Exotic density-wave states and superconductivity in kagome metals and other strongly correlated electron systems

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in collaboration with

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(28 November, NQS2022, Kyoto)

NAGOYA UNIVERSITY

新学術領域研究 令和元年度～５年度

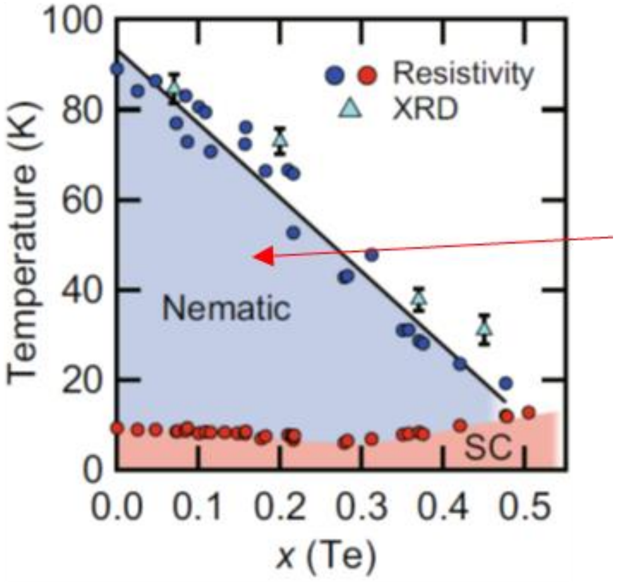
量子液晶の物性科学

Quantum Liquid Crystals

Unconventional orders: non-local, non-s-wave

Fe-based SCs

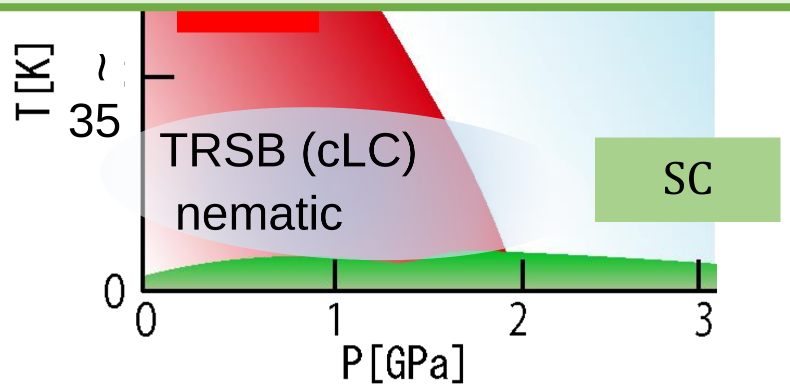
S. Onari and HK, Frontiers in Physics (2022)



kagome metal AV_3Sb_5

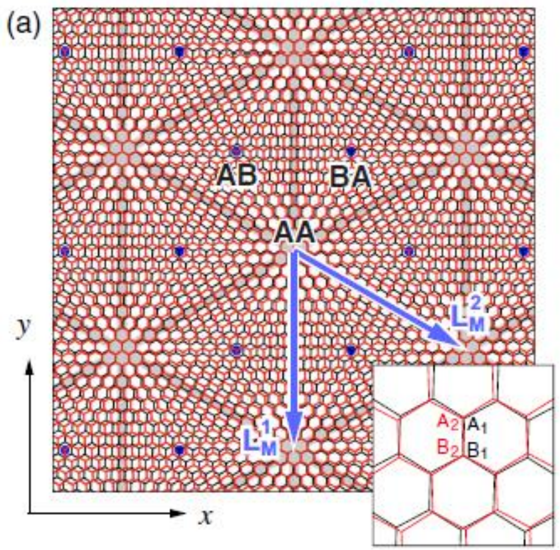
R. Tazai et al, Sci. Adv. 8, abl4108 (2022)

Open issues:
✓Origin of unconventional orders
✓Interplay between different orders



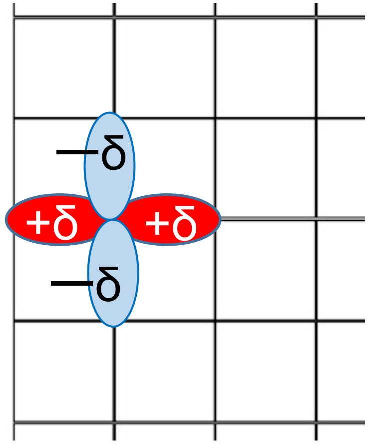
twisted bilayer graphene

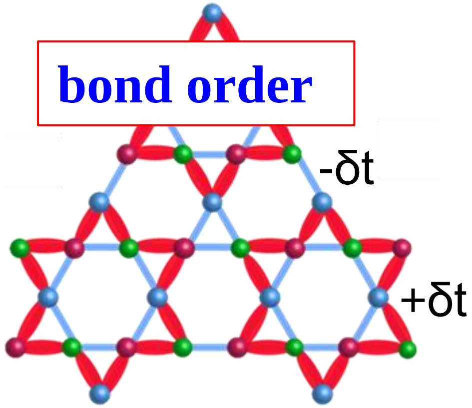
S. Onari and HK, PRL 128, 066401 (2022)



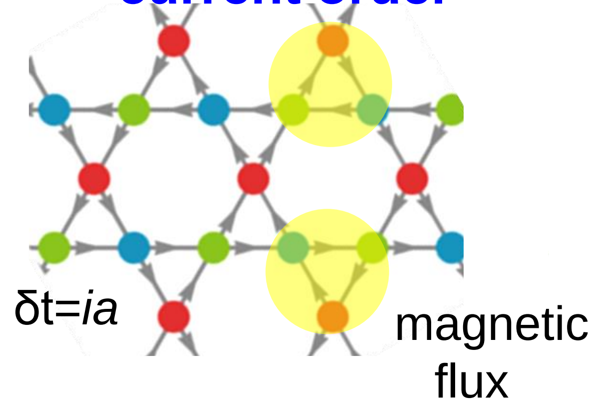
nematic order

Orbital order
+
Bond order
= real hopping modulation δt＝±δ





odd-parity, imaginary = current order



Mean-field approximation (MFA)

1. Multiorbital Hubbard model

l,*m*: orbital

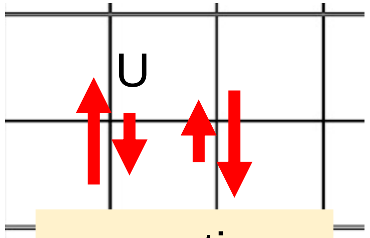
$$\sum_i \left[U \sum_l n_{l\uparrow} n_{l\downarrow} + U' \sum_{l>m} n_l n_m + (J, J') \right]$$

Intra-orbital > Inter-orbital
→spin order →orbital order

MFA →

SDW (local order parameter)

× Orbital order
n_{xz}-n_{yz}≠0



magnetism by on-site U

Beyond-Mean-field theory is needed !

2. U+V Hubbard model

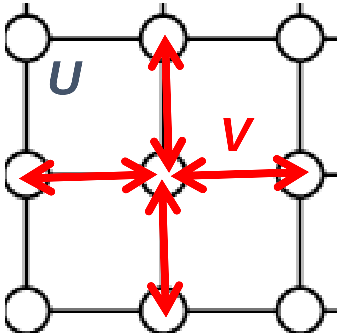
$$V_{\boldsymbol{q}} = 2V[\cos q_x + \cos q_y] \quad \rightarrow \quad V_{\boldsymbol{k}-\boldsymbol{k}'} = 2V \gamma_{\boldsymbol{k}} \gamma_{\boldsymbol{k}'} + \cdots$$

γ_k = cosk_x - cosk_y

d-wave bond-order

cf. eigenvalue decomposition

square lattice



MFA →

Bond order can emerge,
but very large V ($\gtrsim U/2$) is necessary.

Theory 1: Symmetry breaking in the normal self-energy $f_{\boldsymbol{q}}(\boldsymbol{k})$ [~ δt]

R. Tazai, S. Matsubara et al, arXiv:2205.02280

Ground potential (Luttinger-Ward)

$$\Omega = T\sum_{k\sigma}(\ln G_{k\sigma} - G_{k\sigma}\Sigma_{k\sigma}) + \Phi[G]$$

+

$\Sigma_{\boldsymbol{q}}(k) = \Sigma^0(k) + f_{\boldsymbol{q}}(\boldsymbol{k})$: symmetry breaking at $\boldsymbol{q}$ (=form factor)

$$\frac{\delta\Omega[f]}{\delta f} = 0$$

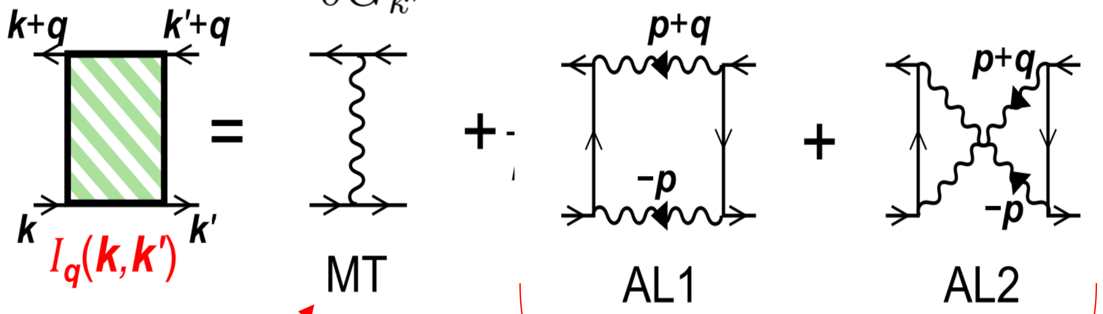
Density-wave (DW) equation:
optimum solution $f_{\boldsymbol{q}}(\boldsymbol{k})$ that minimize Ω.

$$\lambda f(k) = T\sum_{k'}(G^0_{k'})^2 I_{kk'} f(k')$$

S. Onari, *et al.*, PRL **116**, 227001 (2016)~

$$I_{kk'} \equiv \frac{\delta\Sigma_k[G]}{\delta G_{k'}}$$

irreducible 4-point vertex

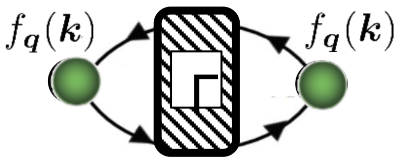


charge current order
R. Tazai et al, PRB, L161112 (2021)
d-wave SC Hirsch et al, PRB ('86)

- orbital order in Fe-based SCs
  R. Tazai et al, arXiv:2205.02280
- bond-order in kagome metals
  R. Tazai et al, Sci. Adv. 8, abl4108 (2022)

