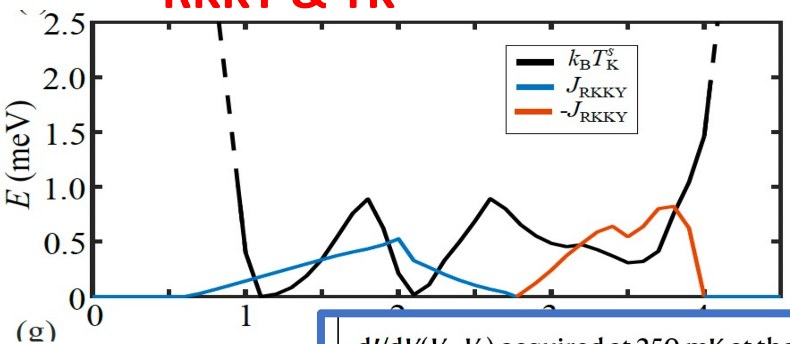
Proposed phase diagram



DMFT Spectrum

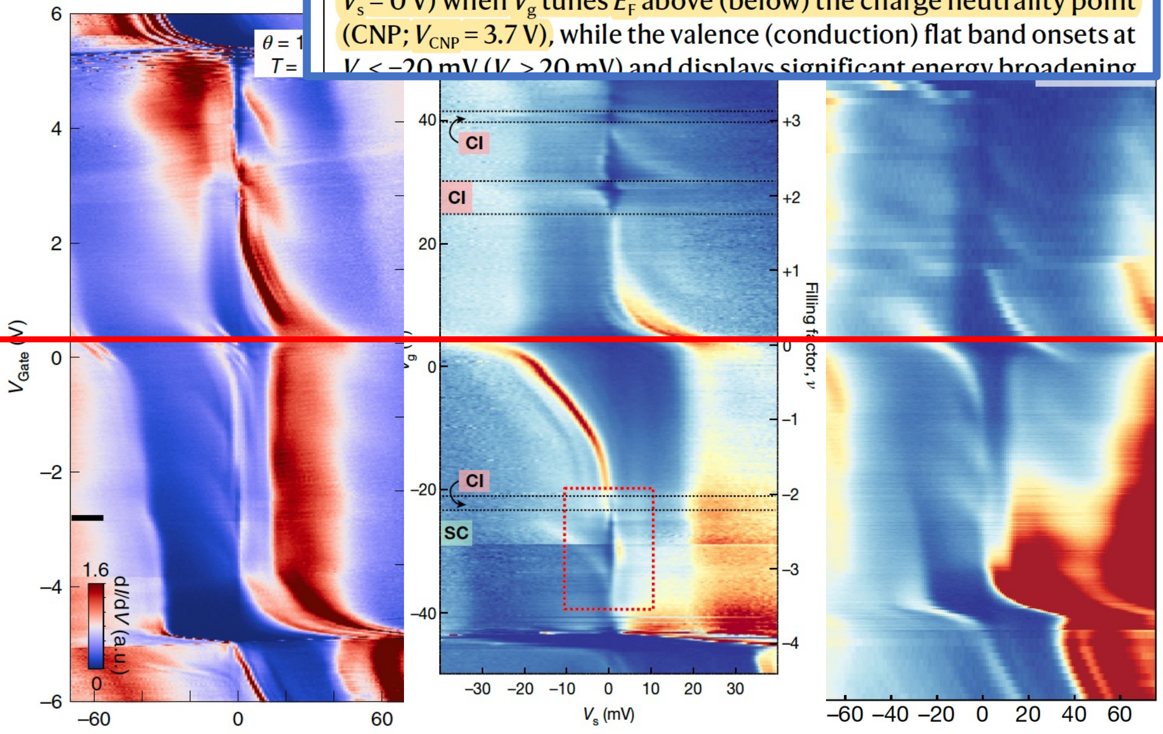


RKKY & TK



$dI/dV(V_s, V_g)$ acquired at 250 mK at the centre of an AA site in device A (see Supplementary Information for AB/BA data). Figure 1c shows that the conduction (valence) flat band is pinned to the Fermi energy (E_F; $V_s = 0$ V) when V_g tunes E_F above (below) the charge neutrality point (CNP; $V_{CNP} = 3.7$ V), while the valence (conduction) flat band onsets at $V_s < -20$ mV ($V_s > 20$ mV) and displays significant energy broadening

EXP Spectrum



Choi et al. 2021

T=400mK

Oh et al. 2021, Nuckolls et al. 2020,

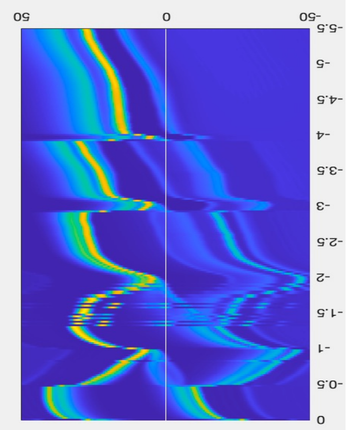
T=250mK

Wong et al. 2020

T=6K

See also:

*Chou, Sas Sarma et al, PRL, **131**, 026501 (2023)*
*Hu, Bernevig et al., PRL. **131**, 166501 (2023)*
*Datta, et al., Nat Commun **14**, 5036 (2023)*
Rai, Bernevig, Georges, et al., arXiv:2309.08529 (2023)
Lau, Coleman, arXiv:2303.02670 (2023)



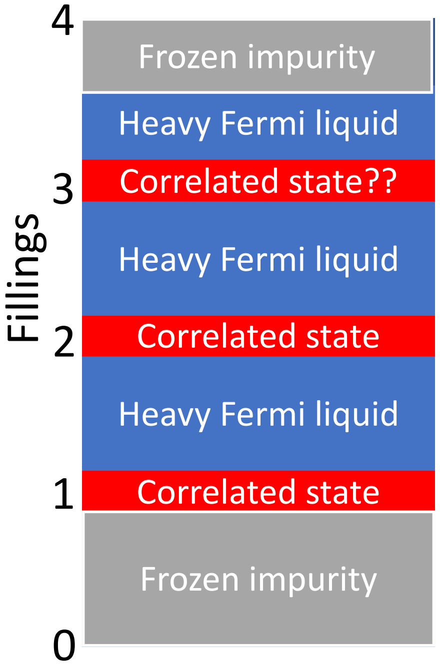
HF spectrum

(correct only at integer filling)

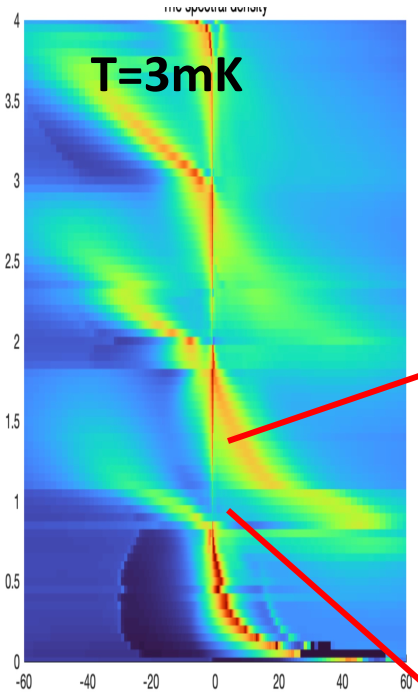
PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

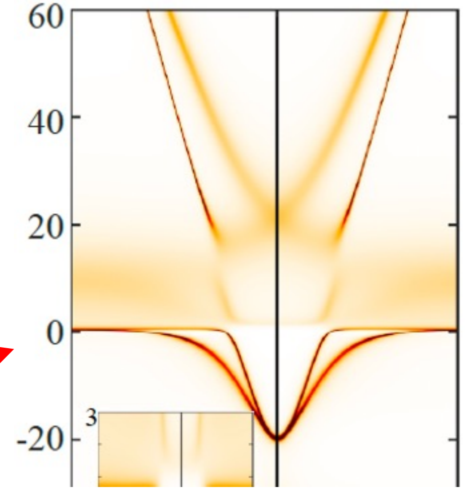
Results from NRG+DMFT

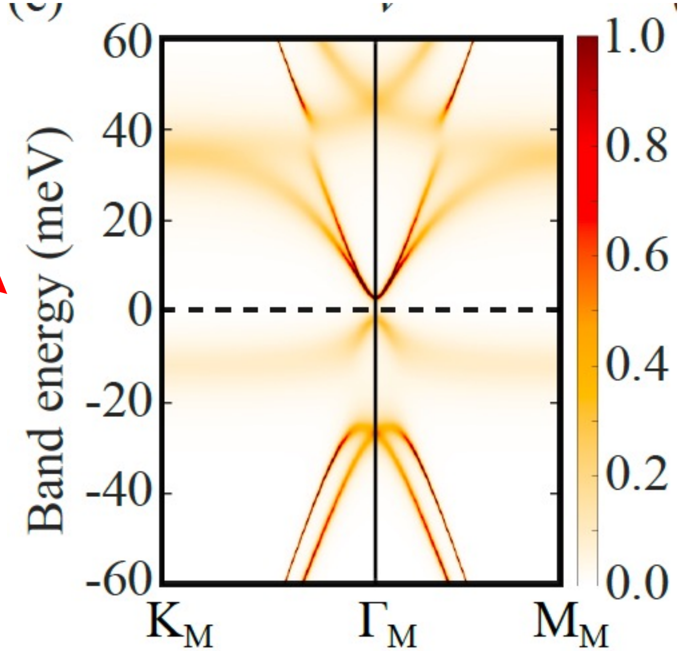
Proposed phase diagram



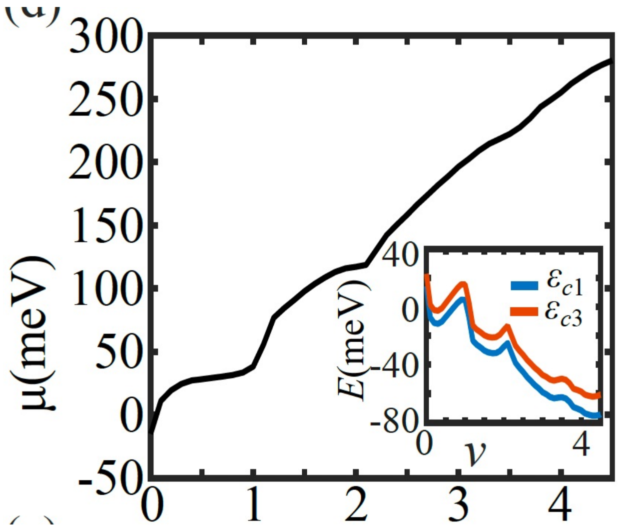
DMFT Spectrum







Compressibility (mu v.s. filling)



