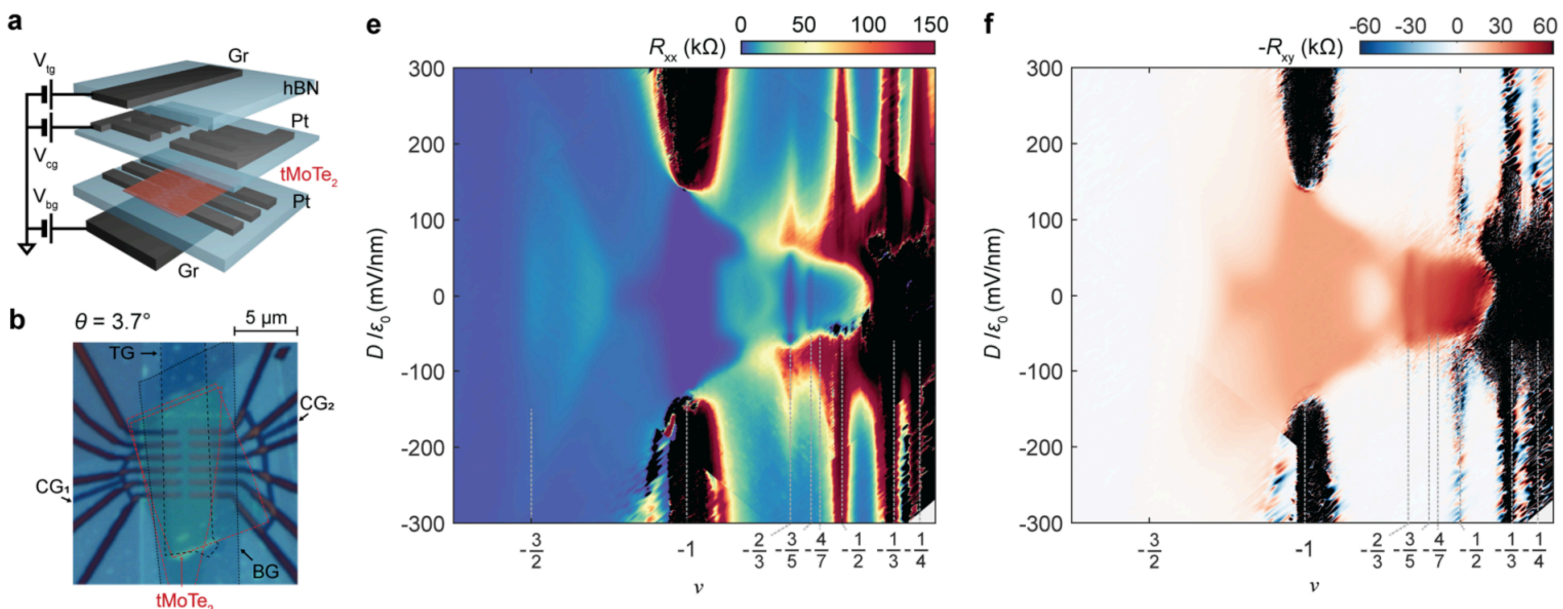
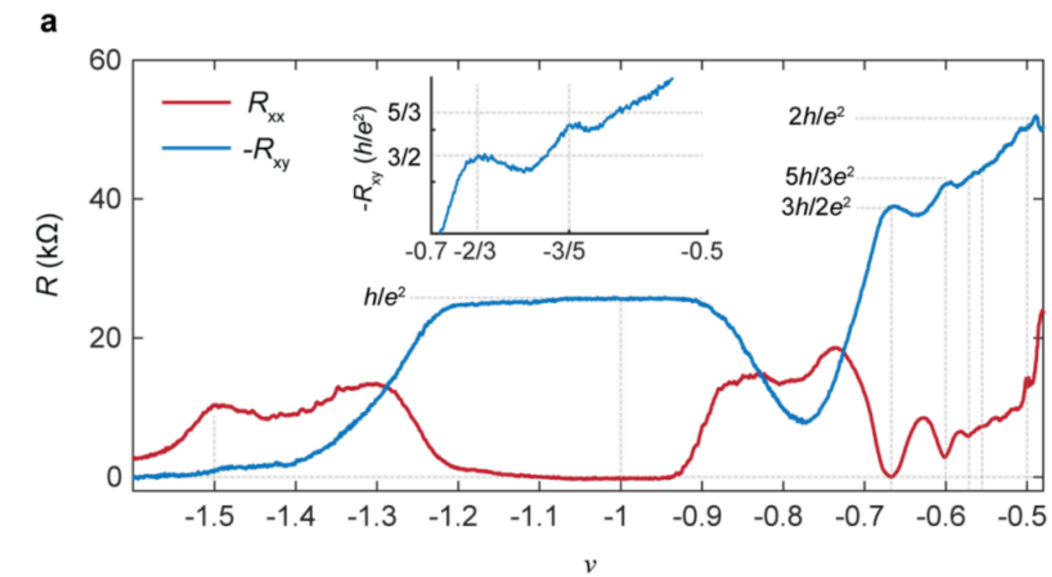
Transitions and Excitations in FCI & TBG

from Quantum Many-Body Computation Perspective

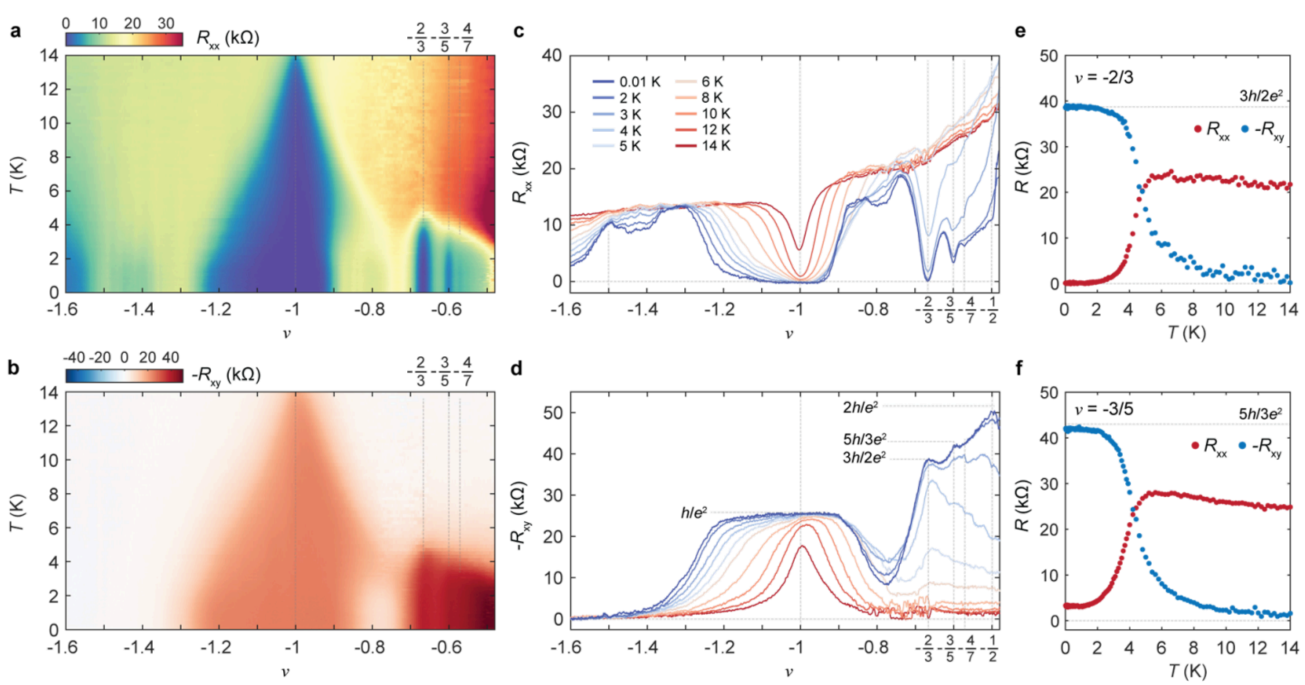
ZI YANG MENG
孟子楊
https://quantummc.xyz/

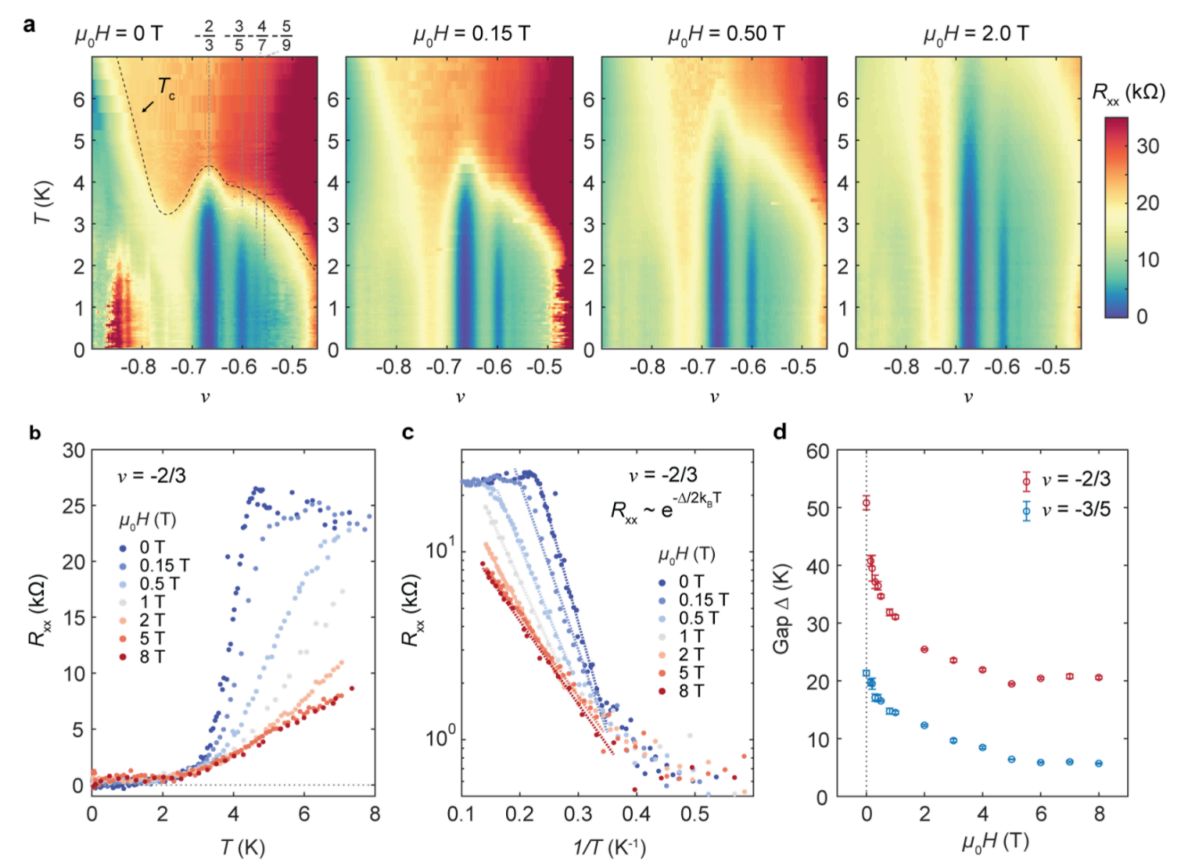
Integer and Fractional Quantum Anomalous Hall Effects





$$-\frac{p}{2p-1}, \quad p = 2,3,4,5$$



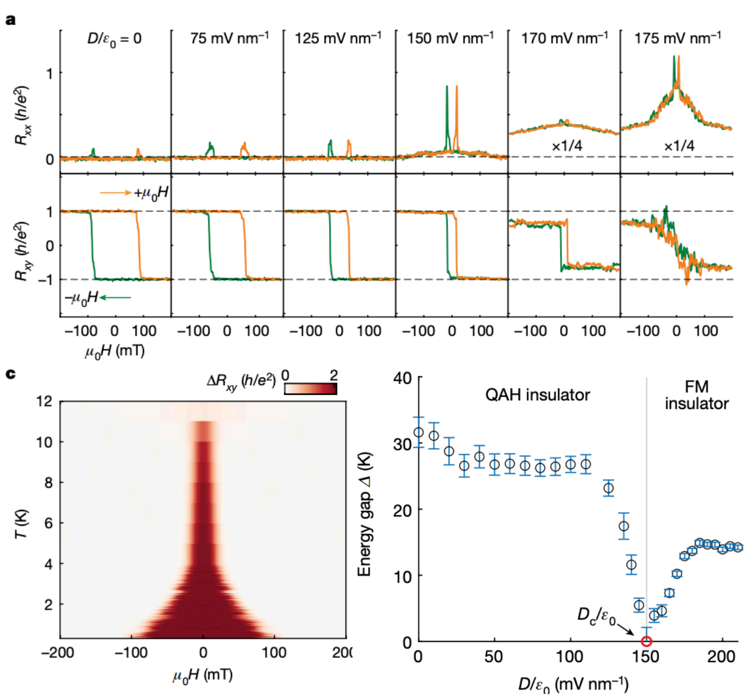


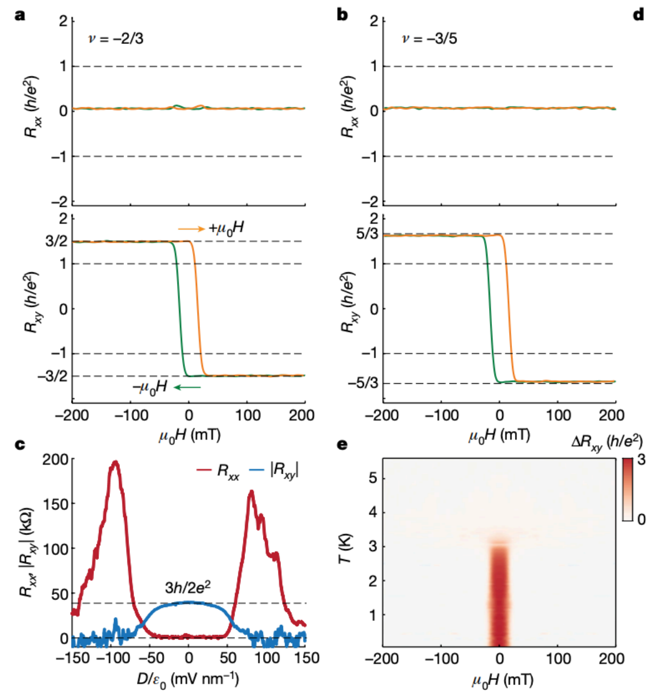
H. Park et al., Observation of High-Temperature Dissipationless Fractional Chern Insulator, arXiv:2503.10989

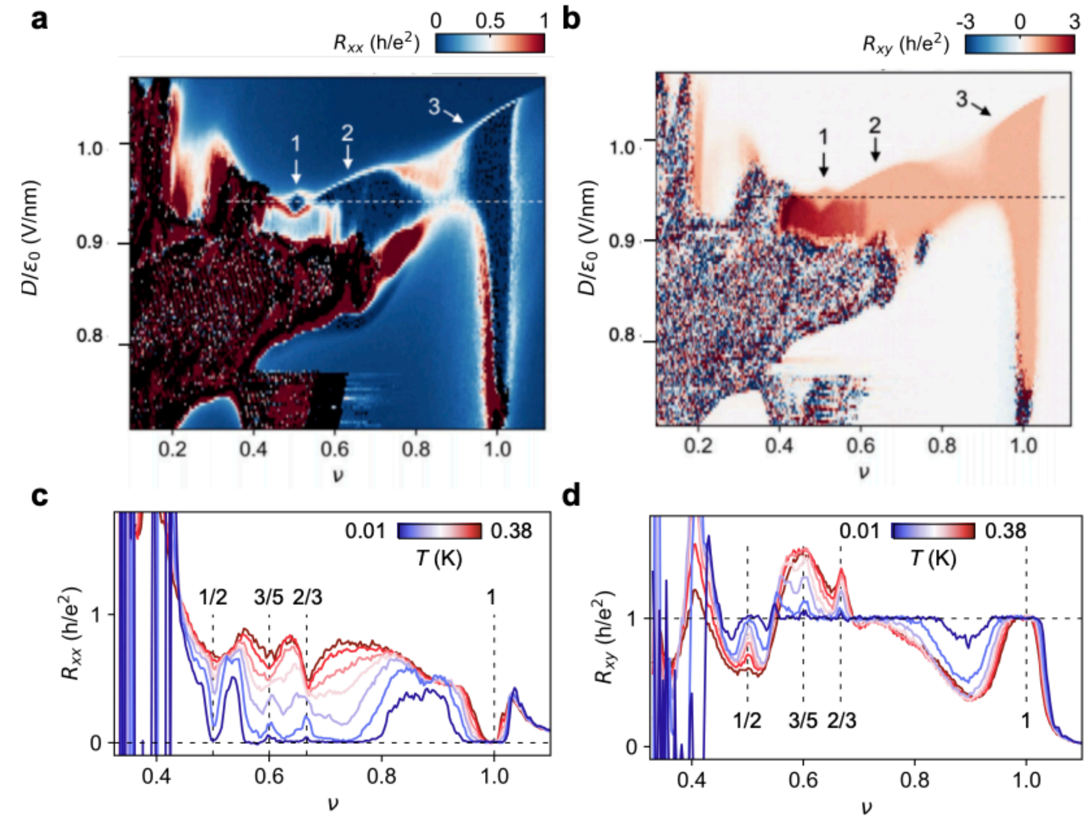
Integer and Fractional Quantum Anomalous Hall Effects

twisted bilayer MoTe2

rhombohedral pentalayer graphene/hBN







difference in temperature/energy scales

energy gap ~ 20 K

FQAH ~ 0.4 K
FQAH - QAH 0.04 K
FQAH - QAH - CDW - FL transitions

- J. Cai et al., Signatures of fractional quantum anomalous Hall states in twisted MoTe2, Nature 622, 63 (2023)
- H. Park et al., Observation of fractionally quantized anomalous Hall effect, Nature 622, 74 (2023)
- Z. Lu et al., Fractional quantum anomalous Hall effect in multilayer Graphene, Nature 626, 759 (2024)
- Z. Lu et al., Extended Quantum Anomalous Hall States in Graphene/hBN moiré superlattices, Nature 637, 1090 (2025)

Fractional Chern Insulator

Phys. Rev. Lett 132, 236502 (2024)

Thermodynamic Response and Neutral Excitations in Integer and Fractional Quantum Anomalous Hall States Emerging from Correlated Flat Bands

Rep. Prog. Phys 87, 108003 (2024)

arXiv: 2404.06745

Continuous transition and gapless roton inside fractional quantum anomalous Hall states

arXiv:2501.00247

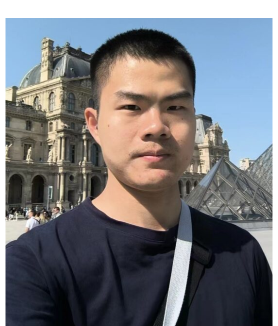
arXiv: 2505.04138

Spectra of Magnetoroton and Chiral Graviton Modes of Fractional Chern Insulator

Phys. Rev. Lett 134, 076601 (2025)

Continuous Transition between Bosonic Fractional Chern Insulator and Superfluid

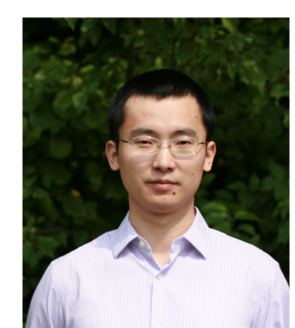
Lattice model, ED, DMRG+TDVP, (Thermal) Tensor-Network


Min Long

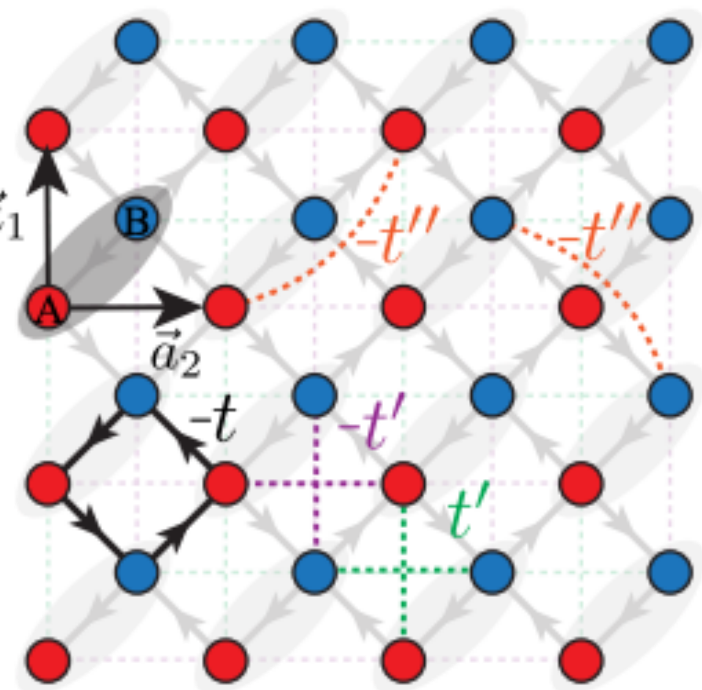

Hongyu Lu


Han-Qing Wu


Bin-Bin Chen


Kai Sun

(a)



$$H = H_0 + H_I$$

$$H_0 = -t \sum_{\langle i,j \rangle} e^{i\phi_{ij}}(c_i^\dagger c_j + h.c.) - \sum_{\langle\langle i,j \rangle\rangle} t'_{ij}(c_i^\dagger c_j + h.c.) - t'' \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} (c_i^\dagger c_j + h.c.)$$

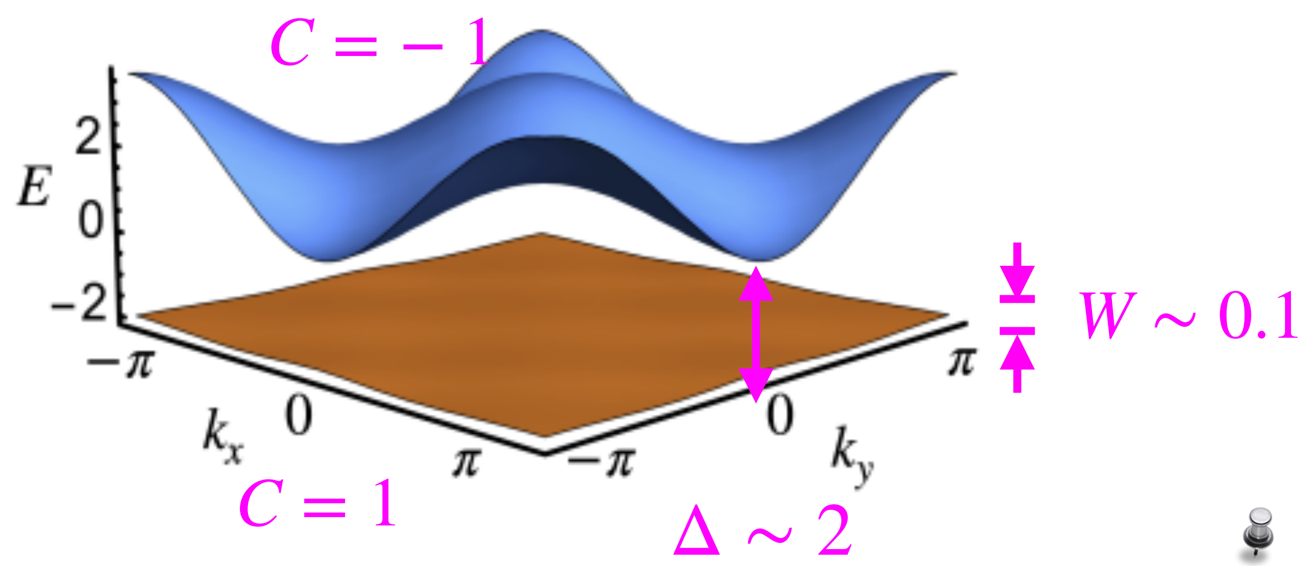
$$t = 1 \qquad t' = \pm \frac{1}{2+\sqrt{2}} \qquad t'' = -\frac{1}{2+2\sqrt{2}}$$

$$\phi_{ij} = \frac{\pi}{4}$$

$$H_I = V_1 \sum_{\langle i,j \rangle} n_i n_j + V_2 \sum_{\langle\langle i,j \rangle\rangle} n_i n_j + V_3 \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} n_i n_j + \mu \sum_i n_i$$

$V_1 = V_2 = V_3 = 0$

(b)



consider filling factors of the flat band

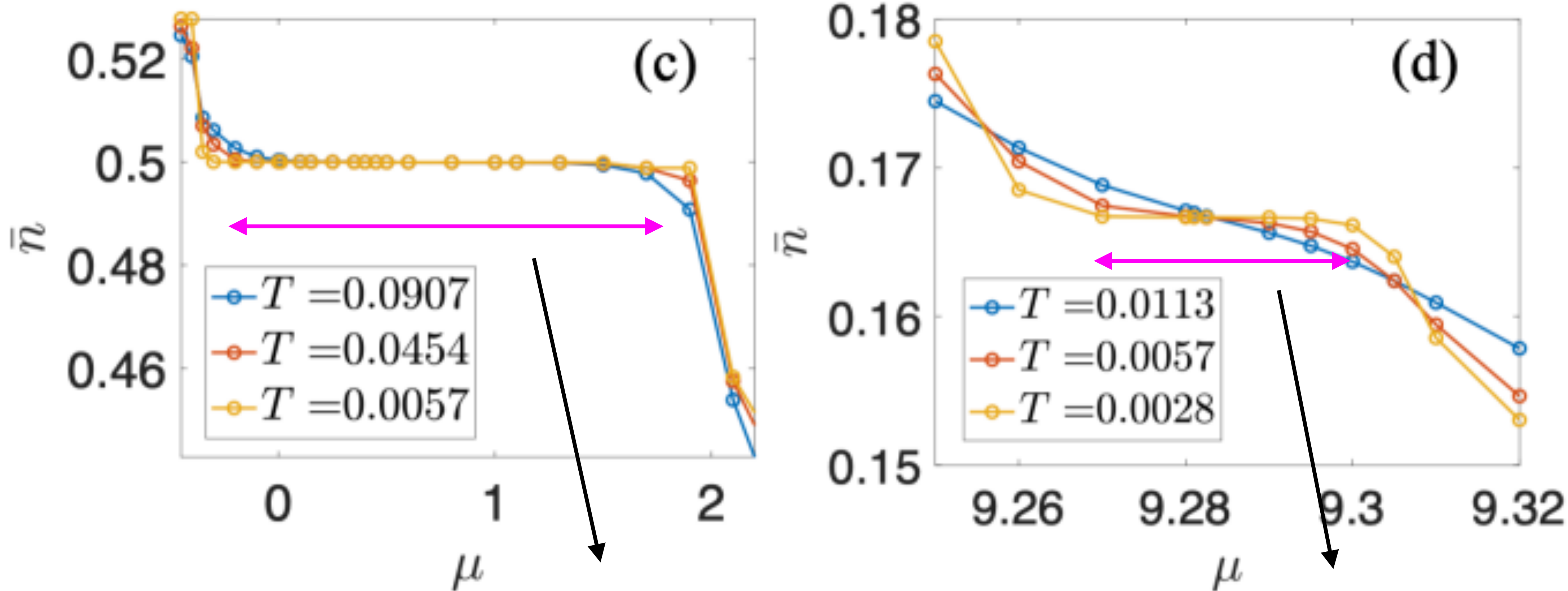
$$\nu = 1 \quad \text{and} \quad \nu = \frac{1}{3}$$

and only consider the interaction V_1

Hongyu Lu et al., PRL 132, 236502 (2024)