Theory 2: Optimization of $\chi_f(\boldsymbol{q})$ using functional RG theory

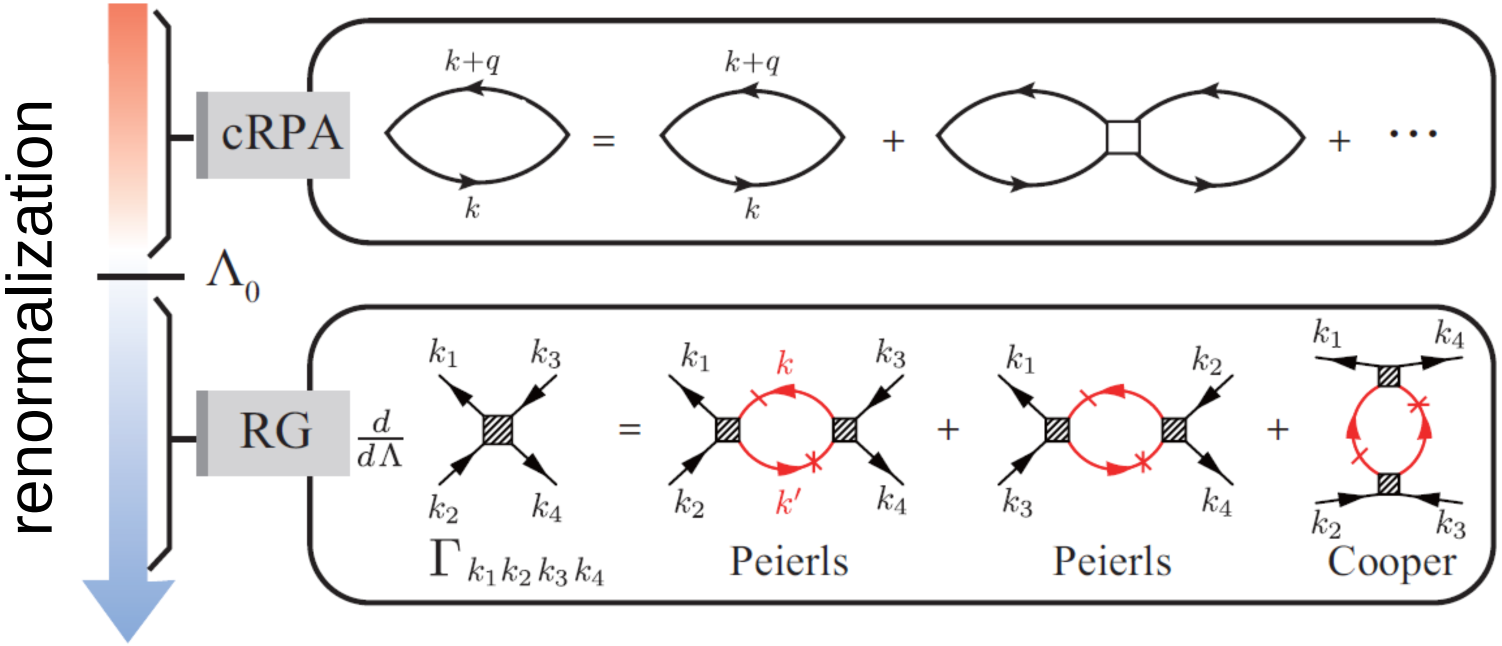
$\chi_f(\boldsymbol{q})=$



Optimized form factor $f_q(k)=$ ●
is realized. (highest T_c)

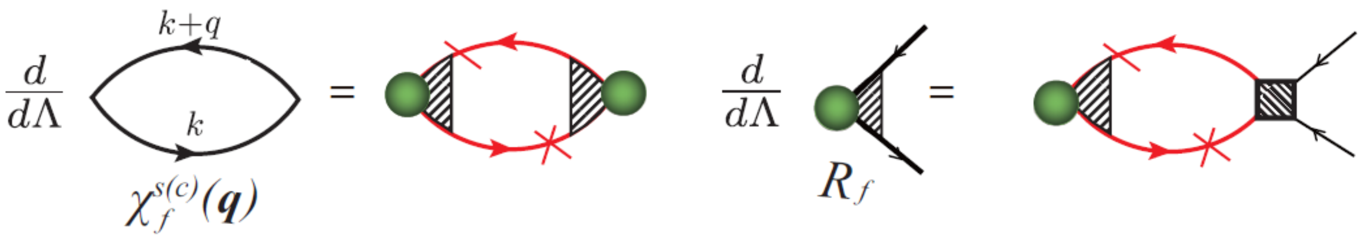
R. Tazai et al.,
PRB 103, L161112 (2021)

Importance of AL interference mechanism!



RG+cRPA theory
M. Tsuchiizu et al, PRL (2013)～

W. Metzner, et al.,
Rev. Mod. Phys. (2012)



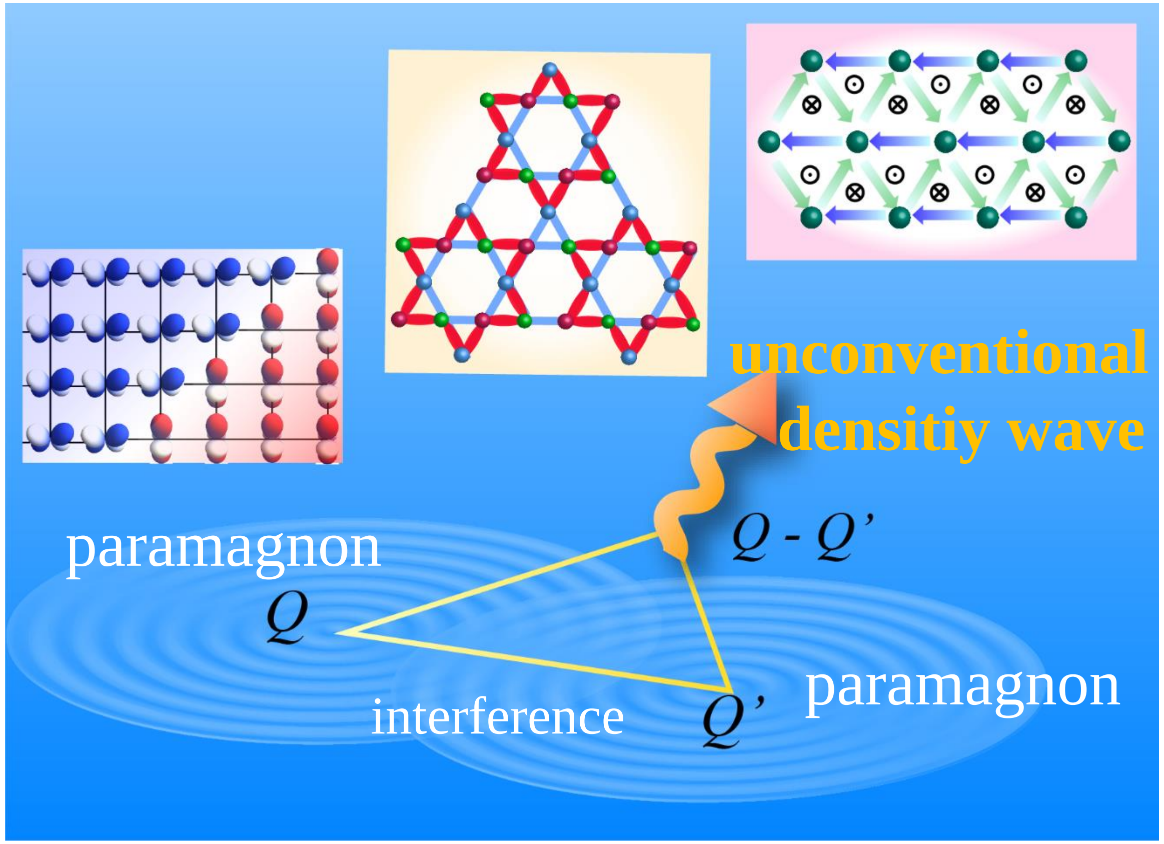
➡ $\chi_f(\boldsymbol{q})$

We optimize $f_q(k)=$ ●
by variational method
using >100 basis

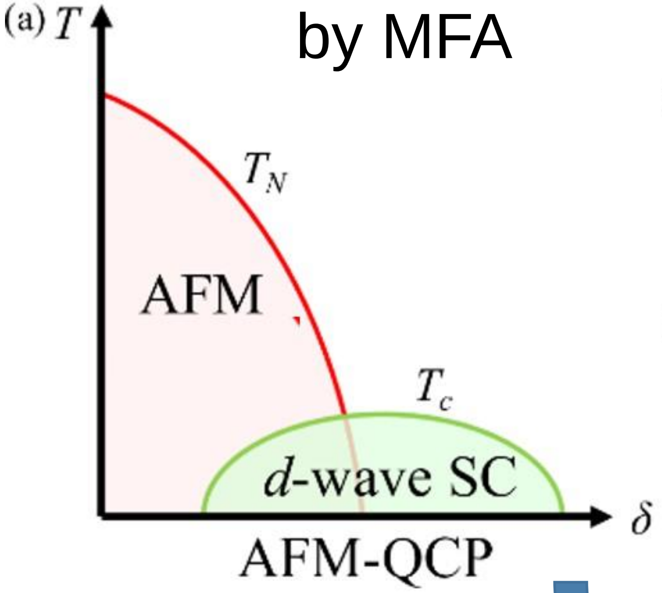
R. Tazai et al., PRB 103, L161112 (2021)

quantum interference mechanism

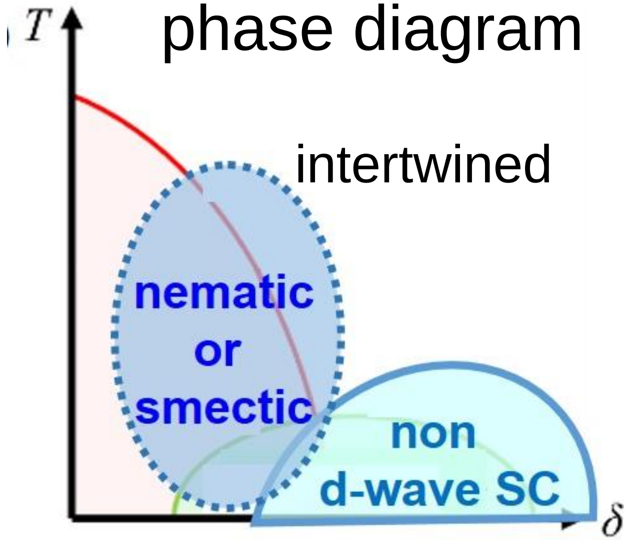
H. Kontani et al., Adv. Phys. (accepted)



