TBA

Liang Fu

Topological Bound and Applications

Liang Fu

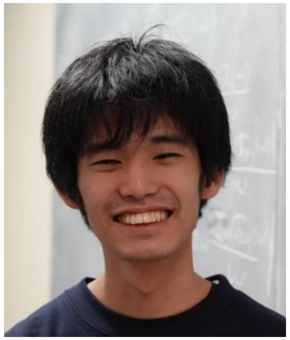
With Yugo Onishi

- topological bound on energy gap
  PRX 14, 011052 (2024)

- thermodynamic bounds on energy gaps
  arXiv:2401.04180

- structure factor & quantum geometry
  arXiv:2406.06783

- topological bound on structure factor
  arXiv:2406.18653



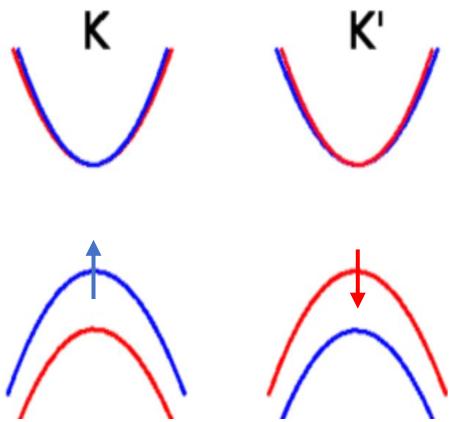
We consider general quantum many-body systems with conserved U(1) charge, e.g., total electron number N or spin S_z.

We study *bulk* properties in the thermodynamic limit, including energy gap and correlation function.

We will derive exact and useful inequality relations based on fundamental principles of physics.

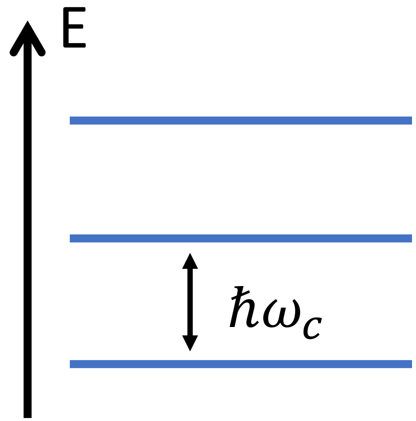
Insulating States with Bulk Energy Gap

Monolayer TMD



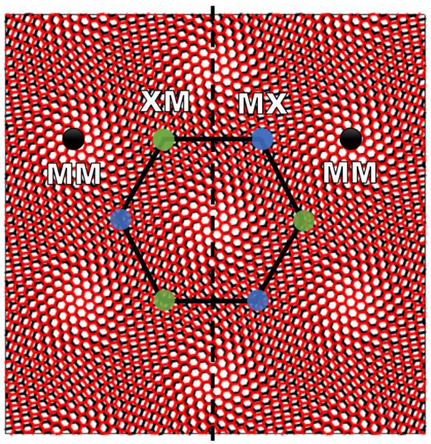
band gap ~ 1eV

Quantum Hall state



cyclotron gap ~ 1meV

QAH (B=0)



topological gap ~10meV

Large topological gap enables high-temperature dissipationless conduction.

Mind the Gap

How large can topological gap be ?

Upper Bound on Topological Gap

Onishi & LF, PRX 14, 011052 (2024)

$$\Delta \leq \frac{2\pi\hbar^2 n}{m|C|}$$

$C \equiv h\sigma_{xy}/e^2$: many-body Chern number (integer or fractional)

for general systems whose Hamiltonians take the form:

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \mathbf{p}_i \cdot \mathbf{A}(\mathbf{r}_i) + U(\mathbf{r}_i) + \sum_{ij} V(\mathbf{r}_i - \mathbf{r}_j)$$

alternative derivation: Batra & Feldman, arXiv:2407.17603

Energy Gap and Structure Factor

$$\Delta_q \leq \frac{\langle[\rho_{\boldsymbol{q}}, [H, \rho_{-\boldsymbol{q}}]]\rangle}{2VS_{\boldsymbol{q}}}$$

Feynman-Bij

Denote the ground state as $|\Psi\rangle$ with $H|\Psi\rangle = E_0|\Psi\rangle$

Construct a variational state at wavevector q:

$$|\Psi_q\rangle = V^{-1/2}S_q^{-1/2}\rho_q|\Psi\rangle$$

with density operator $\rho_q = \sum_k c_{k+q}^{+}c_k$, where

$S_q = \frac{1}{V}\langle\Psi|\rho_q\rho_{-q}|\Psi\rangle$ is static structure factor

$\Delta_q \leq E_q - E_0$

Static Structure Factor ($T = 0$)

$$S_{\boldsymbol{q}} = \frac{1}{V} \langle \rho_{\boldsymbol{q}} \rho_{-\boldsymbol{q}} \rangle$$

equal-time correlation function

$$S_{\boldsymbol{q}=0} = Vn^2 \qquad S_{q=G} \propto V \qquad S_{q\neq G} \propto o(1)$$

In classical limit, electrons are point particles located at lattice sites, leading to $S_{q\neq G} = 0$, with G reciprocal vectors.

$S_{q\neq G} \neq 0$ comes from quantum fluctuation in electron position.

Energy Gap and Structure Factor

$$\Delta_q \leq \frac{\langle [\rho_{\boldsymbol{q}}, [H, \rho_{-\boldsymbol{q}}]] \rangle}{2VS_{\boldsymbol{q}}} = \frac{\hbar^2 n q^2}{2mS_q}$$ Feynman-Bij

(for $H = \sum \frac{p_i^2}{2m} + \cdots$)

For gapped systems,

$$S_q = \frac{1}{4\pi} K q^2 \text{ at } q \to 0 \quad \Rightarrow \quad \Delta_{q\to 0} \leq \frac{(2\pi\hbar^2)n}{mK}$$

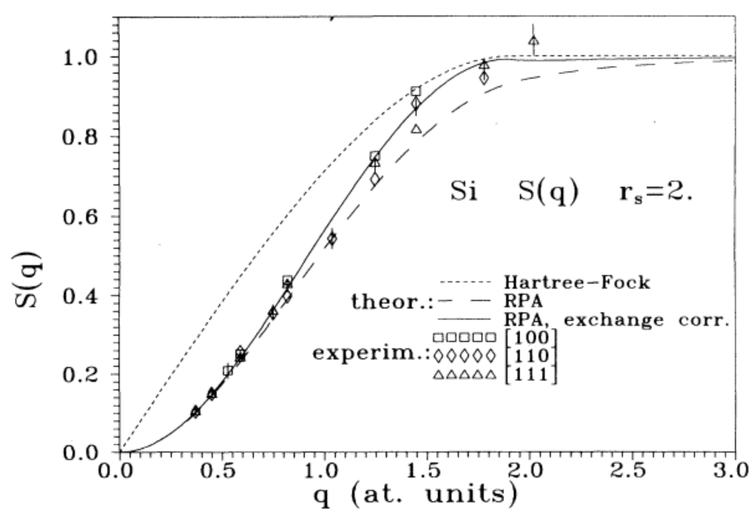
K: "quantum weight"

Structure Factor

$$S(q) = \int d\omega\, S(q,\omega) = 2\hbar \int d\omega\, \mathrm{Im}\, \Pi(q,\omega)$$

(dynamical SF) (density response function)

Experimentally measured by inelastic x-ray scattering.



Topological Bound on Static Structure Factor

$$S_q \geq \frac{1}{4\pi} C q^2 \text{ at } q \to 0$$

for general 2D gapped systems with U(1) symmetry, including fractional Chern insulators.

Charge or spin structure factor has a universal lower bound set by ground state topology: many-body Chern number.