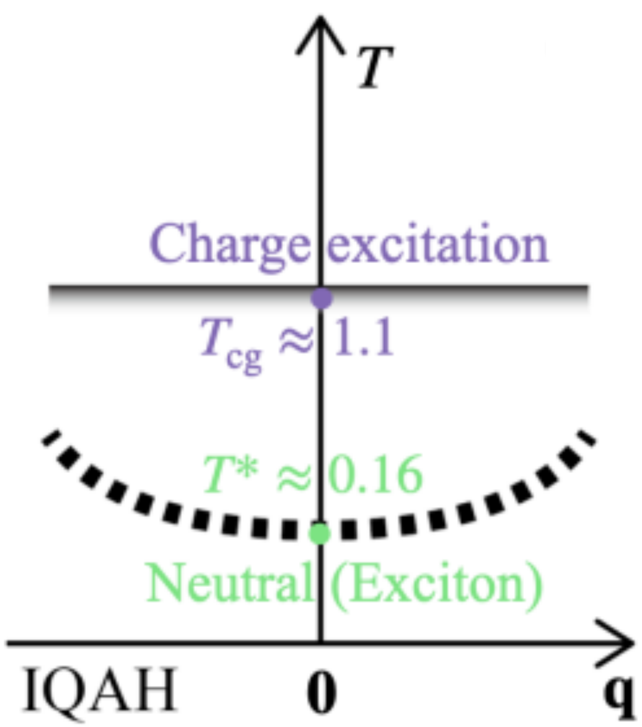
Find the insulating plateaus

$$\bar{n} = \frac{\nu}{2}$$



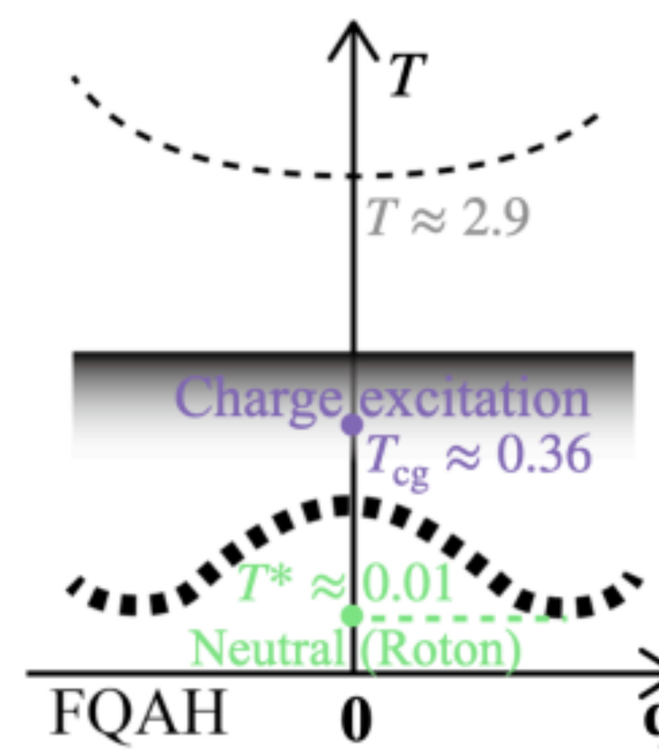
$\Delta_{cg} \sim 1$

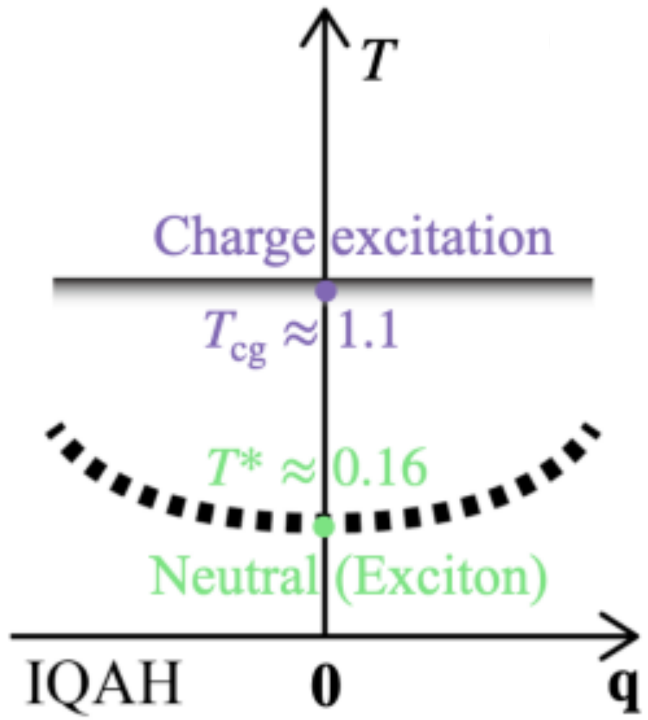
$\Delta_{cg} \sim 0.36$

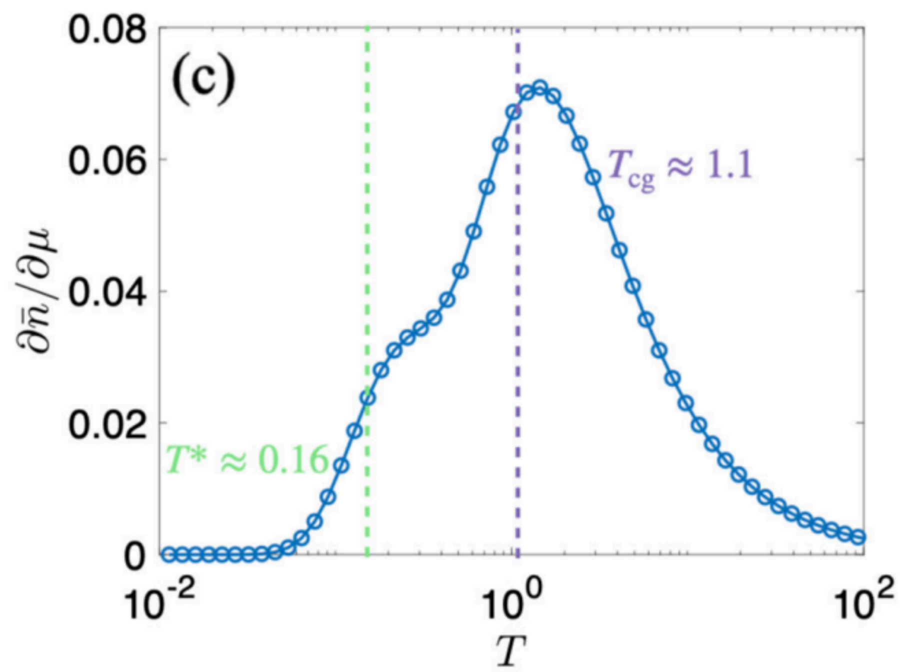


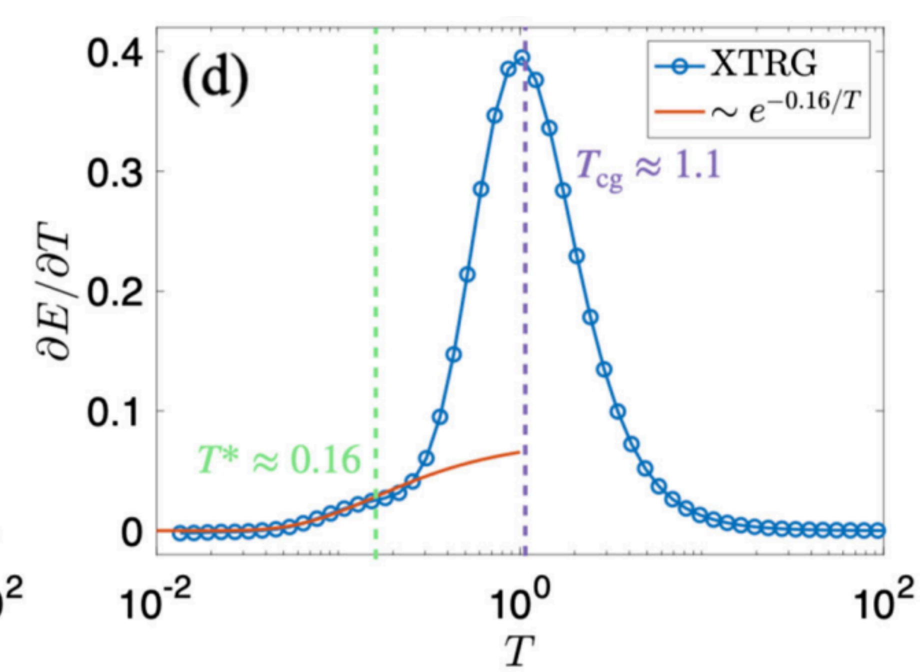
Two questions:

1. Temperature scales
2. Elementary excitations



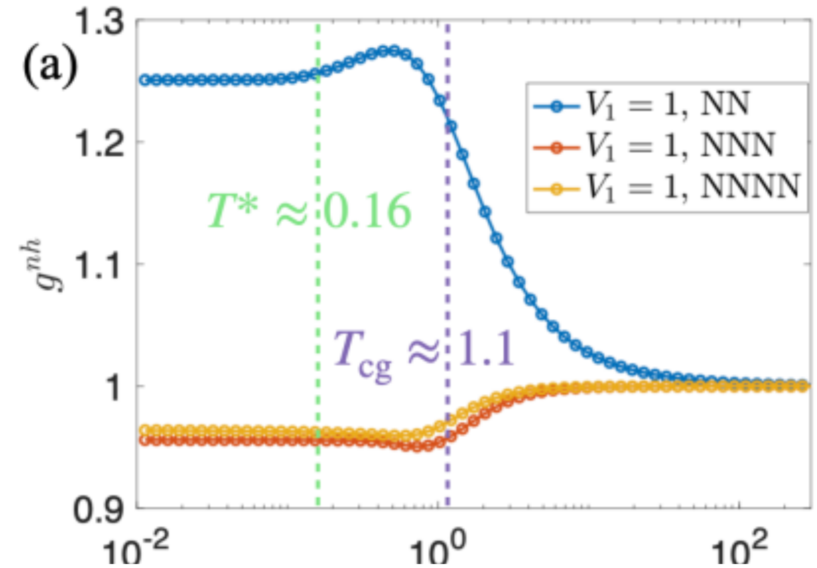




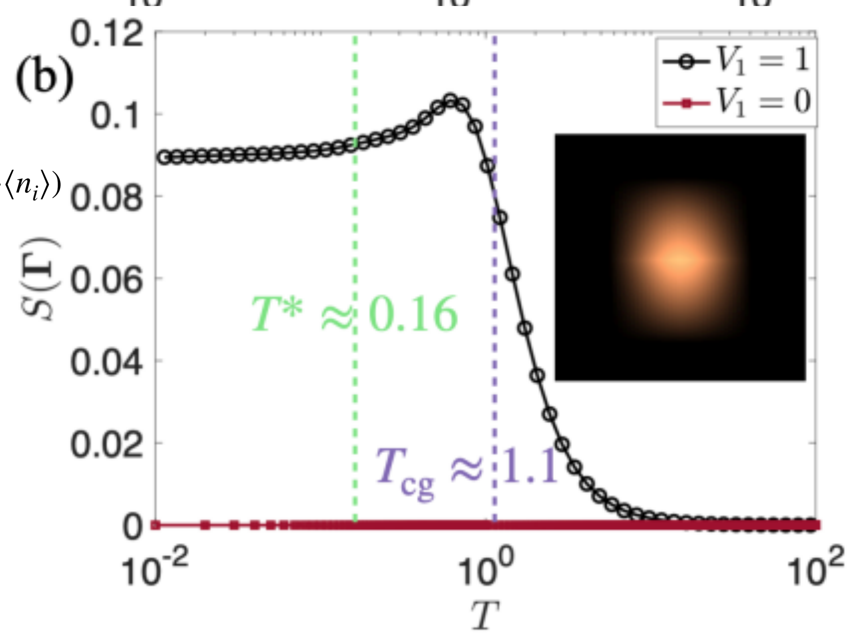


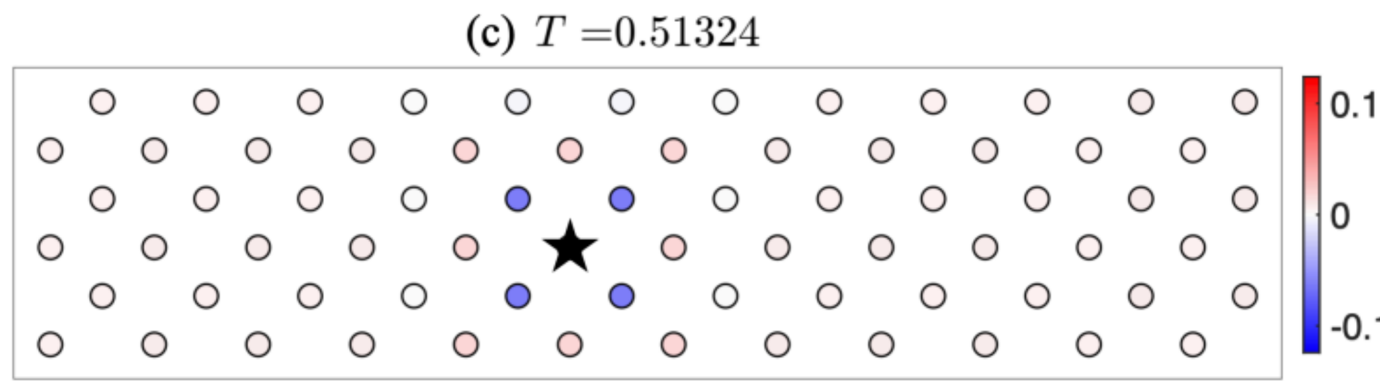
$T^* < T < T_{cg}$ Exciton proliferations, intrinsic correlation effect

$$g^{nh} = \frac{\langle n_0 h_i \rangle_T}{\langle n_0 \rangle_T \langle h_i \rangle_T}$$

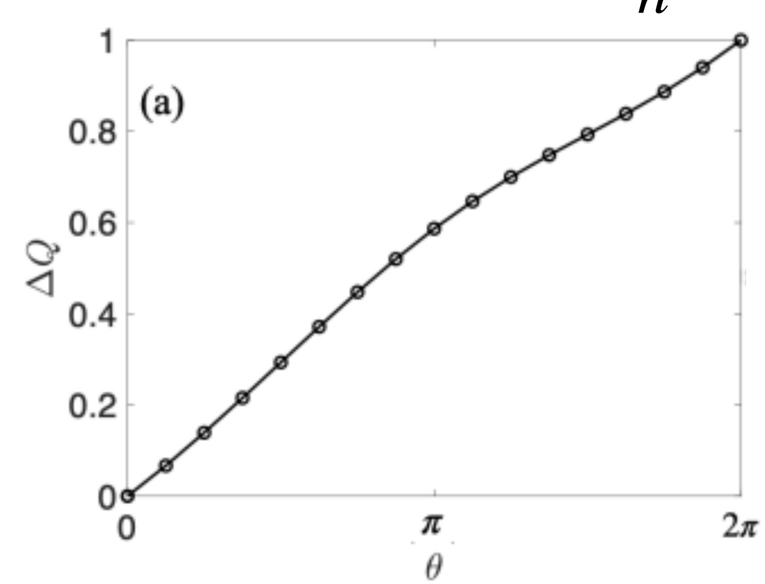


$$S(\mathbf{q}) = \sum_i e^{-i\mathbf{q}\cdot(\mathbf{r_i}-\mathbf{r_0})}(\langle n_o n_i \rangle - \langle n_0 \rangle \langle n_i \rangle)$$

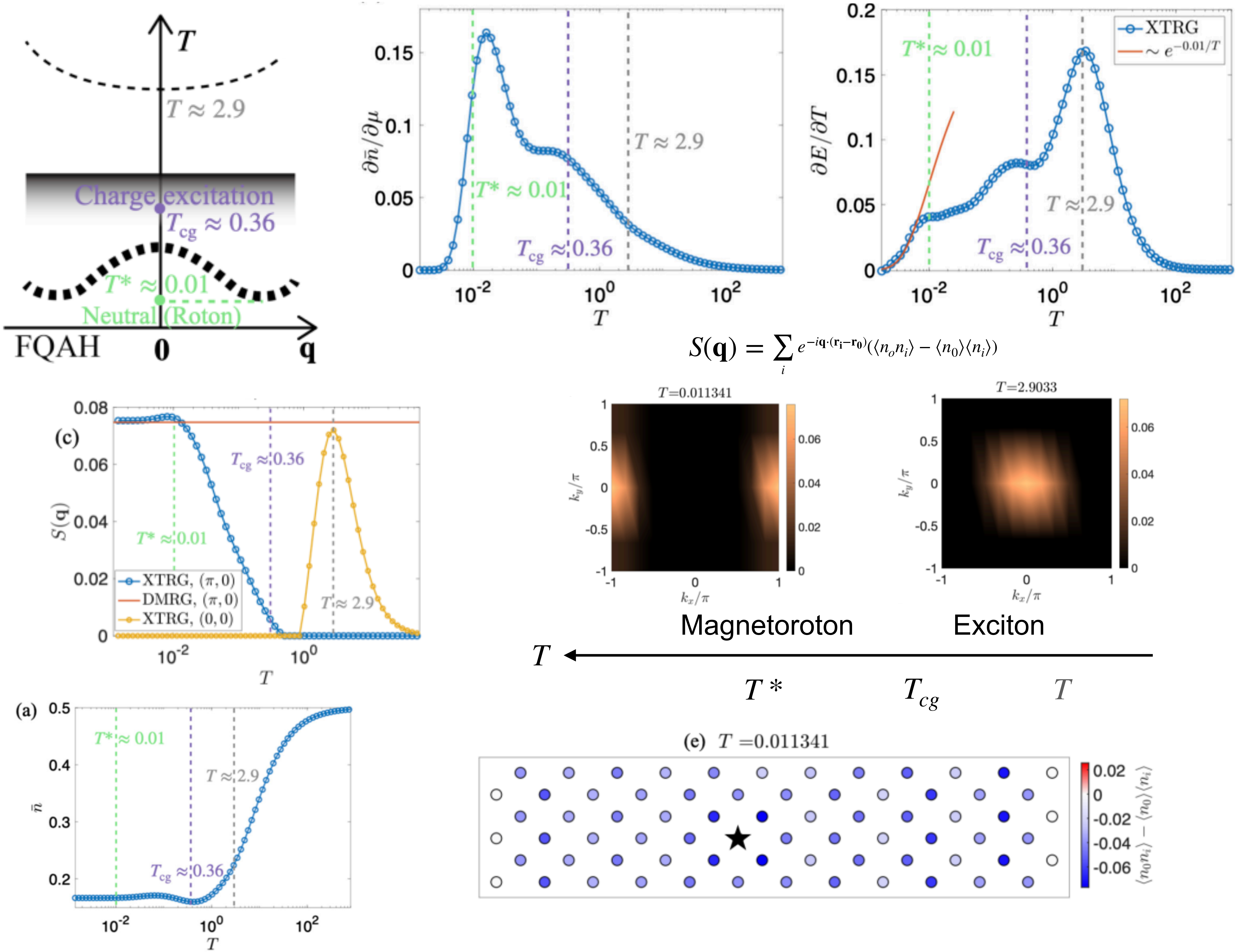




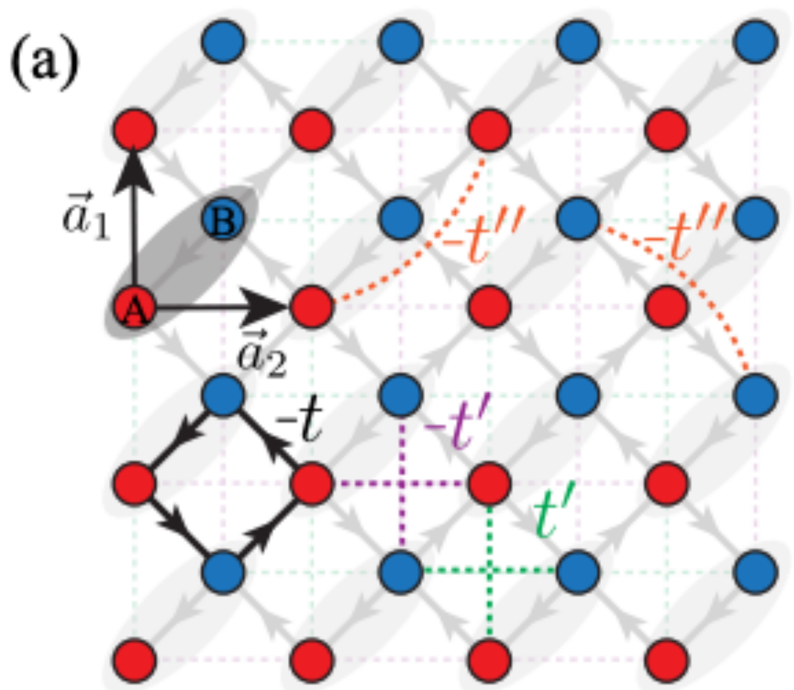
Charge pumping $\sigma_{xy} = \frac{e^2}{h}$



$T = 0$



T
T ≈ 2.9
Charge excitation
T_cg ≈ 0.36
T* ≈ 0.01
Neutral (Roton)
FQAH
0
q
∂n̄/∂μ
∂E/∂T
XTRG
∼ e^{−0.01/T}
S(q) = ∑_i e^{−iq·(r_i−r_0)}(⟨n_o n_i⟩ − ⟨n_0⟩⟨n_i⟩)
T=0.011341
T=2.9033
k_x/π
k_y/π
Magnetoroton
Exciton
T*
T_cg
(c)
S(q)
XTRG, (π, 0)
DMRG, (π, 0)
XTRG, (0, 0)
(a)
n̄
(e) T =0.011341
⟨n_0 n_i⟩ − ⟨n_0⟩⟨n_i⟩



$$H = H_0 + H_I$$

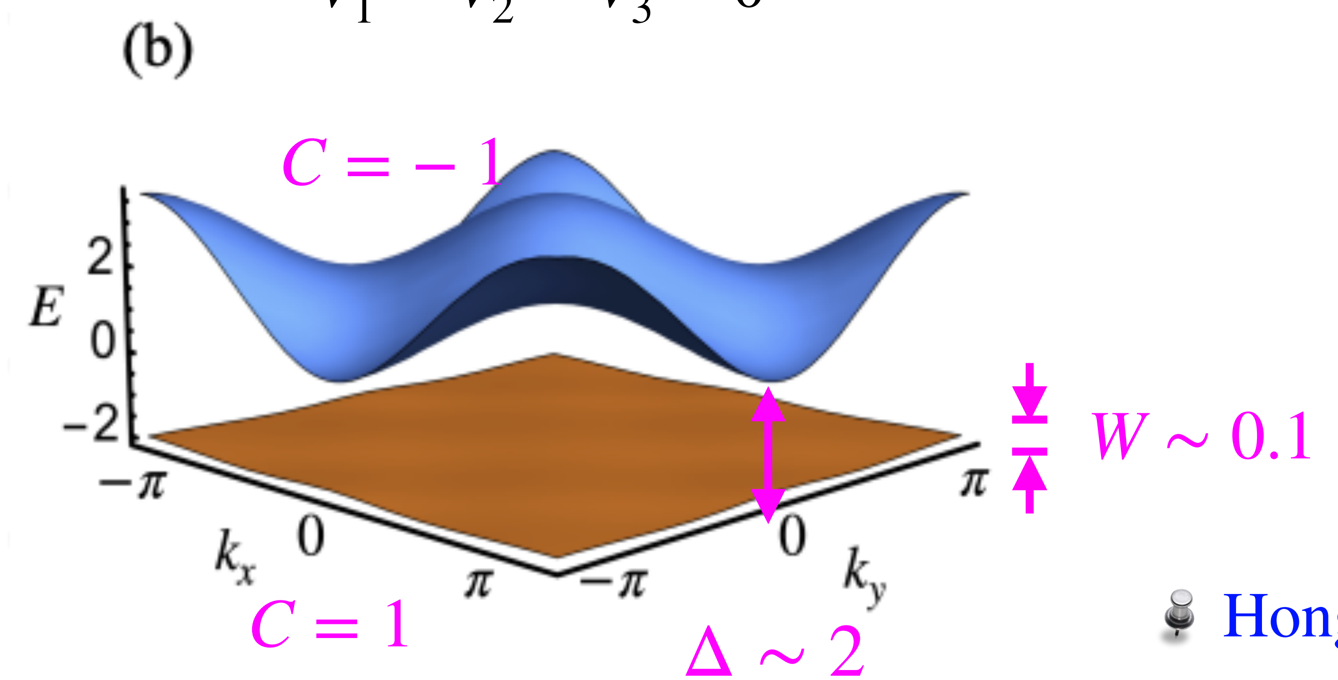
$$H_0 = -t \sum_{\langle i,j \rangle} e^{i\phi_{ij}} (c_i^\dagger c_j + h.c.) - \sum_{\langle\langle i,j \rangle\rangle} t'_{ij} (c_i^\dagger c_j + h.c.) - t'' \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} (c_i^\dagger c_j + h.c.)$$

$$t = 1 \qquad t' = \pm \frac{1}{2+\sqrt{2}} \qquad t'' = -\frac{1}{2+2\sqrt{2}}$$

$$\phi_{ij} = \frac{\pi}{4}$$

$$H_I = V_1 \sum_{\langle i,j \rangle} n_i n_j + V_2 \sum_{\langle\langle i,j \rangle\rangle} n_i n_j + V_3 \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} n_i n_j + \mu \sum_i n_i$$

$$V_1 = V_2 = V_3 = 0$$

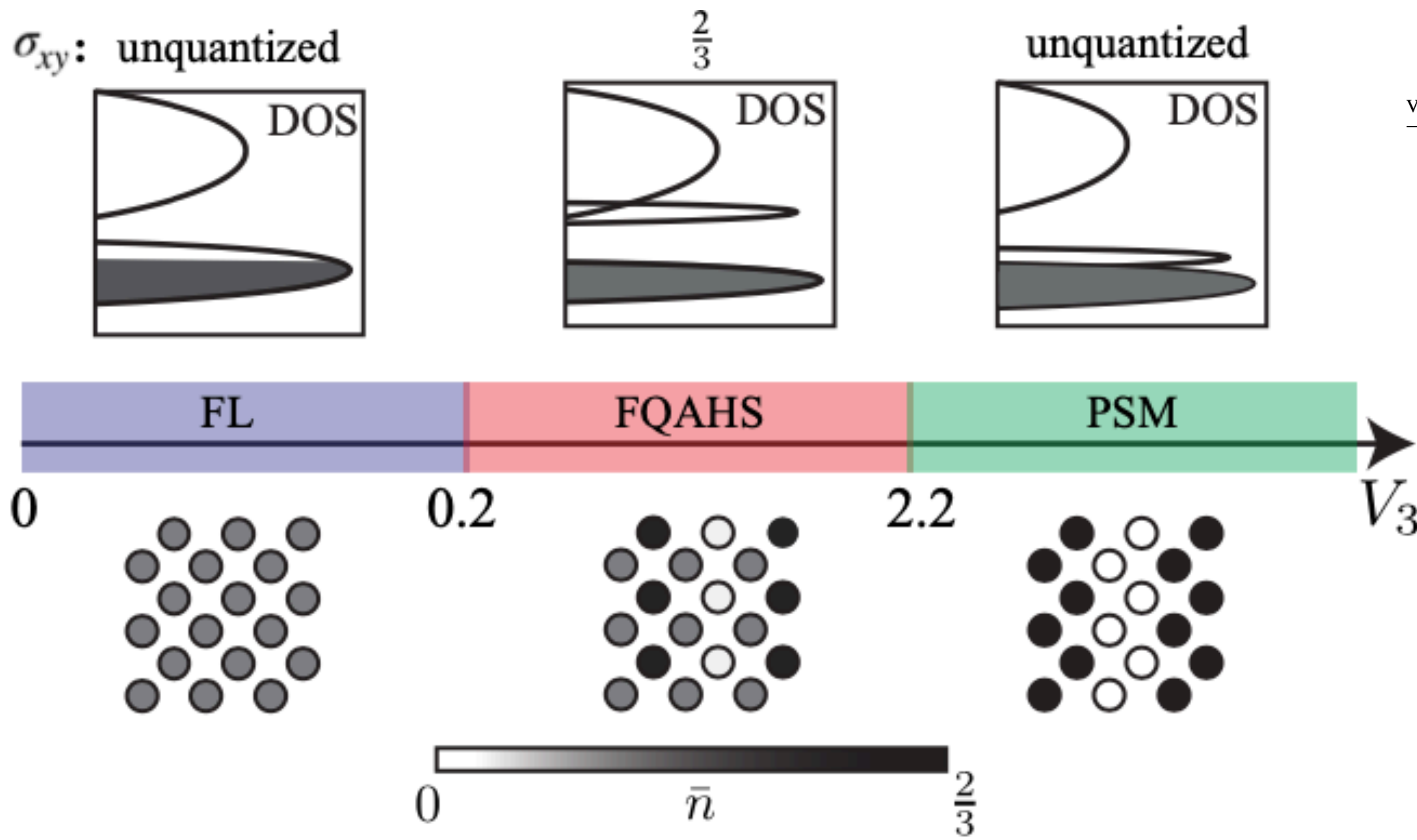


Consider filling factor of the flat band

$$\nu = \frac{2}{3}$$

and consider the NNN interaction V_3

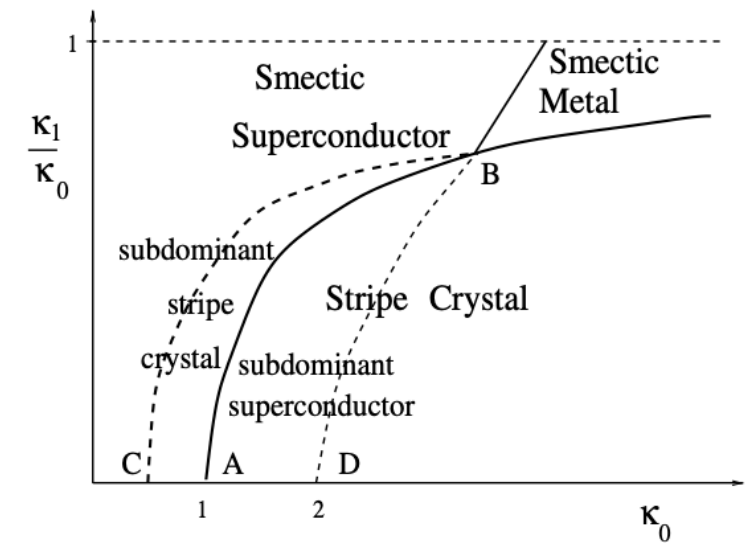
Hongyu Lu et al., Rep. Prog. Phys. 87 (2024) 108003