phase diagram
by MFA

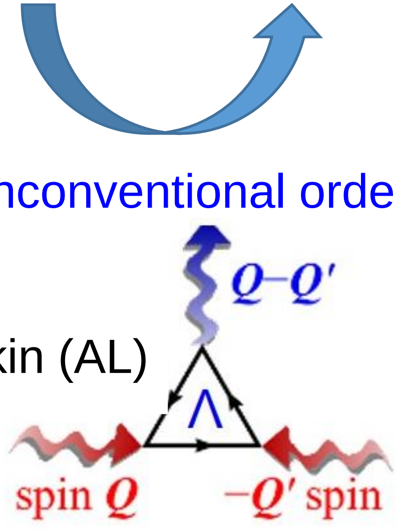


new
phase diagram



unconventional order

Aslamazov-larkin (AL)
interference



Contents

1. Nematiicy in FeSe: Lifshitz transition R. Tazai, S. Matsubara et al, arXiv:2205.02280

2. XY-type nematicity in twisted bilayer graphene S. Onari et al, PRL 128, 066401 (2022)

3. Cascade of exotic orders in kagome metal AV_3Sb_5 (A=Cs,Rb,K)

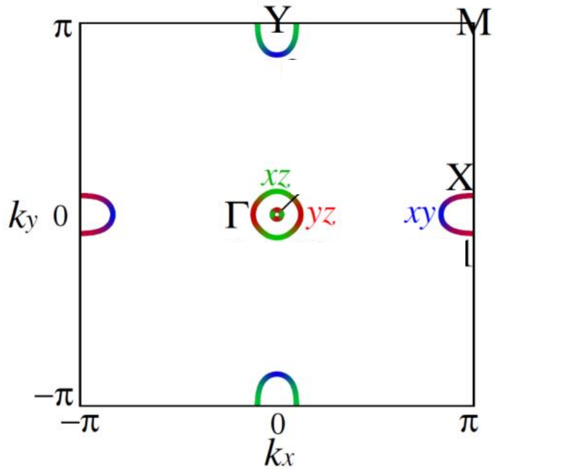
   Bond-order and superconductivity R. Tazai et al, Sci. Adv. 8, abl4108 (2022)

   Charge current order and Z_3 nematicity R. Tazai et al, arXiv:2207.08068

Nematicity in FeSe families

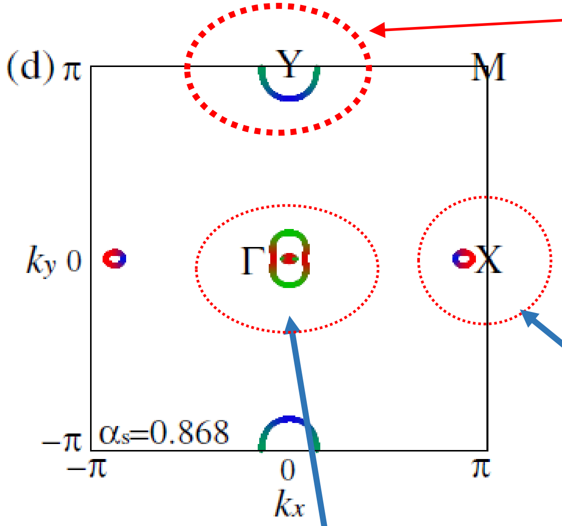
FeSe

C_4 Fermi surface ($T>T_S$)



AL interference mechanism
on xz,yz-orbitals

S. Onari, *et al.*, PRL **116**, 227001 (2016)



Recent ARPES (2019~)

This pocket disappears below T_S

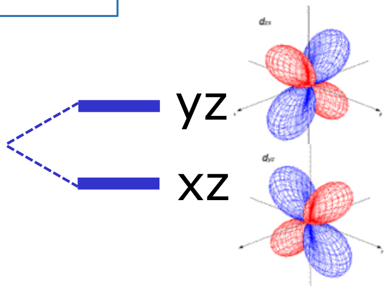
ARPES: S.S. Huh et al,
Commun. Phys. **3**, 52 (2020).

ARPES: M. Yi, et al,
PRX **9**, 041049 (2019).

Elongated along k_x-axis

Elongated along k_y-axis

orbital polarization



Laser ARPES
Y. Suzuki et al.,
RPB 92, 205117 (2015)

We revisit this problem
by including the xy-orbital.
→successful !

R. Tazai, S. Matsubara et al,
arXiv:2205.02280

form factors on xz and xy orbitals

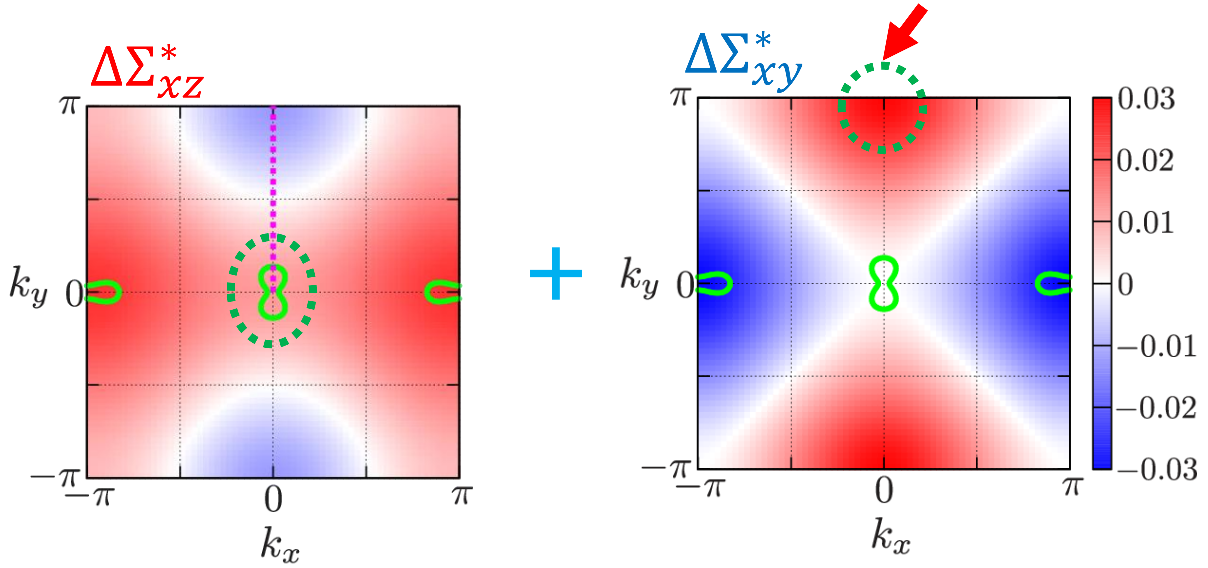
R. Tazai, S. Matsubara et al,
arXiv:2205.02280

disappearance of e-pocket

ARPES: M. Yi, et al, PRX **9**, 041049 (2019).

xz,yz-orbital polarization

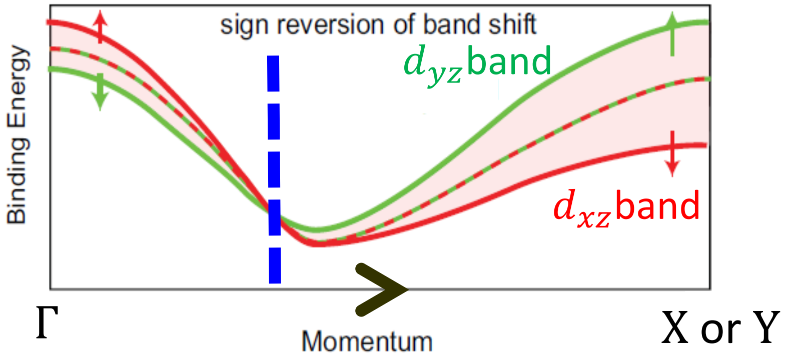
similar to Onari et al, PRL 2016



xy-orbital bond-order

$\propto (\cos k_x - \cos k_y)$

new result !

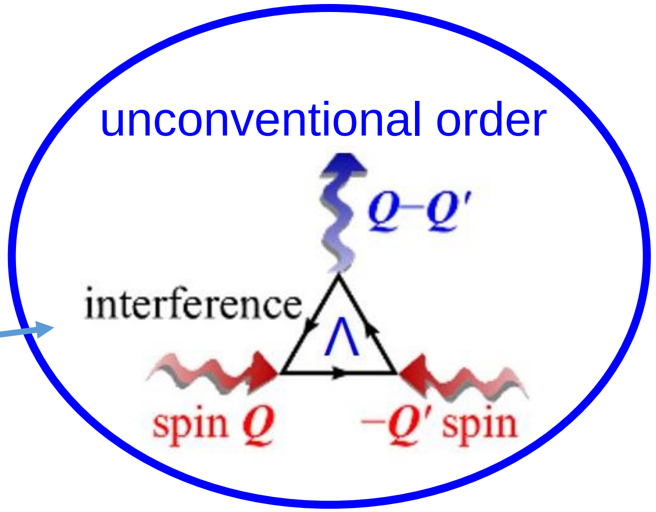


ARPES
Y. Zhang et al, PRB **94** , 115153 (2016).
Y. Suzuki et al, PRB **92**, 205117 (2015).

✓All t_{2g} orbitals are important.

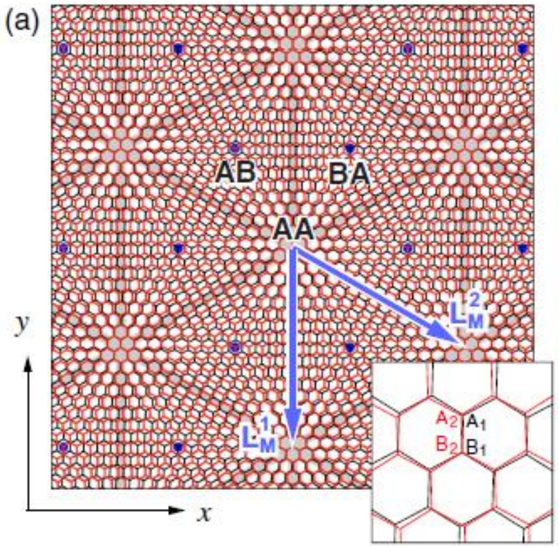
✓No filling parameters except for U.