Onishi & LF, arXiv:2401.13847

Structure Factor and Optical Conductivity

Continuity equation relates conductivity & density response:

$$\Pi(\boldsymbol{q}, \omega) = i \frac{q_\alpha q_\beta \sigma_{\alpha\beta}(\boldsymbol{q}, \omega)}{\omega}$$

Sum rule relates optical conductivity to static structure factor:

$$S(q) = \frac{\hbar}{\pi} q_\alpha q_\beta \int_0^\infty d\omega \, \frac{\mathrm{Re}\, \sigma_{\alpha\beta}(\omega)}{\omega} \text{ at } q \to 0$$

Quantum weight K is related to longitudinal optical response $\sigma_{xx}(\omega)$.

Optical Absorption

$\mathrm{Re}\,\sigma_{xx}$ and $\mathrm{Im}\,\sigma_{xy}$ are dissipative parts of optical response
(T-even) (T-odd)

Under left/right circularly polarized light $\boldsymbol{E} = E(\cos\omega t\,, \pm\sin\omega t)$,

the absorbed power must be non-negative:

$$P_{\pm} = \boldsymbol{j}\cdot\boldsymbol{E} = \left(\mathrm{Re}\,\sigma_{xx}(\omega) \pm \mathrm{Im}\,\sigma_{xy}(\omega)\right)E^2 \geq 0$$

magnetic circular dichroism

$\Rightarrow$ $\mathrm{Re}\,\sigma_{xx} \geq |\mathrm{Im}\,\sigma_{xy}|$ at all ω

Onishi & LF, PRX (2024)

Topological Bound on Static Structure Factor

$$\int_0^\infty d\omega \, \frac{\mathrm{Re}\, \sigma_{xx}}{\omega} \geq \int_0^\infty d\omega \, \frac{\left|\mathrm{Im}\, \sigma_{xy}\right|}{\omega} \geq \left| \int_0^\infty d\omega \, \frac{\mathrm{Im}\, \sigma_{xy}}{\omega} \right|$$

Using Kramers-Kronig relation: $= \frac{\pi}{2} \sigma_{xy}(0) \equiv \frac{1}{4} C \qquad (\hbar = 1)$

$$S(q) = \frac{\hbar}{\pi} q^2 \int_0^\infty d\omega \, \frac{\mathrm{Re}\, \sigma_{xx}(\omega)}{\omega} \geq \frac{1}{4\pi} C q^2 \text{ at } q \to 0$$

Bound is saturated iff optical absorption is 100% chirality selective.

derived solely from nonnegative dissipation & causality !
applicable to general gapped systems even with strong interaction.

Topological Bound on Energy Gap

$S(q) \geq \frac{1}{4\pi} C q^2$ at $q \to 0$

$\Delta_q \leq \frac{\hbar^2 n q^2}{2m S_q}$

$$\Delta \leq \frac{2\pi\hbar^2 n}{m|C|}$$

More generally,

$$\Delta \leq \frac{4W^0}{|C|}$$

$W^0 = \int_0^\infty d\omega \, \mathrm{Re}\, \sigma_{xx}$
optical spectral weight

Onishi & LF, PRX (2024)

Structure Factor of Quantum Hall States

$\nu = 1$: $s(k) = 1 - \exp(-k^2 l^2/2)$

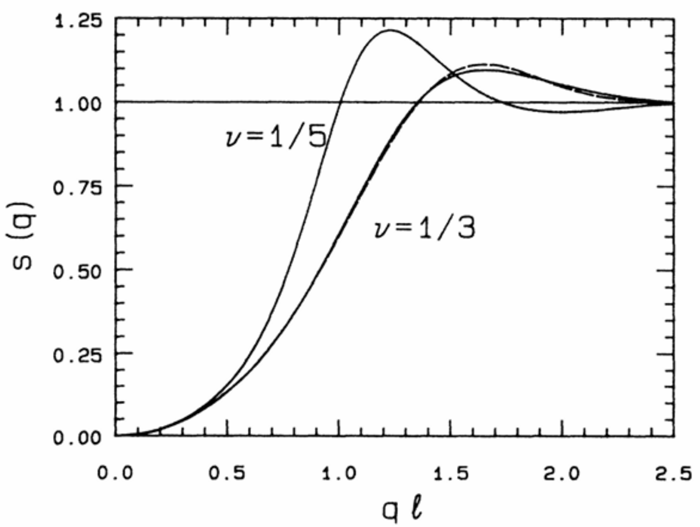


FIG. 2. Static structure factor. Solid line is modified-hypernetted-chain calculation. Dashed line is from fit to Monte Carlo data.

Girvin-MacDonald-Platzman, 1986

For *all* quantum Hall states in LL systems with *Galilean invariance*, Kohn's theorem dictates

$$Re\ \sigma_{xx}(\omega) \propto \delta(\omega - \omega_c)$$

$C = \nu$ (LL filling factor)

$$K = 4\hbar \int_0^\infty d\omega\ \frac{\mathrm{Re}\ \sigma_{xx}(\omega)}{\omega}$$

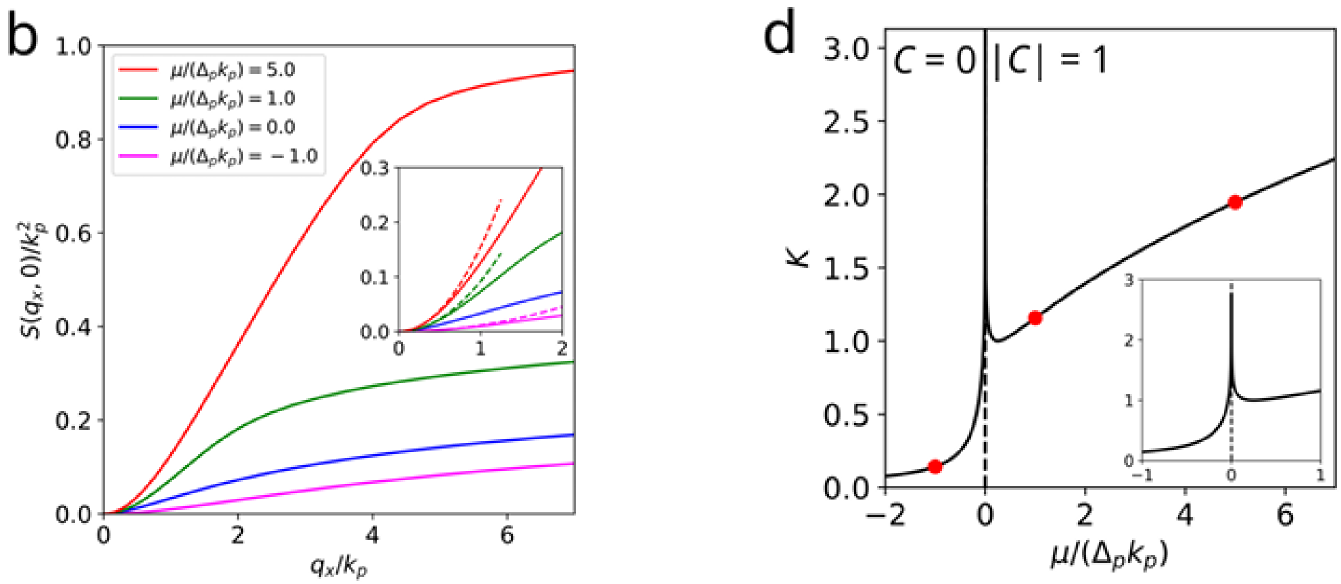
$$= 4\hbar \frac{\int_0^\infty d\omega\ \mathrm{Re}\ \sigma_{xx}(\omega)}{\omega_c} = \frac{hn/m}{eB/m} = \nu$$

$K = C$: lower bound on structure factor is **saturated** (even with LL mixing).