VOLUME 85, NUMBER 10 PHYSICAL REVIEW LETTERS 4 SEPTEMBER 2000

Quantum Theory of the Smectic Metal State in Stripe Phases

V. J. Emery,[1] E. Fradkin,[2] S. A. Kivelson,[3,4] and T. C. Lubensky[5]



FL — Fermi liquid
FQAHS — Fractional quantum anomalous Hall smectic state
PSM — Polar smectic metal

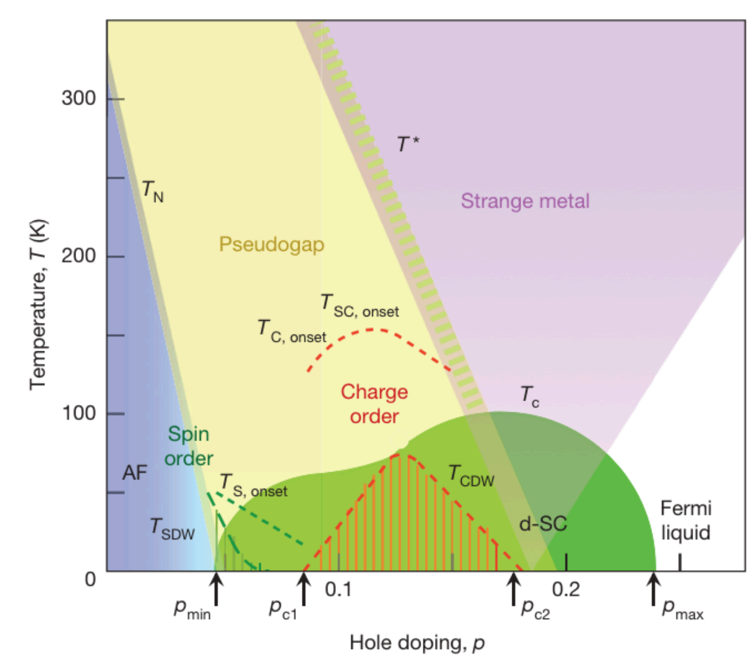
Intertwinement of topological order and Landau order

REVIEW

doi:10.1038/nature14165

From quantum matter to high-temperature superconductivity in copper oxides

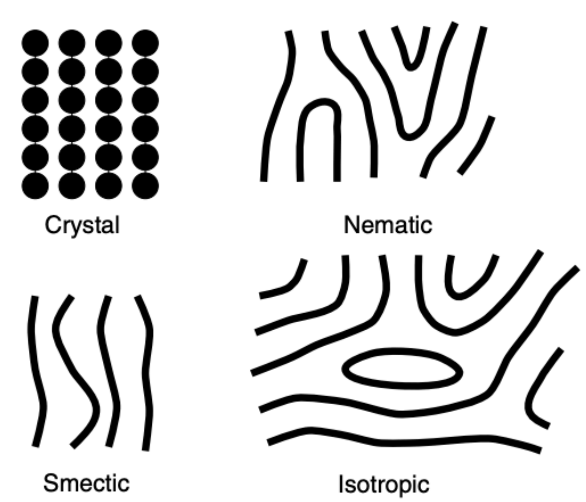
B. Keimer[1], S. A. Kivelson[2], M. R. Norman[3], S. Uchida[4] & J. Zaanen[5]



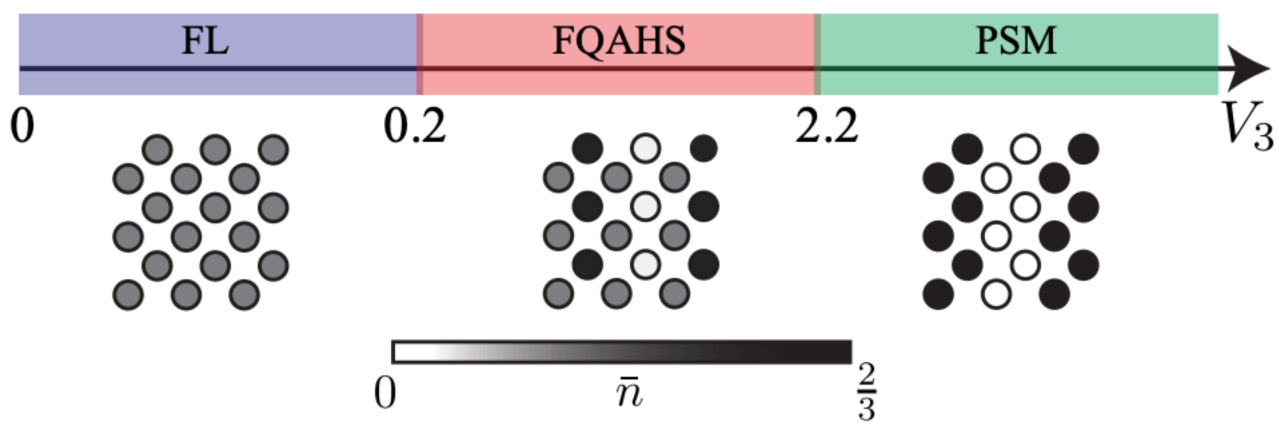
Electronic liquid-crystal phases of a doped Mott insulator

S. A. Kivelson*, E. Fradkin† & V. J. Emery‡

Nature 393, 550 (1998)



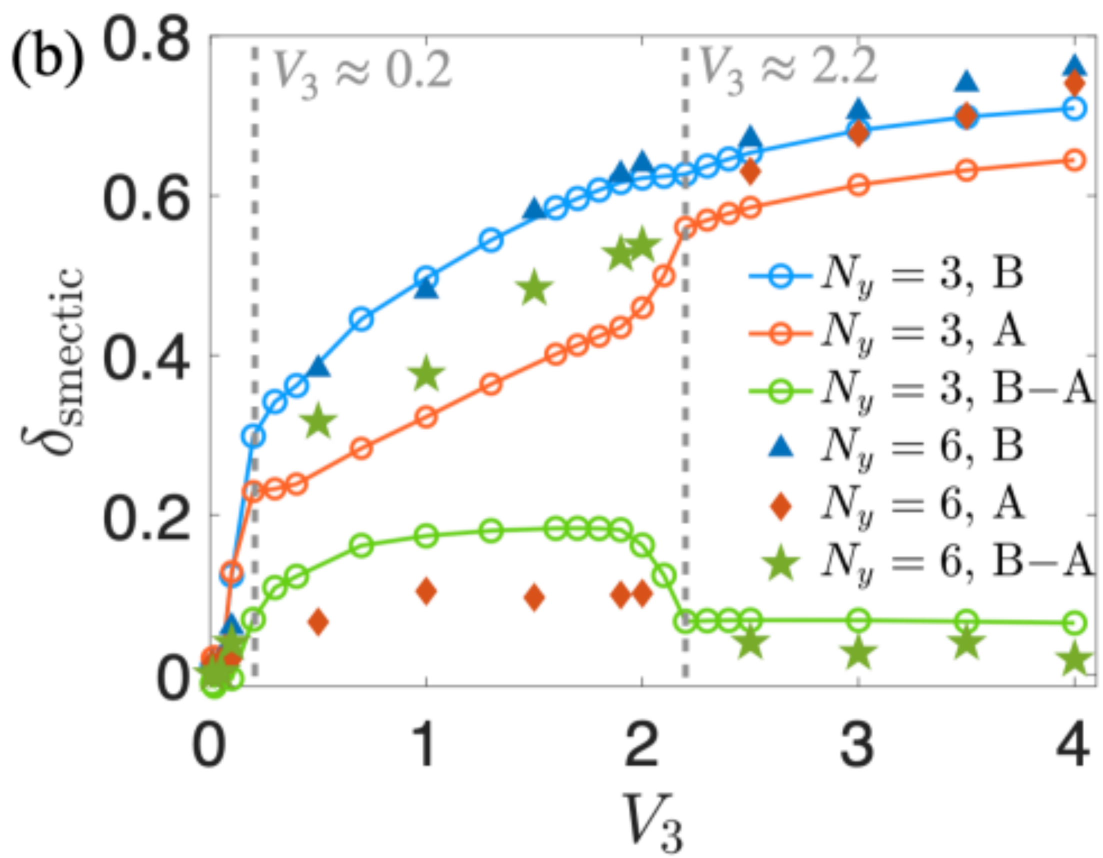
Hongyu Lu et al., Rep. Prog. Phys. 87 (2024) 108003

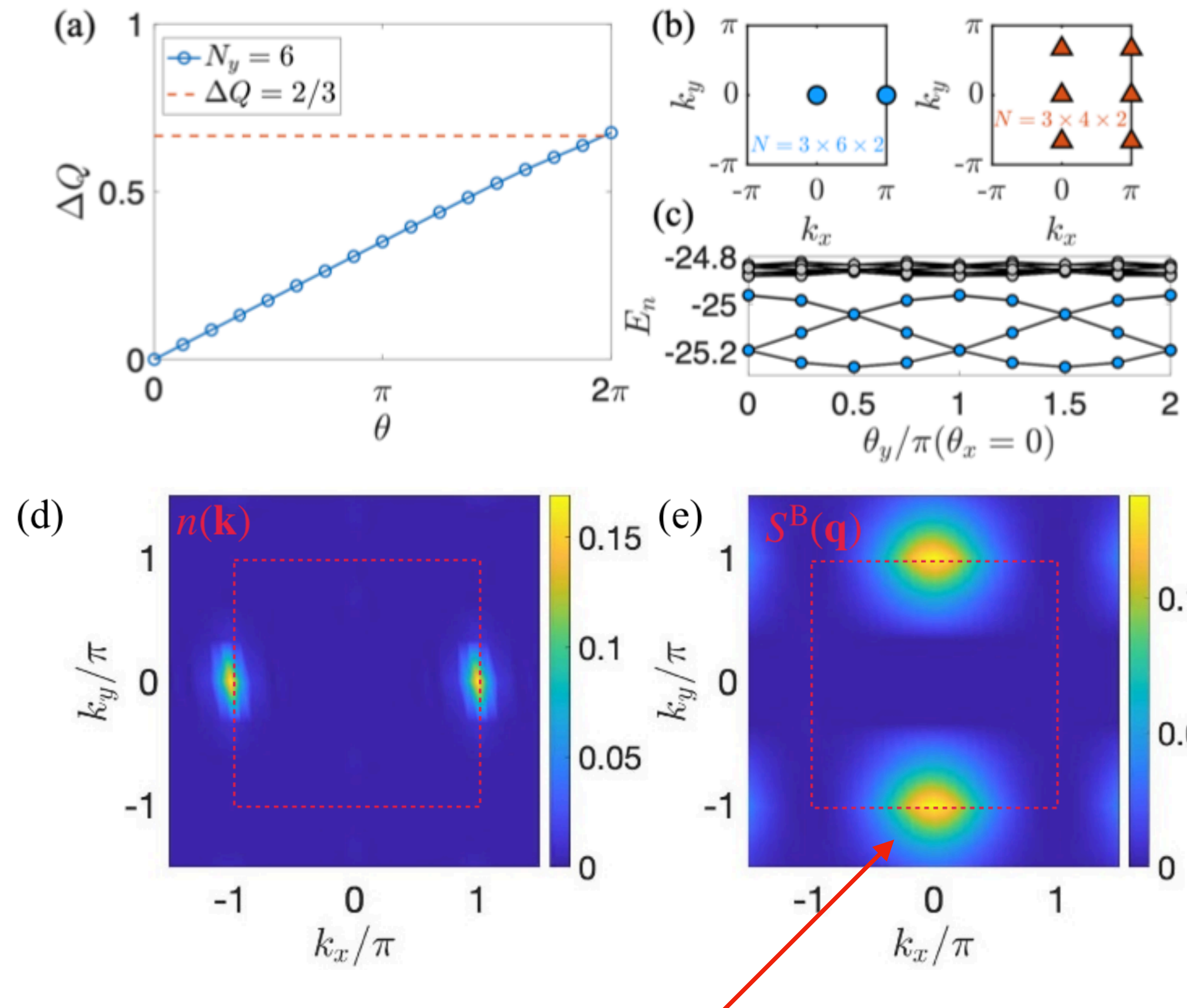


Charge pumping

$$\sigma_{xy} = \frac{2}{3}\frac{e^2}{h}$$

6-fold degeneracy





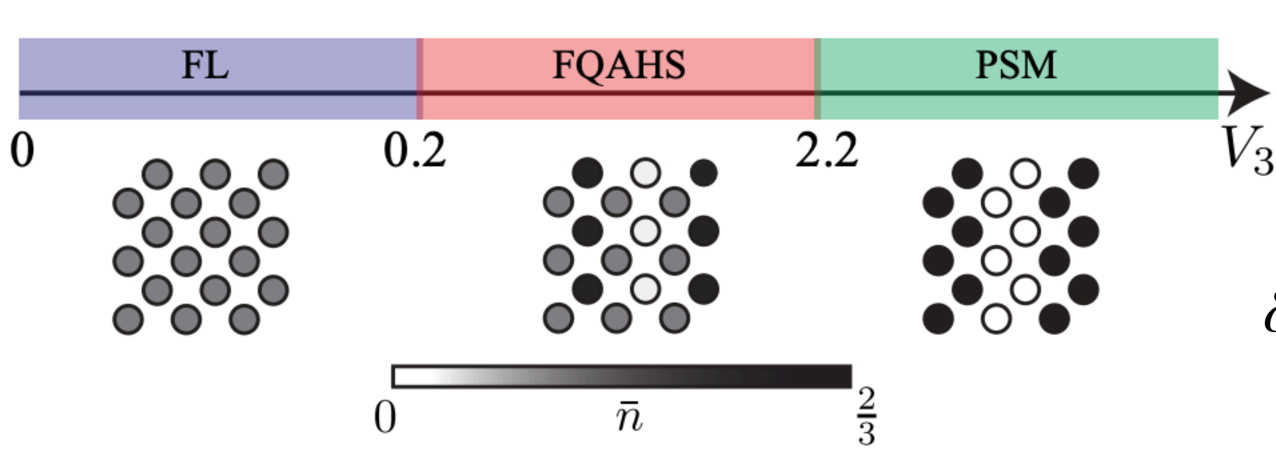
Charge-neutral magnetoroton

$$\delta^{A/B}_{smectic} = \frac{1}{N}\sum_i (-1)^{x_i}\, n_i^{A/B} \qquad i \text{ unit cell}$$

$$S^{A/B}(\mathbf{q}) = \sum_i e^{-i\mathbf{q}\cdot(\mathbf{r_i}-\mathbf{r_0})}(\langle n_0^{A/B} n_i^{A/B}\rangle - \langle n_0^{A/B}\rangle\langle n_i^{A/B}\rangle)$$

Hongyu Lu et al., PRL 132, 236502 (2024)

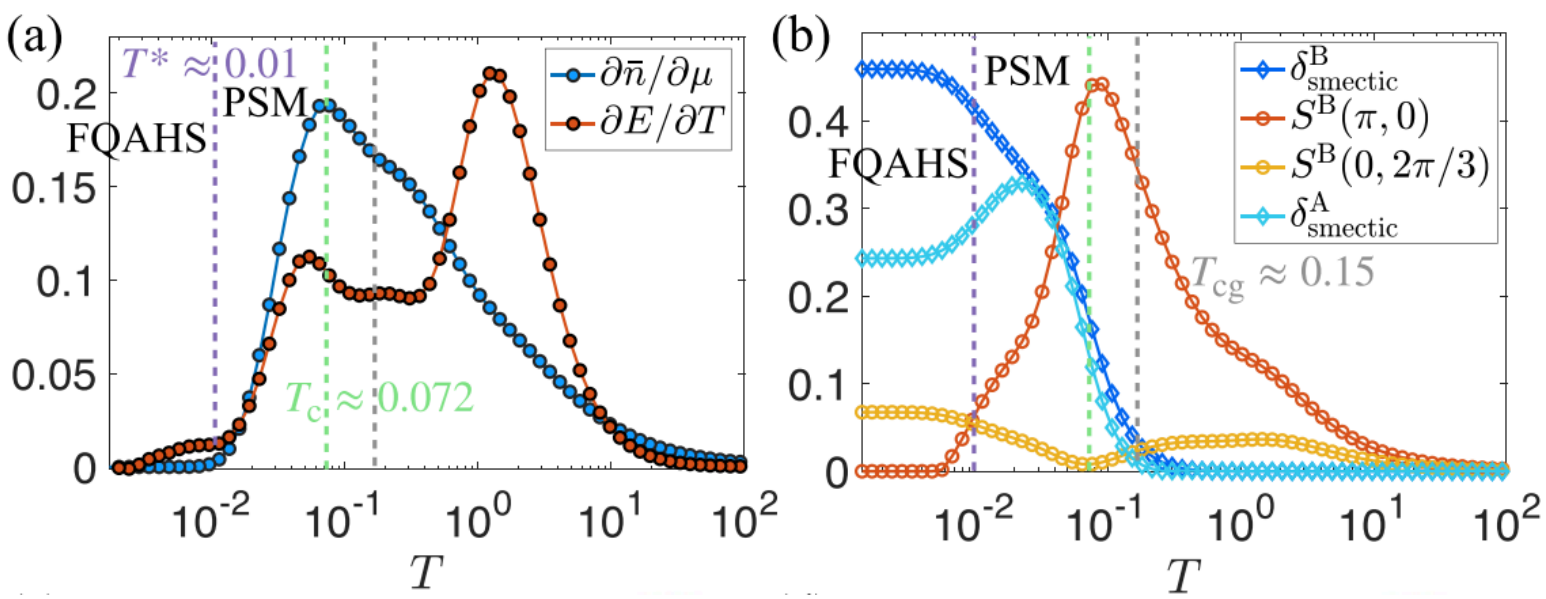
Hongyu Lu et al., Rep. Prog. Phys. 87 (2024) 108003

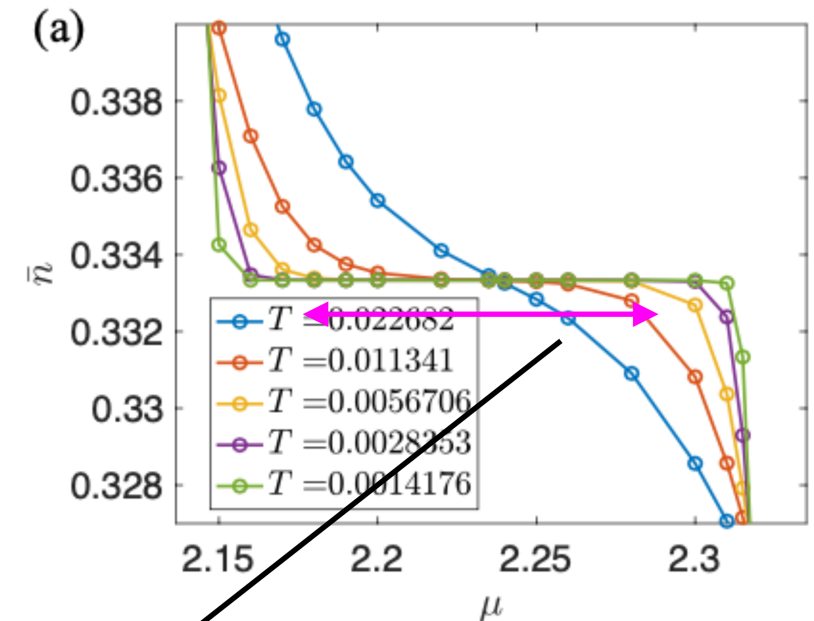


$$\delta^{A/B}_{smectic} = \frac{1}{N}\sum_i (-1)^{x_i}\, n_i^{A/B}$$

$$S^{A/B}(\mathbf{q}) = \sum_i e^{-i\mathbf{q}\cdot(\mathbf{r_i}-\mathbf{r_0})}(\langle n_0^{A/B} n_i^{A/B}\rangle - \langle n_0^{A/B}\rangle\langle n_i^{A/B}\rangle)$$

$V_3 = 1$

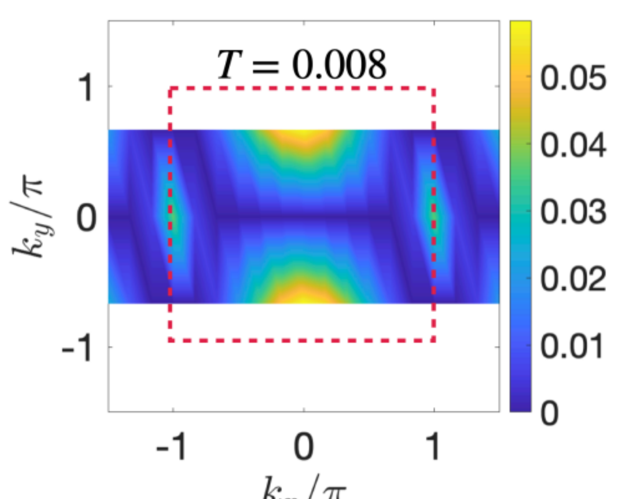


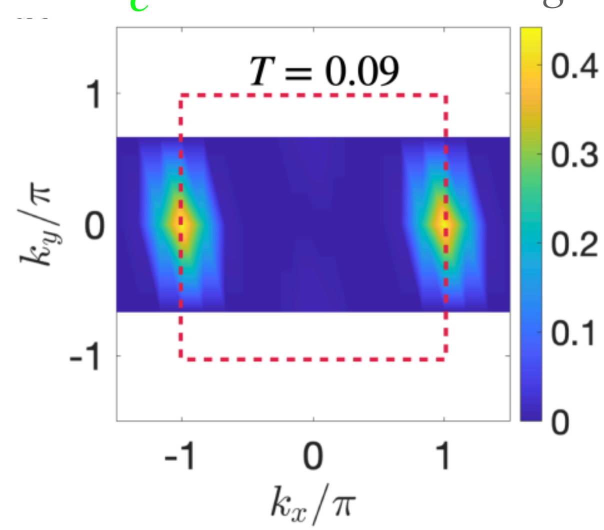


Magnetoroton Smectic order

T ←

T^* T_c $T_{cg} \sim \Delta_{cg} \sim 0.15$

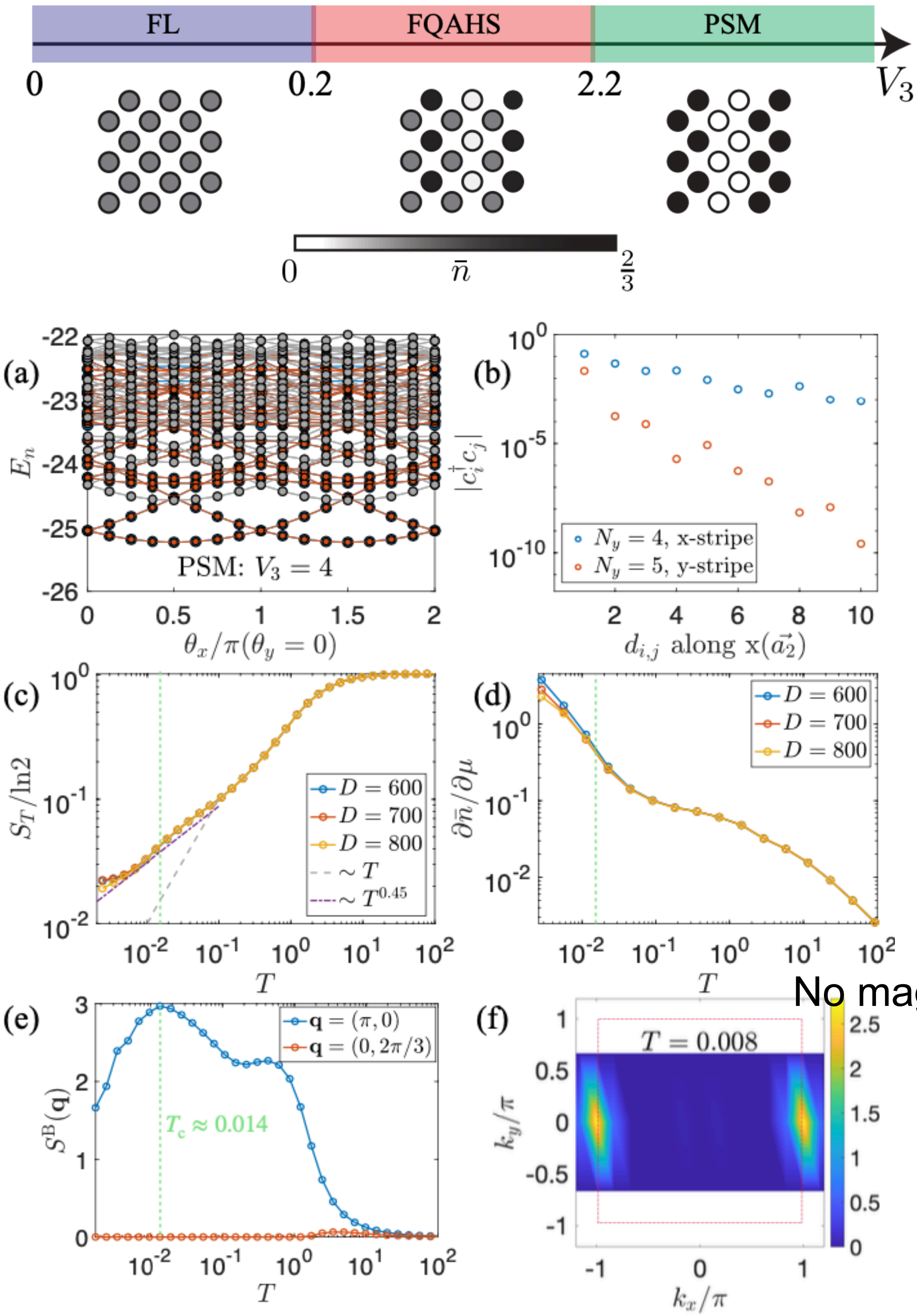




Roton gap determines the onset temperature of FCI

Hongyu Lu et al., PRL 132, 236502 (2024)