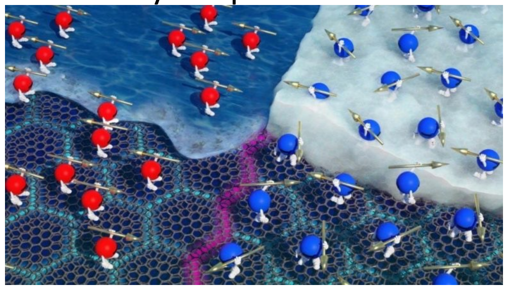
PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

"Pomeranchuck effect" around nu=+-1

Pomeranchuk effect

large entropy in the ordered phase, which disappear under magnetic field

→ loosely coupled local moments

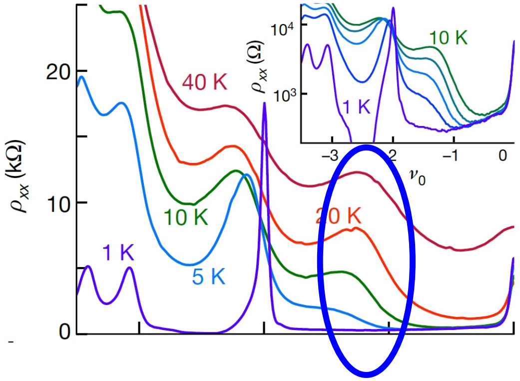


Low T: liquid

High T: *barely coupled moments*

Rozen et al. 2021, Saito et al. 2021

Transport

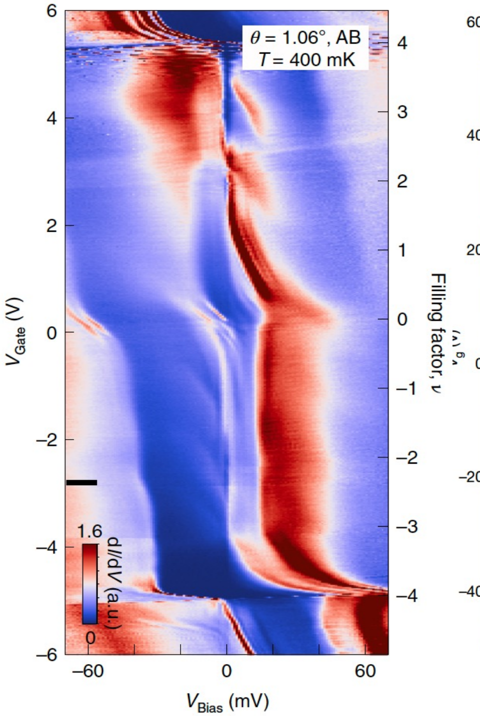


Low T: no resistance peak

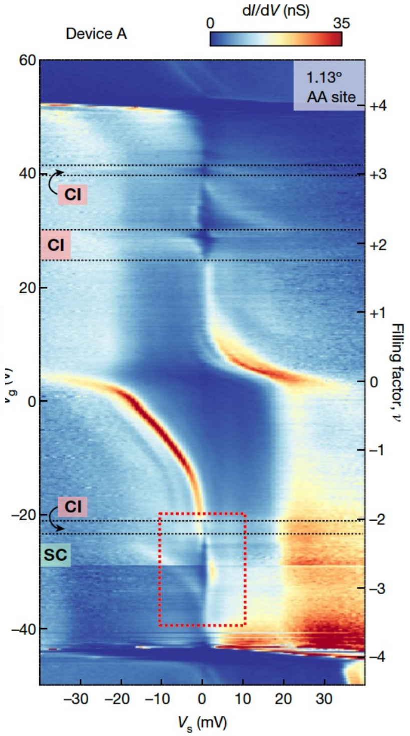
High T: resistance peak

Saito et al. 2021

Zero-energy peak at low T



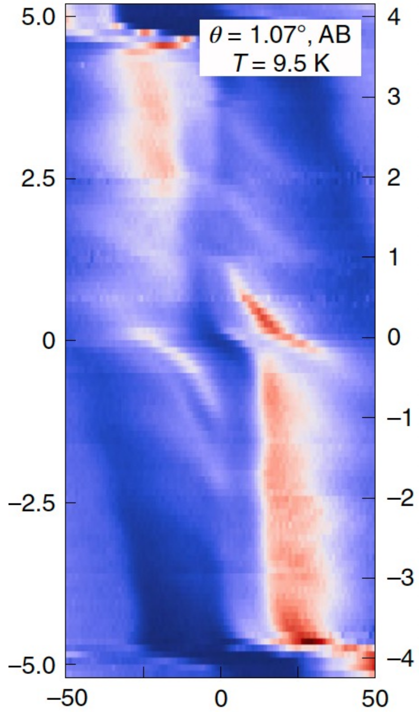
Choi et al. 2021



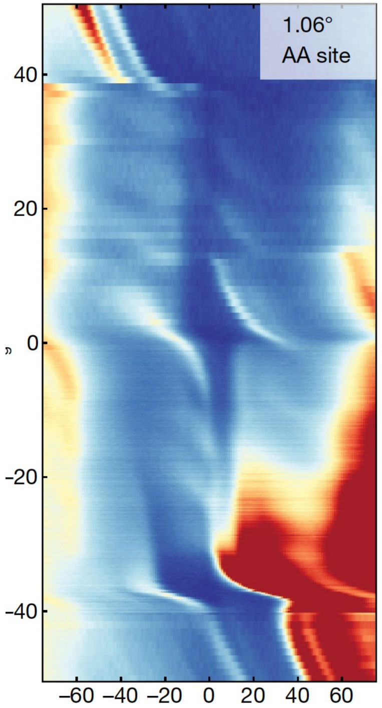
Oh et al. 2021,

Nuckolls et al. 2020,

Quantum dot behavior at high T



Choi et al. 2021

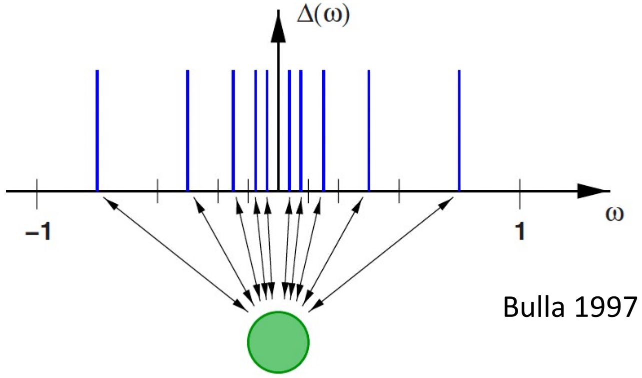


Wong et al. 2020

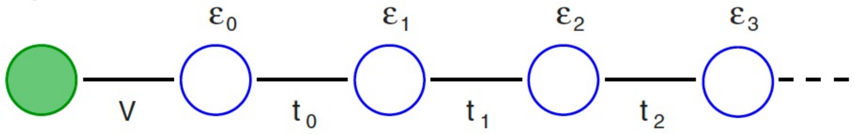
PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

NRG calculation

Wilson chain:



Bulla 1997 RMP



f-site

Free-fermion chain

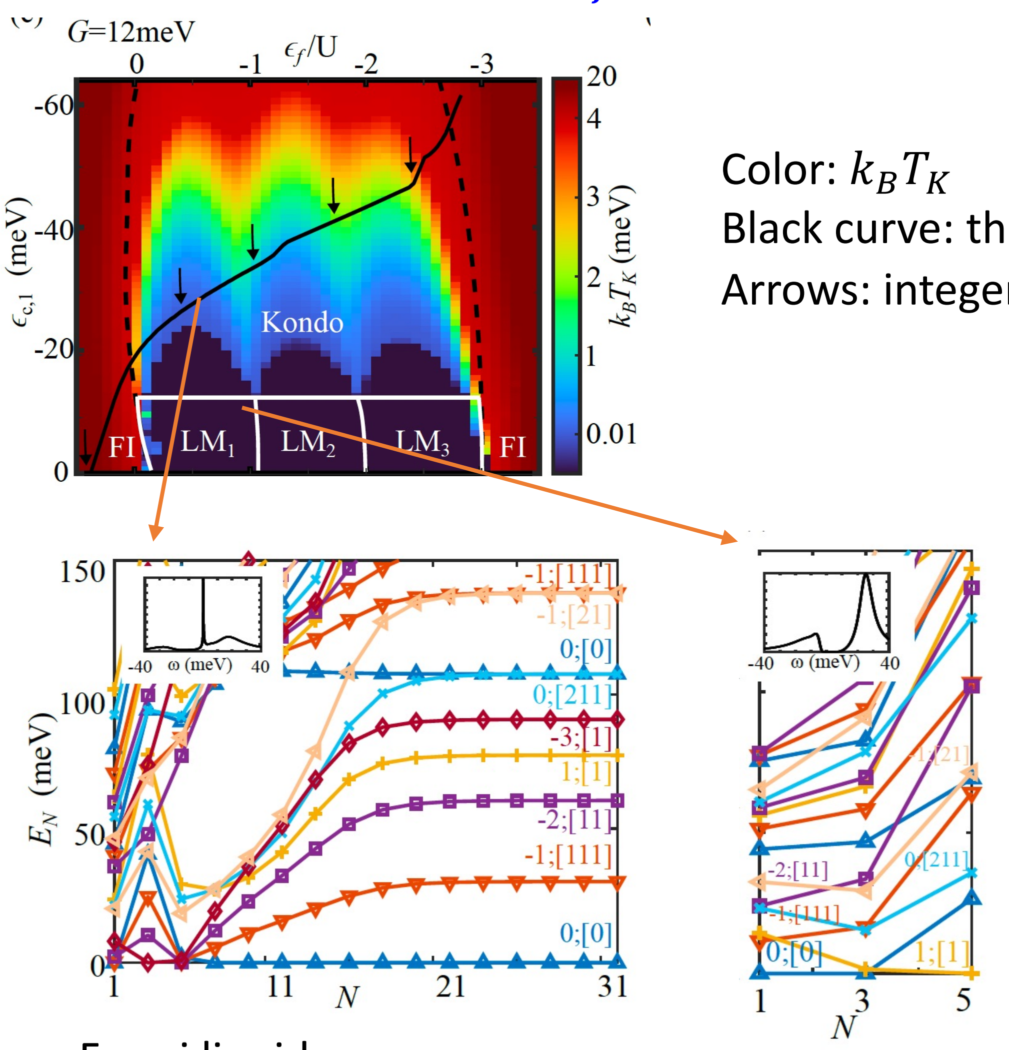
ϵ_n and t_n are determined by $\Delta(\omega)$

RG Process: $\widetilde{H}_N = (\Lambda)^{\frac{1}{2}N-1}\hat{H}_N$

$$\widetilde{H}_{N+1} = \Lambda^{\frac{1}{2}}\widetilde{H}_N + \Lambda^{\frac{1}{2}(N-1)}\sum_{\alpha s}\left(\epsilon_{N+1}d^\dagger_{N+1,\alpha s}d_{N+1,\alpha s} + t_N d^\dagger_{N+1,\alpha s}d_{N,\alpha s} + t_N d^\dagger_{N,\alpha s}d_{N+1,\alpha s}\right).$$

Truncate Hilbert space every step

Phase diagram in (ϵ_c, ϵ_f) space



Color: $k_B T_K$
Black curve: the SCF $\boldsymbol{\epsilon_c}, \boldsymbol{\epsilon_f}$
Arrows: integer fillings

Fermi liquid
Kondo resonance

Local moment
Hubbard bands

At an early stage (higher temp), lowest state is LM [1] (U(4) irrep)
➔ “Pomeranchuck effect” in experiments ?

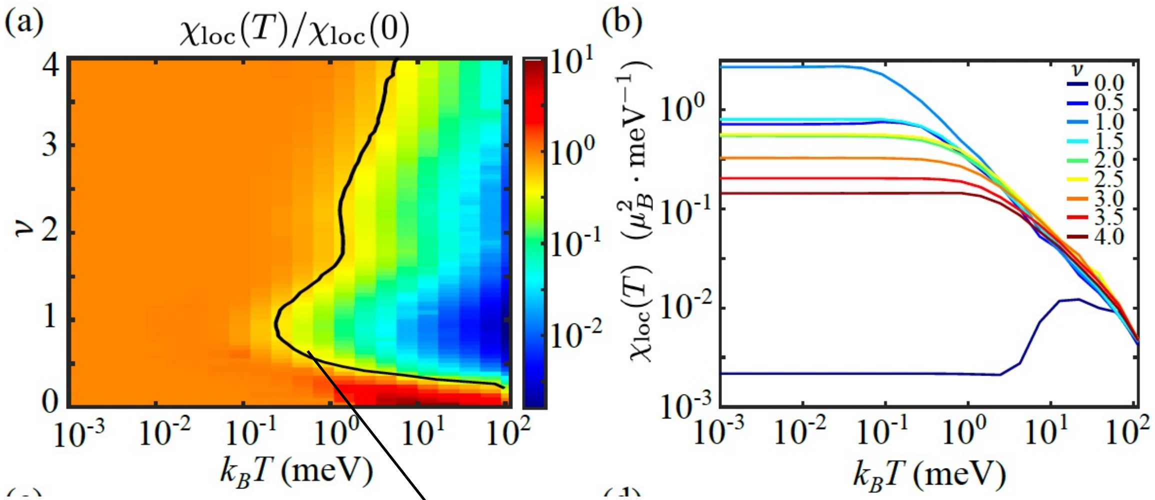
Local moments

At nu=1,

- local moments at early stage RG → LM at higher T
- Fermi liquid at later stage RG → FL at lower T
- => **Not pomeranchuck (a phase transition), but a cross-over from Kondo screening to free moments!**

Spin-susceptibility

- const. as T → 0, FL phase
- Cuire's law at higher T, LM phase

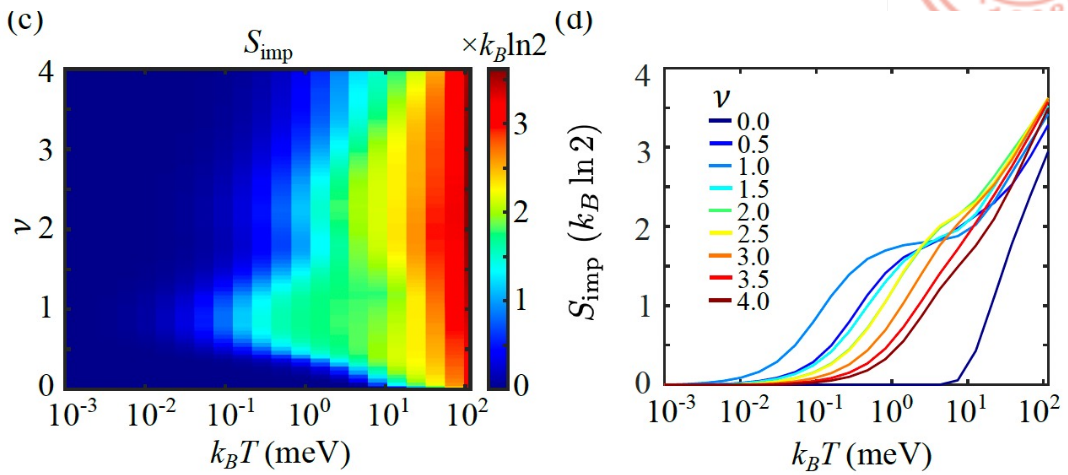


Kondo Temp

Rozen et al. 2021, Saito et al. 2021

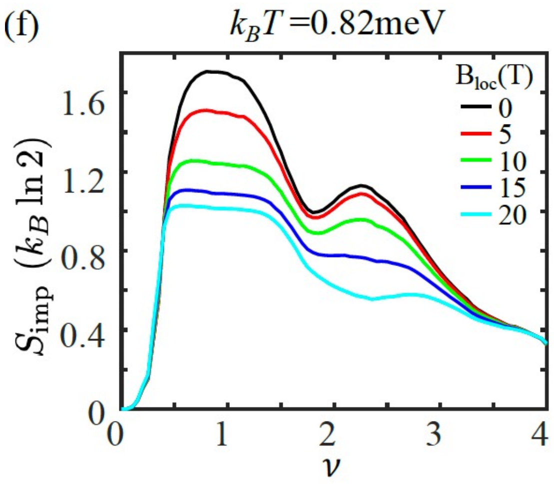
Entropy

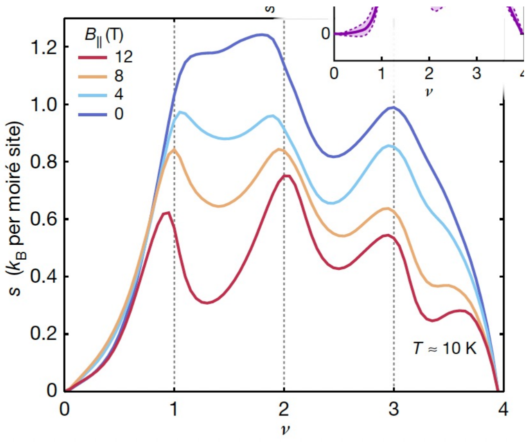
- 0 as T → 0, FL phase
- At nu=1, log 4 around T~10K, due to the four fold LM1