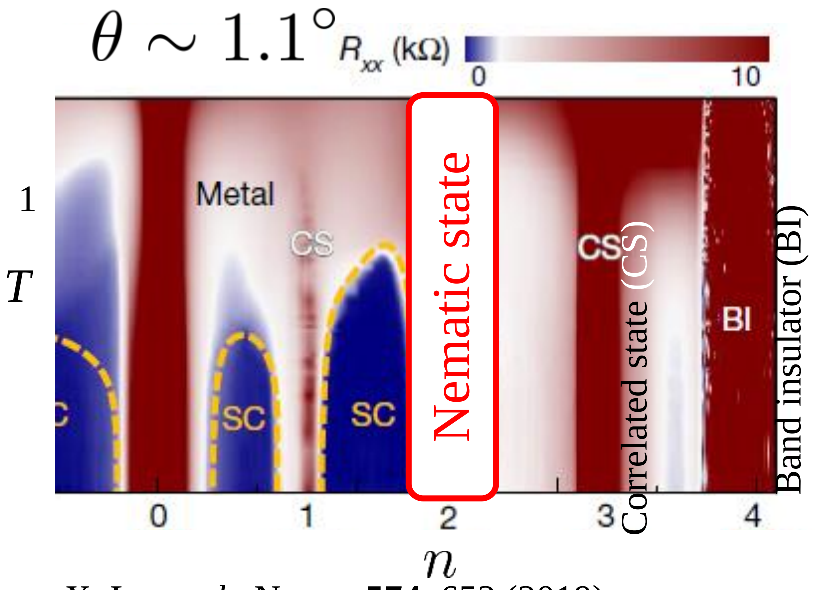
✓Success of
AL-type Interference mechanism !



Magic angle twisted bilayer graphene (MATBG)

Moire superlattice
(large molecular orbitals)

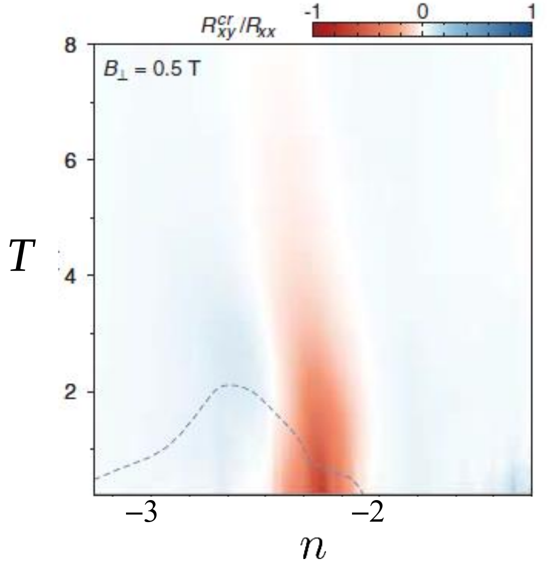




X. Lu *et al*., Nature **574**, 653 (2019)

Phase diagram

Nematicity in MATBG is an important unsolved problems!



in-plane anisotropy of ρ

$$\propto \frac{\rho_1 - \rho_2}{\rho_1 + \rho_2}$$

Y. Cao *et al*., Sciencce **372**, 264 (2021)

Ex.1: Acoustic-phonon ($\boldsymbol{q}$=**0**) mechanism

R. M. Fernandes *et al*., Sci. Adv. **6**, eaba8834 (2020)

However, $\boldsymbol{q}$-dependence is not studied

Ex.2: parquet-RG theory (6-vHS model)

D. V. Chichinadze *et al*., PRB **102**, 125120 (2020).

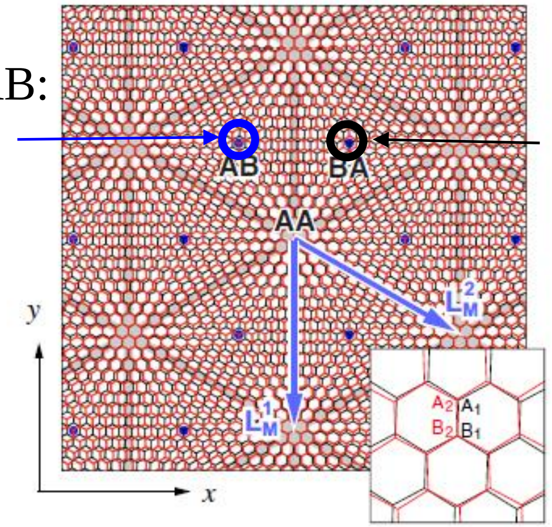
However, nematic instability is very weak.

4-sublattice Hubbard model of MATBG

Moire superlattice

Wannier orbital on AB: valley degrees of freedom $\xi=\pm 1$

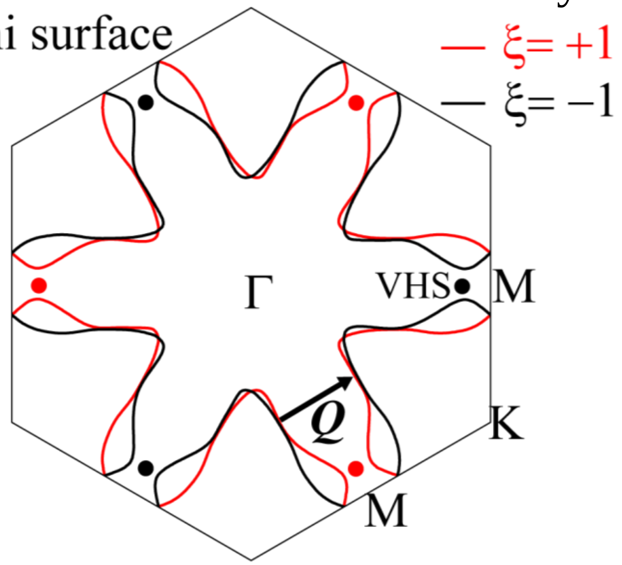
$\psi_{\xi=+1}(\boldsymbol{r}) = \{\psi_{\xi=-1}(\boldsymbol{r})\}^*$



Wannier orbital on BA: $\xi=\pm 1$

Fermi surface

Six VHS points



On-site Coulomb
(σ=±1)×(ξ=±1)

$$\frac{U}{16}\left[-\sum_{\mu,\nu}^{0\sim 3}(\hat{O}^i_{\mu,\nu})^2+4(\hat{O}^i_{0,0})^2\right]$$

SU(4) symmetry
U=*U'*, *J*=0

spin×valley operator: $\hat{O}^i_{\mu,\nu}=\sum_{\rho,\xi}(\hat{\sigma}_\mu\hat{\tau}_\nu)_{\rho\xi,\rho'\xi'}c^\dagger_{i\rho\xi}c_{i\rho'\xi'}$ $\quad \mu,\nu=0\sim 3$

$\hat{\sigma}_m$:spin Pauli matrix

$\hat{\tau}_n$:valley Pauli matrix

Similarity to multipolar f-electron CeB_6

R. Tazai and H. Kontani, RPB 100, 241103 (2019)

SU(4) spin+valley susceptibility and nematicity

S. Onari and HK,
PRL 128, 066401 (2022)

15-channel susceptibilities $\chi_{\mu,\nu}(\boldsymbol{q}) = \frac{1}{2}\int_0^\beta du \langle T_u \hat{O}_{\mu,\nu}(\boldsymbol{q},u)\hat{O}_{\mu,\nu}(-\boldsymbol{q},0)\rangle$

$\chi_{m,0}$: Spin (3)

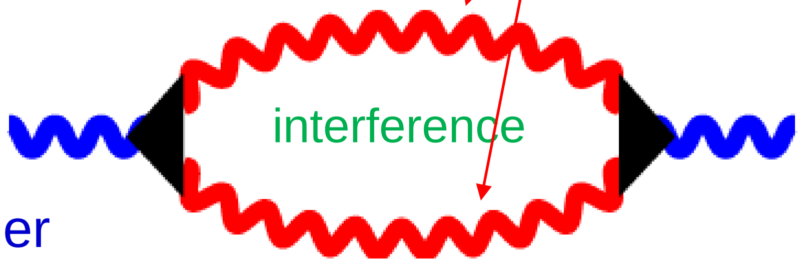
inherent in MATBG:

$\chi_{0,n}$: Valley (3)

$\chi_{m,n}$: spin-valley quadrupole (9)

SU(4) fluctuations develop.

Interference between SU(4) fluctuations

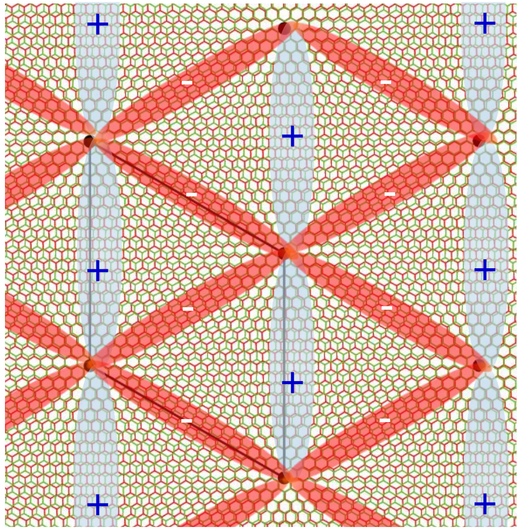


XY nematic order
at ***q*=0** in $O_{0,0}$ channel

$$\hat{f}_{\boldsymbol{k}} = (f_{x^2-y^2}(\boldsymbol{k}), f_{xy}(\boldsymbol{k}))\hat{O}_{0,0}$$

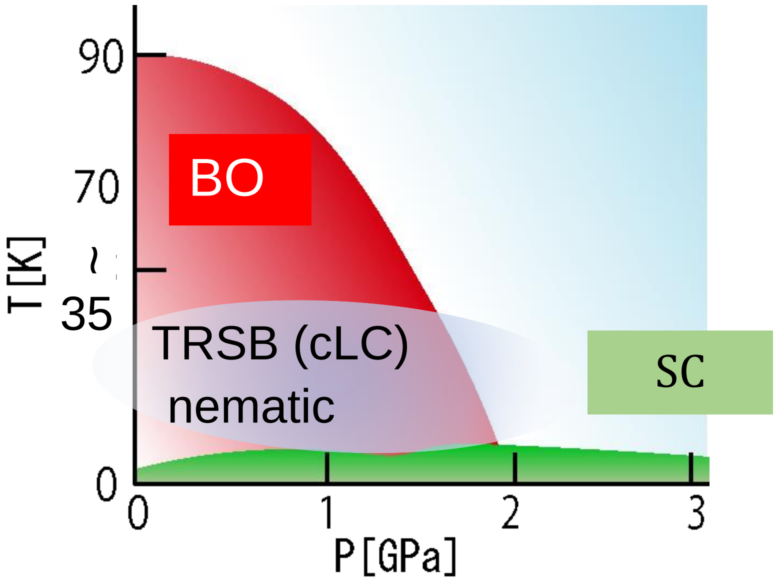
E-symmetry bond order

nematicity in MATBG !