Chern Insulators/Superconductors

BCS Hamiltonian: $H = \sum_k \xi_k (c_{k\uparrow}^{+} c_{k\uparrow} + c_{k\downarrow}^{+} c_{k\downarrow}) + (\Delta_k c_{k\uparrow}^{+} c_{-k\downarrow}^{+} + h.c)$

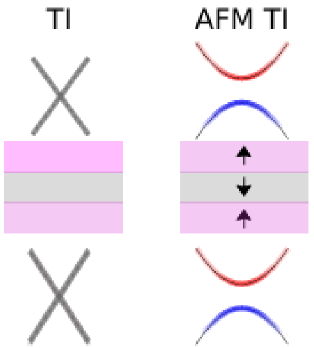
with $\xi_k = \frac{k^2}{2m} - \mu$ and $\Delta_k = k_x + i k_y$

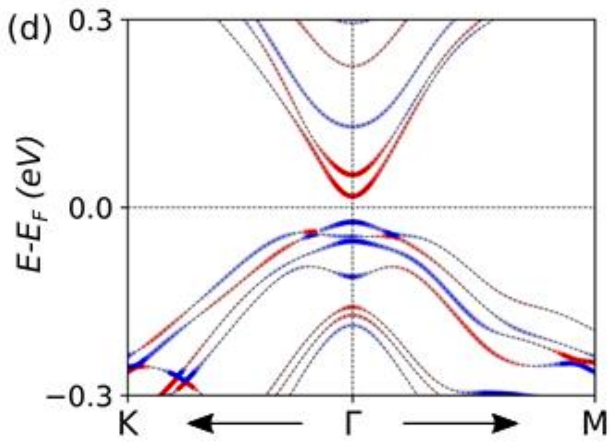


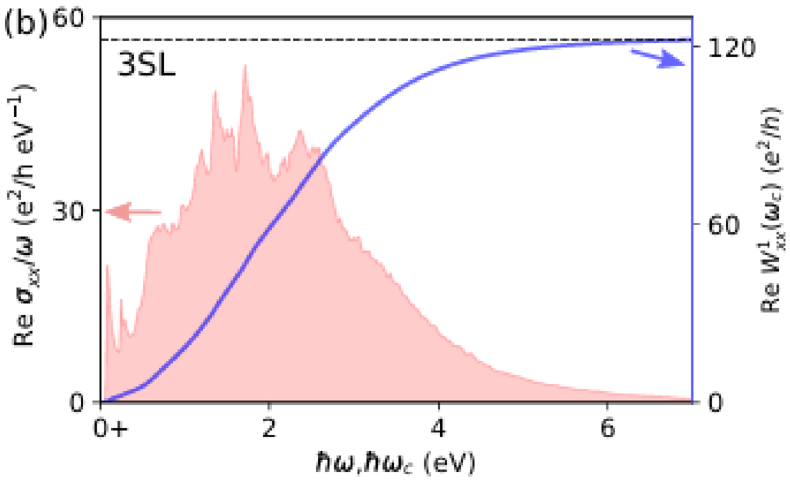
Divergence of quantum weight at topological phase transition:
$K \sim |\log \mu|$ consistent with $\sigma(\omega)$ = const for massless Dirac fermion

Real Materials

3SL $MnBi_2Te_4$:

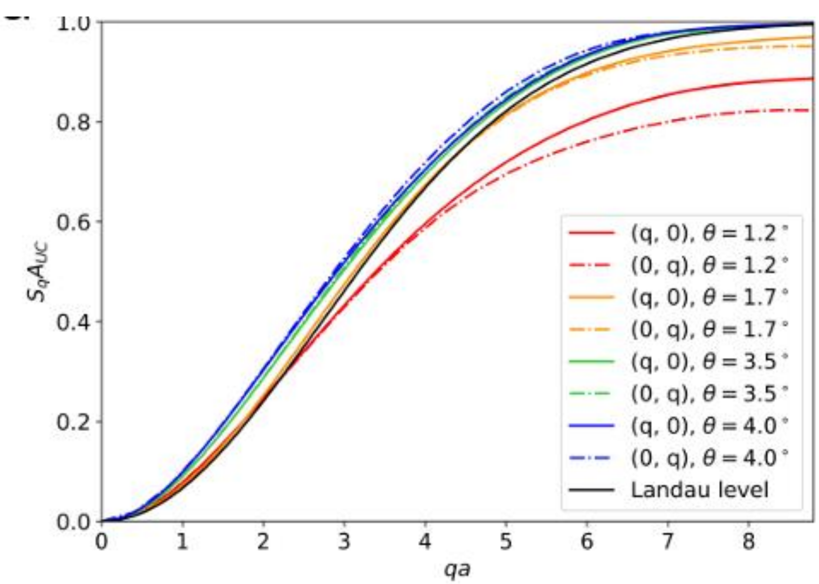


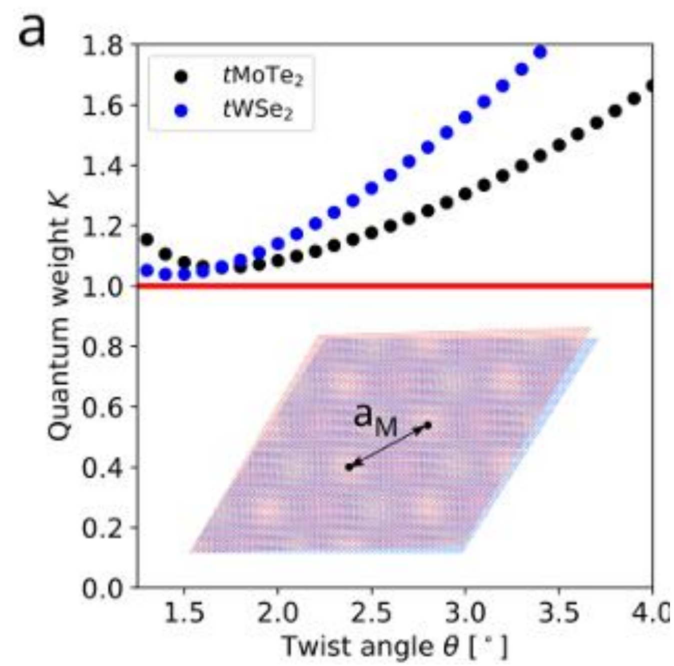




Gosh, Onishi, LF & Bansil, arXiv:2401.09689

Twisted TMD Bilayers





New Result: Fractional Chern Insulator

From band-projected exact diagonalization on N=27 cluster

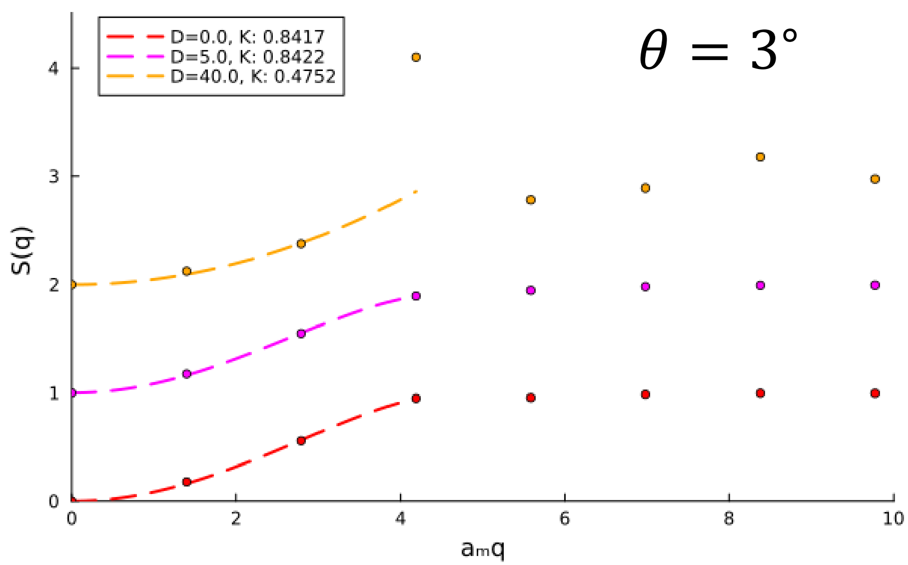
Materials	ϕ (deg)	V (meV)	w (meV)	m (m_e)	a_0 (Å)
tMoTe_2	-91	11.2	-13.3	0.62	3.52