Hongyu Lu et al., Rep. Prog. Phys. 87 (2024) 108003

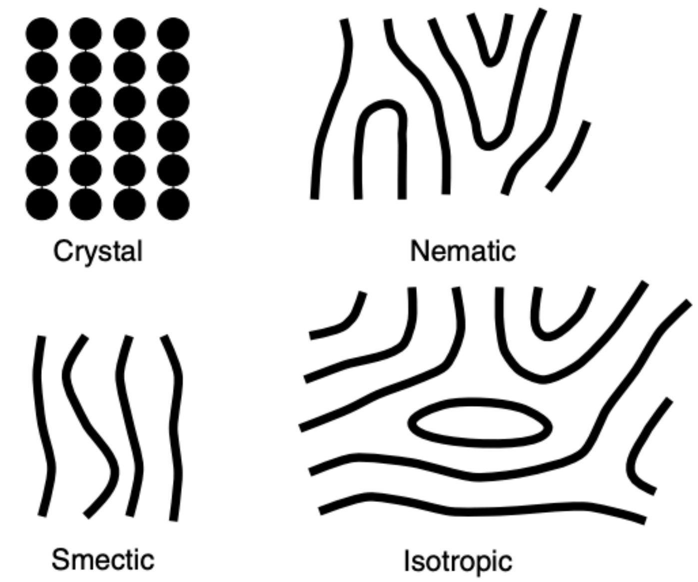


No magnetoroton

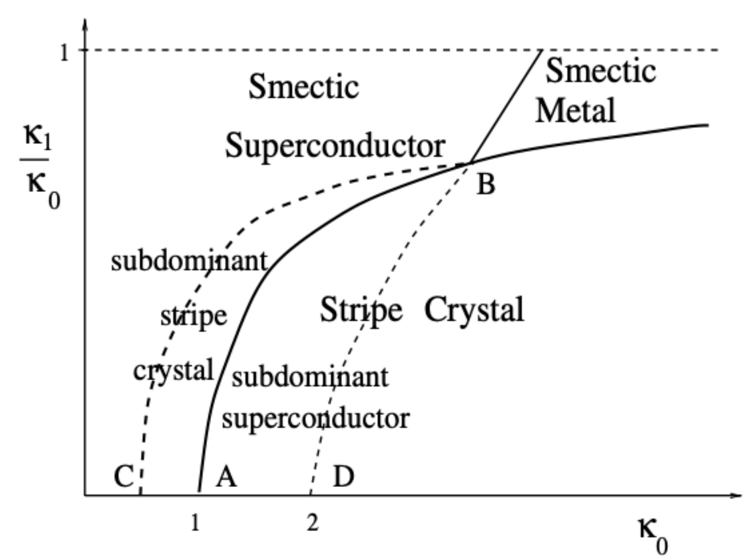
Electronic liquid-crystal phases of a doped Mott insulator

Nature 393, 550 (1998)

S. A. Kivelson*, E. Fradkin† & V. J. Emery‡



Coupled Luttinger liquid (non-Fermi liquid)

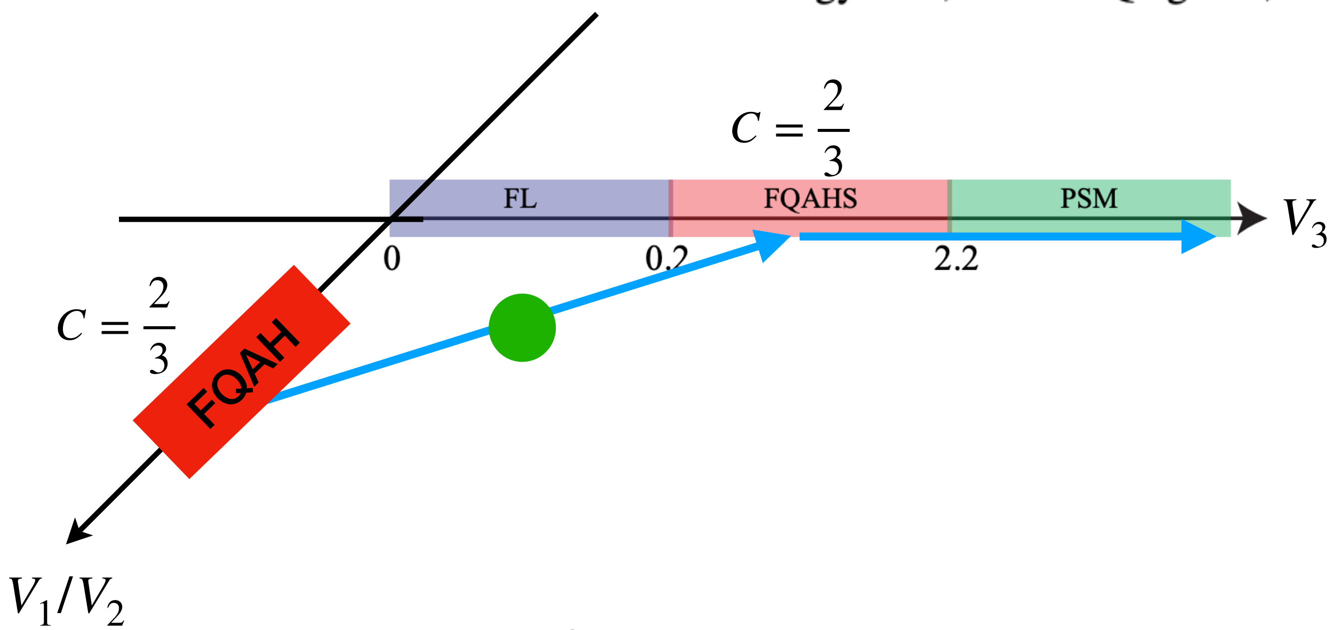


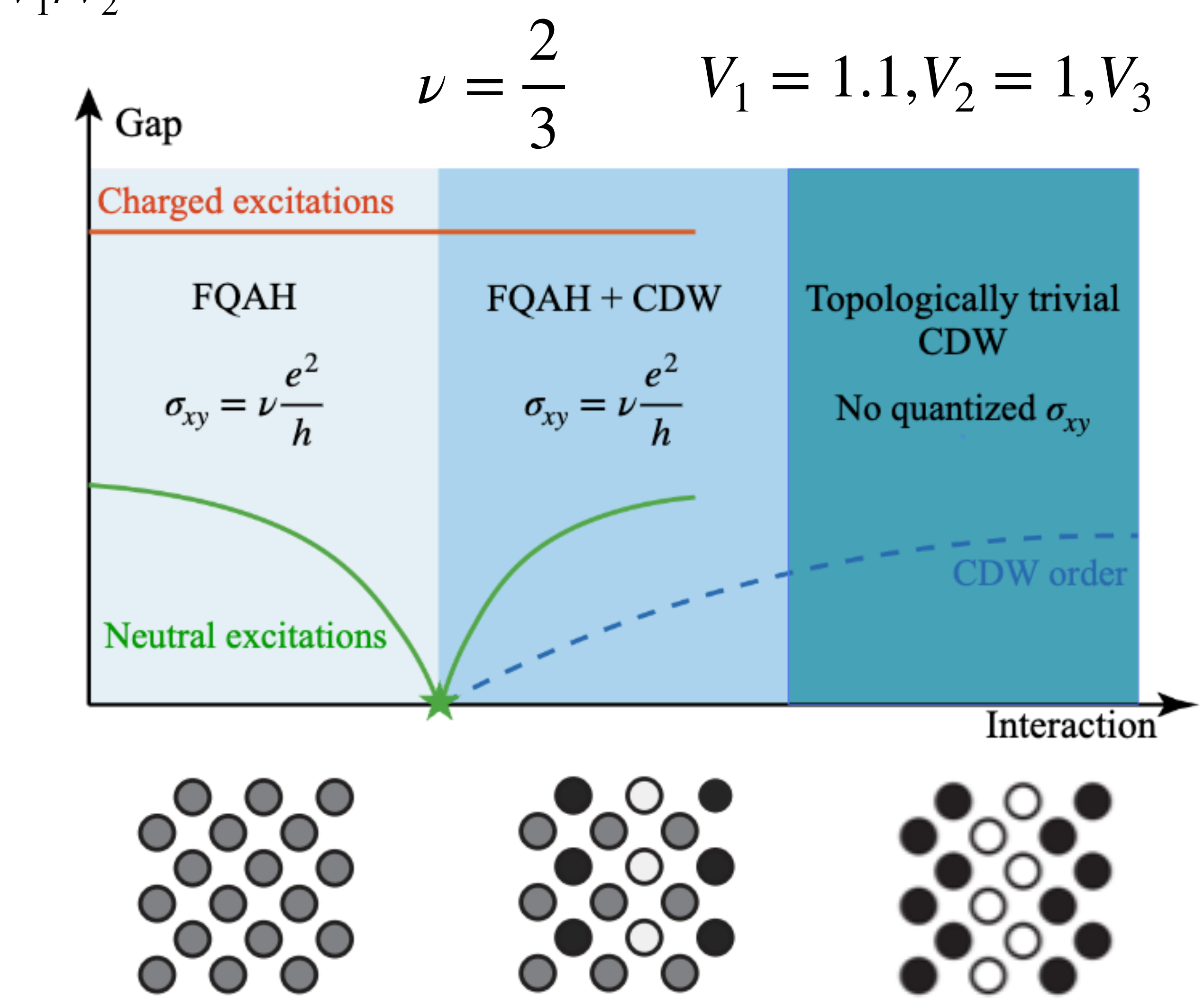
Emery, Fradkin, Kivelson, Lubensky, PRL 85, 2160 (2000)

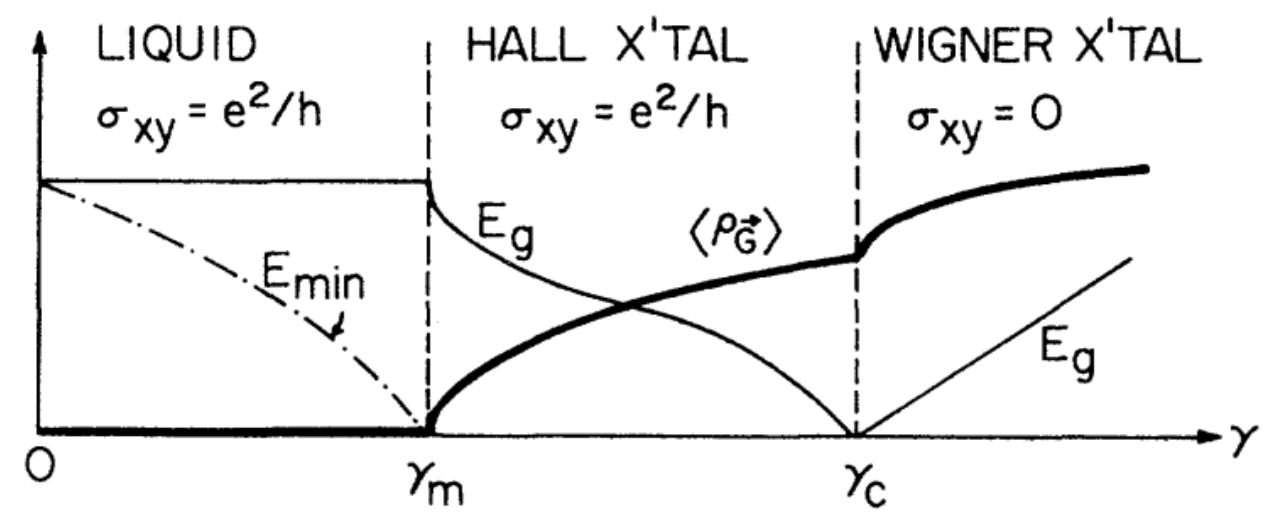
arXiv:2404.06745

Continuous transition and gapless roton inside fractional quantum anomalous Hall states

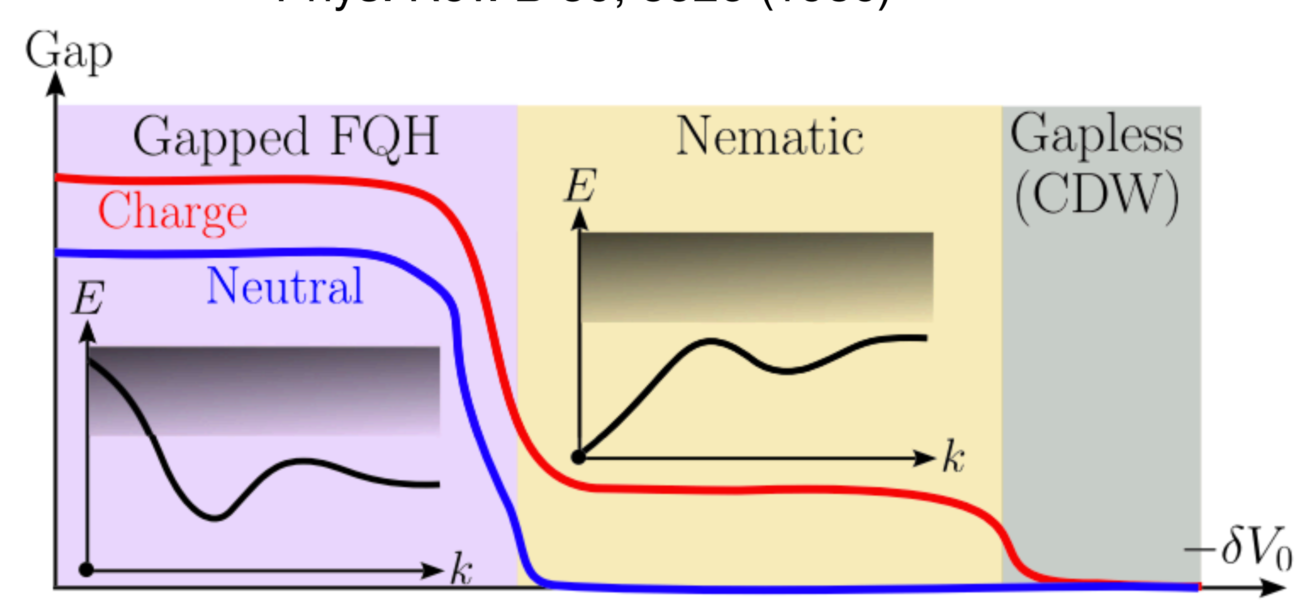
Hongyu Lu,[1,*] Han-Qing Wu,[2,*] Bin-Bin Chen,[3] and Zi Yang Meng[1,†]



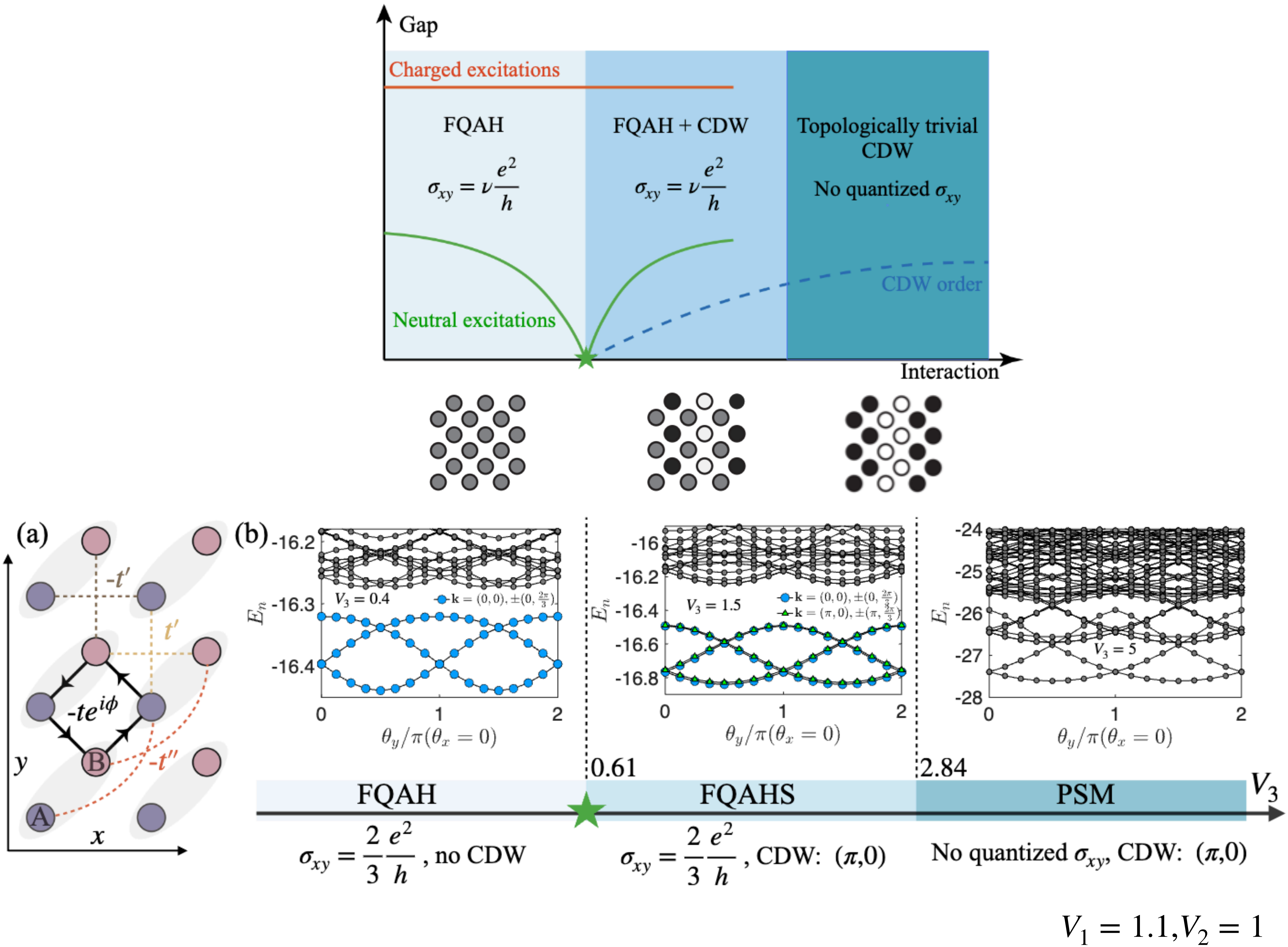




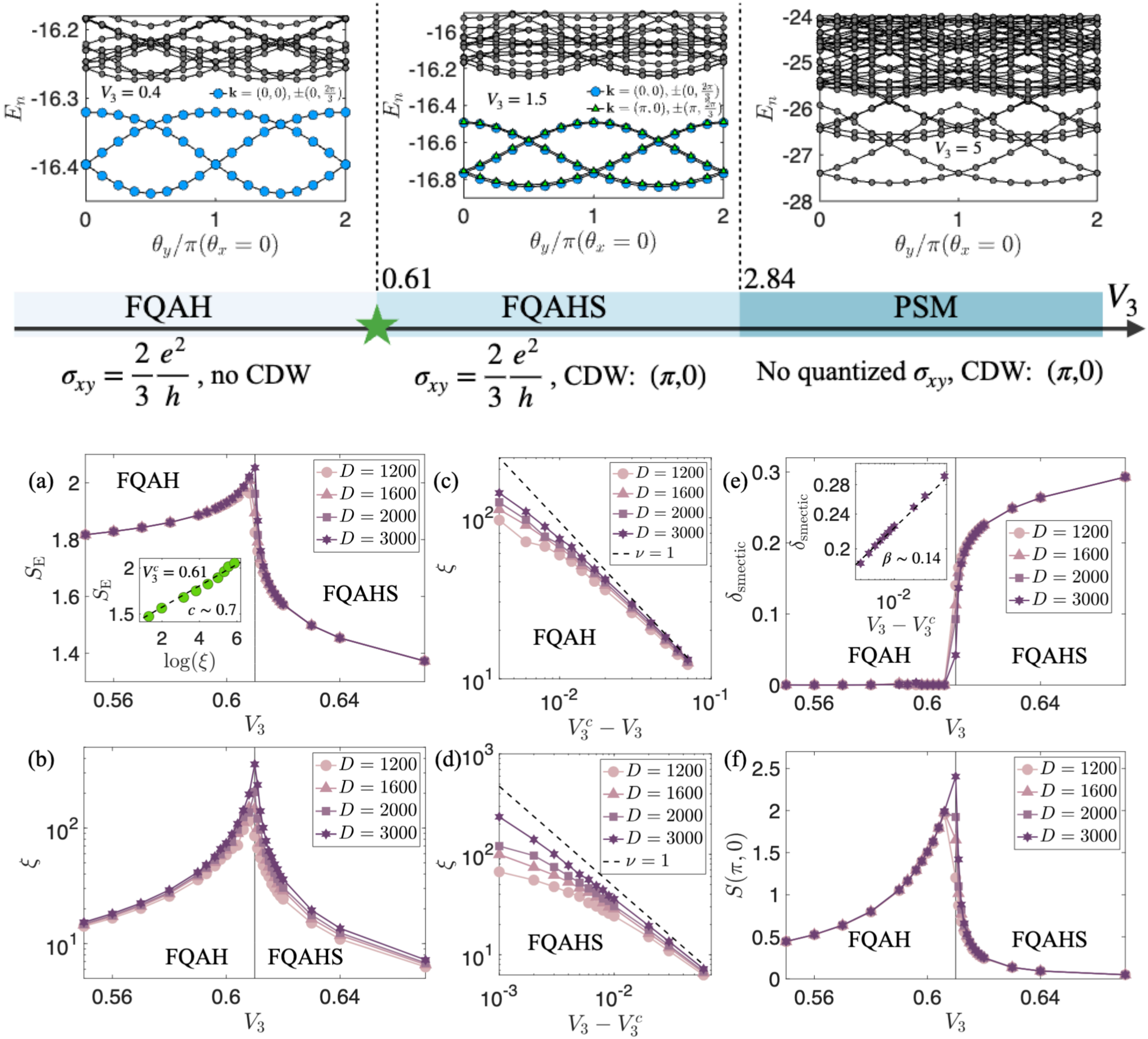
Tesanovic, Axel, Halperin,
“Hall crystal” versus Wigner crystal,
Phys. Rev. B 39, 8525 (1989)



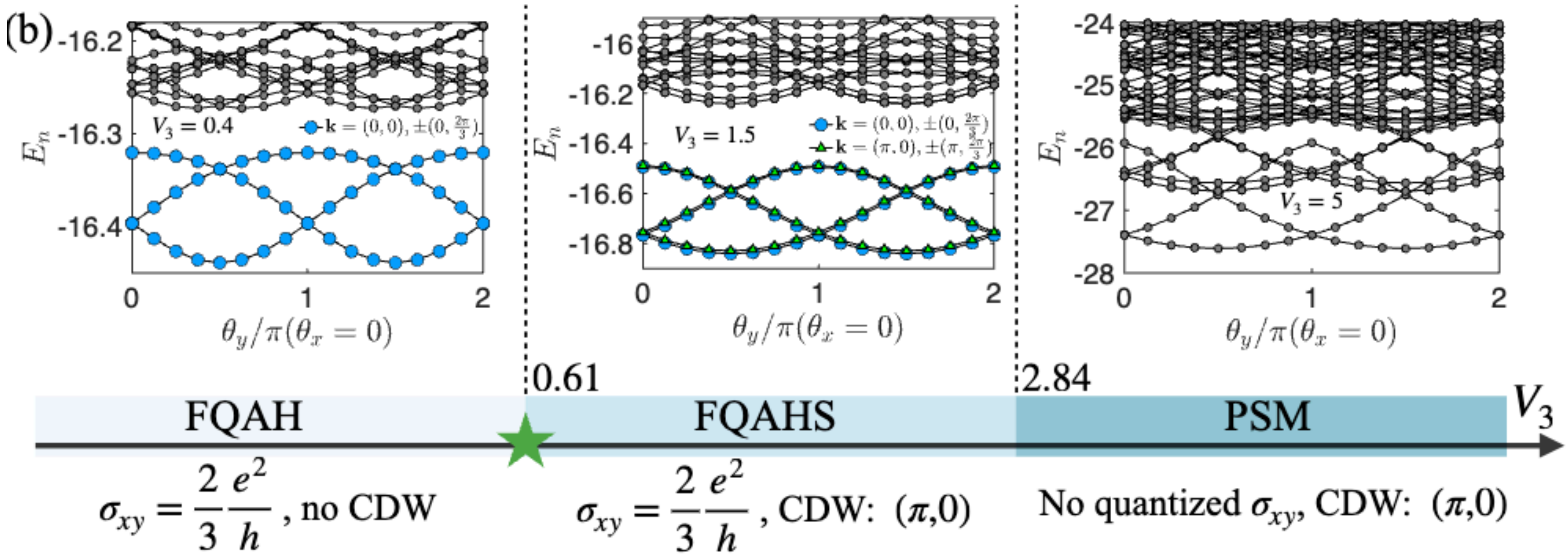
Pu, Balram, Taylor, Fradkin, Papic,
Microscopic Model for Fractional Quantum Hall Nematics,
Phys. Rev. Lett. 132, 236503 (2024)