Comparision with Exps

Entropy curve as a function of nu at T~10K





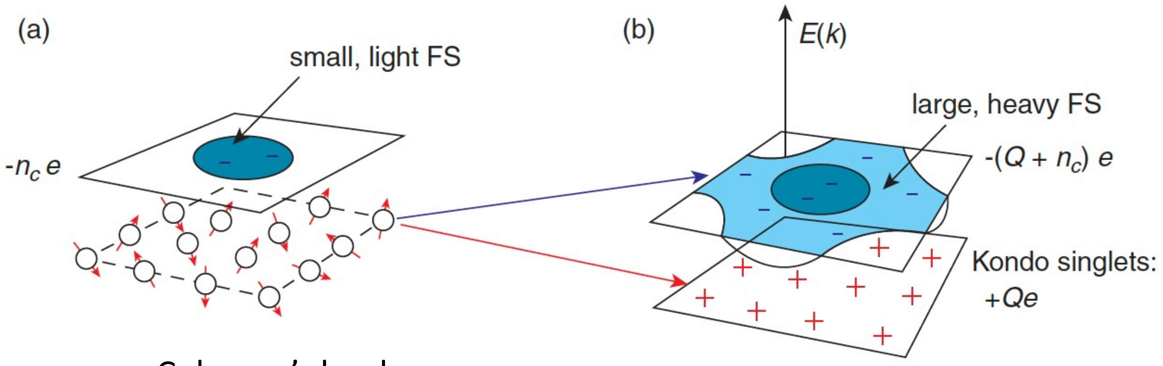
Rozen et al. 2021

Two-peak-one-dip feature: non-monotonous TK

PRL 129, 047601 (2022), PRB 109, 045419 (2024), arXiv:2402.00869 (2024)

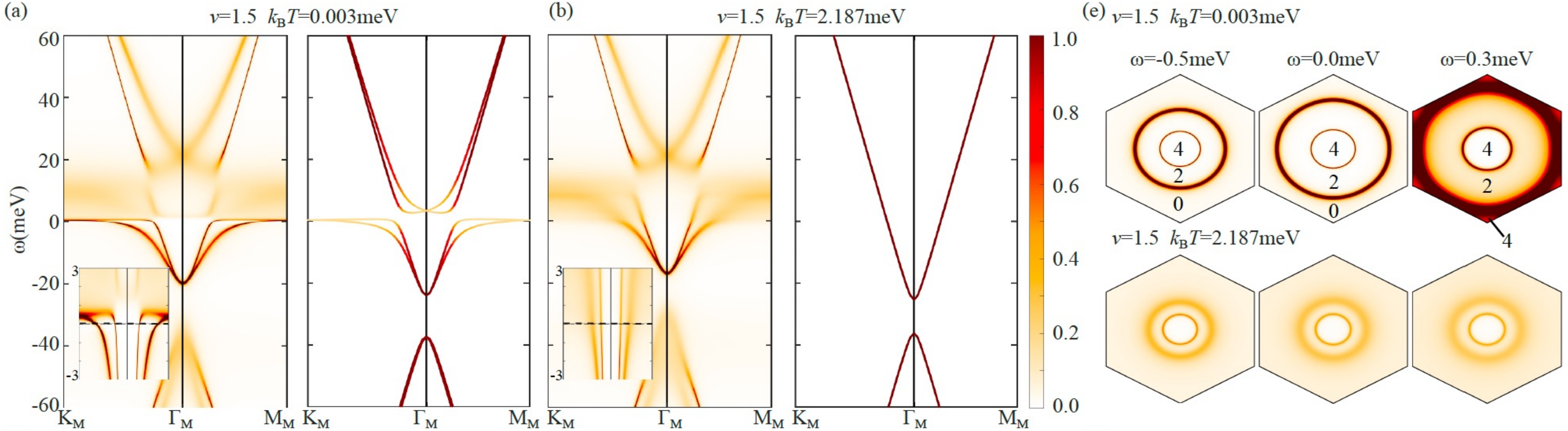
Experimental predictions

Temperature dependent energy surfaces



Coleman's book

DMFT bands **DMFT Fermi surface**



arXiv:2402.00869 (2024)

- ***Construction of Topological Heavy-Fermion Model***
- ***Summary of the correlation physics***
- ***Pairing mechanism***
- ***Superconductor phase***

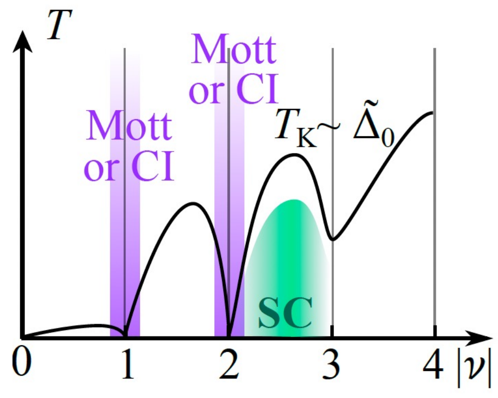
arXiv:2402.00869 (2024)

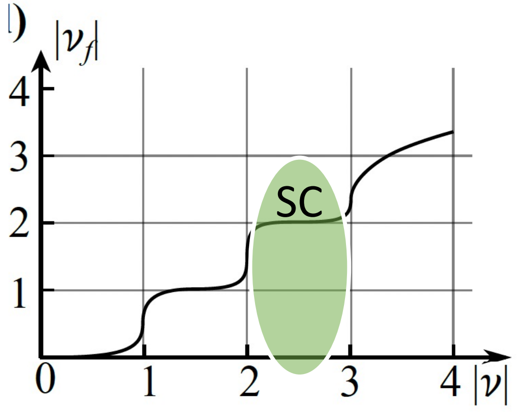
A single-site problem

Motivation: Onsite pairing as in A_3C_{60}?

*Dodaro, Kivelson et al., PRB **98**, 075154 (2018)*
*Angeli, Fabrizio et al., PRX **9**, 041010 (2019), Blason, Fabrizio, PRB **106**, 235112 (2022)*

Stating point: Anderson impurity model from self-consistent DMFT





Parameters:

- F-occupation: $|\nu_f| \approx 2$
- Kondo temperature T_K

Effective action

$$S_0 = -\sum_{\omega}\sum_{\alpha\eta s} f^\dagger_{\alpha\eta s}(\omega)(-i\omega + \epsilon_f - i\Delta(\omega)) f_{\alpha\eta s}(\omega)$$

$f^\dagger_{\beta\eta s}$

- orbital a.m. $(-)^{\beta-1}\eta$ (mod 3)
- valley charge $\eta = \pm$
- spin $s = \uparrow, \downarrow$

$\Delta(\omega) \approx \Delta_0 \cdot \mathrm{sgn}(\omega)$

Hubbard U

$$H_{I1} = \frac{U}{2}\sum_{\alpha\eta s}\sum_{\alpha'\eta' s'} f^\dagger_{\alpha\eta s} f^\dagger_{\alpha'\eta' s'} f_{\alpha'\eta' s'} f_{\alpha\eta s}$$

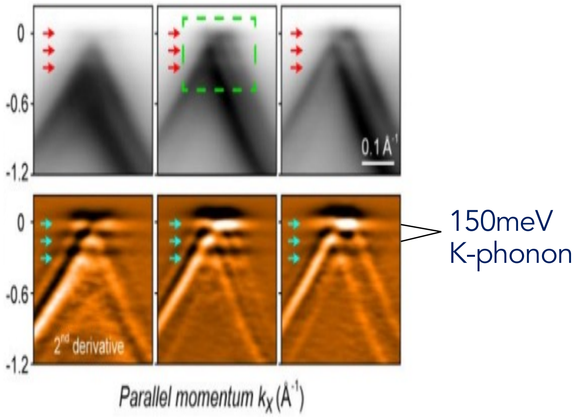
$U \approx 58$meV

$S_0 + H_{I1}$ faithfully characterizes low energy Kondo physics

arXiv:2402.00869 (2024)

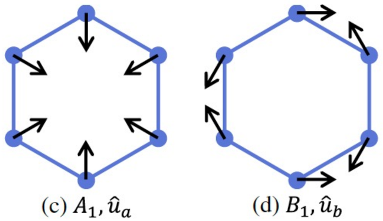
Other interactions

Electron-phonon coupling: (K-phonon)



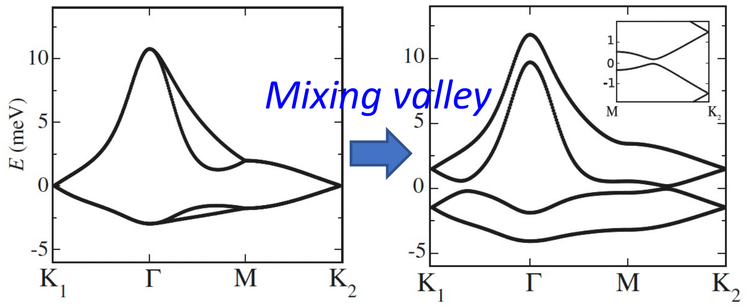
Strong EPC

Cheng et al. (2023) arXiv



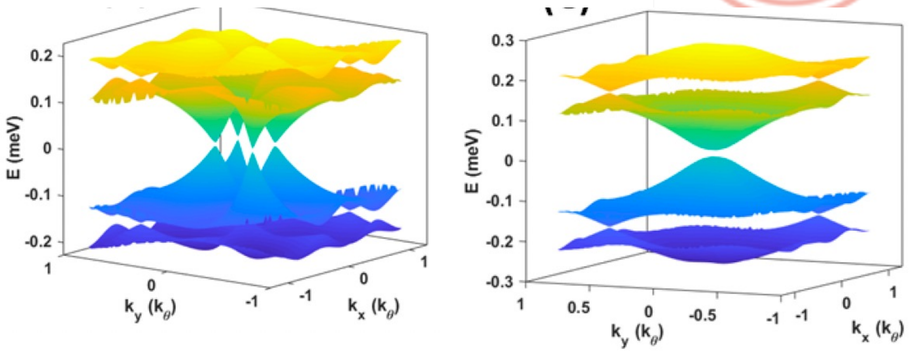
*Wu, MacDonald et al., PRL **121**, 257001 (2018)*