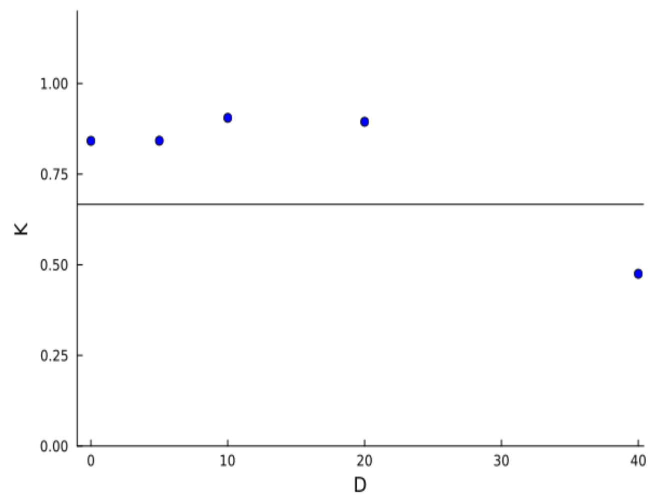
Reddy … Zhang & LF, PRB (2023)

Timothy Zakalama

FCI-CDW transition at $\nu = 2/3$ driven by displacement field:

$\theta = 3°$

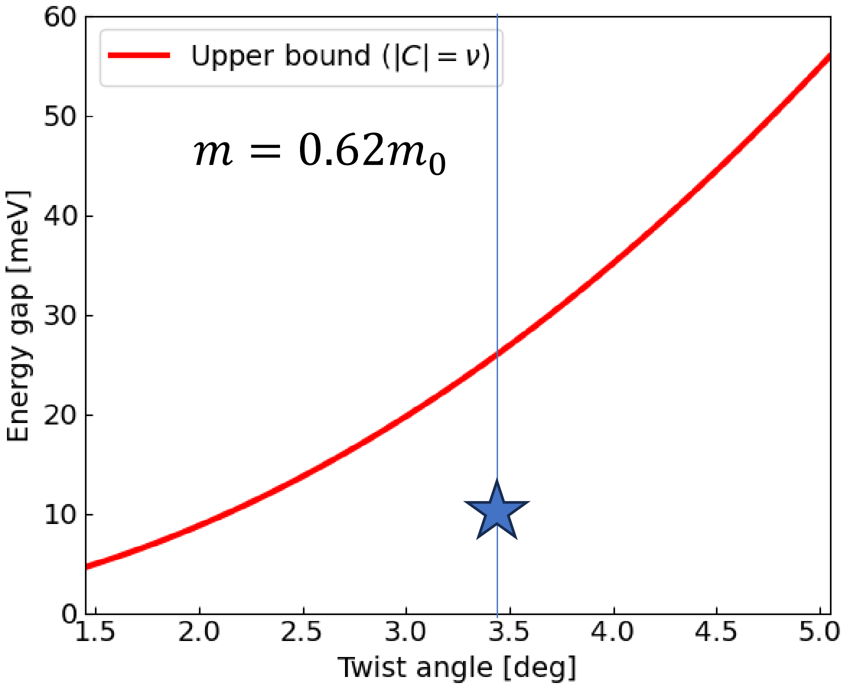




Topological Gap Bound

For Chern insulators with $C = \nu$ in twisted semiconductors,

the **maximum possible** gap is $\frac{2\pi\hbar^2}{mA_\theta}$.



Topology Sets Bounds

- Topology has wider consequences for diverse physical properties beyond quantized responses.

- Topological bound on $S(q)$: analog of minimal surface

- When interaction is not too long-ranged (excluding Coulomb in 3D), $S_{q\to 0}$ is directly related to *many-body* quantum metric.

- For 3D Coulomb systems, lower and upper bounds of $S_{q\to 0}$ set by *inverse* dielectric constant & *plasmon* gaps Onishi & LF, arXiv:2406.18653

(different from quantum metric) Komissarov, Holder & Queiroz, 2024
Souza, Martin, Stengel, 2024

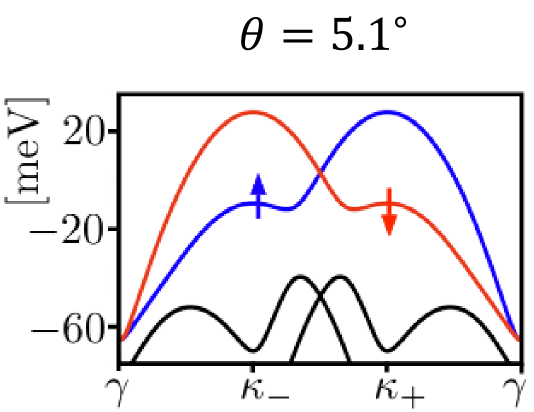
relation with corner entanglement:
Estienne, Stéphan & Witczak-Krempa, 2022
Tam, Herzog-Arbeitman & Yu, 2023
Wu, Cai, Cheng & Kumar, 2023

Tuning Magnetic Orders in Twisted TMD Bilayers

Implications for SC and QAH

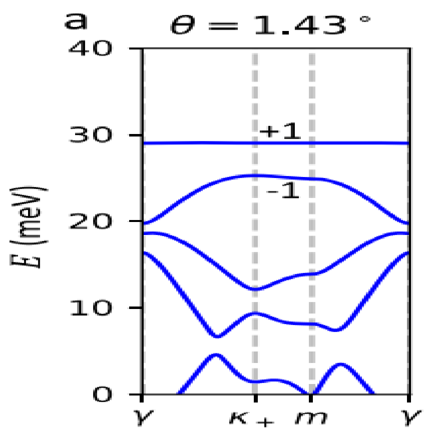
large angle: van-Hove singularity

- 120° easy-plane (xy) AFM
- superconductivity



small angle: topological flat band

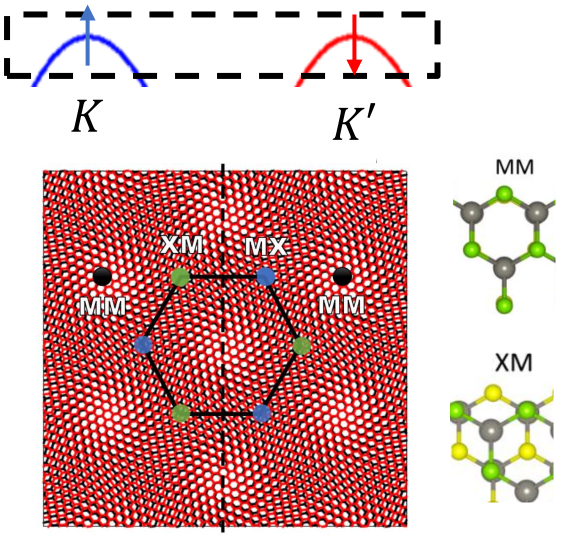
- Ising ferromagnetism
- fractionalization



new result: QAH + canted AFM

Topological Bands in Twisted TMD

Wu, Lovorn, Tutuc, Martin and MacDonald (2019)



$$H_{\uparrow} = \begin{pmatrix} \frac{\hbar^2 k^2}{2m} + V_1(r) & t(r) \\ t^\dagger(r) & \frac{\hbar^2 k^2}{2m} + V_2(r) \end{pmatrix}$$