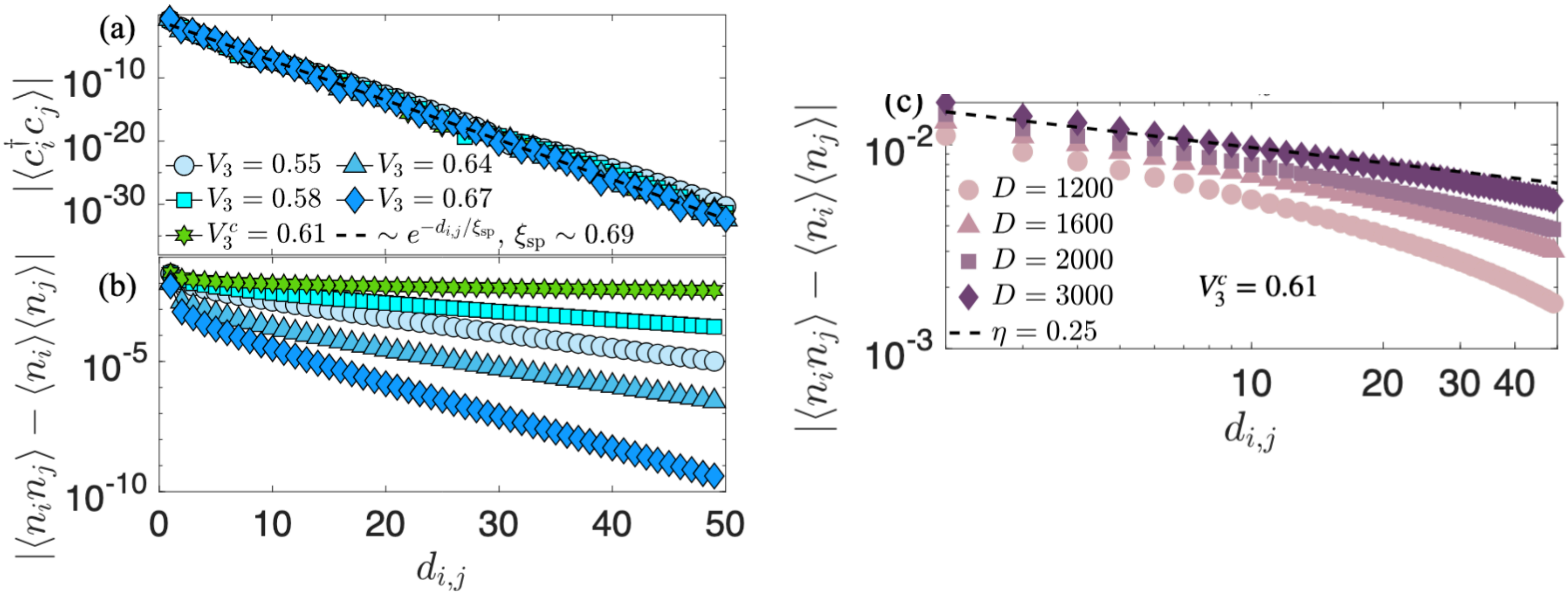


Gap
Charged excitations
FQAH
$\sigma_{xy} = \nu \frac{e^2}{h}$
FQAH + CDW
$\sigma_{xy} = \nu \frac{e^2}{h}$
Topologically trivial CDW
No quantized σ_{xy}
CDW order
Neutral excitations
Interaction
(a)
-t′
t′
$-te^{i\phi}$
-t″
A
B
y
x
(b)
$V_3 = 0.4$
$\mathbf{k} = (0,0), \pm(0, \frac{2\pi}{3})$
$V_3 = 1.5$
$\mathbf{k} = (0,0), \pm(0, \frac{2\pi}{3})$
$\mathbf{k} = (\pi,0), \pm(\pi, \frac{2\pi}{3})$
$V_3 = 5$
E_n
$\theta_y/\pi(\theta_x = 0)$
0.61
2.84
FQAH
FQAHS
PSM
V_3
$\sigma_{xy} = \frac{2}{3}\frac{e^2}{h}$, no CDW
$\sigma_{xy} = \frac{2}{3}\frac{e^2}{h}$, CDW: $(\pi,0)$
No quantized σ_{xy}, CDW: $(\pi,0)$
$V_1 = 1.1, V_2 = 1$



$V_3 = 0.4$
$\mathbf{k} = (0,0), \pm(0, \frac{2\pi}{3})$
E_n
$\theta_y/\pi(\theta_x = 0)$
$V_3 = 1.5$
$\mathbf{k} = (\pi,0), \pm(\pi, \frac{2\pi}{3})$
$V_3 = 5$
0.61
2.84
FQAH
FQAHS
PSM
V_3
$\sigma_{xy} = \frac{2}{3}\frac{e^2}{h}$, no CDW
$\sigma_{xy} = \frac{2}{3}\frac{e^2}{h}$, CDW: $(\pi,0)$
No quantized σ_{xy}, CDW: $(\pi,0)$
(a)
(b)
(c)
(d)
(e)
(f)
$D = 1200$
$D = 1600$
$D = 2000$
$D = 3000$
S_E
$V_3^c = 0.61$
$c \sim 0.7$
$\log(\xi)$
ξ
$\nu = 1$
$V_3^c - V_3$
$V_3 - V_3^c$
$\delta_{\mathrm{smectic}}$
$\beta \sim 0.14$
$S(\pi, 0)$

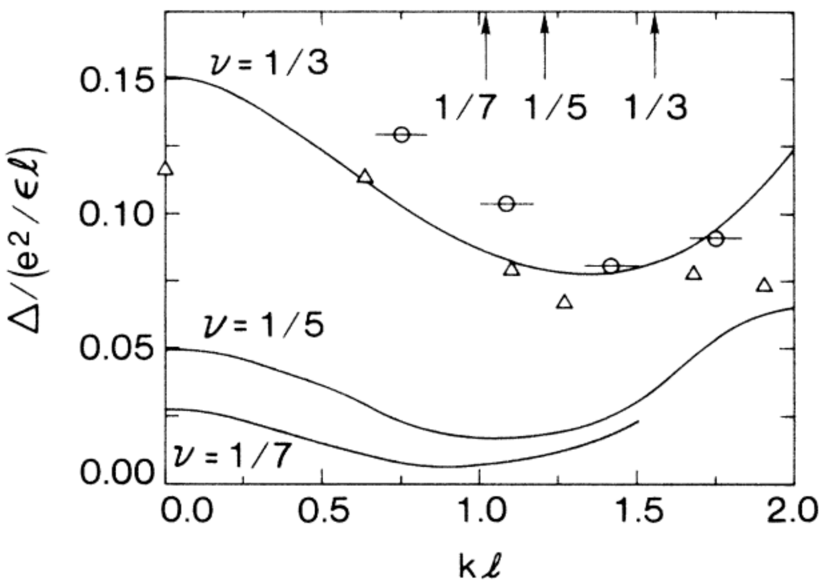

(b)
$V_3 = 0.4$
$\mathbf{k} = (0,0), \pm(0, \frac{2\pi}{3})$
E_n
$\theta_y/\pi(\theta_x = 0)$
$V_3 = 1.5$
$\mathbf{k} = (\pi,0), \pm(\pi, \frac{2\pi}{3})$
$V_3 = 5$
0.61
2.84
FQAH
FQAHS
PSM
V_3
$\sigma_{xy} = \frac{2}{3}\frac{e^2}{h}$, no CDW
$\sigma_{xy} = \frac{2}{3}\frac{e^2}{h}$, CDW: $(\pi,0)$
No quantized σ_{xy}, CDW: $(\pi,0)$


(a)
$|\langle c_i^\dagger c_j \rangle|$
$V_3 = 0.55$
$V_3 = 0.64$
$V_3 = 0.58$
$V_3 = 0.67$
$V_3^c = 0.61$
$\sim e^{-d_{i,j}/\xi_{\rm sp}}$, $\xi_{\rm sp} \sim 0.69$
(b)
$|\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle|$
$d_{i,j}$
(c)
$D = 1200$
$D = 1600$
$D = 2000$
$D = 3000$
$\eta = 0.25$
$V_3^c = 0.61$

PHYSICAL REVIEW B VOLUME 33, NUMBER 4 15 FEBRUARY 1986

Magneto-roton theory of collective excitations in the fractional quantum Hall effect

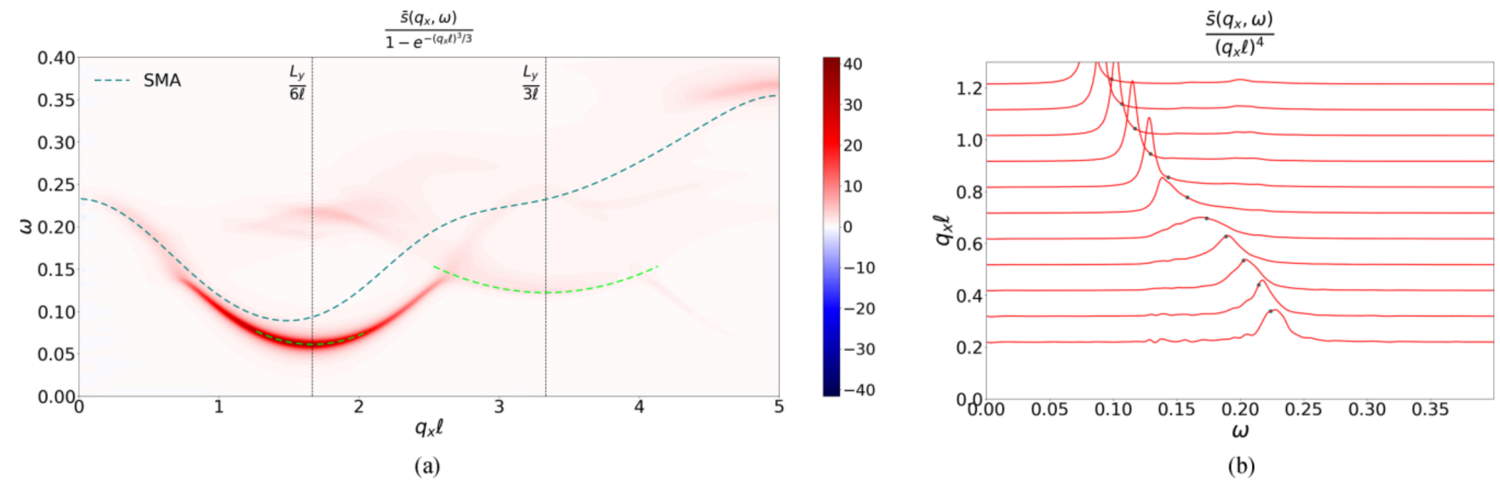
S. M. Girvin A. H. MacDonald P. M. Platzman



PHYSICAL REVIEW B **106**, 075116 (2022)

Neutral excitations of quantum Hall states: A density matrix renormalization group study

Prashant Kumar and F. D. M. Haldane



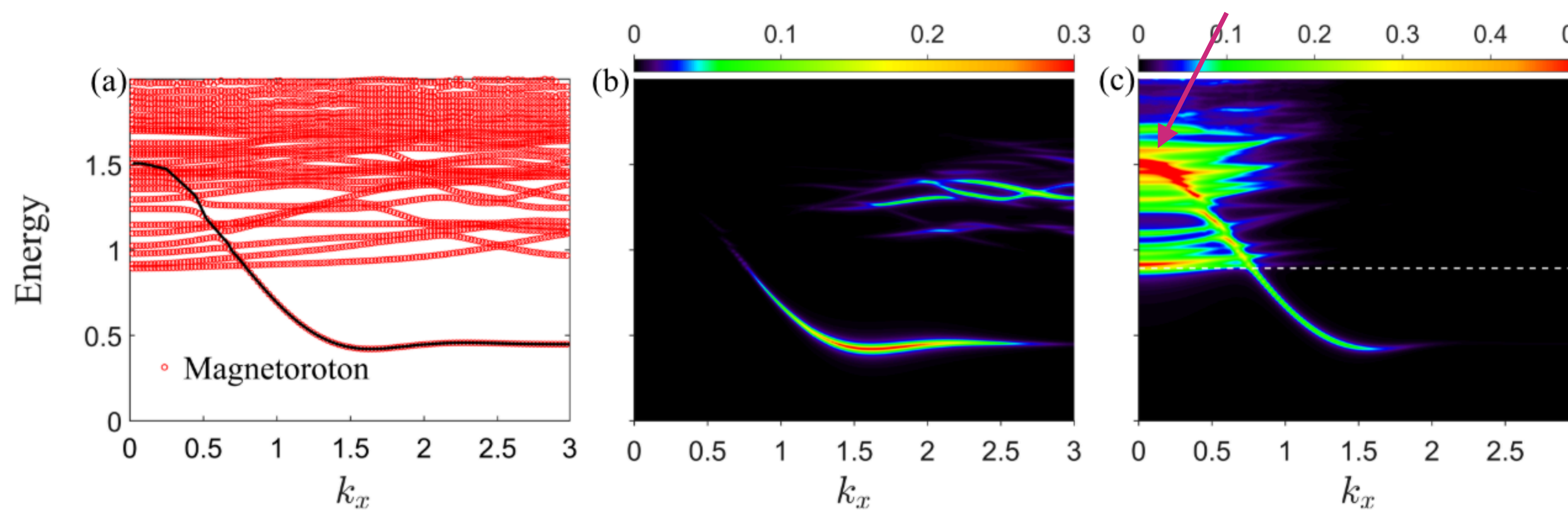
The dynamical structure factor of $\nu = 1/3$ Laughlin FQH state at $L_y = 10l$ for V_1 Haldane pseudopotential.

PHYSICAL REVIEW B **110**, 195137 (2024)

Resolving geometric excitations of fractional quantum Hall states

Yang Liu,[1,2] Tongzhou Zhao,[1] and T. Xiang[1,2,*]

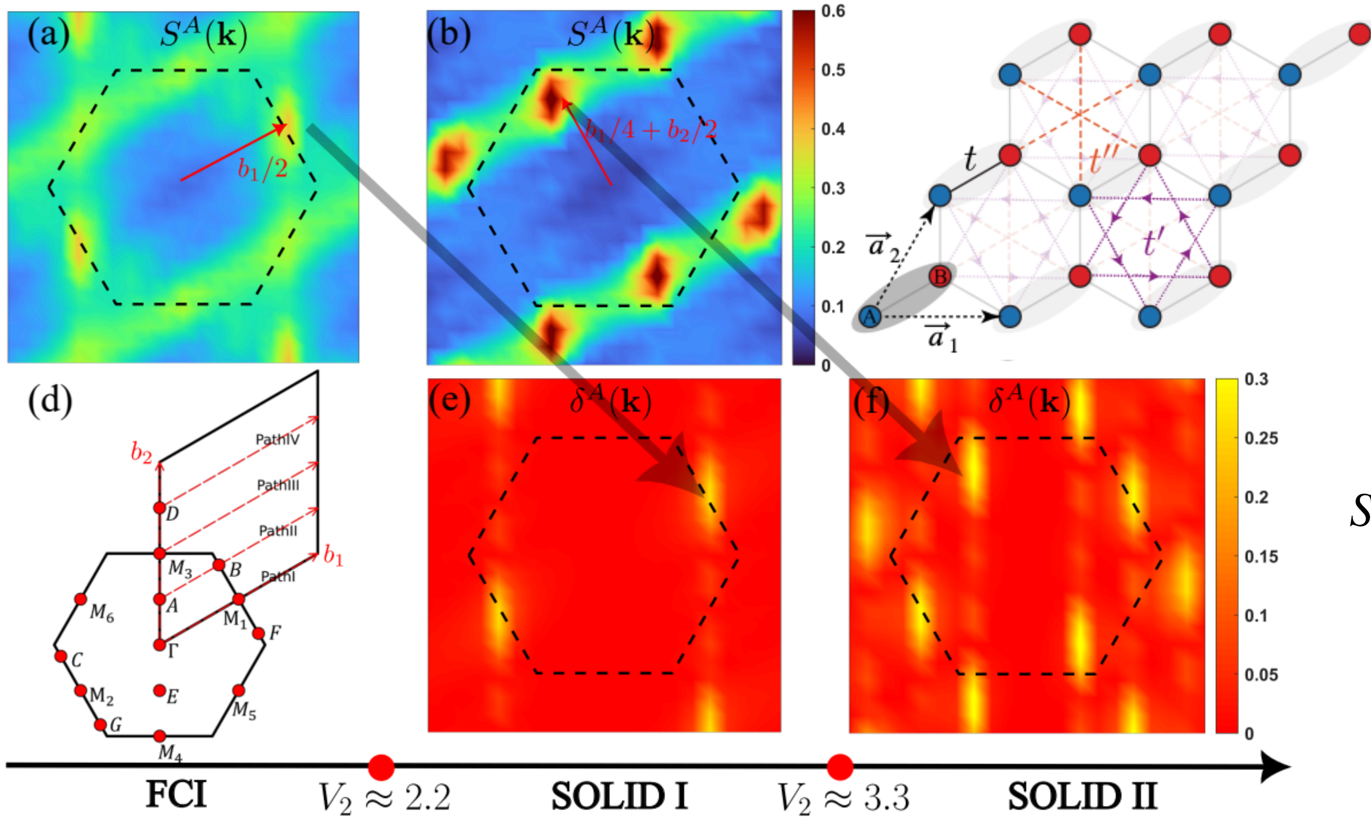
$k = 0,\ S = -2,\ \{d_{x^2-y^2},\ d_{xy}\}$



arXiv:2501.00247

Spectra of Magnetoroton and Chiral Graviton Modes of Fractional Chern Insulator

Min Long,[1] Hongyu Lu,[1] Han-Qing Wu,[2] and Zi Yang Meng[1,*]



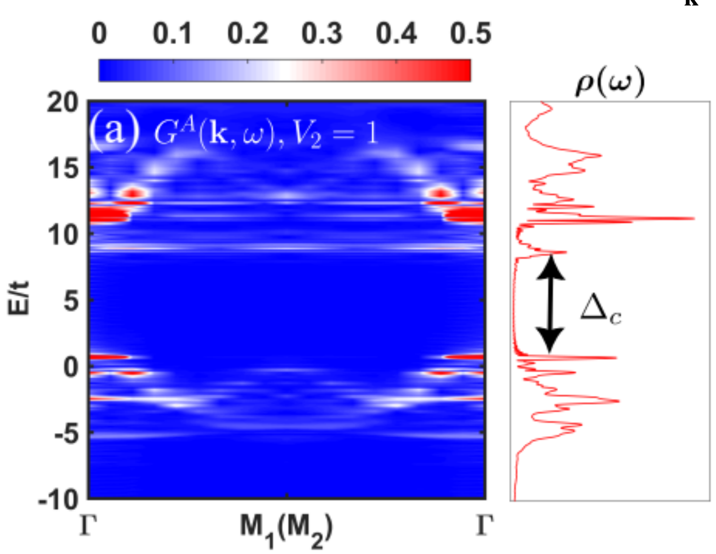
$$H = -t\sum_{\langle i,j\rangle}\left(b_i^\dagger b_j e^{i\phi_{ij}} + \mathrm{H.c.}\right) - t'\sum_{\langle\langle i,j\rangle\rangle}\left(b_i^\dagger b_j + \mathrm{H.c.}\right) - t''\sum_{\langle\langle\langle i,j\rangle\rangle\rangle}\left(b_i^\dagger b_j + \mathrm{H.c.}\right) + V_1\sum_{\langle i,j\rangle} n_i n_j + V_2\sum_{\langle\langle i,j\rangle\rangle} n_i n_j$$

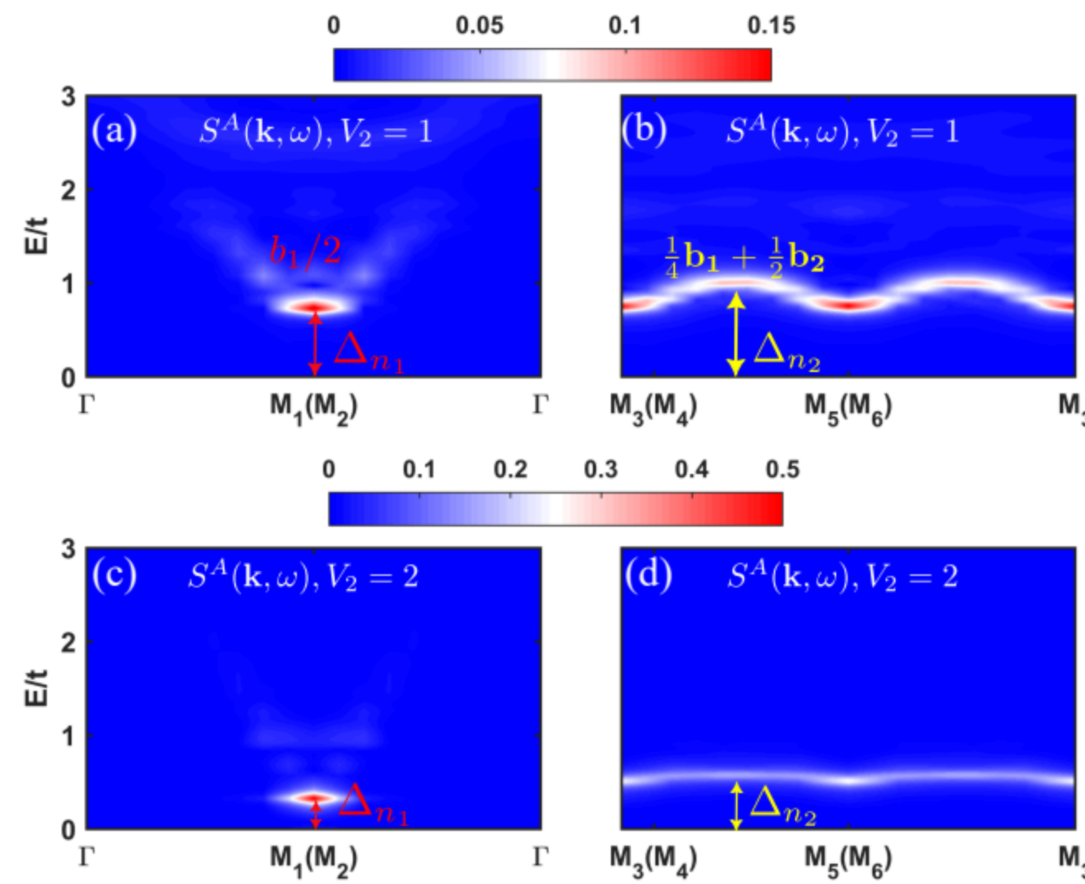
$t = 1$ $\quad t' = 0.6$ $\quad t'' = -0.58$ $\quad \phi = 0.4\pi$

Roton spectrum in FCI

$$S^A(\mathbf{k},\omega) = \frac{1}{\sqrt{N_t N_A}}\sum_{j,l} e^{i(\omega t_l - \mathbf{k}\cdot(\mathbf{x_j}-\mathbf{x}_0))}\left(\langle n_{j,A}(t_l) n_{0,A} - \langle n_{j,A}\rangle\langle n_{0,A}\rangle\right)$$

$G^A(\mathbf{k},\omega)$ $\quad \rho(\omega) = \frac{1}{N_k}\sum_{\mathbf{k}} G^A(\mathbf{k},\omega)$





arXiv:2501.00247

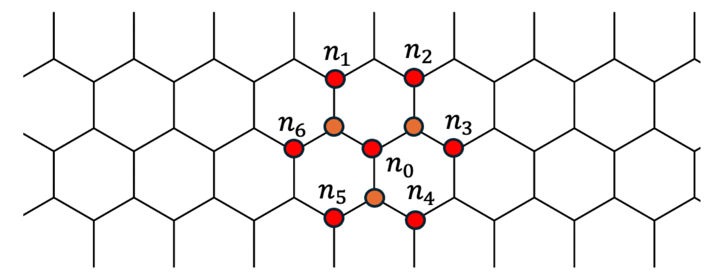
Spectra of Magnetoroton and Chiral Graviton Modes of Fractional Chern Insulator

Min Long,[1] Hongyu Lu,[1] Han-Qing Wu,[2] and Zi Yang Meng[1,*]

chiral Graviton spectrum in FCI

$$O_j^{\pm} = \sum_{l=1}^{6} e^{\pm i L_z \phi_l} n_j n_{j+\delta_l}, \quad L_z = 2, \quad \phi_l = l\frac{\pi}{3}$$

$$G^{\pm}(\mathbf{k}, \omega) = \frac{1}{\sqrt{N_t N_A}} \sum_{j,l} e^{i(\omega t_l - \mathbf{k}\cdot(\mathbf{x_j} - \mathbf{x_0}))} \langle O_j^{\mp}(t_l) O_0^{\pm} \rangle$$



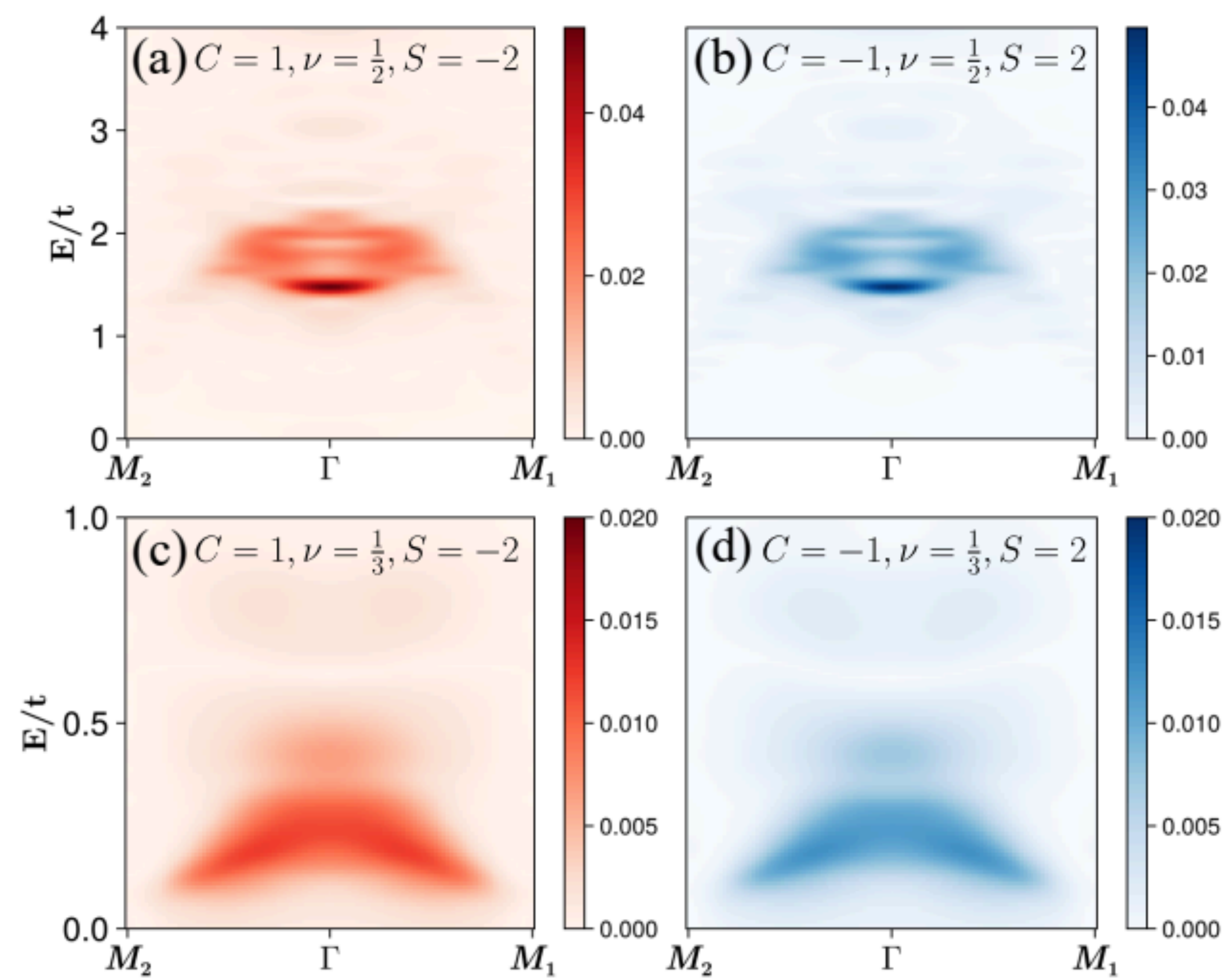
6 NNN neighbors on the same sublattice

$$g^{+}(\mathbf{k}, \omega) = G^{+}(\mathbf{k}, \omega) - G^{-}(\mathbf{k}, \omega)$$

probes S=2 signal

$$g^{-}(\mathbf{k}, \omega) = G^{-}(\mathbf{k}, \omega) - G^{+}(\mathbf{k}, \omega)$$