~150meV



Valley Jahn-Teller effect:

*Angeli, Fabrizio et al., PRX **9**, 041010 (2019)*



BCS pairing (assuming U=0)
s-wave is more favored than d-wave

*Wu, MacDonald et al., PRL **121**, 257001 (2018)*
Liu, Bernevig, arXiv:2303.15551 (2023)

Effective interaction on heavy fermion basis

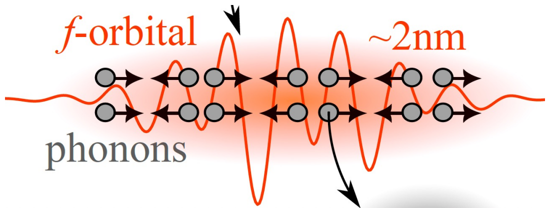
Favor inter-valley singlets

$$H_{I3} = \frac{J_A}{4}\sum_\eta \hat{N}_\eta \hat{N}_{\overline{\eta}} + J_A \sum_\eta \hat{\mathbf{S}}_\eta \cdot \hat{\mathbf{S}}_{\overline{\eta}} - \frac{J_A}{2}\sum_{\alpha\eta s s'} f^\dagger_{\alpha\eta s} f^\dagger_{\overline{\alpha}\eta s'} f_{\alpha\overline{\eta}s'} f_{\alpha\eta s}$$

Anti-Hund's coupling:

- JA = 1.3meV << U=58meV
- JA may be enhanced by 1-3 times by renormalization

*Basko, PRB **77**, 041409 (2008)*

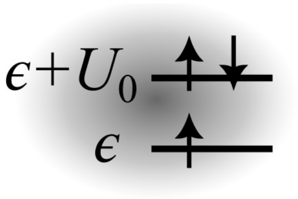


Mesoscopic orbitals coupled to microscopic phonons <-> A3C60

arXiv:2402.00869 (2024)

Other interactions

Hubbard U_0 at carbon atom



Parameter: U0 ~ 3-9eV
Role: forbid double occupation

Wehling et al., PRL 106, 236805 (2011),
*Wu, MacDonald et al., PRL **121**, 257001 (2018)*
Zhang, Liu et al., PRL 128 026403 (2022)

Penalty to intra-orbital singlet

$$\frac{J_H}{2}\hat{N} + \frac{J_H}{4}\sum_\alpha \hat{N}_\alpha^2 - J_H \sum_\alpha \hat{\mathbf{S}}_\alpha \cdot \hat{\mathbf{S}}_\alpha$$

$$\frac{J'_H}{4}\sum_\alpha \hat{N}_\alpha \hat{N}_{\bar{\alpha}} - J'_H \sum_\alpha \hat{\mathbf{S}}_\alpha \cdot \hat{\mathbf{S}}_{\bar{\alpha}}$$

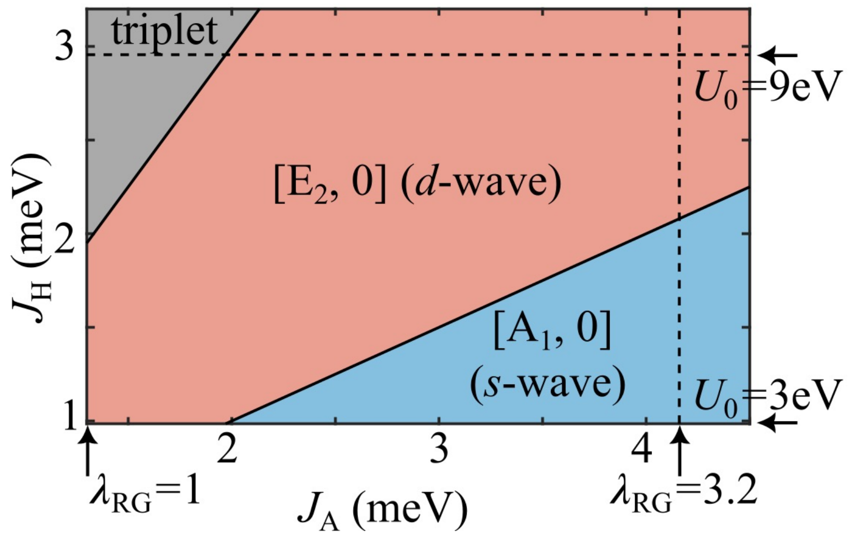
Penalty to inter-orbital singlet

Hund's coupling:
J_H ~ 1- 3meV
$J_H' \approx \frac{J_H}{3}$

Large overlap between $\alpha = 1, 2$ and AB sublattice!!!

A two particle problem

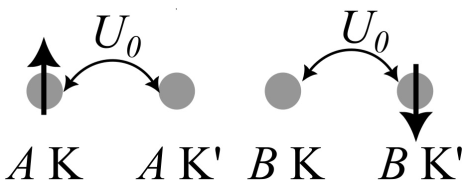
motivated by $|\nu_f| \approx 2$



!!! NO PAIRING DUE TO PROHIBITIVE U !!!

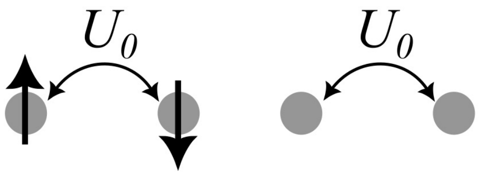
E_2 states $f^\dagger_{\alpha+\uparrow} f^\dagger_{\bar{\alpha}-\downarrow} - (\uparrow\leftrightarrow\downarrow)$

$E = U - 2J_A + 8/3 J_H$



A_1 state $f^\dagger_{1+\uparrow} f^\dagger_{1-\downarrow} + f^\dagger_{2+\uparrow} f^\dagger_{2-\downarrow} - (\uparrow\leftrightarrow\downarrow)$

$E = U - J_A + 2/3 J_H$



arXiv:2402.00869 (2024)

An (almost) SOLVABLE limit: $T_K \ll J_{A,H}$

Local Fermi Liquid

Nozières et al. (1980)
Hewson (1993)

- T_K defines a ***single*** energy scale of the problem
- All renormalized parameters ~ T_K

Renormalized S0

$$\sum_\omega \tilde{f}_I^\dagger(\omega)(-i\omega - i\tilde{\Delta}_0 \cdot \mathrm{sgn}(\omega) + \tilde{\epsilon}_f)\tilde{f}_I(\omega)$$

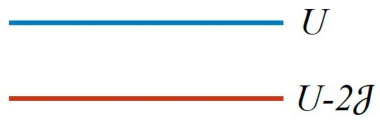
- $\tilde{f} = z^{-\frac{1}{2}} f$
- $\tilde{\Delta}_0 = z\,\Delta_0$
- $\frac{\tilde{\epsilon}_f}{\tilde{\Delta}_0} = \cot\frac{\pi(4+\nu_f)}{8}$
- $z = 1 - \partial_{i\omega}\Sigma(\omega)$

Physical parameters:

- $\tilde{\Delta}_0 \sim T_K$ ~0.1-1meV
- $z \sim 0.1 - 0.3$

Projector interaction: $U(1)^{\times 4} \times SU(2)^{\times 2}$ symmetry

- Interaction → ***Projector*** to the E_2 states
- Most generic interaction

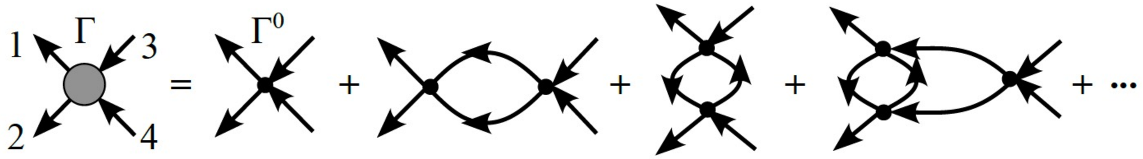


$$S_I = \frac{1}{2}\int d\tau \sum_{\alpha\eta}\left(\left(U_1 + \frac{\mathcal{J}}{2}\right)N_{\alpha\eta}N_{\overline{\alpha\eta}} + U_2 N_{\alpha\eta}N_{\alpha\overline{\eta}} + U_3 N_{\alpha\eta}N_{\overline{\alpha}\eta} + U_4 N_{\alpha\eta}^2 + 2\mathcal{J}\cdot\mathbf{S}_{\alpha\eta}\cdot\mathbf{S}_{\overline{\alpha\eta}}\right)$$

- Bare values: $U_{1,2,3,4} = U$, $\mathcal{J} \sim J_A$
- Generators: $\tau^{0,z}\sigma^{0,z}$, $(\tau^0\sigma^0 \pm \tau^z\sigma^z)s^{x,y,z}$

Renormalized Interaction

- $\tilde{U}_i = z^2\Gamma_{Ui}$
- $\tilde{J} = z^2\,\Gamma_J$
- Γ is divergent $\sim z^{-1}$



We need to derive the ***exact*** Γ

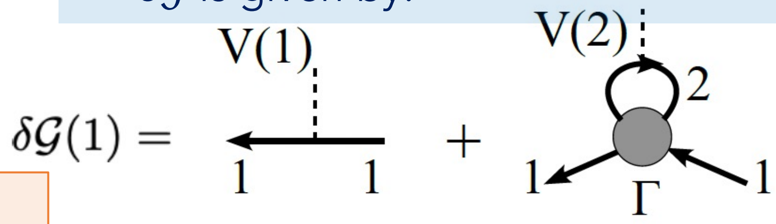
arXiv:2402.00869 (2024)