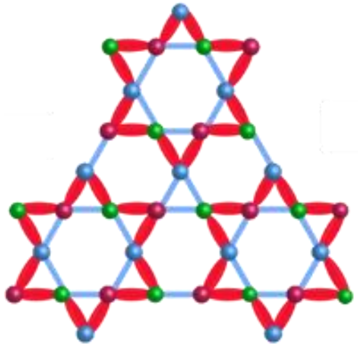
kagome superconductor AV_3Sb_5 (A=K,Rb,Cs)

2019～



bond order (BO)

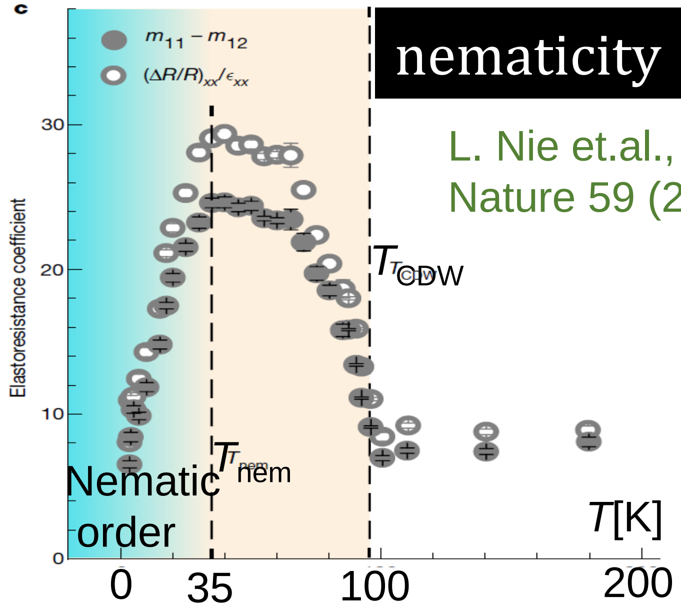
2×2



STM study

Jiang, YX., *et al.* *Nat. Mater.* (2021)

nematicity

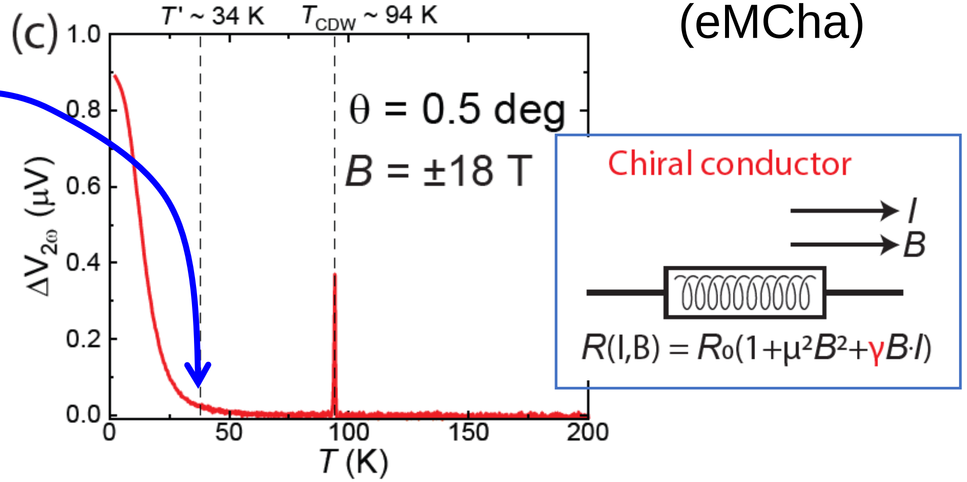


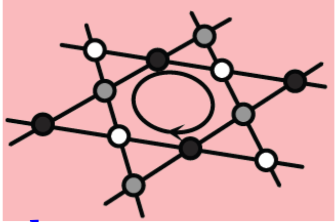
L. Nie et.al., Nature 59 (2022)

C. Guo et al., arXiv:2203.09593

electronic magneto-chiral anisotropy (eMCha)

violation of chiral symmetry





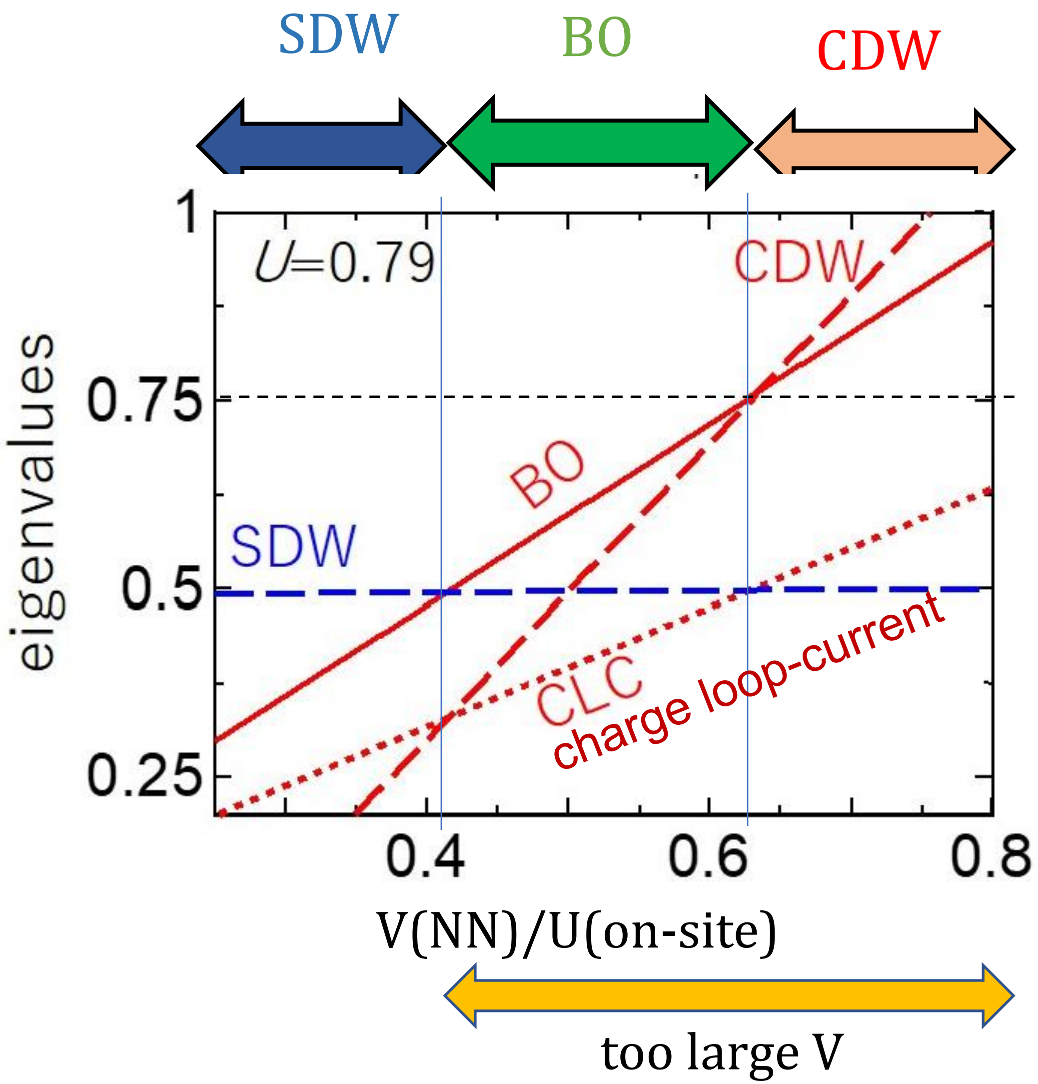
loop current

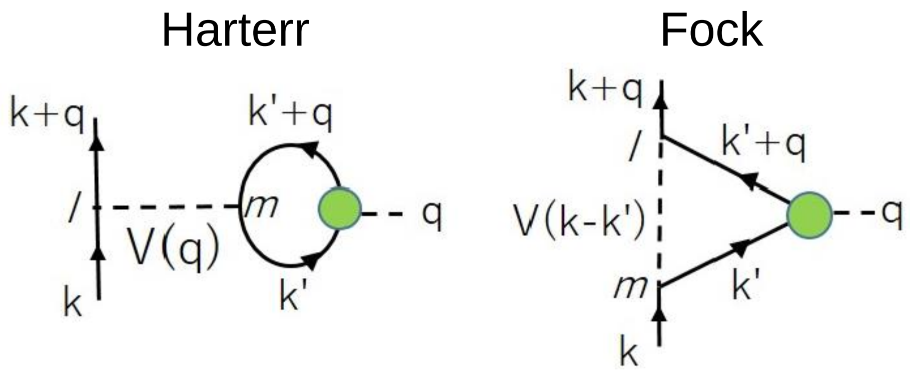
unsolved problems

✓Origin of
- BO phase?
- nematicity ?
- loop curent ?
- SC state ?

Interplay between these phases?

Limitation of the MFA: *U*+*V* Hubbard model





- ✓ Large V/U is needed for BO.
- ✓ cLC instability is always small.
- ✓ Absence of nematicity
- ✓ Superconductivity?

"Beyond-MFA" theory is demanded!

Theoretical model of AV_3Sb_5

X. Wu, Phys. Rev. Lett. 127, 177001 (2021)

$$H = \sum_{kij} \epsilon_k c^\dagger_{ki} c_{kj} + \sum_i U n_{i\uparrow} n_{i\downarrow}$$

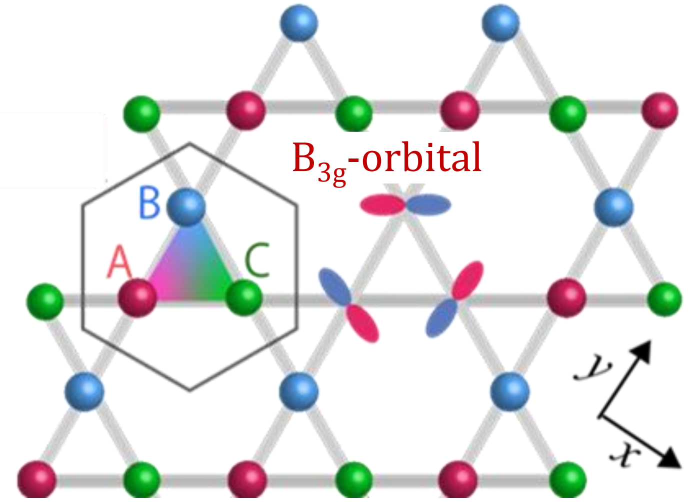
kinetic term — on-site Coulomb

i, j : sublattice$(= \mathrm{A, B, C})$

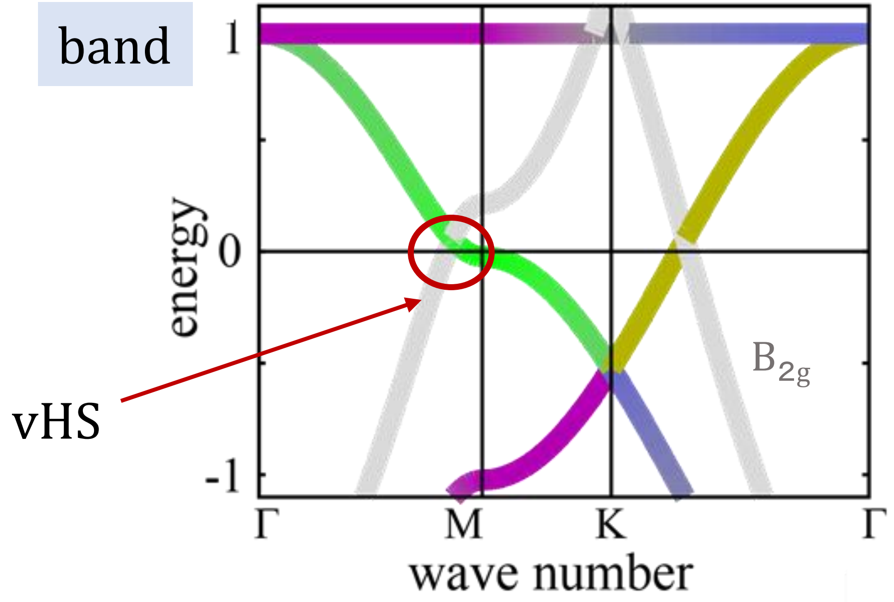
$t = 0.5$

long range V=0

unit: [eV]