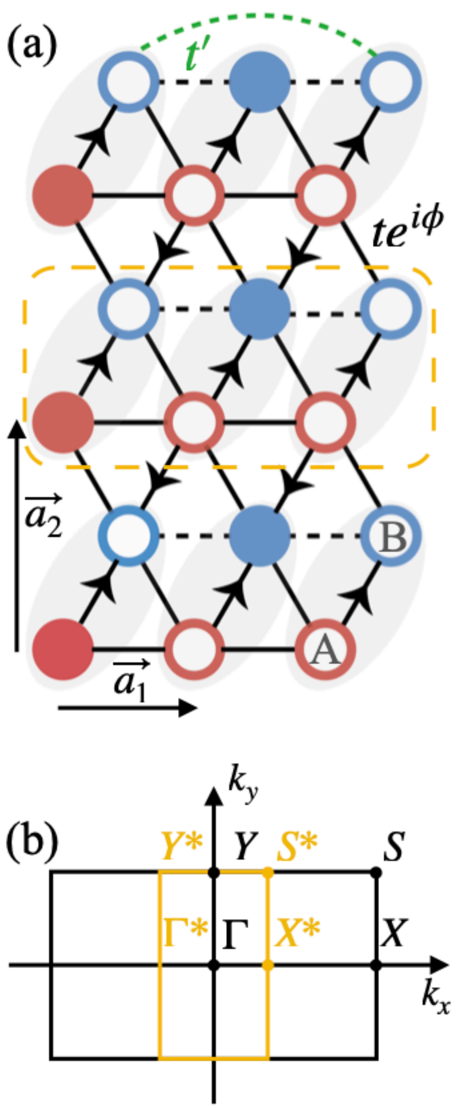
probes S=-2 signal



arXiv: 2505.04138

Generic (fractional) quantum anomalous Hall crystals from interaction-driven band folding

Hongyu Lu,[1] Han-Qing Wu,[2] Bin-Bin Chen,[3] Wang Yao,[4] and Zi Yang Meng[1,*]



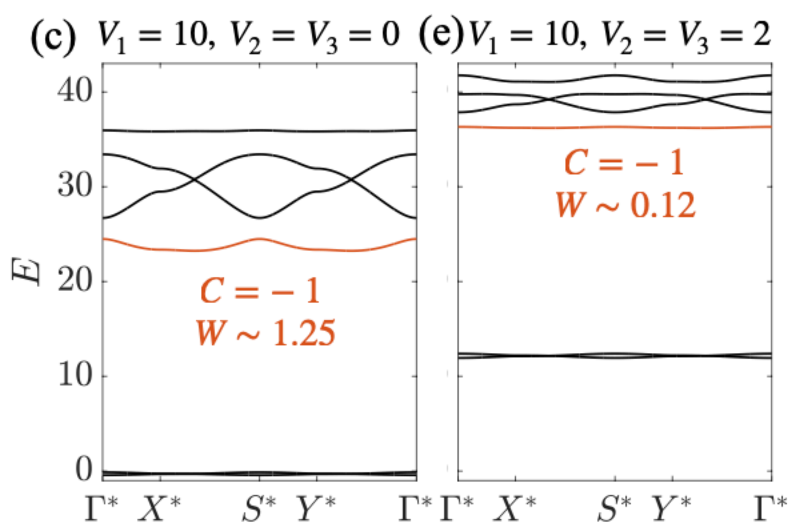
$$H=\sum_{\langle i,j\rangle} te^{i\phi_{ij}}(c_i^\dagger c_j+h.c.)+\sum_{\langle\langle\langle i,j\rangle\rangle\rangle} t'(c_i^\dagger c_j+h.c.)+V_1\sum_{\langle i,j\rangle} n_in_j+V_{ij}\sum_{\langle\langle i,j\rangle\rangle} n_in_j+V_{ij}\sum_{\langle\langle\langle i,j\rangle\rangle\rangle} n_in_j$$

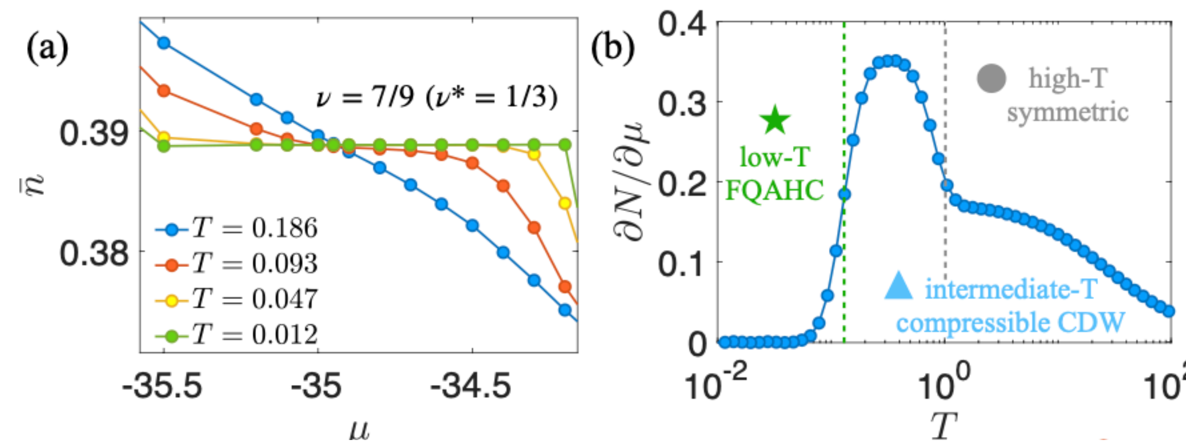
$\sigma_H \neq \nu$ filling of the original flat band

PRB 86, 235118 (2012)

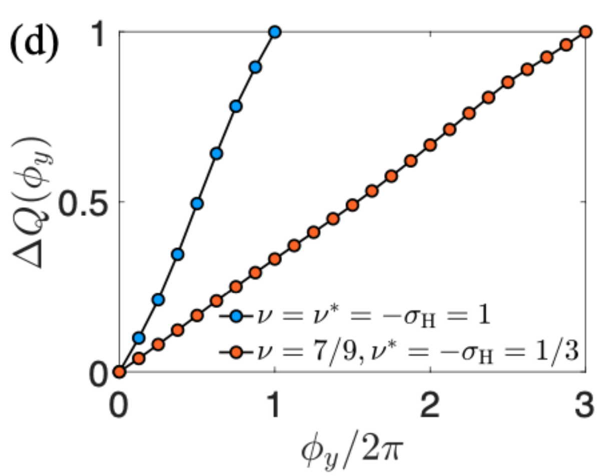
PRL 113, 216404 (2014)

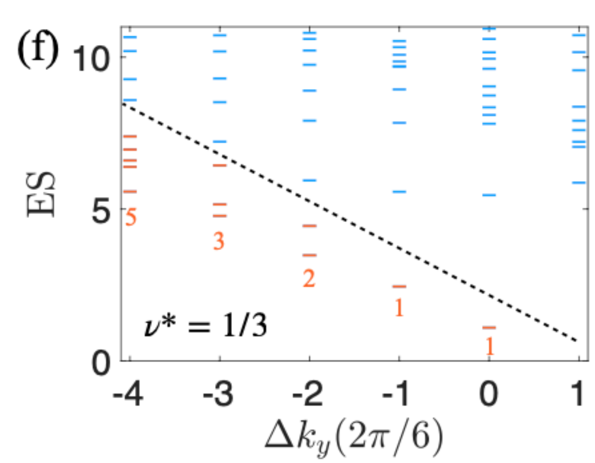
$\nu = 2/3$

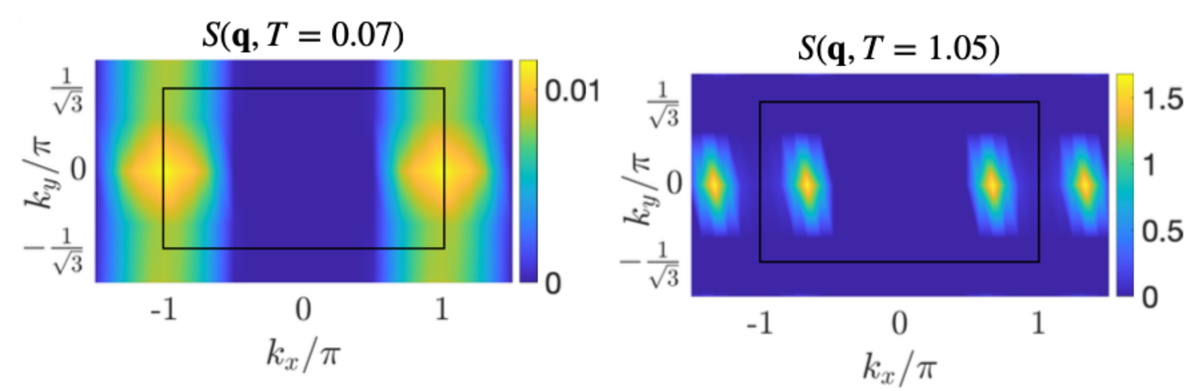




$\sigma_H = \nu^* = 3\nu - 2$





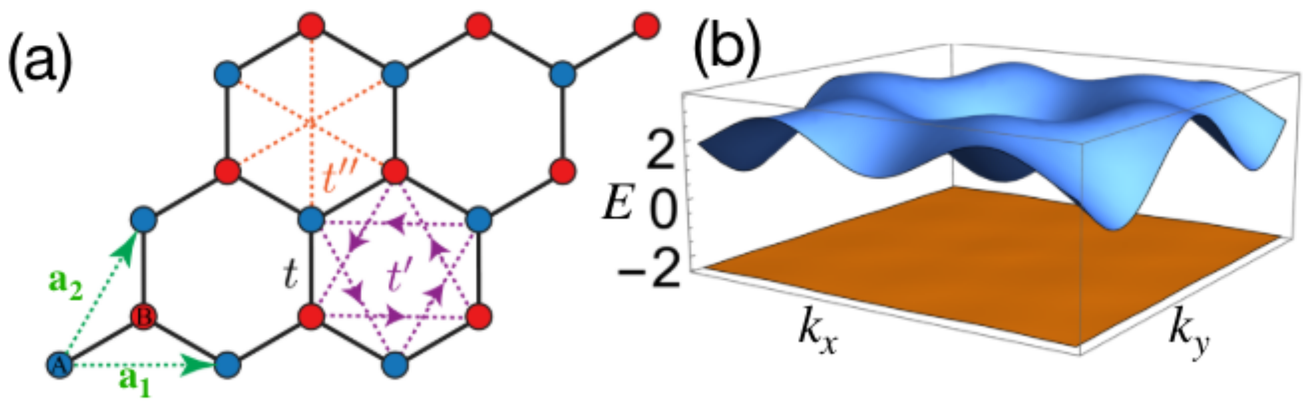


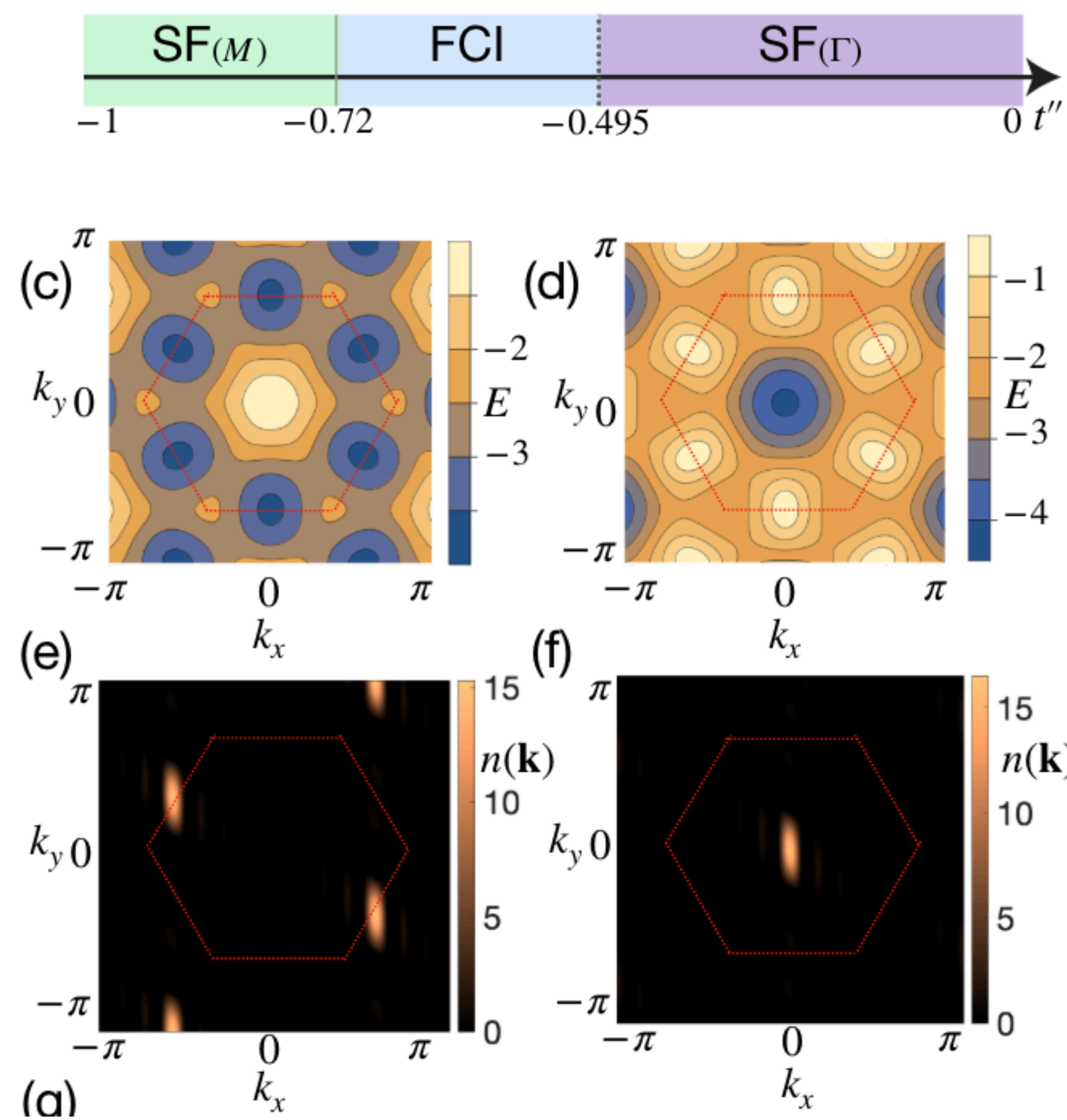
Hongyu Lu et al., Phys. Rev. Lett 132, 236502 (2024)

Phys. Rev. Lett. 134, 076601 (2025)

Continuous Transition between Bosonic Fractional Chern Insulator and Superfluid

Hongyu Lu,[1] Han-Qing Wu,[2] Bin-Bin Chen,[1,*] and Zi Yang Meng[1,†]





$$H = -\sum_{\langle i,j\rangle} t(b_i^\dagger b_j + \text{H.c.}) - \sum_{\langle\langle i,j\rangle\rangle} t'(e^{i\phi} b_i^\dagger b_j + \text{H.c.}) - \sum_{\langle\langle\langle i,j\rangle\rangle\rangle} t''(b_i^\dagger b_j + \text{H.c.}) + V_1 \sum_{\langle i,j\rangle} n_i n_j + V_2 \sum_{\langle\langle i,j\rangle\rangle} n_i n_j$$

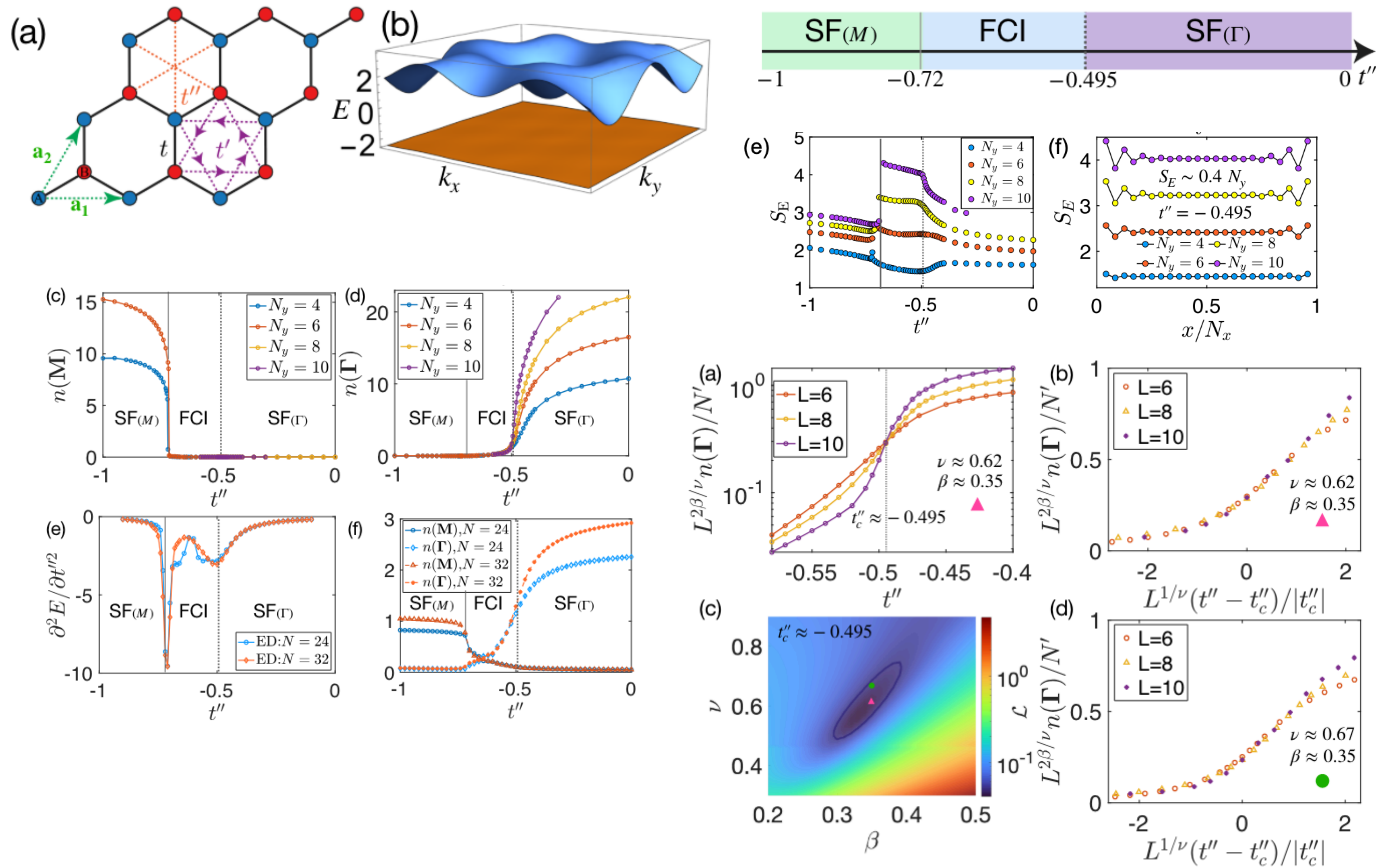
$t = 1 \quad t' = 0.6 \quad t'' = -0.58 \quad \phi = 0.4\pi$

Hard-core boson $V_1 = V_2 = 0$

Phys. Rev. Lett. 134, 076601 (2025)

Continuous Transition between Bosonic Fractional Chern Insulator and Superfluid

Hongyu Lu[1], Han-Qing Wu[2], Bin-Bin Chen[1,*] and Zi Yang Meng[1,†]



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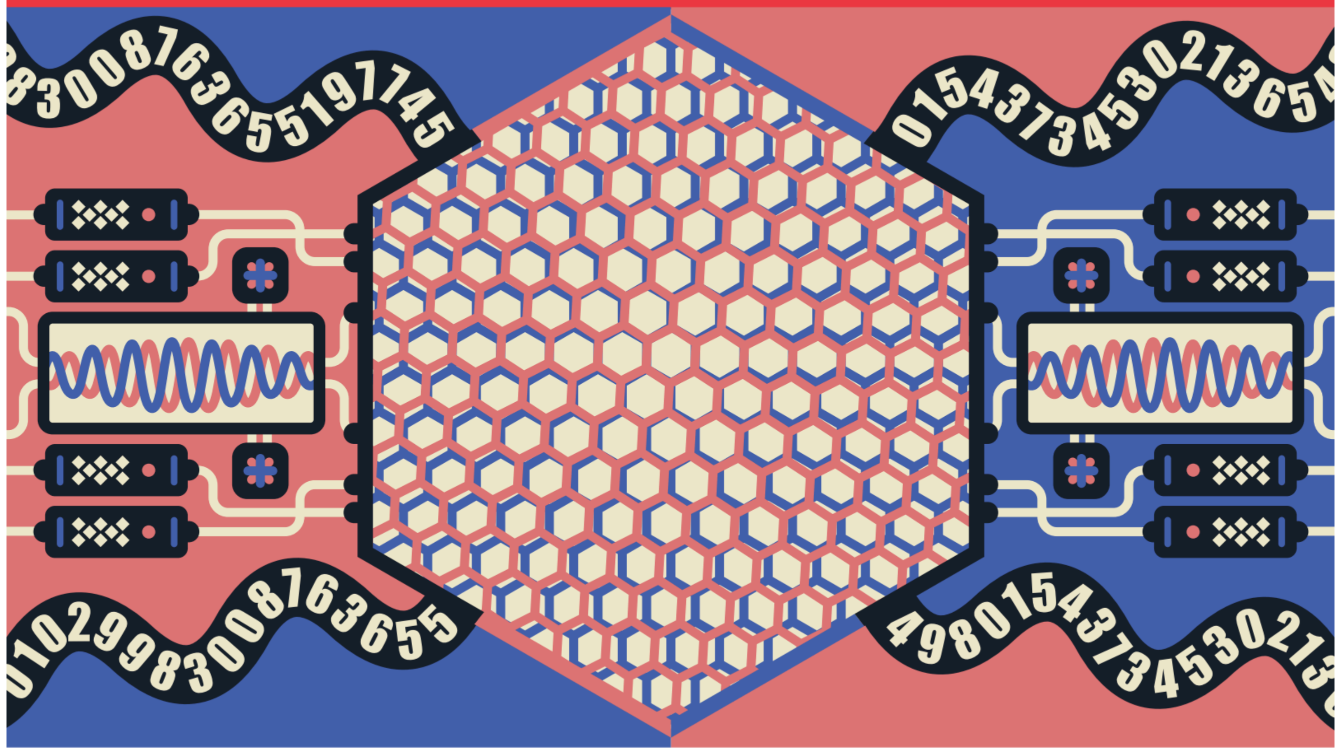


4 — 7 September 2025

University of Hong Kong

Fractional Chern insulators

Course director

Zi Yang Meng
University of Hong Kong

Organising committee

Kin Fai Mak, Cornell University
Zi Yang Meng, University of Hong Kong
Adrian Po, Hong Kong University of Science and Technology
Kai Sun, University of Michigan
Senthil Todadri, Massachusetts Institute of Technology

Speakers

Andrei Bernevig
Dmitri Efetov
Nicolas Regnault
Subir Sachdev
Jie Shan
Kun Yang

More details are available at:

Twisted Bilayer Graphene

Chin. Phys. Lett 38, 077305 (2021)   Phys. Rev. Lett 130, 016401 (2023)

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

Phys. Rev. B 107, L241105 (2023)

Polynomial sign problem and topological Mott insulator in twisted bilayer graphene

Phys. Rev. B 109, 125404 (2024)

Evolution from quantum anomalous Hall insulator to heavy-fermion semimetal in magic-angle twisted bilayer graphene

arXiv: 2412.11382 (to appear in Nat. Commun.)