An (almost) SOLVABLE limit: $T_K << J_{A,H}$

Ward identity

- Gauge transform: $f' = e^{i\,\tau\,\nu O} f$
- O is symmetry generator
- $\mathcal{G}'(\tau) = e^{i\,\tau\,\nu\,O}\mathcal{G}(\tau)$
- $\mathcal{G}'(\tau) - \mathcal{G}(\tau)$

- $S[f,f] = S'[f'] = S[f'] + V[f']$
- $\delta\mathcal{G}$ is given by:



- Exact relation between $\delta\Sigma[V] \sim \Gamma$
- $\delta\Sigma[V]$ is related to susceptibilities

Exact susceptibilities

$\tilde{\Gamma} = z^2\Gamma$: renormalized interaction

Conserved quantity

Filling fraction

$$\chi^O = \frac{\sin^2\delta_f}{\pi\,\tilde{\Delta}_0}\left[\mathrm{Tr}[O^2] - \frac{\sin^2\delta_f}{\pi\tilde{\Delta}_0}\mathrm{Tr}[O\cdot\tilde{\Gamma}\cdot O]\right]$$

Yoshimori (1976)

Kondo temperature

Our model:

- Charge, $O = 1$
- Spin, $O = s^z$
- Valley, $O = \tau^z$
- Orbital, $O = \sigma^z$
- Angular momentum, $O = \tau^z\sigma^z$

- $\mathrm{Tr}[O\cdot\tilde{\Gamma}\cdot O] = 2\tilde{U}_1 + 2\tilde{U}_2 + 2\tilde{U}_3 + \tilde{U}_4 + \tilde{J}$
- $\mathrm{Tr}[O\cdot\tilde{\Gamma}\cdot O] = -\tilde{U}_4 + \tilde{J}$
- $\mathrm{Tr}[O\cdot\tilde{\Gamma}\cdot O] = -2\tilde{U}_1 - 2\tilde{U}_2 + 2\tilde{U}_3 + \tilde{U}_4 - \tilde{J}$
- $\mathrm{Tr}[O\cdot\tilde{\Gamma}\cdot O] = -2\tilde{U}_1 + 2\tilde{U}_2 - 2\tilde{U}_3 + \tilde{U}_4 - \tilde{J}$
- $\mathrm{Tr}[O\cdot\tilde{\Gamma}\cdot O] = 2\tilde{U}_1 - 2\tilde{U}_2 - 2\tilde{U}_3 + \tilde{U}_4 + \tilde{J}$

arXiv:2402.00869 (2024)

An (almost) SOLVABLE limit: $T_K << J_{A,H}$

Physical susceptibilities

As T_K << J, only the ground (E2) states participate Kondo screening

$$f^\dagger_{\alpha+\uparrow} f^\dagger_{\overline{\alpha}-\downarrow} - (\uparrow\leftrightarrow\downarrow)$$

A 2D Hilbert space

- Frozen charge ➔ $\chi^c = 0\ (\ll T_K^{-1})$
- Frozen spin ➔ $\chi^s = 0$
- Frozen orbital ➔ $\chi^o = 0$
- Frozen valley ➔ $\chi^v = 0$
- Fluctuating angular momentum ➔ $\chi^a \sim T_K^{-1}$

$$\widetilde{U}_1 = -2\pi\widetilde{\Delta}_0, \quad \widetilde{U}_{2,3} = 2\pi\widetilde{\Delta}_0 - \frac{\widetilde{\mathcal{J}}}{2}, \quad \widetilde{U}_4 = -2\pi\widetilde{\Delta}_0 + \widetilde{\mathcal{J}}$$

Applying this to standard Anderson impurity

- $\widetilde{U} = \pi\widetilde{\Delta}_0$: same as Bethe ansatz solution
- Applicable to U(n)XSU(2) model

Hewson (1993), Nishikawa (2010)

Two-particle energies

- Inter-valley E_2 singlet: $-2\pi\,\widetilde{\Delta}_0 - \tilde{\mathcal{J}}$
- Inter-valley E_2 triplet: $-2\pi\,\widetilde{\Delta}_0 + \tilde{\mathcal{J}}$
- Intra-valley intra orbital singlet: $-2\pi\,\widetilde{\Delta}_0 + \tilde{\mathcal{J}}$
- Inter-valley intra-orbital: $2\pi\,\widetilde{\Delta}_0 - \frac{1}{2}\tilde{\mathcal{J}}$
- Inter-valley intra-orbital: $2\pi\,\widetilde{\Delta}_0 + \frac{1}{2}\tilde{\mathcal{J}}$

One of them must be negative !!
Hence renormalized interaction has pairing channel!

- Stability of the Fermi liquid requires:
- $\tilde{\mathcal{J}} = k\cdot\widetilde{\Delta}_0 > 0,\ \ k \in (4.6, 10.3)$
- k should be a universal constant
- ➔ **The *E_2 singlet* is most favored.**

arXiv:2402.00869 (2024)

Crossover from $T_K << J_{A,H}$ to $J_{A,H} << T_K << U$

The $J_{A,H} << T_K << U$ limit

As J << TK << U, multiplet splitting is irrelevant ➔ ***an approximate U(8) symmetry at T_K scale***

- $\mathcal{J} = 0$ $(<<T_K)$
- $U_{1,2,3,4} = U$
- Frozen charge ➔ $\chi^o = 0$
- *No pairing*

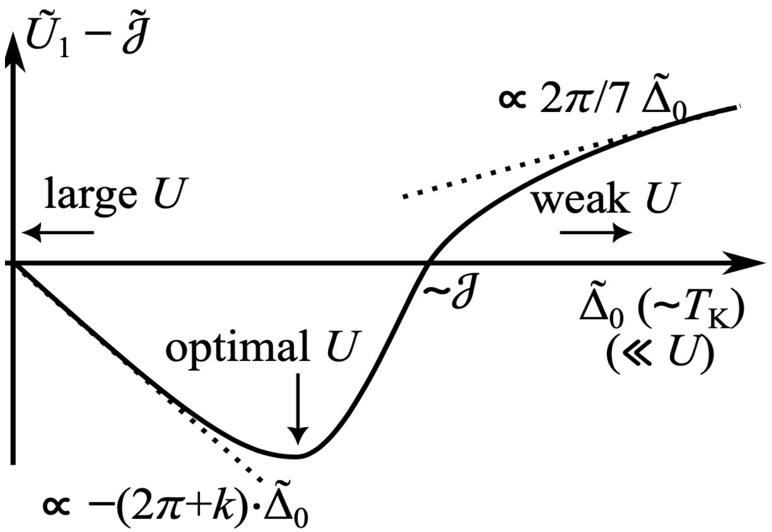
$$\widetilde{U}_{1,2,3,4} = \frac{2\pi}{7}\widetilde{\Delta}_0$$

previously obtained in by Nishikawa, Hewson et al. (2010)

Crossover

Renormalized pairing potential

- **$T_K << J_{A,H}$** : $-(2\pi + k)\widetilde{\Delta}_0$



- **$J_{A,H} << T_K << U$** : $\frac{2\pi}{7}\widetilde{\Delta}_0$
- **$T_K > U$** : U

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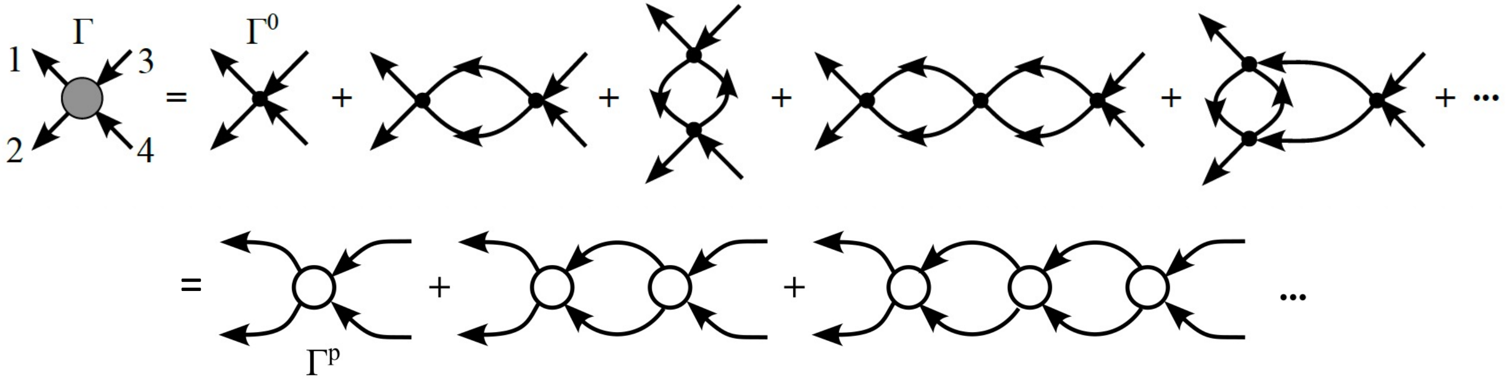
Irreducible vertex in pairing channel

Full vertex can be decomposed into 2PI diagrams



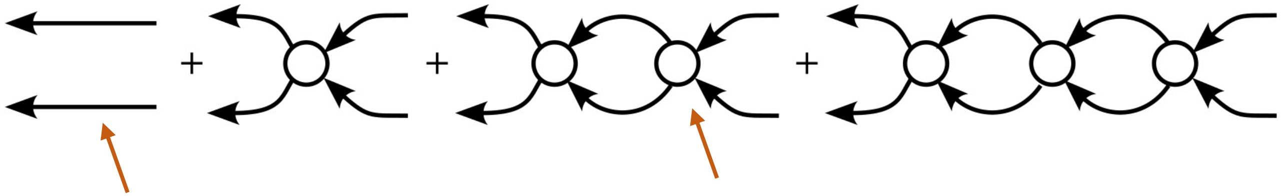
$$U_1^{\mathrm{p}} - \mathcal{J}^{\mathrm{p}} = \frac{\widetilde{U}_1 - \widetilde{\mathcal{J}}}{1 - \frac{1}{4\widetilde{\Delta}_0}(\widetilde{U}_1 - \widetilde{\mathcal{J}})} = -\frac{(2\pi + k)}{1 + \frac{2\pi + k}{4}}\widetilde{\Delta}_0$$