$$= \frac{p^2}{2m} + J\boldsymbol{n}(\boldsymbol{r}) \cdot \boldsymbol{\sigma}$$

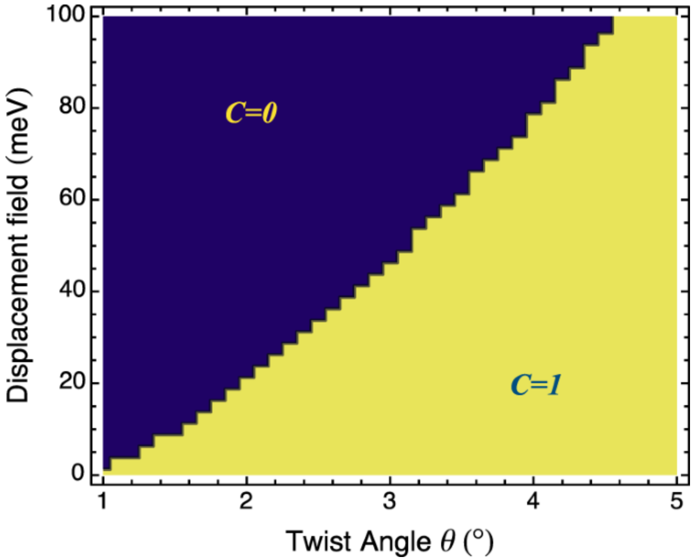
$$H_{\downarrow} = H_{\uparrow}^*$$

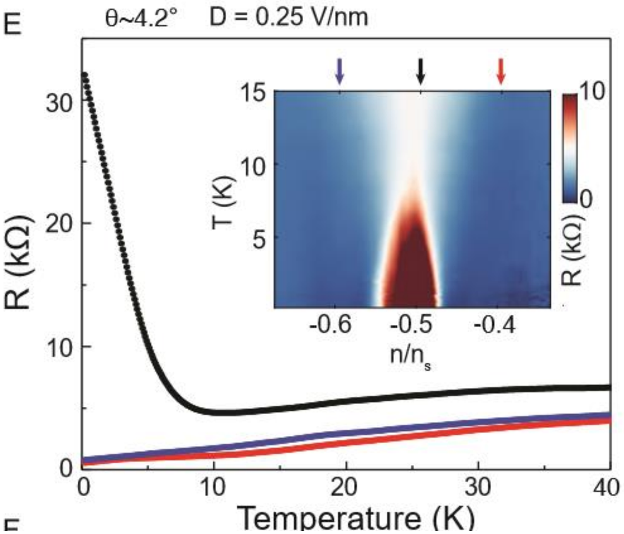
"Zeeman" field due to interlayer tunneling & moire potential

Layer-pseudospin texture is topologically nontrivial and produces emergent "magnetic" field that is opposite for spin ↑and ↓.

⇒ time-reversed pair of spin ↑and ↓ Chern bands (Kane-Mele type)

Band Topology is NOT Enough for QAH





Wang et al, Nat. Mat. (2020)

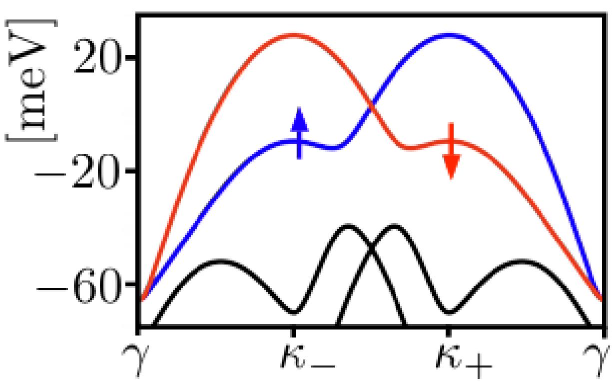
Insulating states at n=1 without AHE

Twisted WSe_2: $\theta > 4°$

correlated insulator at $\nu = 1$

$\frac{e^2}{\epsilon a_M} \sim W$: 50meV ($\epsilon$=5) >> insulating gap ~ 30K

vHS in dispersive band



Symmetry of normal state: $U(1) \times Z_2^T$

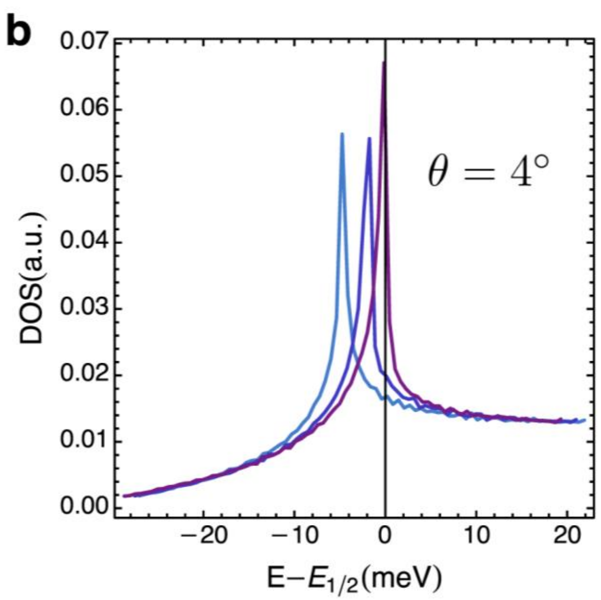
Two competing states at $n = 1$:

- Ising ferromagnet
  $\langle c_\uparrow^+ c_\uparrow - c_\downarrow^+ c_\downarrow \rangle \neq 0$ & $\sigma_{xy} \neq 0$
- 120° spiral SDW = xy AFM
  $\langle c_{k+Q\uparrow}^+ c_{k\downarrow} \rangle \neq 0$ & $\sigma_{xy} = 0$

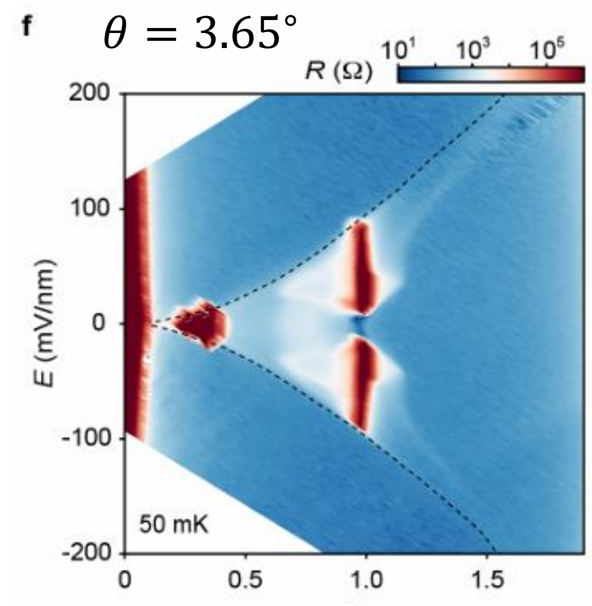
Weak-coupling nesting favors over xy AFM

Bi & LF, Nat. Commun. (2021)

New Experiments



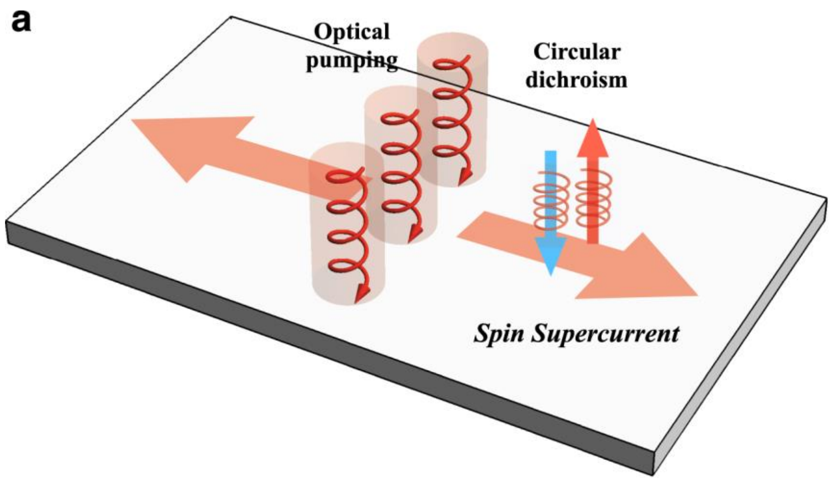
Bi & LF, Nat. Commun. (2021)