band



Fermi surface

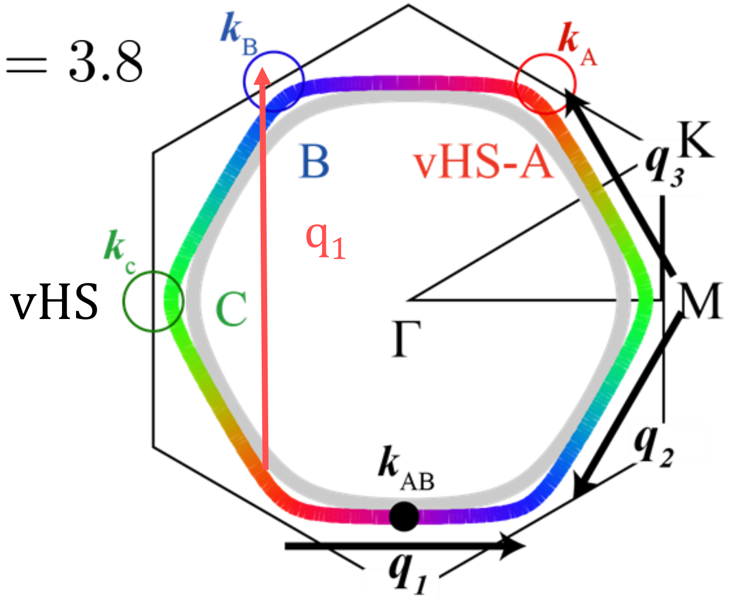
vHS ⇔ pure A,B,C sublattice

↓

Spin fluctuations:

Intra-sublattice at ***q*=0**

$n = 3.8$

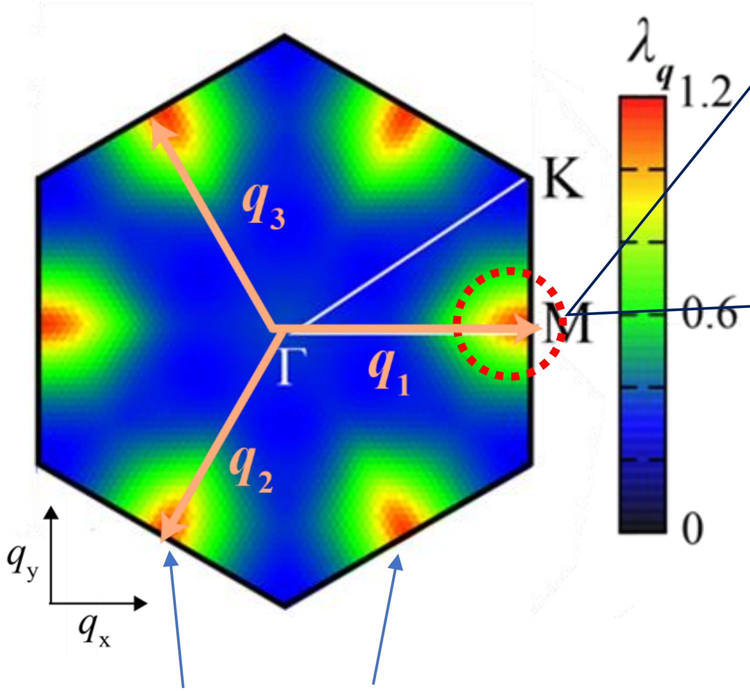


Emergence of bond-order

R. Tazai et al,
Sci. Adv. 8, abl4108 (2022)

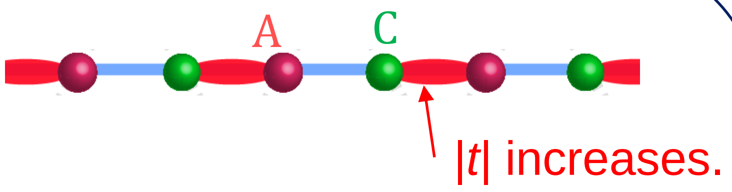
eigenvalue of DW equation

λ_q by AL term

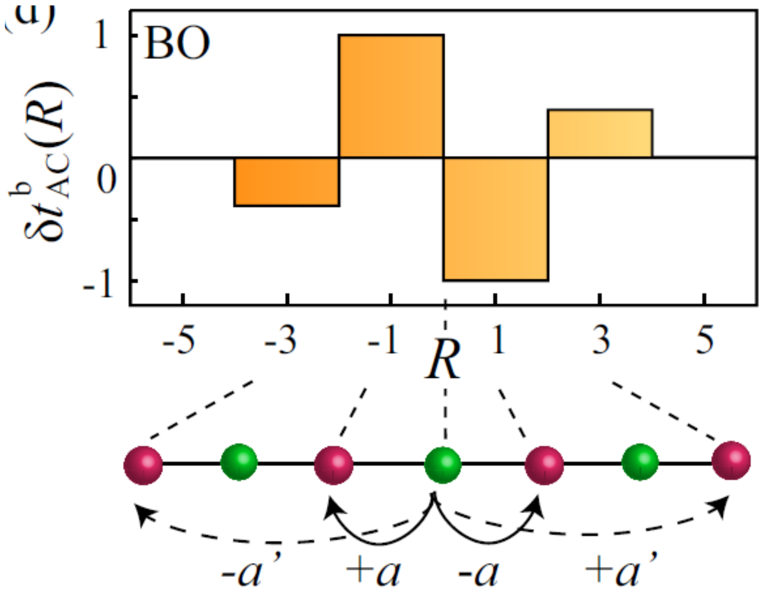


A density-wave
at $\boldsymbol{q}=\boldsymbol{q}_{n.}$ (n=1,2,3)

DW = bond-order



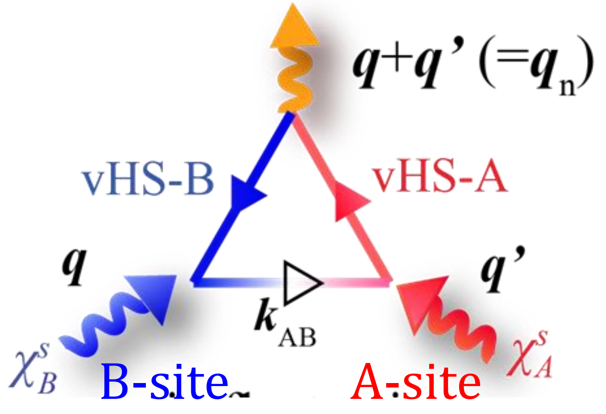
form factor in real space



t=-0.5

interference among
site A and site B

BO among A and B



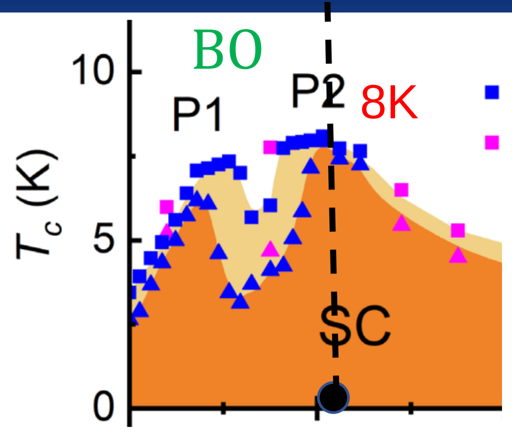
GL theory

✓ 3Q BO is favorable in energy.

A. Ogawa *et al*., in preparation

Triplet and Singlet SC phase

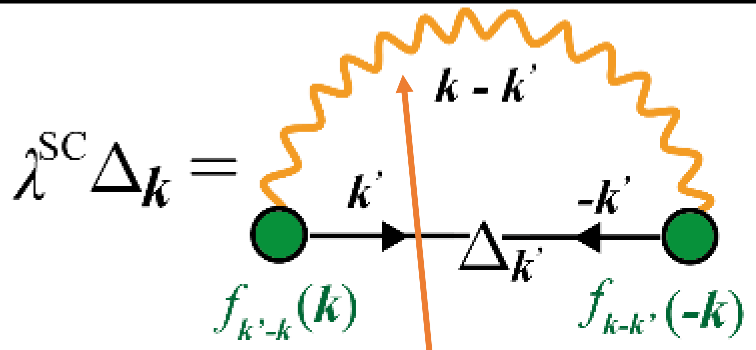
R. Tazai et al,
Sci. Adv. 8, abl4108 (2022)



BO fluctuations should be important.