- Slightly weaker than full vertex

2PI serves as effective interaction on lattice

Georges, Kotliar, et al., RMP (1996)

- SC susceptibility on lattice:



Lattice green's function

Sum $U_1^p - \mathcal{J}^p$ over sites

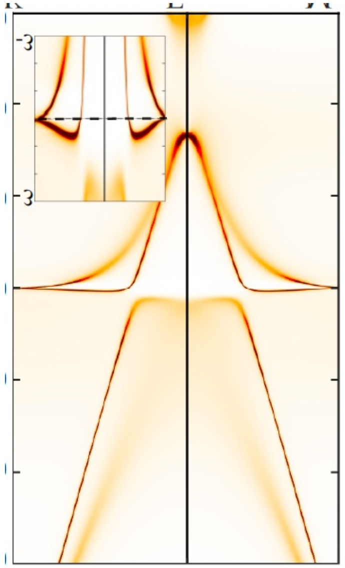
The local pairing fluctuation ➔ SC on lattice

- ***Construction of Topological Heavy-Fermion Model***
- ***Summary of the correlation physics***
- ***Pairing mechanism***
- ***Superconductor phase***

arXiv:2402.00869 (2024)

Renormalized lattice model

The free part: heavy Fermi liquid



$$\epsilon_f \sum_{\mathbf{k}} \tilde{f}^\dagger_{\mathbf{k}} \tilde{f}_{\mathbf{k}} + c^\dagger_{\mathbf{k}} \mathcal{H}^{(c)}(\mathbf{k}) c_{\mathbf{k}} + z^{\frac{1}{2}} \left[c^\dagger_{\mathbf{k}} \mathcal{H}^{(cf)}(\mathbf{k}) \tilde{f}_{\mathbf{k}} + h.c. \right]$$

- Parameters:
- TK=0.1-1meV
- Z=0.1-0.3

- The quasi-particle part is characterized by a bilinear term
- $\tilde{f} = z^{-\frac{1}{2}} f$ is quasi-particle
- cf hybridization is suppressed by $z^{\frac{1}{2}}$

Chiral-d solution

$$\tilde{f}^\dagger_{\mathbf{k}\alpha+\uparrow} \tilde{f}^\dagger_{-\mathbf{k}\overline{\alpha}-\downarrow} - (\uparrow \leftrightarrow \downarrow)$$

Interacting part

the E2 singlet state

$$= \frac{U_1^{\mathrm{p}} - \mathcal{J}^{\mathrm{p}}}{2} \sum_{\mathbf{R}} \sum_{\eta} (\tilde{f}^\dagger_{\mathbf{R}2\overline{\eta}\downarrow} \tilde{f}^\dagger_{\mathbf{R}1\eta\uparrow} - \tilde{f}^\dagger_{\mathbf{R}2\overline{\eta}\uparrow} \tilde{f}^\dagger_{\mathbf{R}1\eta\downarrow})(\tilde{f}_{\mathbf{R}1\eta\uparrow} \tilde{f}_{\mathbf{R}2\overline{\eta}\downarrow} - \tilde{f}_{\mathbf{R}1\eta\downarrow} \tilde{f}_{\mathbf{R}2\overline{\eta}\uparrow})$$

- $U_1^p - \mathcal{J}^p$ is the 2PI vertex

$$U_1^{\mathrm{p}} - \mathcal{J}^{\mathrm{p}} = \frac{\widetilde{U}_1 - \widetilde{\mathcal{J}}}{1 - \frac{1}{4\widetilde{\Delta}_0}(\widetilde{U}_1 - \widetilde{\mathcal{J}})} = -\frac{(2\pi + k)}{1 + \frac{2\pi + k}{4}} \widetilde{\Delta}_0$$

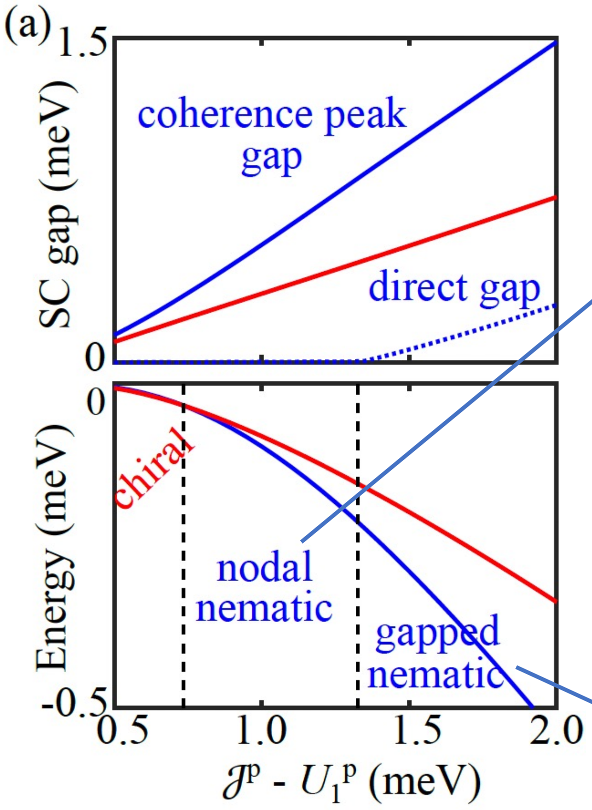
Nematic-d solution

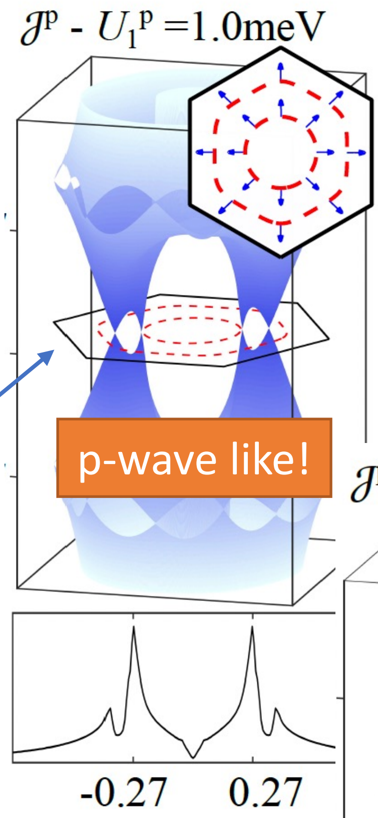
$$e^{-i\varphi} \tilde{f}^\dagger_{\mathbf{k}1+\uparrow} \tilde{f}^\dagger_{-\mathbf{k}2-\downarrow} + e^{i\varphi} \tilde{f}^\dagger_{\mathbf{k}2+\uparrow} \tilde{f}^\dagger_{-\mathbf{k}1-\downarrow} - (\uparrow \leftrightarrow \downarrow)$$

- φ: orientation of nematic order
- TRS preserving
- C3 breaking

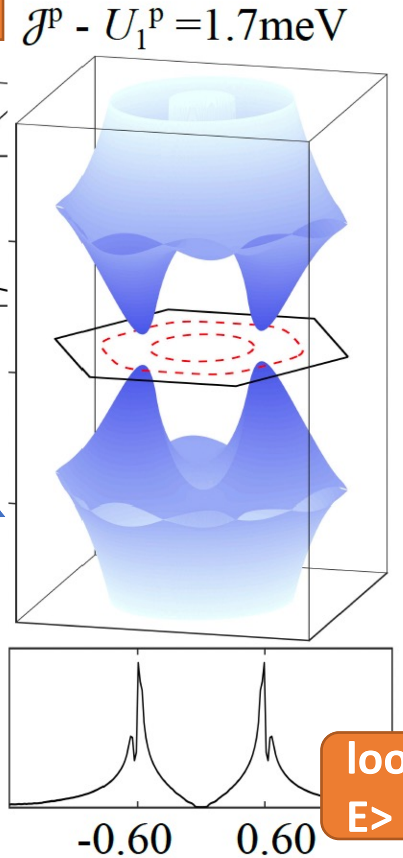
Phase diagram

arXiv:2402.00869 (2024)





p-wave like!



looks V-shaped at E> gap, E < Δ_0

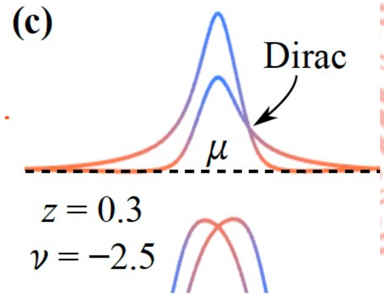
Berry's phase enforced nodes

$$(C_{2z}T)\psi^\dagger_{\mathbf{k}+s}(C_{2z}T)^{-1} = \psi^\dagger_{\mathbf{k}+s}e^{i\phi_\mathbf{k}}$$

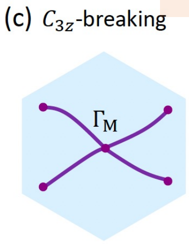
$$\cos(\phi_\mathbf{k}+\varphi)\cdot\psi^\dagger_{\mathbf{k}+\uparrow}\psi^\dagger_{-\mathbf{k}-\downarrow} - (\uparrow\leftrightarrow\downarrow)$$