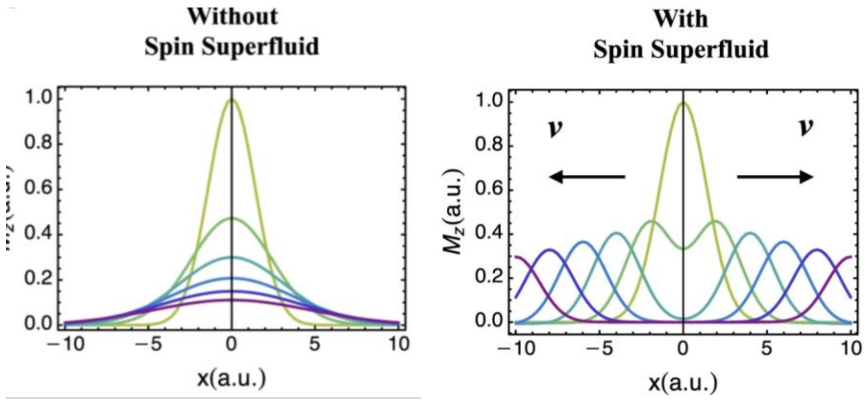


Xia … Shan & Mak, arXiv:2405.14784
Guo .. Dean, arXiv:2406.03418

- vHS tunable by filling and electric field
- correlated insulator $\nu = 1$ induced by vHS

XY AFM = Spin Superfluid





Correlated insulator should have linearly dispersing magnons (Goldstone mode) and support collective spin transport.

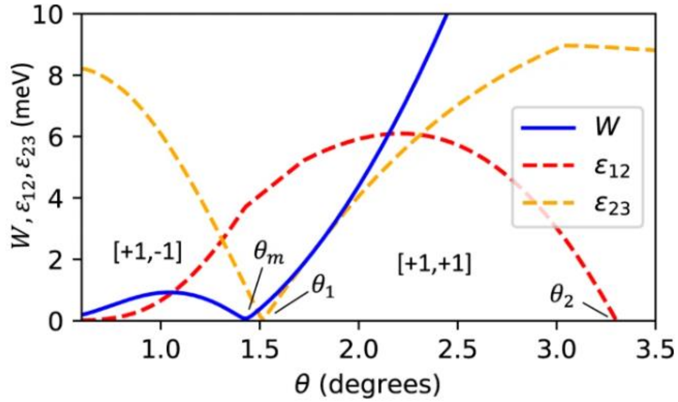
optical imaging of spin diffusion in TMD monolayer:
Jin … Wang, Science (2018)

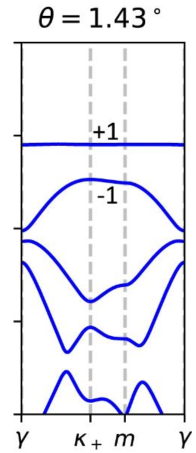
Proximity to xy AFM drives p-wave SC near vHS

Schrade & LF, arXiv:2110.10172 (PRB 2024)

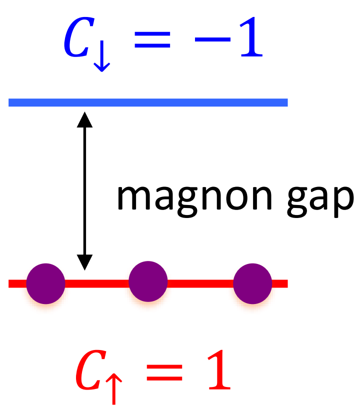
Integer & Fractional QAH in Small-Twist-Angle TMD Bilayers

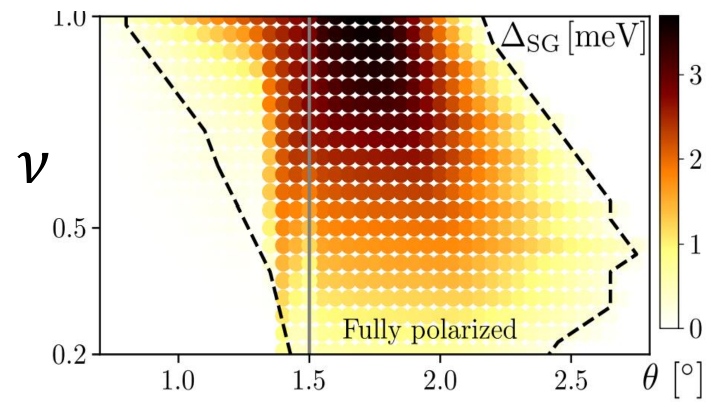
Magic angle in $tWSe_2$





Ising FM

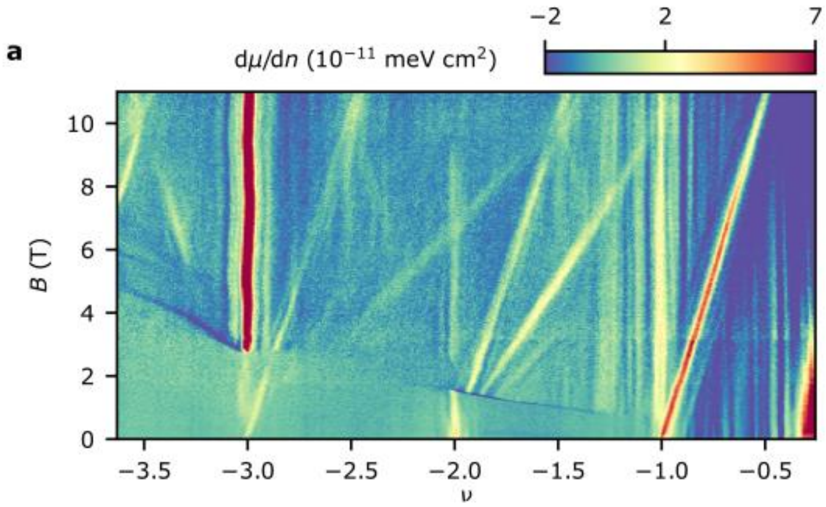


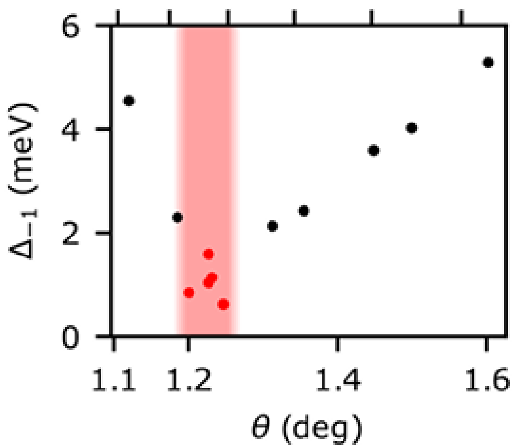


Devakul, Crepel, Zhang & LF, Nat. Comm. (2021) See also Li, Kumar, Sun & Lin (PRR 2021)

Crepel & LF, arXiv:2207.08895 (PRB 2023)