F. H. Yu et al., Nat. Comm. **12**, 3645 (2021).

beyond Migdal-Eliashberg gap equation



Bond fluctuations give large pairing glue.

$$V^{sing} = -\frac{3}{2}V_s + V_{bond}$$

$$V^{trip} = \frac{1}{2}V_s + V_{bond}$$

spin fluctuation

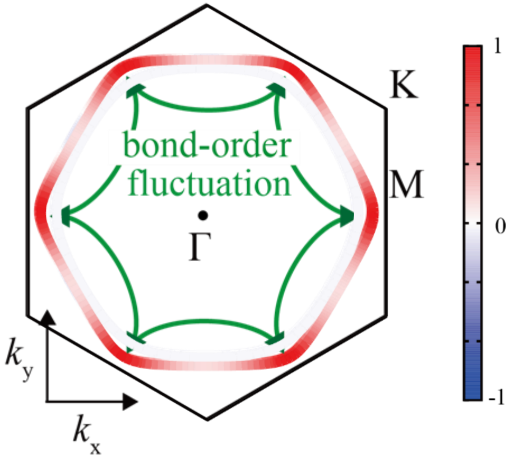
bond fluctuation

$$V_{bond} = \frac{g_{um} f_k f'_k}{1 - \lambda_{k-k'}}$$

g_{um} >>U

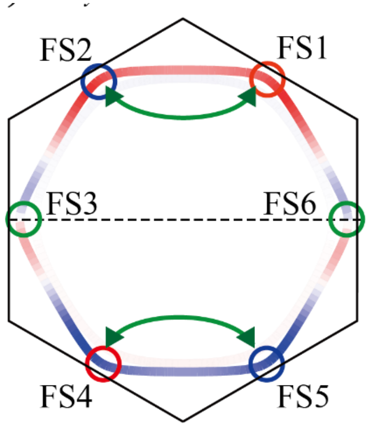
1. anisotropic s-wave gap

$\chi^{bond} > \chi^{s}$



2. p-wave gap

$\chi^{bond} \approx \chi^{s}$



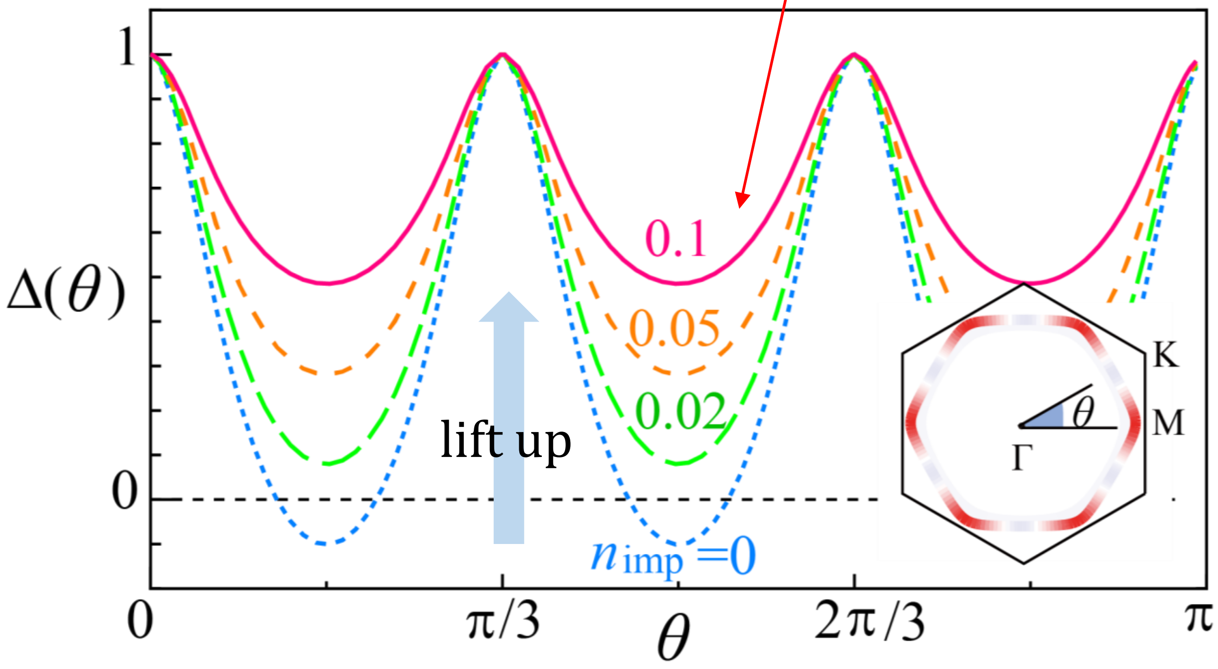
R. Tazai et al., Sci. Adv (2022)

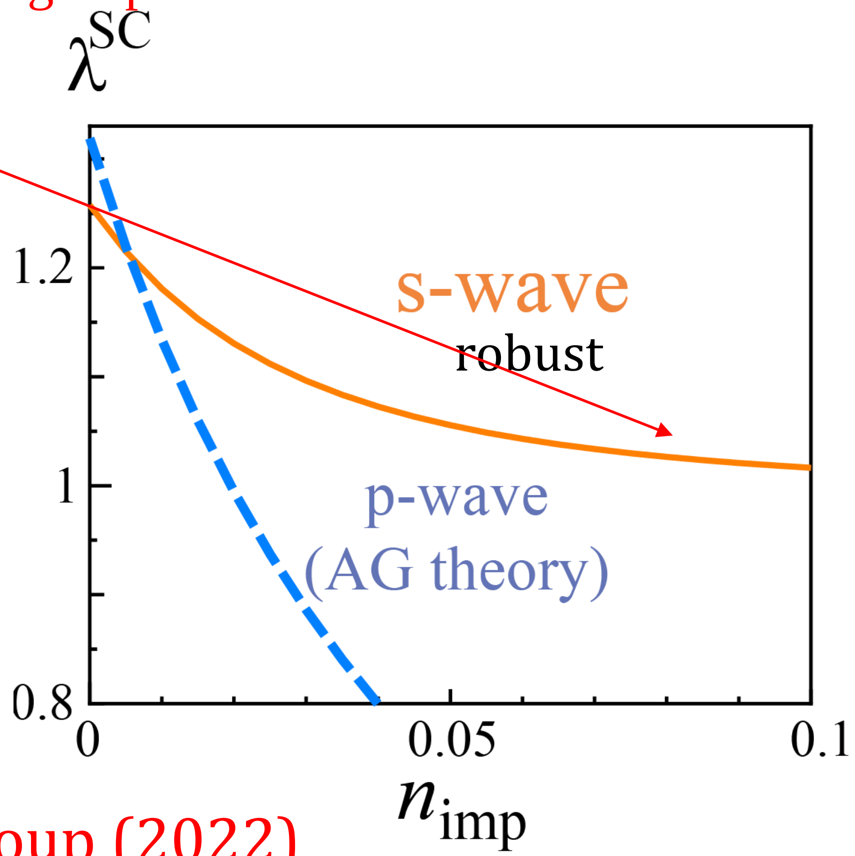
Impurity effect on SC

R. Tazai et al, Sci. Adv. 8, abl4108 (2022)

T-matrix approximation $\hat{T} = \frac{\hat{I}_{\mathrm{imp}}}{\hat{1} - \hat{g}\hat{I}_{\mathrm{imp}}}$ $\hat{\Sigma}^n = n_{\mathrm{imp}}\hat{T}$ self-energy

Impurity effect study by Shibauchi group

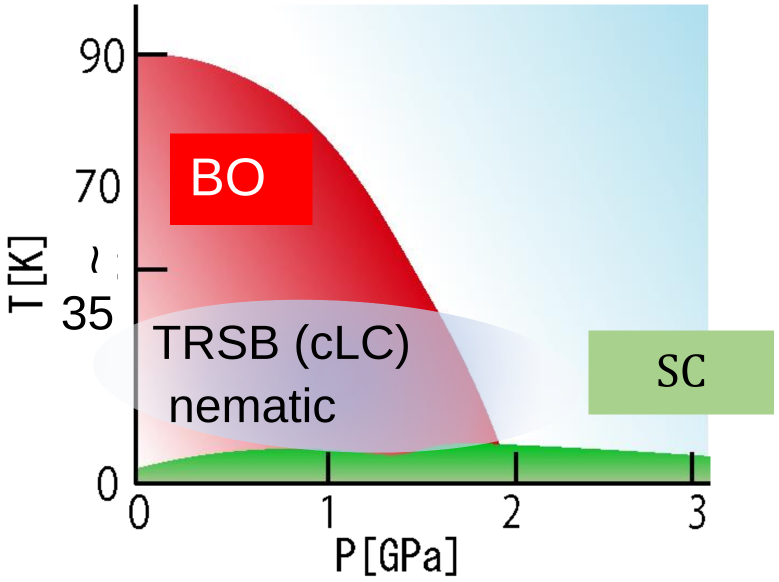




experiment: Shibauchi group (2022)

Tc of nodal SC (p,nodal s) suddenly decrease, while full s-wave SC is robust.

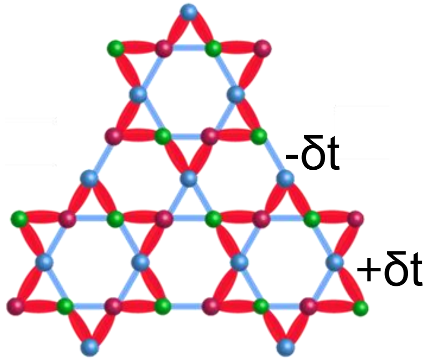
Current order and Z_3 nematcity in kagome metal



Z_3 nematic order

- χ_{nem}(T) by elastoresistance (T_{nem} ~ 35K)
  S.-Y. Yang et al, Sci. Adv. 6, eabb6003 (2020).
- Scanning birefringence (T_{nem} ~ 90K)
  Y. Xu et al., arXiv:2204.10116
- STM (QPI)
  H. Li et al, Nat. Phys. 18, 265 (2022)

(anti) star of David bond-order (SoD BO)



Theory

R. Tazai et al,
Sci. Adv. (2022)

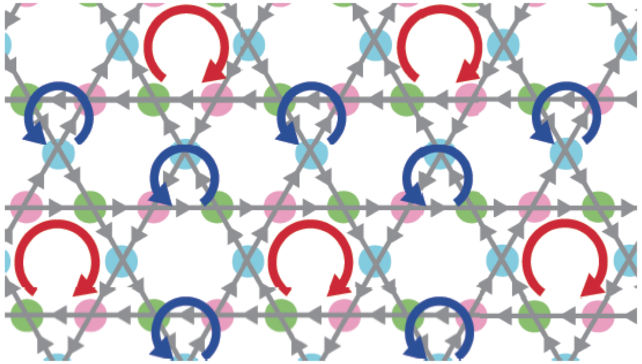
time reversal symmetry breaking (TRSB)

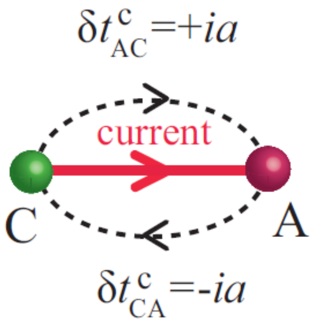
- Kerr effect (T_{TRSB} ~ 90K)
  Q. Wu et al., arXiv: 2110.11306
- μSR (T_{TRSB} ~ 35K, 70K)
  C. Mielke et al., Nature 602, 245 (2022).
- eMCha study (T_{nem} ~ 35K)
  C. Gio et al., ArXiv:2203.09593
- giant AHE (T_{TRSB} ~ 35K)
  Y-X Jiang et al., Nat. Mat. (2021).