Euler's pairing obstruction

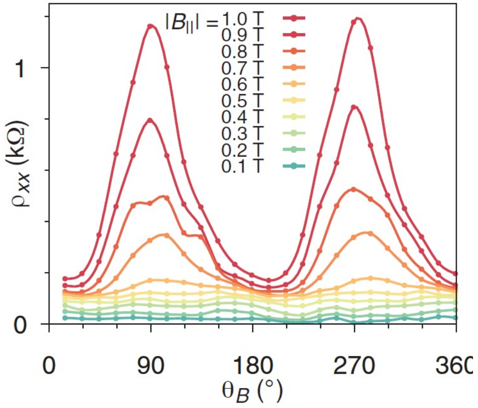
Yu, Das Sarma, et al. (2022), arXiv:2202.02353



- ϕ_k winds 2pi on FS

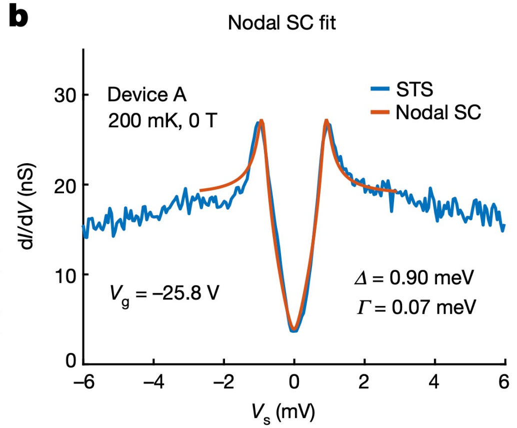


✓ Nematicity



Cao et al. (2021) Science

✓ V-shaped gap

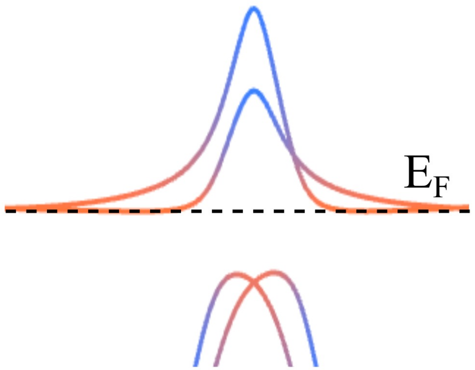


Oh et al. (2021) Nature

arXiv:2402.00869 (2024)

Strong coupling features

Energy scale

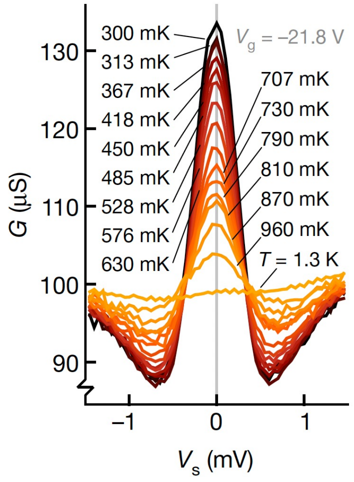


- $E_F \sim T_K$
- $U_p - J_p \sim 4\, T_K > E_F$

- *BEC rather than BCS!*

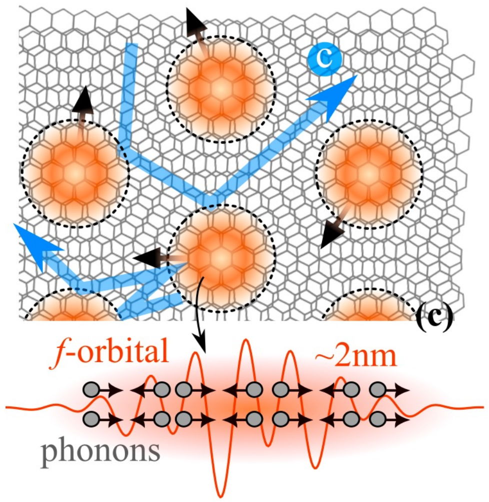
✓ Gap ~ 25 Tc

Oh et al. (2021) Nature



Coherence establishes at lower energy than pairing

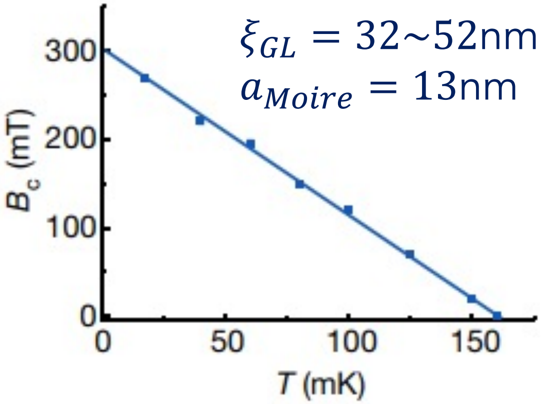
Real space picture



- *Coherence length:*
- *Kondo cloud*

$$\frac{v_F}{T_K} \sim \frac{1}{k_F} \sim \text{a few } a_M$$

✓ Small coherence length



Cao et al. (2018) Nature
Lu et al. (2019) Nature

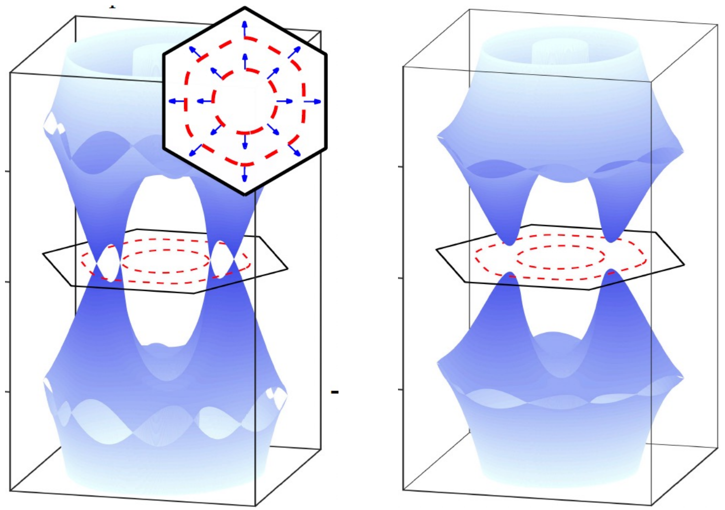
arXiv:2402.00869 (2024)

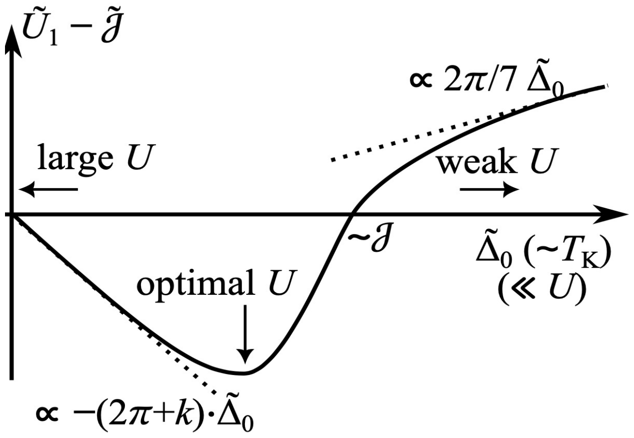
Summary

- Explain how the weak attraction wins over U
- Consistent with the following experiments:
  - Nematicity
  - V-shaped gap
  - Tc >> gap
  - Small coherence length
  - SC enhanced by suppressing U, introducing SOC

Predictions

- The (gapped) p-wave like nodal structure
- Non-monotonous dependence of Tc on U





arXiv:2402.00869 (2024)

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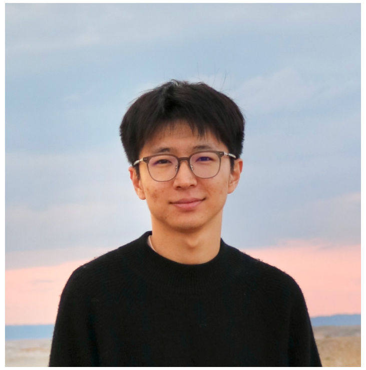

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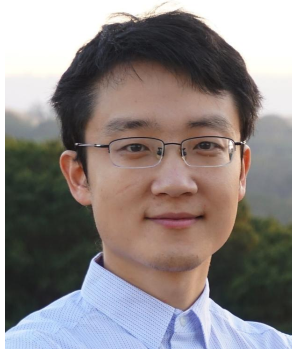

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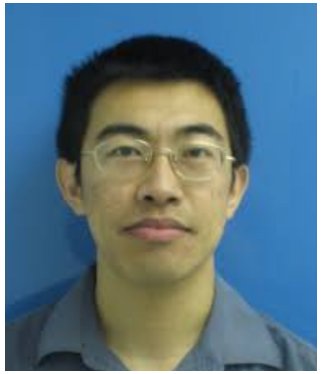

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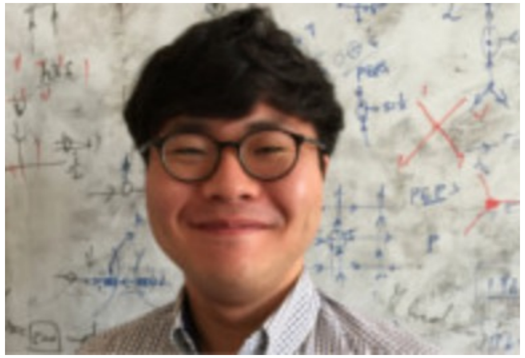

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