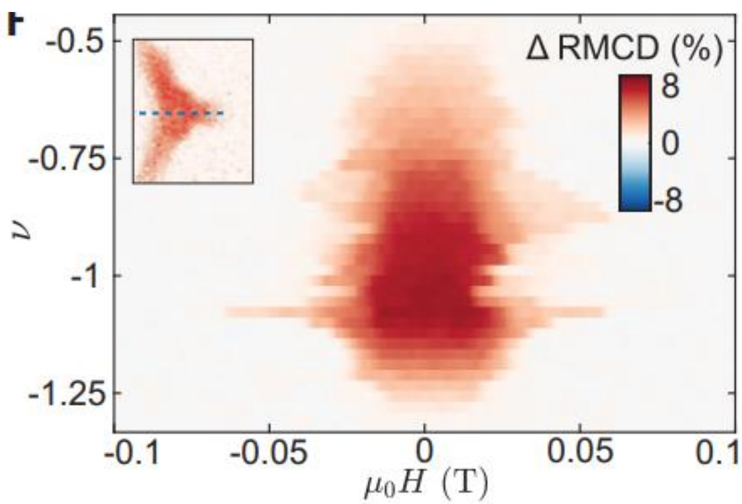
QAH in Twisted TMD Bilayers



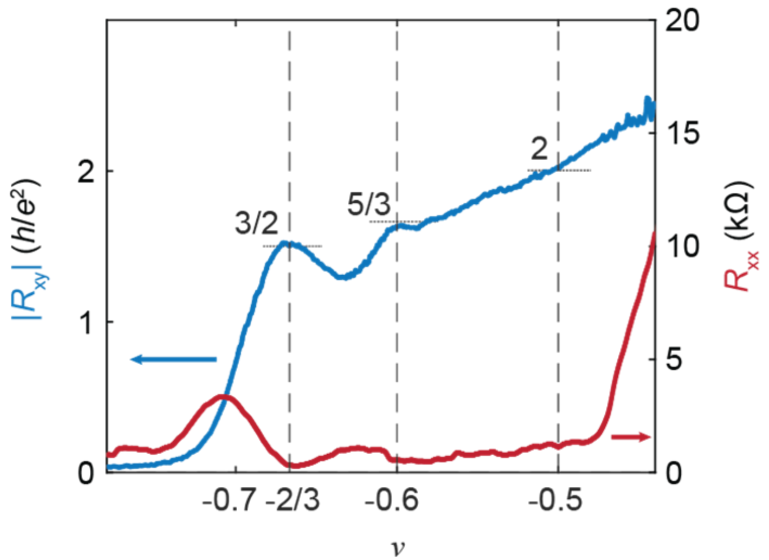


Fouty … LF, Feldman, Science (2024)

FM and FQAH in Twisted TMD Bilayers



Anderson … Xu, Science (2023)



Park … Xu, Nature (2023)

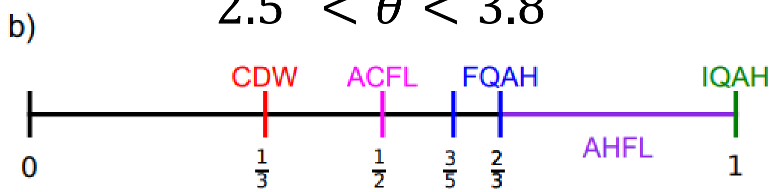
Xu … Li, PRX (2023)

optical signatures from UW & Cornell

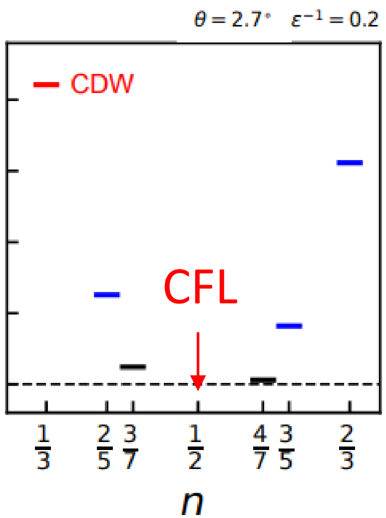
Global Phase Diagram

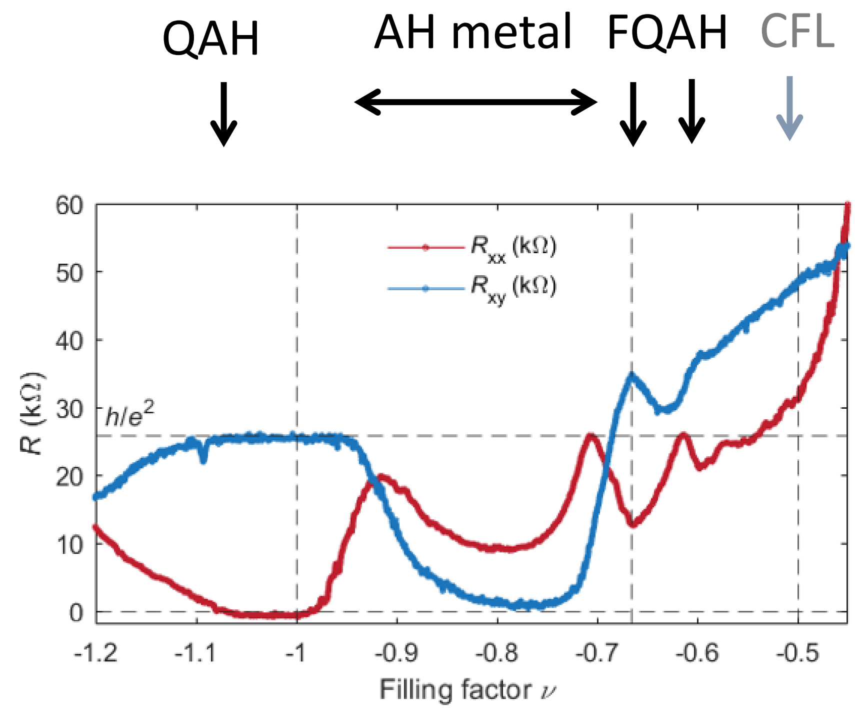
above magic angle

$2.5° < \theta < 3.8°$



$\theta = 3.7°$

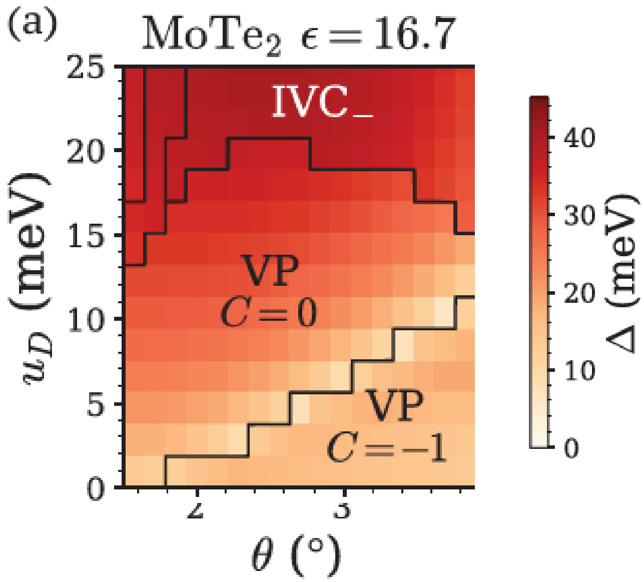


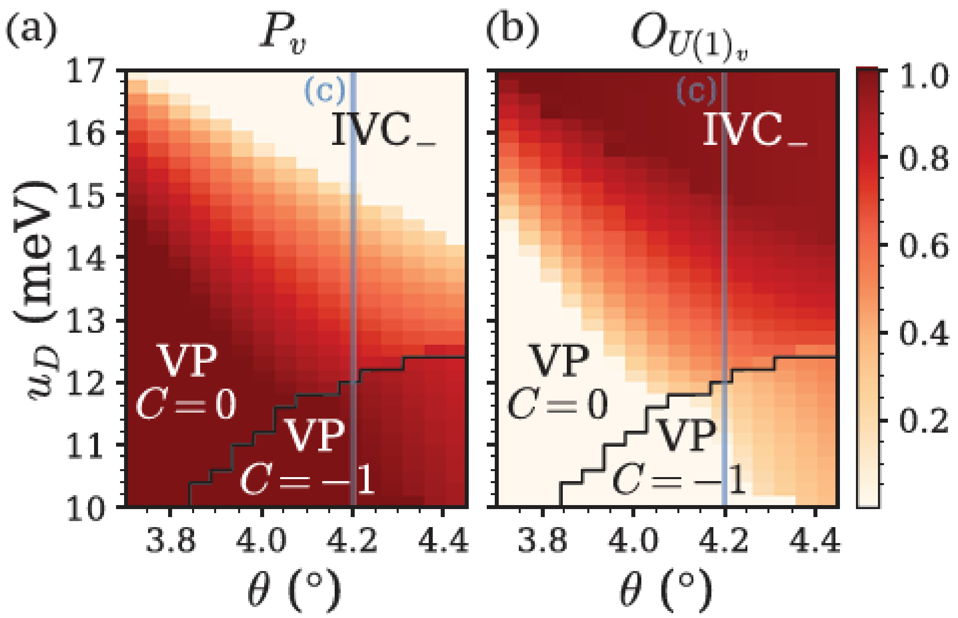


- FCI at $\nu = \frac{2}{3}$ versus CDW at $\nu = \frac{1}{3}$
- FM Fermi liquid at $\frac{2}{3} < \nu < 1$