We focus on the common BO phase

Charge loop current order mediated by bond-order fluctuations and emergent Z_3 nematic order in kagome metal AV_3Sb_5 (A=Cs,Rb,K)

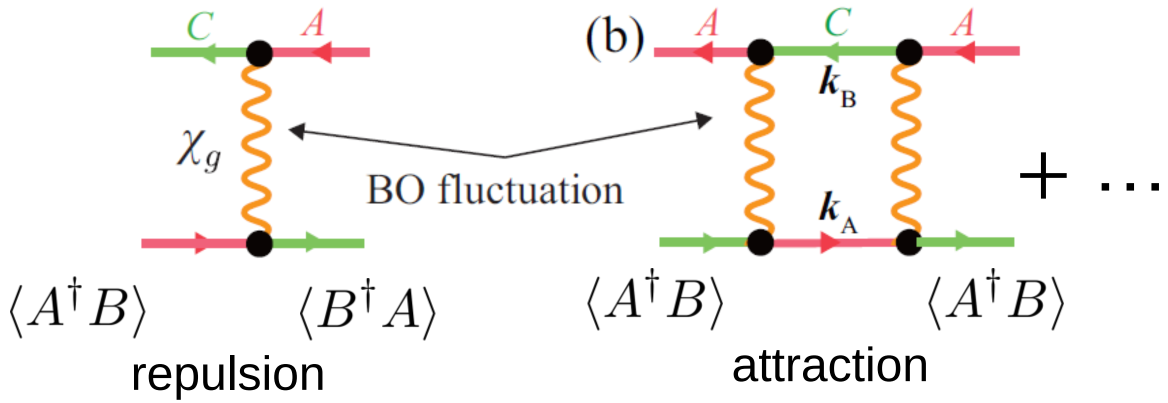
R. Tazai et al, arXiv:2207.08068

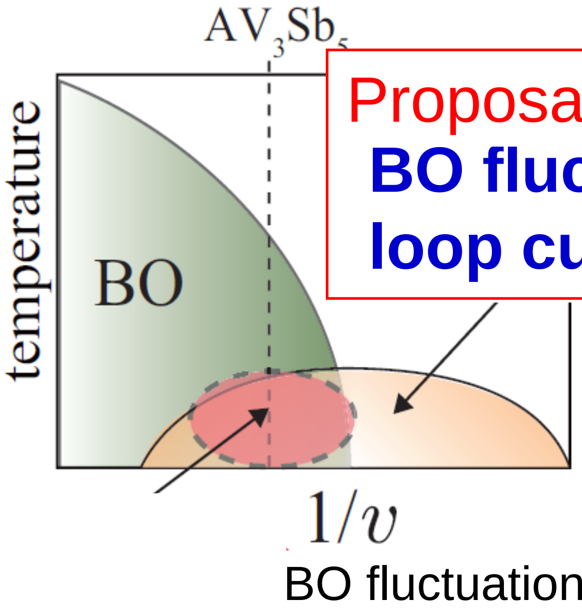




imaginary order parameter
→Berry phase

Proposal 1: Bond-order fluctuations mediate the charge current (and SC)





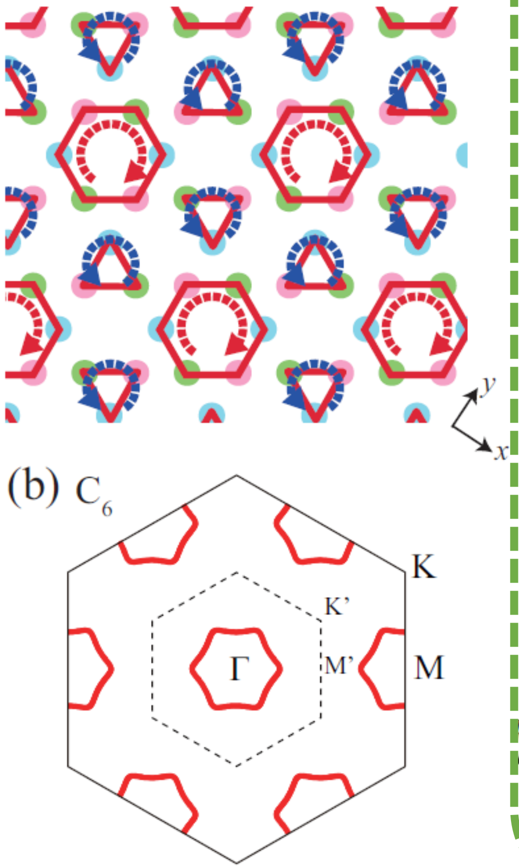
Proposal 1:
BO fluctuation mediated loop current

$$\langle A^\dagger B\rangle = -\langle B^\dagger A\rangle$$: odd-parity p-h condensation = current order

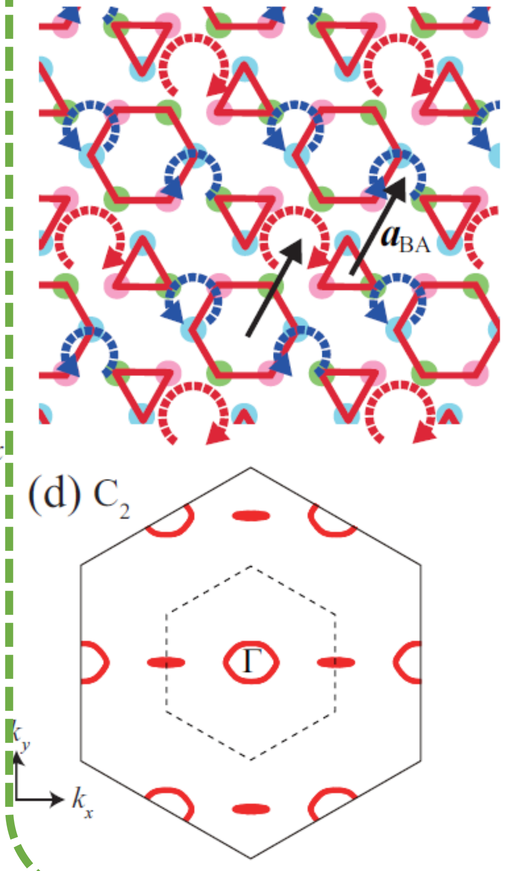
pure imaginary

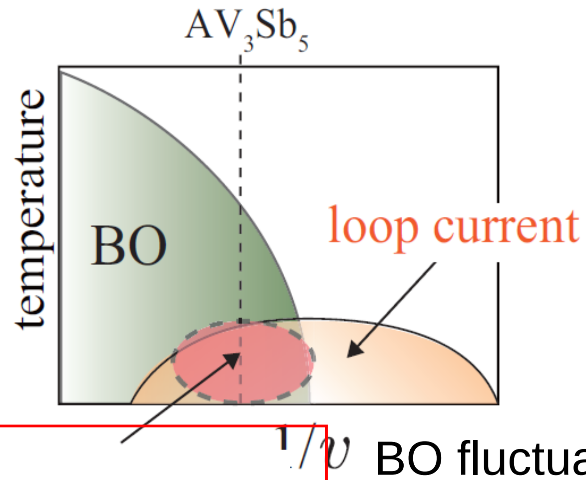
possible BO+cLC states

C_6



C_2





BO fluctuation strength

Proposal 2:
Z_3 nematic BO+cLC state

Z_3 nematic state is stable in the GL free energy argument (The 3rd order term)

R. Tazai et al, arXiv:2207.08068

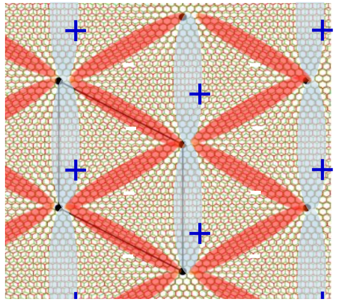
Summary

新学術領域研究 令和元年度～５年度
量子液晶の物性科学
Quantum Liquid Crystals

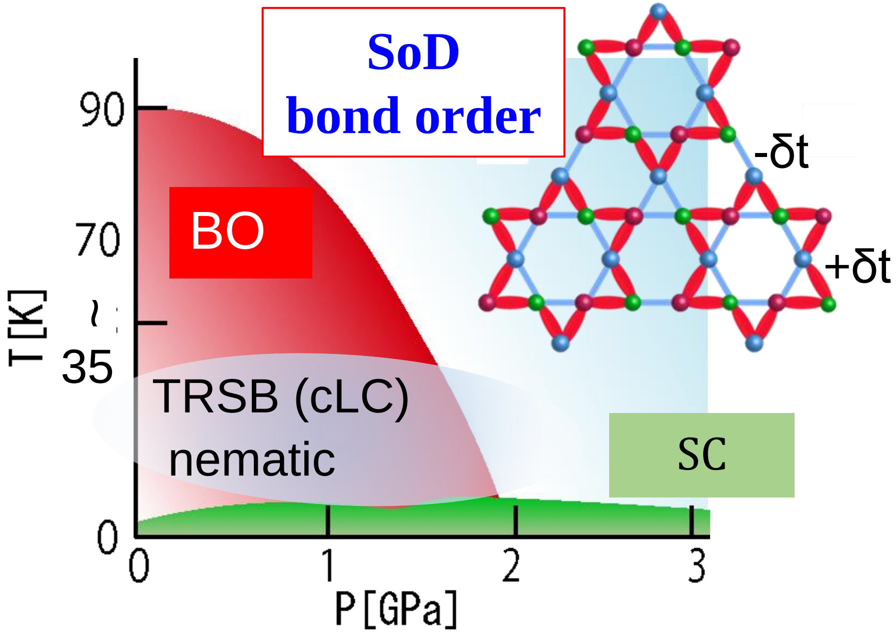
Rich unconventional
p-h condensations
due to strong correlations

1. Lifshitz transition in FeSe
arXiv:2205.02280

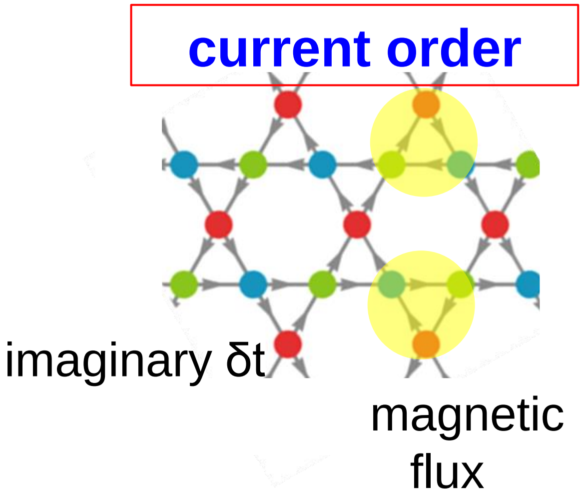
2.XY nematicity in MATBG
PRL 128, 066401 (2022)



Sci. Adv. 8, abl4108 (2022)



arXiv:2207.08068



Proposal 1:
✓ Correlation-drive SoD BO

Proposal 3:
✓Enhancement of cLC order
under H (in SoD state)

Proposal 2:
✓BO fluctuations mediate
charge current and SC
✓Z_3 nematic BO+cLC state