Angle-Tuned Gross-Neveu Quantum Criticality in Twisted Bilayer Graphe A Quantum Monte Carlo Study

Cheng Huang

Xu Zhang

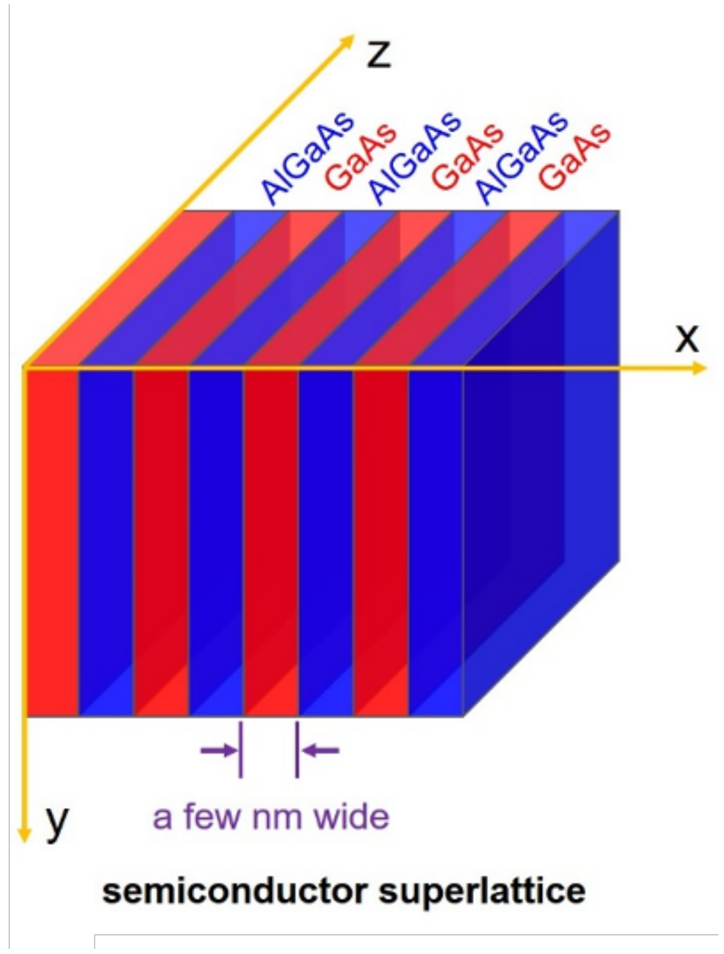
Laura Classen

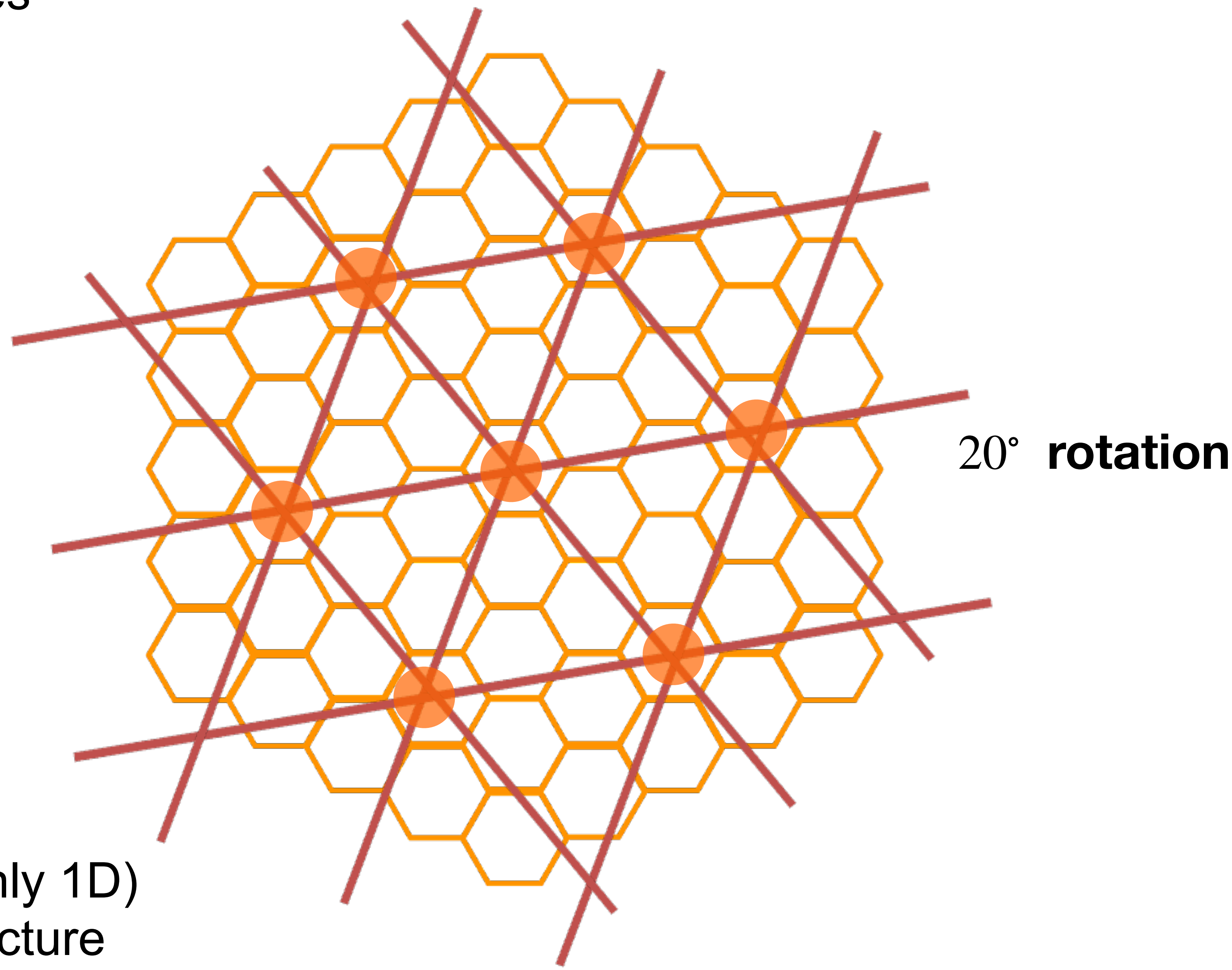
Fakher Assaad

Quantum moiré materials are superlattice of 2D materials (e.g. graphene)

Moiré: stack, twist & new physics emerges
crystal from crystals
ideal playground & challenge for quantum many-body physics

Semiconductor industry,
Quantum dots / wires technologies



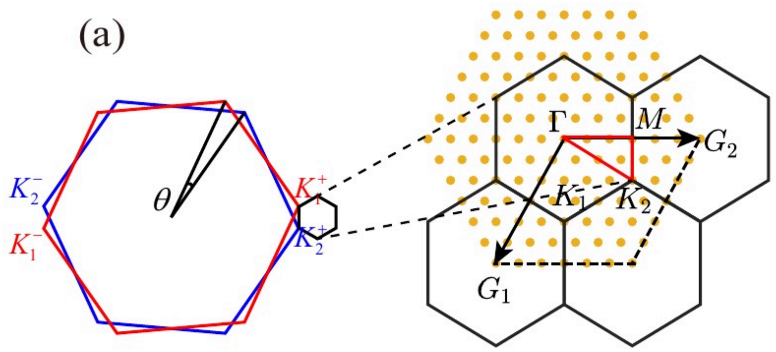


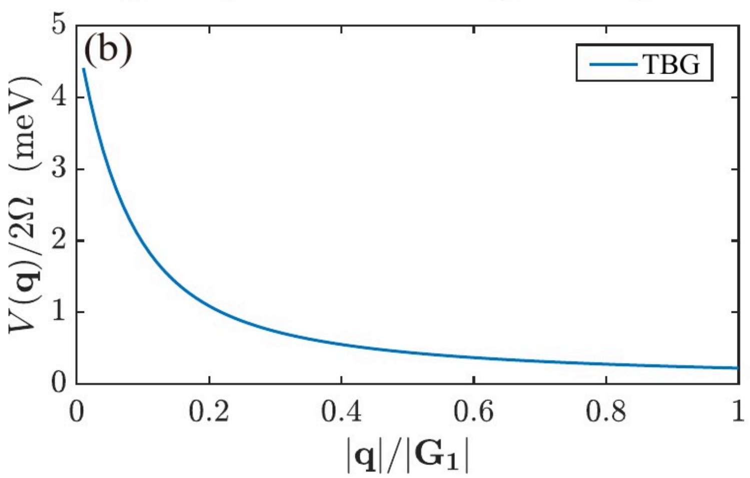
- Periodic in growth direction (mainly 1D)
- Based on free electron band structure

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

Xu Zhang(张栩)[1†], Gaopei Pan(潘高培)[2,3†], Yi Zhang(张燚)[4],
Jian Kang(康健)[5], and Zi Yang Meng(孟子杨)[1,2*]

CPL 38, 077305 (2021)





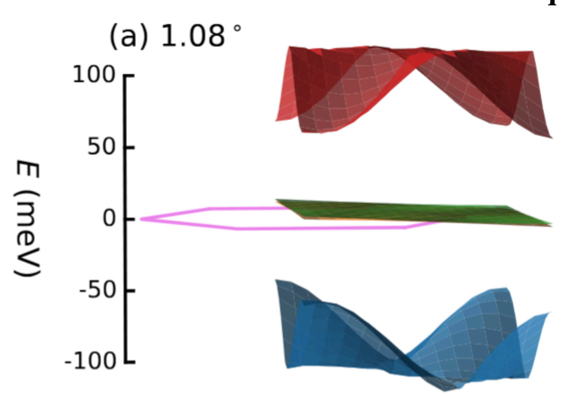
$$H = \underbrace{\sum_{s,\eta,\mathbf{k},m} \epsilon^{s,\eta}_{\mathbf{k},m} c^{\dagger}_{s,\eta,\mathbf{k},m} c_{s,\eta,\mathbf{k},m}}_{H_0} + \underbrace{\frac{1}{2\Omega} \sum_{\mathbf{q}\in mBZ,\mathbf{G}} V(\mathbf{q}+\mathbf{G}) \delta\rho_{\mathbf{q}+\mathbf{G}} \delta\rho_{-\mathbf{q}-\mathbf{G}}}_{H_{int}}$$

$$|\mathbf{G_1}|, |\mathbf{G_2}| = \frac{8\pi}{3a}\sin(\frac{\theta}{2})$$

$$\mathbf{G} = n_1\mathbf{G}_1 + n_2\mathbf{G}_2$$

Gate-screened Coulomb potential $V(\mathbf{Q}) = \frac{e^2}{2\epsilon|\mathbf{Q}|}(1 - e^{-|\mathbf{Q}|d})$

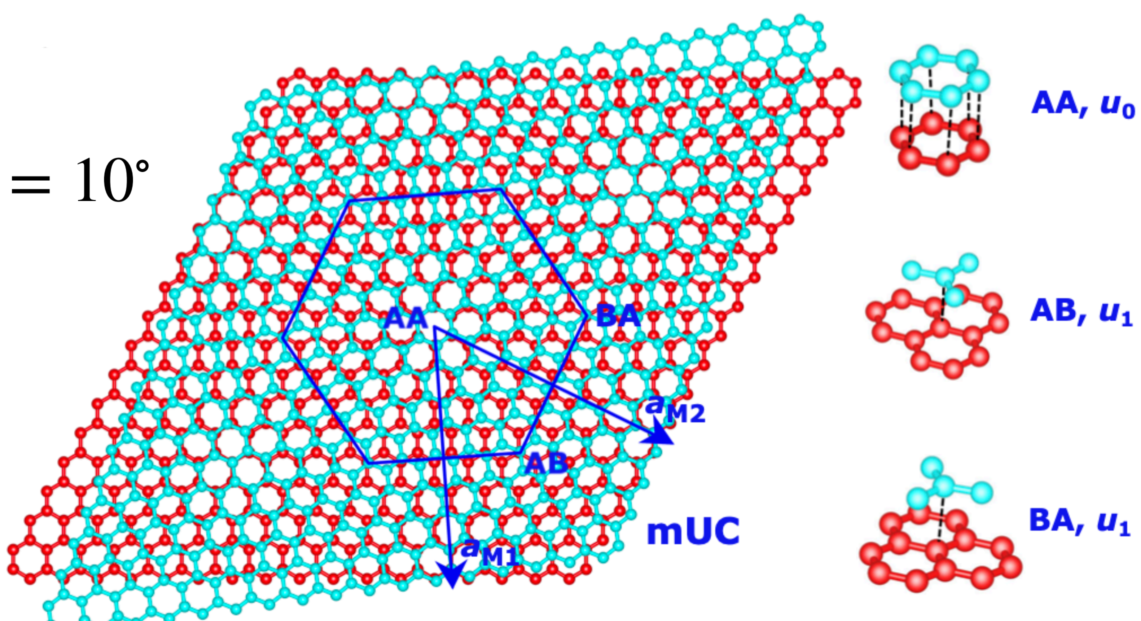
$$\delta\rho_{\mathbf{q}+\mathbf{G}} = \sum_{s,\eta,\mathbf{k},m_1,m_2} \lambda^{s,\eta}_{m_1,m_2}(\mathbf{k}, \mathbf{k}+\mathbf{q}+\mathbf{G}) \left(c^{\dagger}_{s,\eta,\mathbf{k},m_1} c_{s,\eta,\mathbf{k}+\mathbf{q}+\mathbf{G},m_2} - \frac{\nu+4}{8}\delta_{\mathbf{q},0}\delta_{m_1,m_2}\right)$$

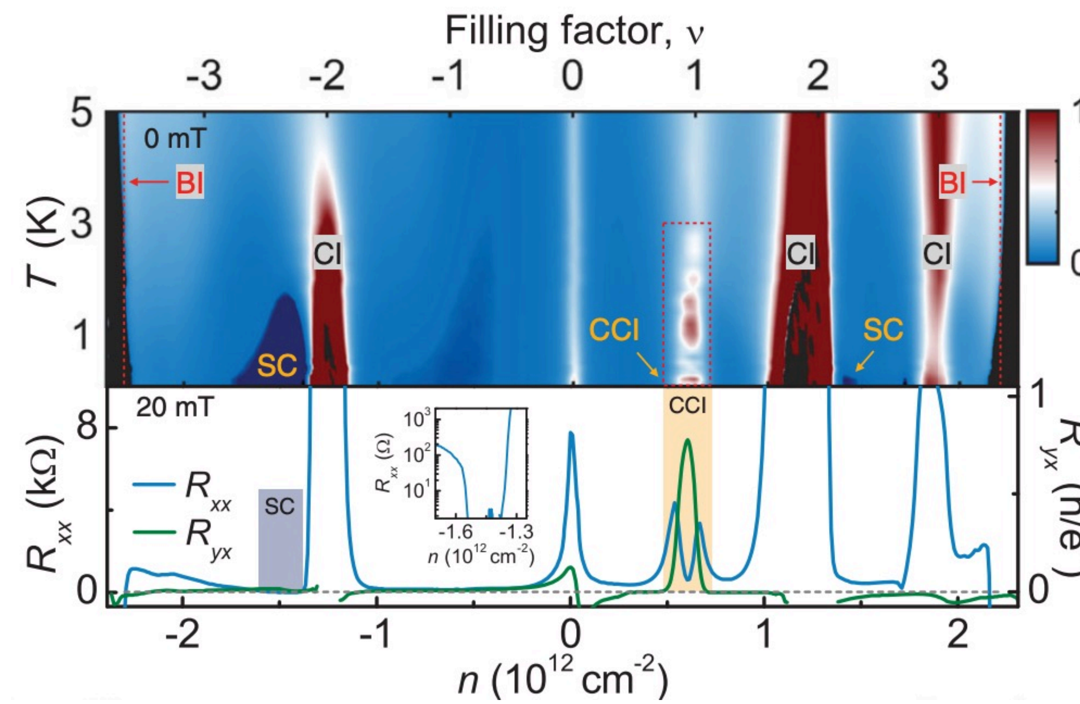


Form factors from Bloch WF

$$\lambda^{s,\eta}_{m_1,m_2}(\mathbf{k}, \mathbf{k}+\mathbf{q}+\mathbf{G}) \equiv \langle u^{s,\eta}_{\mathbf{k},m_1} | u^{s,\eta}_{\mathbf{k}+\mathbf{q}+\mathbf{G},m_2} \rangle$$

$\theta = 10^{\circ}$

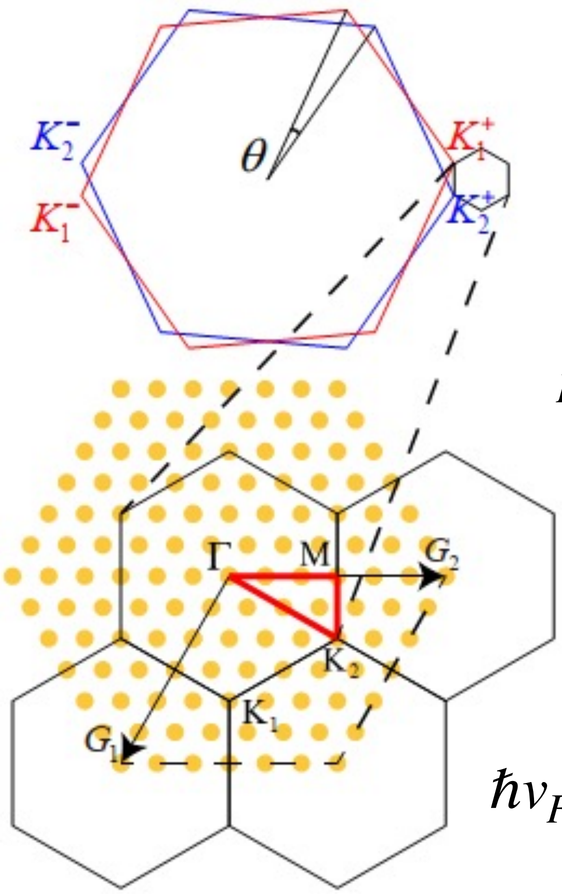




Stepanov … Efetov, PRL 127, 197701 (2021)

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

Xu Zhang(张栩)[1†], Gaopei Pan(潘高培)[2,3†], Yi Zhang(张燚)[4],
Jian Kang(康健)[5], and Zi Yang Meng(孟子杨)[1,2*]



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

CPL 38, 077305 (2021)

- Trambly de Laissardiere et al., Nano Lett. 2010
- Bistritzer & MacDonald, PNAS 2011 BM Hamiltonian

$\eta = \pm$ valley

Pauli for sublattices

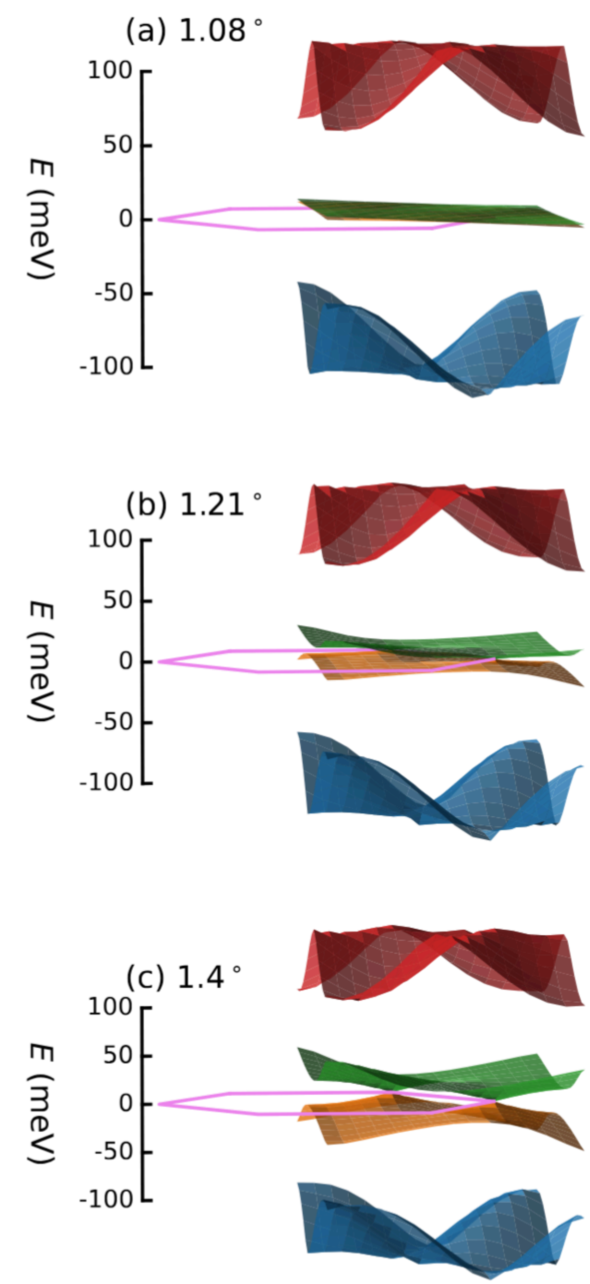
$$\Lambda^\eta = (\eta\Lambda_x, \Lambda_y)$$

$$H_O^{s,\eta}(\mathbf{k})_{\mathbf{G},\mathbf{G}'} = \delta_{\mathbf{G},\mathbf{G}'}\hbar v_F \begin{pmatrix} -(\mathbf{k}+\mathbf{G}-\mathbf{K}_1^\eta)\cdot\Lambda^\eta & 0 \\ 0 & -(\mathbf{k}+\mathbf{G}-\mathbf{K}_2^\eta)\cdot\Lambda^\eta \end{pmatrix} + \begin{pmatrix} 0 & T_1^\eta \\ T_2^{\eta\dagger} & 0 \end{pmatrix}$$

$$T_l^\eta = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix}\delta_{\mathbf{G},\mathbf{G}'} + \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi}{3}\eta} \\ u_1 e^{-i\frac{2\pi}{3}\eta} & u_0 \end{pmatrix}\delta_{\mathbf{G},\mathbf{G}'+(-1)^l\eta\mathbf{G}_1}$$

$$+\begin{pmatrix} u_0 & u_1 e^{i\frac{2\pi}{3}\eta} \\ u_1 e^{-i\frac{2\pi}{3}\eta} & 0 \end{pmatrix}\delta_{\mathbf{G},\mathbf{G}'+(-1)^l\eta(\mathbf{G}_1+\mathbf{G}_2)}$$

$\hbar v_F / a = 2377.45$ meV



$\theta = 1.08^\circ$ 1st magic angle $L_M \approx a/(2\sin(\theta/2)) \sim 10$ nm

$$|\mathbf{G}_1|, |\mathbf{G}_2| = \frac{8\pi}{3a}\sin(\frac{\theta}{2})$$

$u_1 = 110$ meV

$u_0 = 0$ chiral limit

$u_0 \sim 60$ meV, realistic cases

interlayer, intrasublattice hopping

$$\begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix}$$

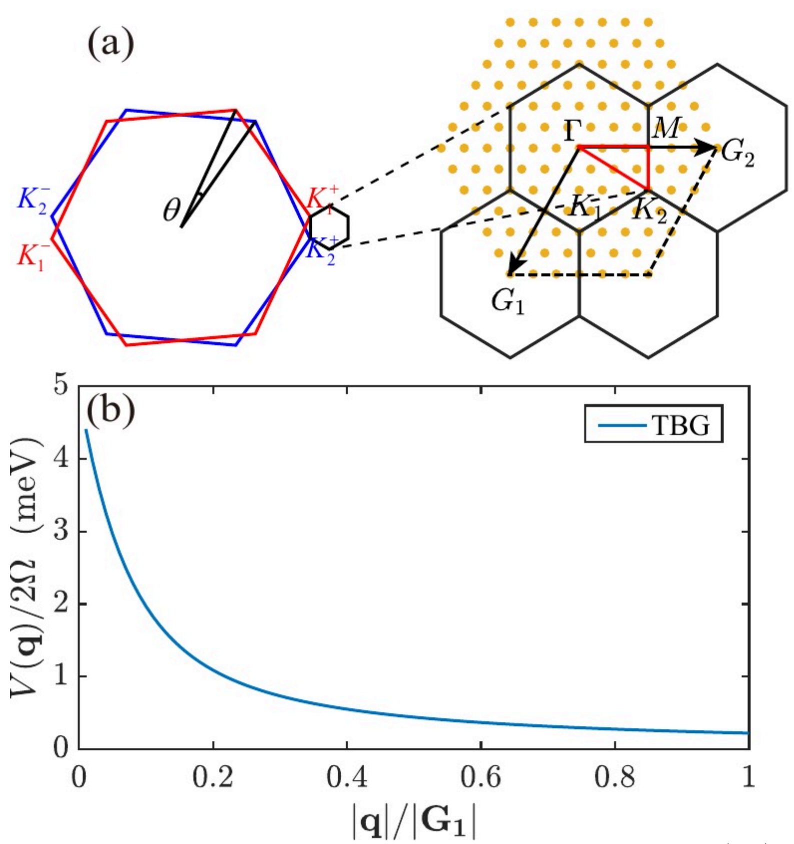
interlayer, intersublattice hopping

$$H_0 = \sum_{s,\eta,\mathbf{k},m} \epsilon_{\mathbf{k},m}^{s,\eta} c_{s,\eta,\mathbf{k},m}^\dagger c_{s,\eta,\mathbf{k},m}$$

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

Xu Zhang(张栩)[1†], Gaopei Pan(潘高培)[2,3†], Yi Zhang(张燚)[4],
Jian Kang(康健)[5], and Zi Yang Meng(孟子杨)[1,2*]

CPL 38, 077305 (2021)



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

$$H_{int} = \frac{1}{2\Omega}\sum_{\mathbf{G}}\sum_{\mathbf{q}\in mBZ} V(\mathbf{q}+\mathbf{G})\delta\rho_{\mathbf{q}+\mathbf{G}}\delta\rho_{-\mathbf{q}-\mathbf{G}}$$

$$\delta\rho_{\mathbf{q}+\mathbf{G}} = \sum_{s,\eta,\mathbf{k},m_1,m_2} \lambda^{s,\eta}_{m_1,m_2}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})\left(c^\dagger_{s,\eta,\mathbf{k},m_1} c_{s,\eta,\mathbf{k}+\mathbf{q}+\mathbf{G},m_2} - \frac{\nu+4}{8}\delta_{\mathbf{q},0}\delta_{m_1,m_2}\right)$$

$$\lambda^{s,\eta}_{m_1,m_2}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}) \equiv \langle u^{s,\eta}_{\mathbf{k},m_1} | u^{s,\eta}_{\mathbf{k}+\mathbf{q}+\mathbf{G},m_2}\rangle$$

overlap of H_0 eigenstate

$$V(\mathbf{q}) = \frac{e^2}{4\pi\varepsilon}\int d^2\mathbf{r}\left(\frac{1}{\mathbf{r}} - \frac{1}{\sqrt{\mathbf{r}^2+d^2}}\right) e^{i\mathbf{q}\cdot\mathbf{r}} = \frac{e^2}{2\varepsilon|\mathbf{q}|}(1-e^{-|\mathbf{q}|d})$$

Single gate

$\frac{d}{2} = 20$ nm

$$\Omega = N_{\mathbf{k}}\frac{\sqrt{3}}{2}L_M^2 \qquad N_{\mathbf{k}} = 6\times 6,\ 9\times 9,\ 12\times 12,\ 15\times 15$$

$\varepsilon = 7\varepsilon_0$

$$= \sum_{\mathbf{G},\mathbf{q}\in mBZ}\frac{V(\mathbf{q}+\mathbf{G})}{2}\left[(\delta\rho_{-\mathbf{q}-\mathbf{G}}+\delta\rho_{\mathbf{q}+\mathbf{G}})^2 - (\delta\rho_{-\mathbf{q}-\mathbf{G}}-\delta\rho_{\mathbf{q}+\mathbf{G}})^2\right]$$

Momentum-Space Quantum Monte Carlo

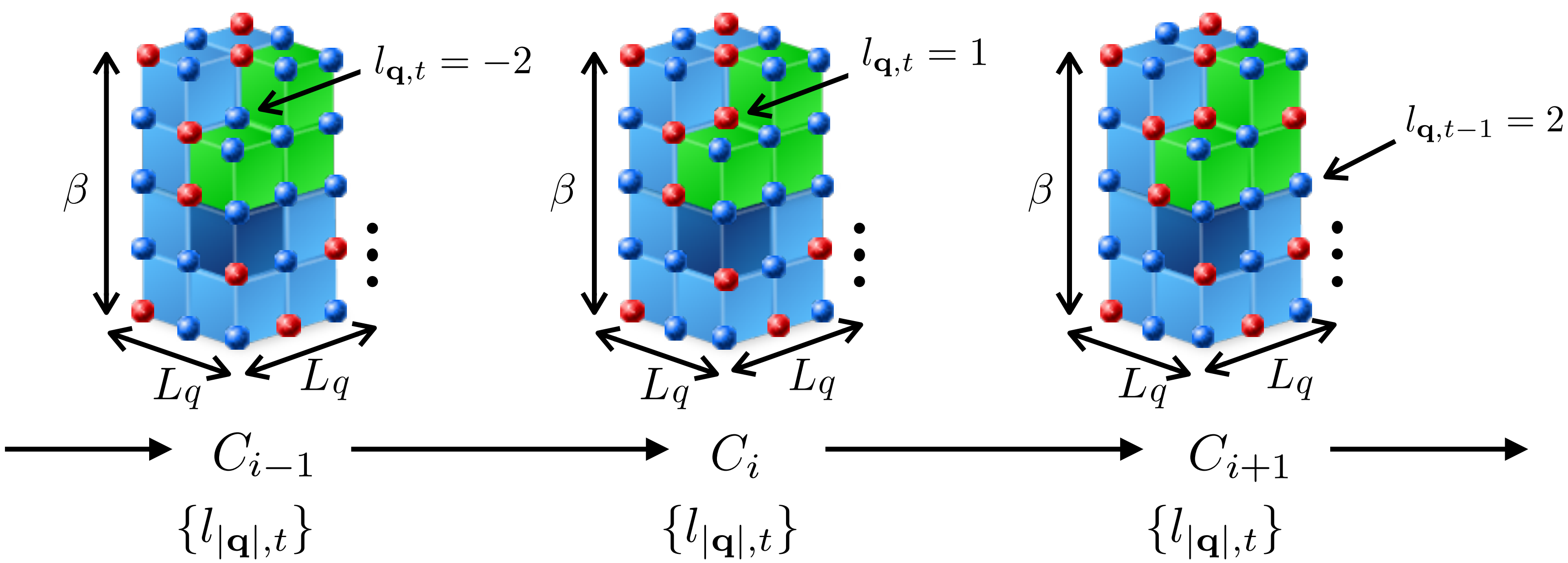
CPL 38, 077305 (2021)