Reddy, Alsallom, Zhang, Devakul & LF, PRB (2023)

Phase Diagram at n=1





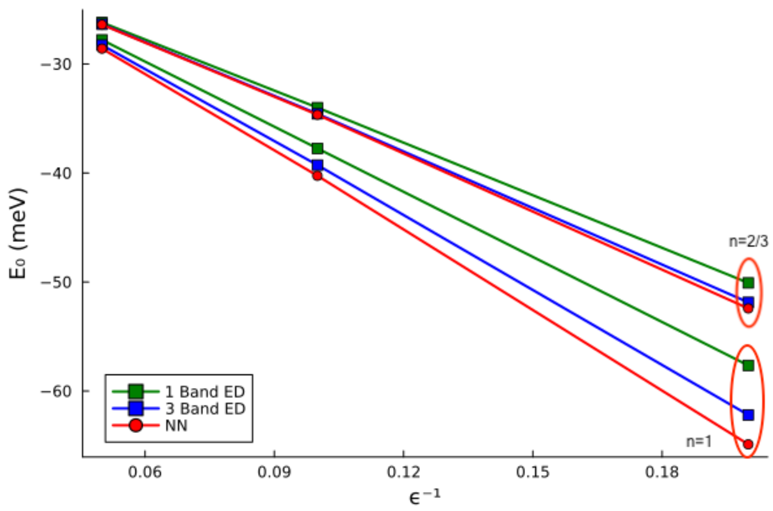
new result: QAH + canted AFM

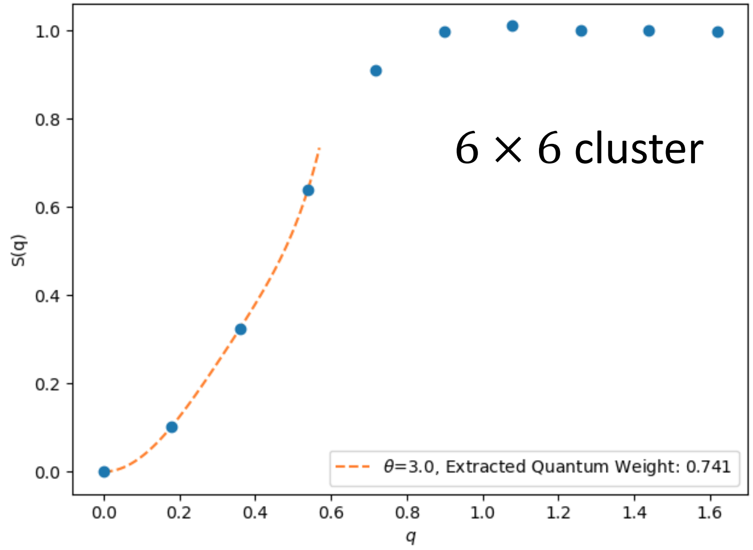
Taige Wang, Devakul, Zaletel & LF, arXiv:2306.02501

Solving FCI with Neural Network

Variational Monte Carlo + NN quantum states

NN result of full continuum model with Coulomb interaction

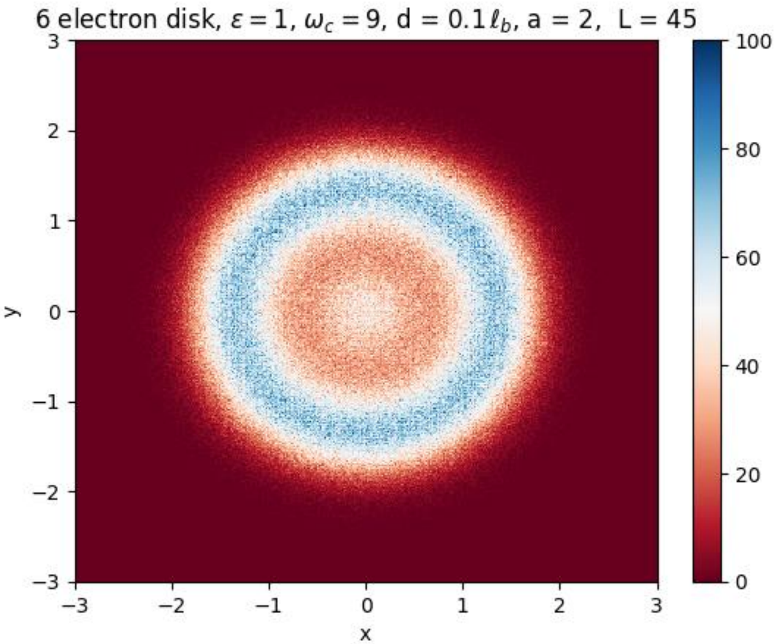


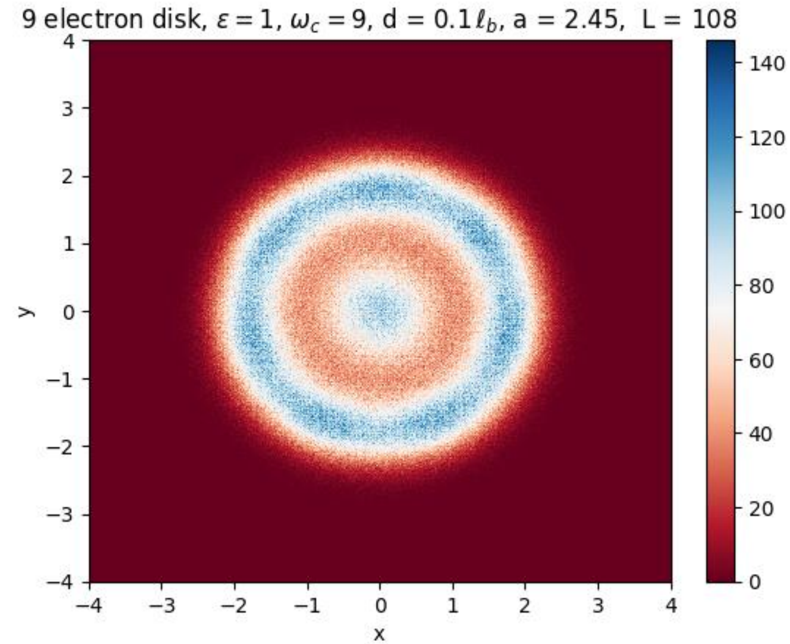


Di Luo

Timothy Zakalama

Solving FQH with Neural Network





Yi Teng
(Cambridge)

David Dai

Inaugural Northeast Quantum Forum (NEQT)

https://sites.usnh.edu/neqt/

Invited Speakers

Allan MacDonald (UT Austin)
Xiaodong Xu (UW)
Chia-Ling Chien (JHU)
Peter Armitage (JHU)
Kin Fai Mak (Cornell)
Jie Shan (Cornell)
Andy Kent (NYU)

Lucas Caretta (Brown)
Gregory Fiete (Northeastern)
Luqiao Liu (MIT)
Qiong Ma (Boston College)
Kemp Plumb (Brown)
Nian Sun (Northeastern)
Fazel Tafti (Boston College)
Ziqiang Wang (Boston College)
Mingzhong Wu (Northeastern)
Suyang Xu (Harvard)