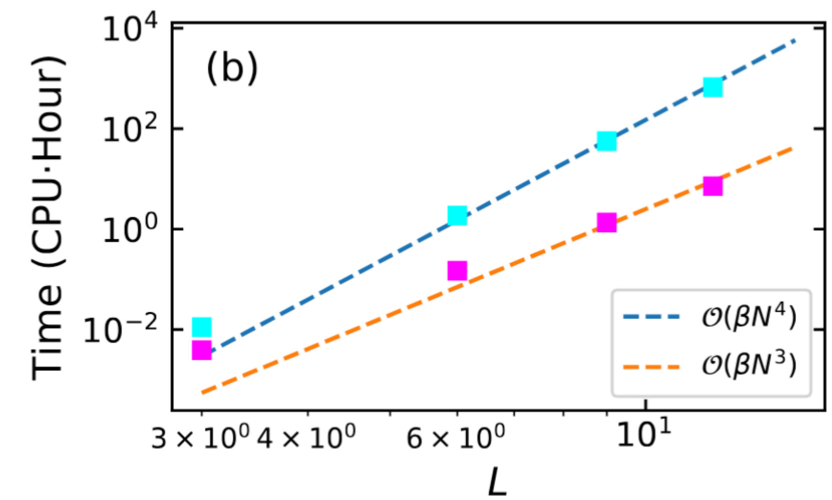
$$Z = \mathrm{Tr}\{\prod_{\tau} e^{-\Delta\tau\, H_{int}(\tau)}\} = \mathrm{Tr}\{\prod_{\tau} \exp\{-\frac{\Delta\tau}{4\Omega} \sum_{\mathbf{G},\mathbf{q}\in mBZ} V(\mathbf{q}+\mathbf{G}) \cdot [\underbrace{(\delta\rho_{-\mathbf{q}-\mathbf{G}} + \delta\rho_{\mathbf{q}+\mathbf{G}})^2}_{A_{\mathbf{Q}}} - \underbrace{(\delta\rho_{-\mathbf{q}-\mathbf{G}} - \delta\rho_{\mathbf{q}+\mathbf{G}})^2}_{B_{\mathbf{Q}}}]\}\}$$

$$\exp(-\alpha_1(\mathbf{Q})A_{\mathbf{Q}}^2) = \frac{1}{4}\sum_{\{l_{\mathbf{Q},\tau,1}\}} \gamma(l_{\mathbf{Q},\tau,1})\ \exp(i\eta(l_{\mathbf{Q},\tau,1})\sqrt{\alpha_1(\mathbf{Q})}\ A_{\mathbf{Q}})) + O(\Delta\tau^4) \qquad \{l_{\mathbf{Q},\tau,1}, l_{\mathbf{Q},\tau,2}\} \qquad \alpha_1(\mathbf{Q}) = \frac{\Delta\tau V(\mathbf{Q})}{4\Omega}$$

$$= \det[\mathbb{1} + \Delta(\mathbb{1} - G_s(\tau))]$$

Δ circulant matrix





Update a single site and update the Green's function, entire space-time update

$O(N^3)$ $\qquad$ $O(\beta N^4)$

Cheng Huang et al., arXiv: 2412.11382

Momentum Space Quantum Monte Carlo on Twisted Bilayer Graphene

Xu Zhang(张栩)[1†], Gaopei Pan(潘高培)[2,3†], Yi Zhang(张燚)[4],
Jian Kang(康健)[5], and Zi Yang Meng(孟子杨)[1,2*]

CPL 38, 077305 (2021) Express Letter

$C_{2z}T$ symmetry $\quad \lambda_{m,n,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}) = \lambda^*_{m,n,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})$

$C_{2z}P$ symmetry $\quad \lambda_{m,n,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}) = m * n * \lambda_{-m,-n,-\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})$

$$\begin{aligned}
\delta\rho_{\mathbf{q}+\mathbf{G},-\tau} &= \sum_{\mathbf{k},m,n} \lambda_{m,n,-\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})(c^\dagger_{\mathbf{k},m,-\tau}c_{\mathbf{k}+\mathbf{q},n,-\tau} - \frac{1}{2}\delta_{\mathbf{q},0}\delta_{m,n}) \\
&= \sum_{\mathbf{k},m,n} -m \times n \times \lambda_{m,n,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})(c_{\mathbf{k}+\mathbf{q},-n,-\tau}c^\dagger_{\mathbf{k},-m,-\tau} - \frac{1}{2}\delta_{\mathbf{q},0}\delta_{m,n}) \\
&= \sum_{\mathbf{k},m,n} -\lambda_{m,n,\tau}(\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G})(\tilde{c}^\dagger_{\mathbf{k}+\mathbf{q},n,-\tau}c_{\mathbf{k},m,-\tau} - \frac{1}{2}\delta_{\mathbf{q},0}\delta_{m,n}) \\
&= \sum_{\mathbf{k},m,n} -\lambda^*_{n,m,\tau}(\mathbf{k},\mathbf{k}-\mathbf{q}-\mathbf{G})(\tilde{c}^\dagger_{\mathbf{k},n,-\tau}c_{\mathbf{k}-\mathbf{q},m,-\tau} - \frac{1}{2}\delta_{\mathbf{q},0}\delta_{m,n}) \\
&= -\delta\rho_{-\mathbf{q}-\mathbf{G},\tau}
\end{aligned}$$

$$\tilde{c}_{\mathbf{k},m,-\tau} = m \times c^\dagger_{\mathbf{k},-m,-\tau}$$

$$B_{\mathbf{Q},-\tau} + iA_{\mathbf{Q},-\tau} = B_{\mathbf{Q},\tau} - iA_{\mathbf{Q},\tau}$$

$$\mathrm{Tr}\{\prod_t B(\{l_{|\mathbf{q}|,t}\})\} = \sum_{\{l_{|\mathbf{q}|,t}\}} D_\tau(\{l_{|\mathbf{q}|,t}\})D_{-\tau}(\{l_{|\mathbf{q}|,t}\}) = \sum_{\{l_{|\mathbf{q}|,t}\}} D_\tau(\{l_{|\mathbf{q}|,t}\})D^*_\tau(\{l_{|\mathbf{q}|,t}\})$$

No sign-problem

decoupled Hamiltonian is traceless anti-Hermitian matrix →

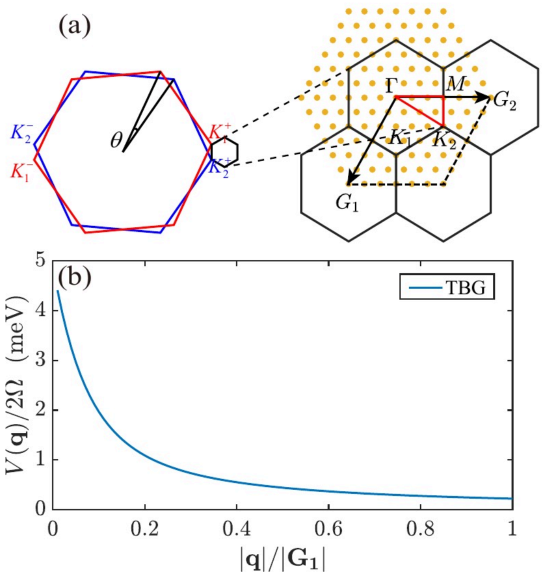
Degrees of freedom	Kinetic terms	Sign structure
Single valley single spin	No	Real
Single valley double spin	No	Non-negative
Double valley single spin	Flat bands	Non-negative
Double valley double spin	Flat bands	Non-negative

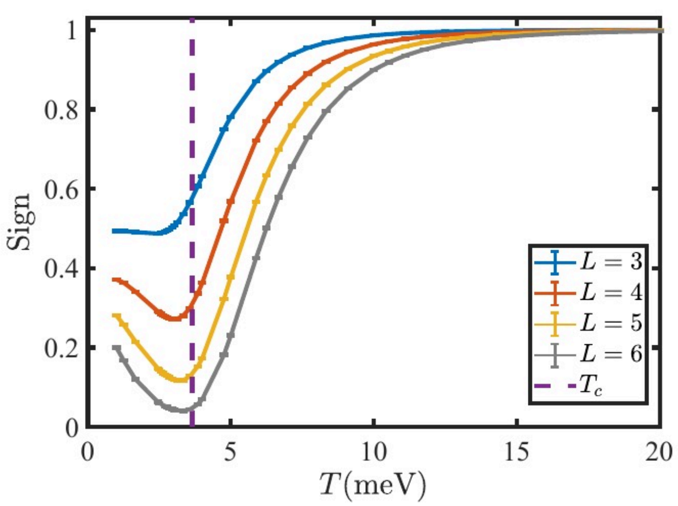
Thermodynamic characteristic for correlated flat-band system with quantum anomalous Hall ground state

Gaopei Pan,[1,2] Xu Zhang,[3] Hongyu Lu,[3] Heqiu Li,[4] Bin-Bin Chen,[3] Kai Sun,[5,*] and Zi Yang Meng[3,†]

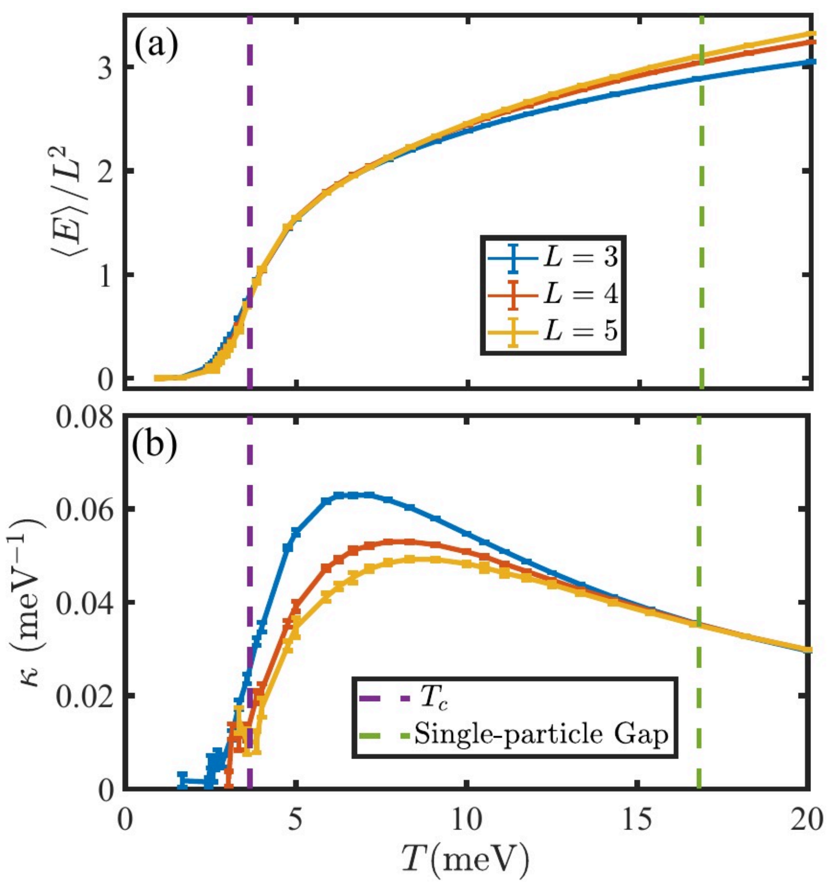
PRL 130, 016401 (2023)

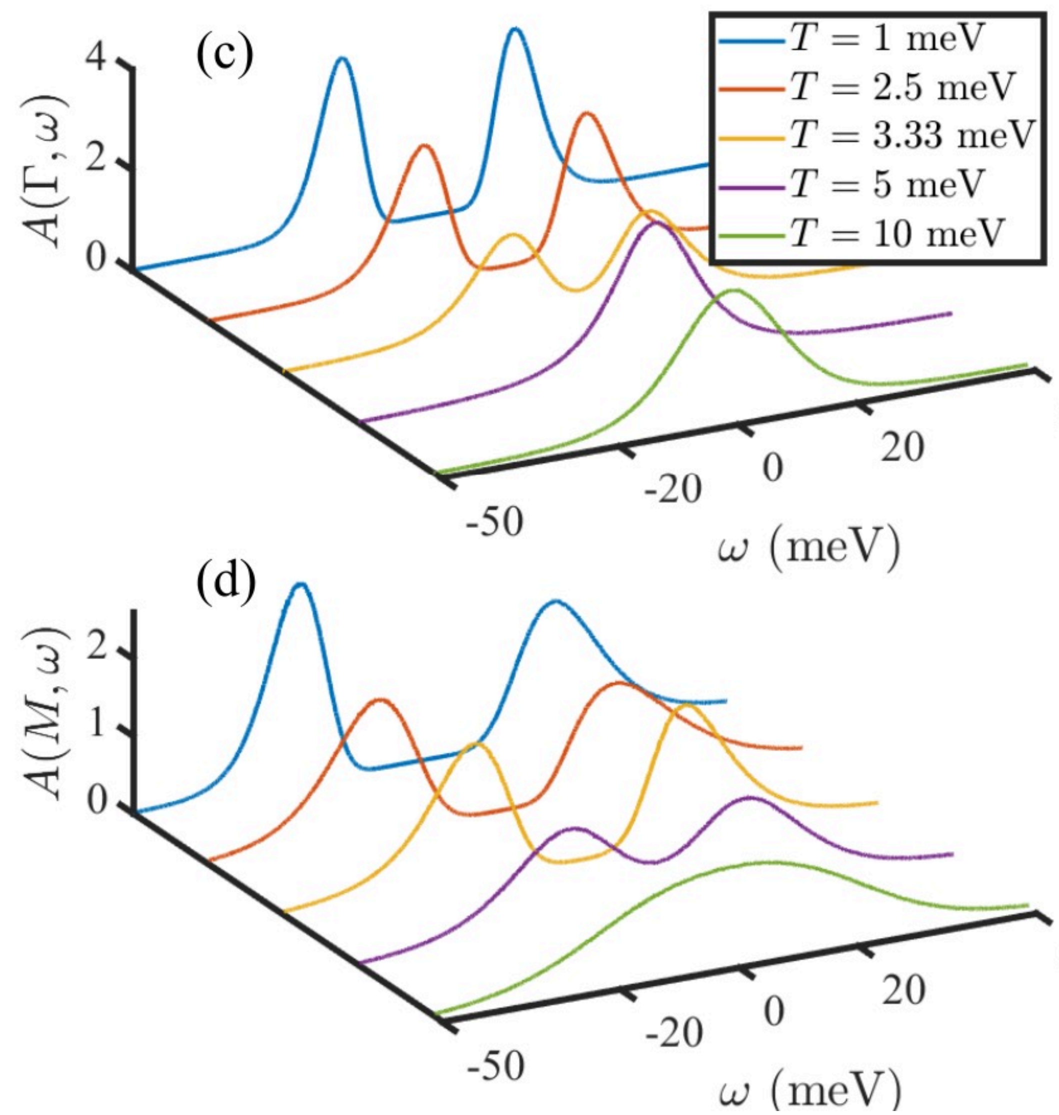
momentum-space QMC
Single valley and single spin





$T_c = 3.65(5)$ meV





$$\kappa = \frac{\partial n}{\partial \mu} = \frac{\langle N^2\rangle - \langle N\rangle^2}{TN}$$

measured via
quantum capacitance

measured via
STM

Thermodynamic characteristic for correlated flat-band system with quantum anomalous Hall ground state

Gaopei Pan,[1,2] Xu Zhang,[3] Hongyu Lu,[3] Heqiu Li,[4] Bin-Bin Chen,[3] Kai Sun,[5,*] and Zi Yang Meng[3,†]

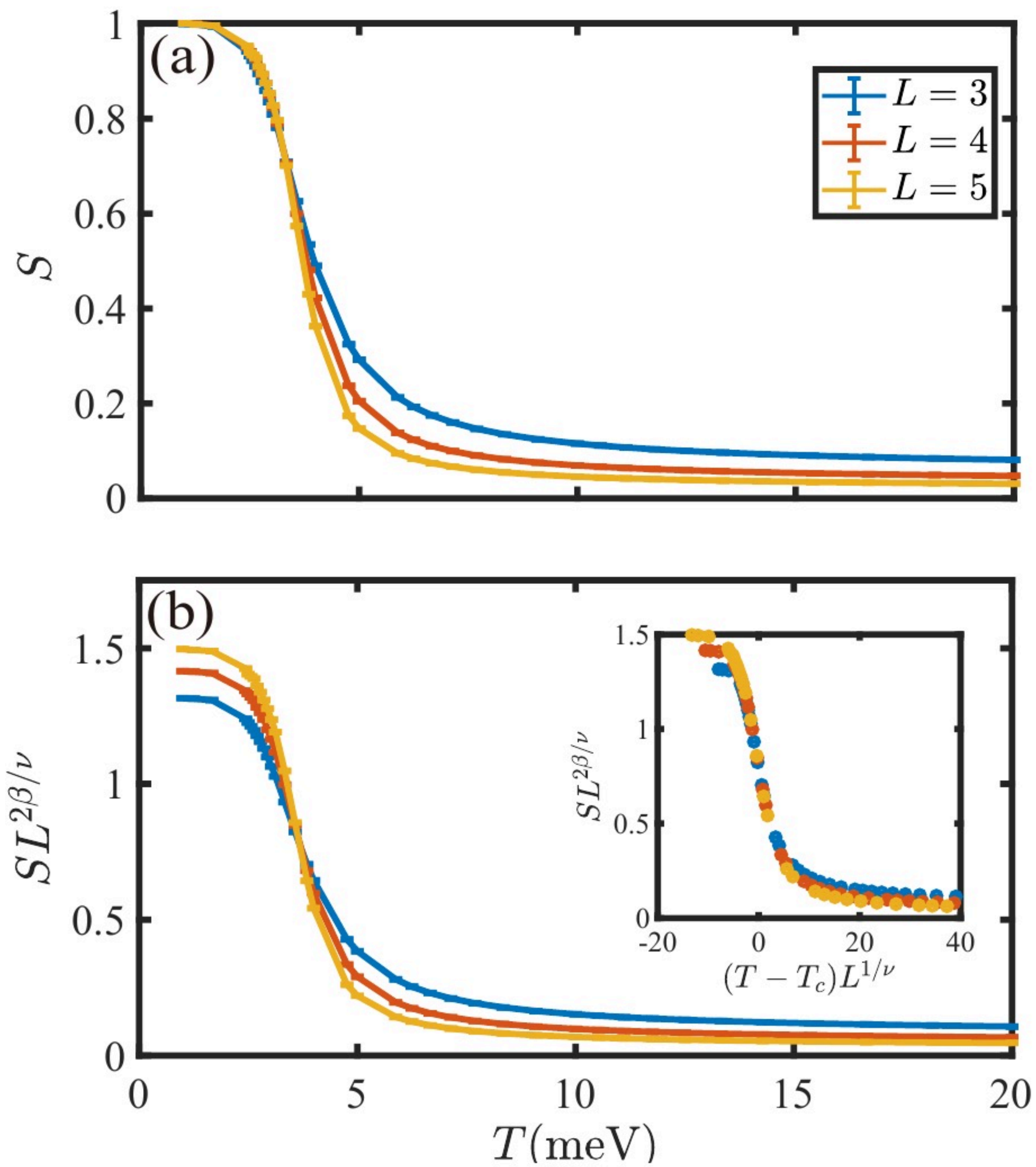
PRL 130, 016401 (2023)

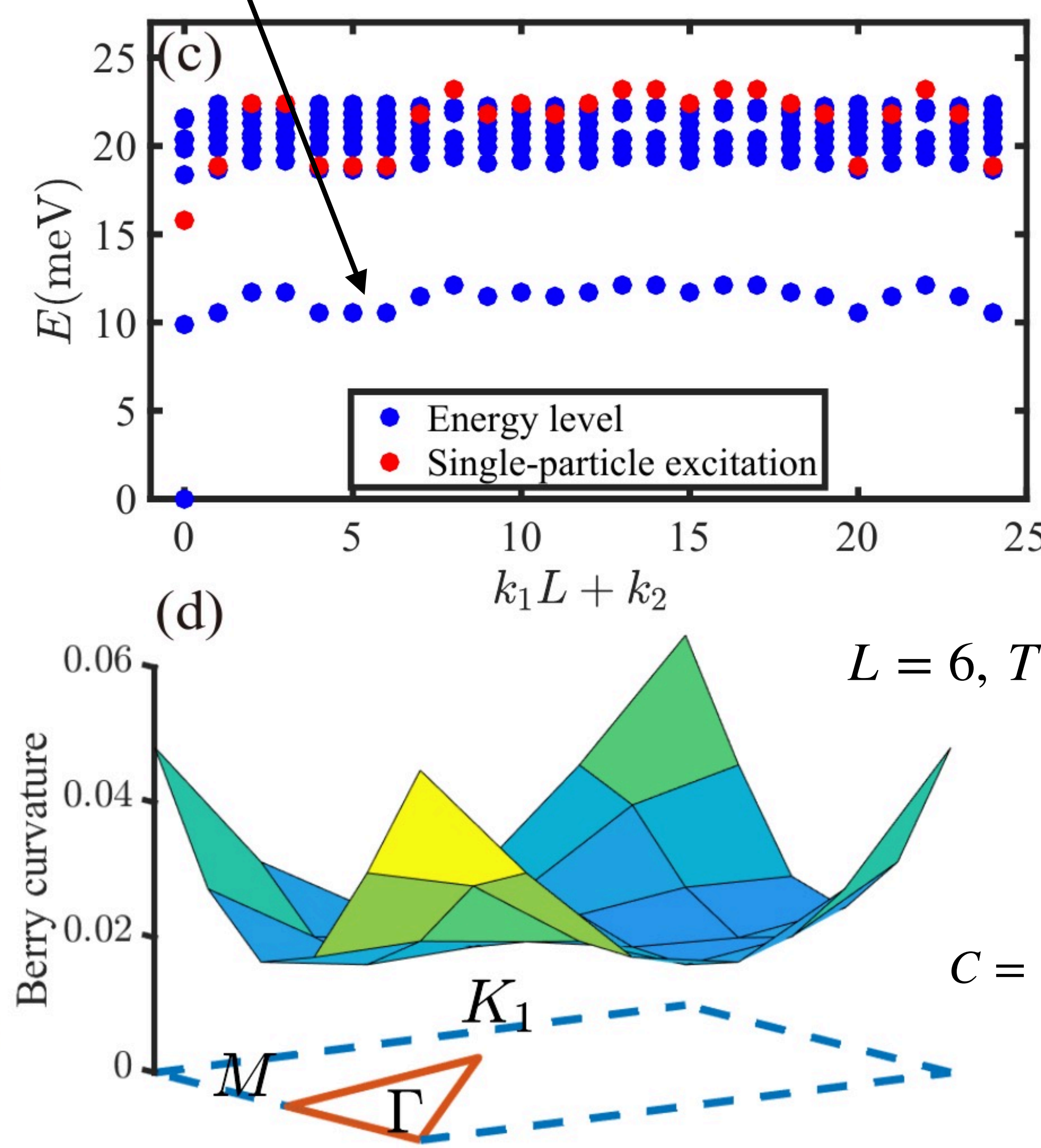
momentum-space QMC & exact diagonalization

$$S = \frac{1}{N^2}\langle (N_+ - N_-)^2 \rangle$$

Gapped excitons restore time-reversal

$L = 5$





$L = 6,\ T = 1.25$ meV

$$C = \sum F_{\square} = 1$$

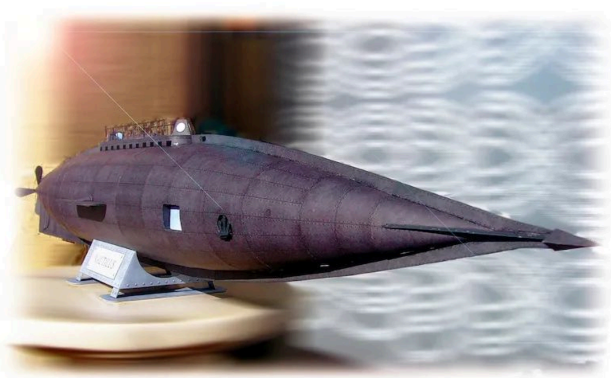
$T_c = 3.65(5)$ meV

Detective Dr. Dragon on the Monte Carlo Sign Problem

Xu Zhang

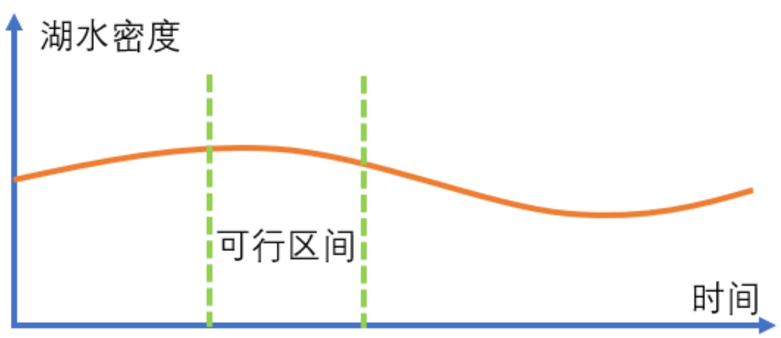
$$\langle \hat{O} \rangle = \frac{\sum_l W_l \langle \hat{O} \rangle_l}{\sum_l W_l} = \frac{\frac{\sum_l |\mathrm{Re}(W_l)| \frac{W_l \langle \hat{O} \rangle_l}{|\mathrm{Re}(W_l)|}}{\sum_l |\mathrm{Re}(W_l)|}}{\frac{\sum_l W_l}{\sum_l |\mathrm{Re}(W_l)|}} \equiv \frac{\langle \hat{O} \rangle_{|\mathrm{Re}(W_l)|}}{\langle \mathrm{sign} \rangle}$$

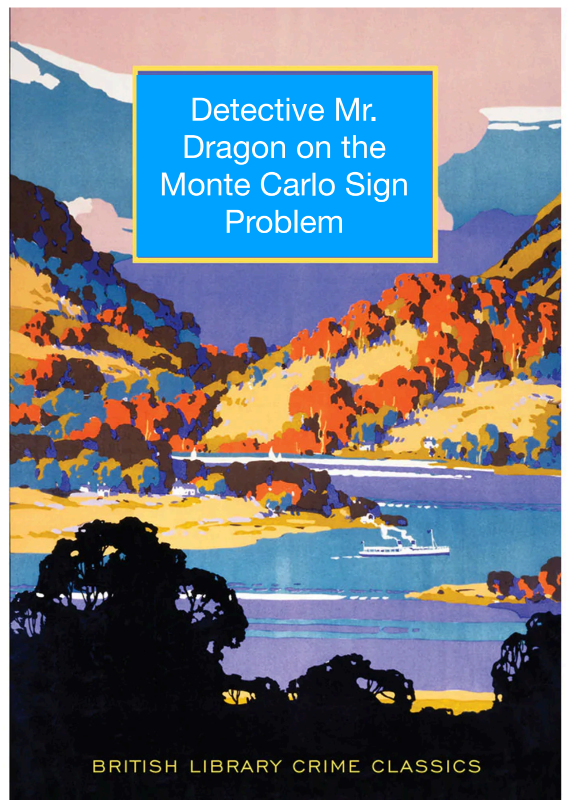
$$\langle sign \rangle \sim e^{-\beta N}$$



$$\langle sign \rangle = \frac{\sum_l W_l}{\sum_l |Re(W_l)|} = \frac{\langle W \rangle}{\langle |Re(W)| \rangle}$$

$$\langle |Re(W)| \rangle \leq \langle |W| \rangle \leq \sqrt{\langle |W|^2 \rangle}$$





$$\langle sign \rangle \geq \frac{\langle W \rangle}{\langle |W| \rangle} = \frac{Z_W}{Z_{|W|}} = \frac{g_W}{g_{|W|}} e^{-\beta(\langle E \rangle_W - \langle E \rangle_{|W|})}$$

$$\langle sign \rangle \geq \frac{\langle W \rangle}{\sqrt{\langle |W|^2 \rangle}} = \frac{Z_W}{\sqrt{Z_{|W|^2}}} = \frac{g_W}{\sqrt{g_{|W|^2}}} e^{-\beta(\langle E \rangle_W - \langle E \rangle_{|W|^2}/2)}$$

Correlated flat-bands have sign bound

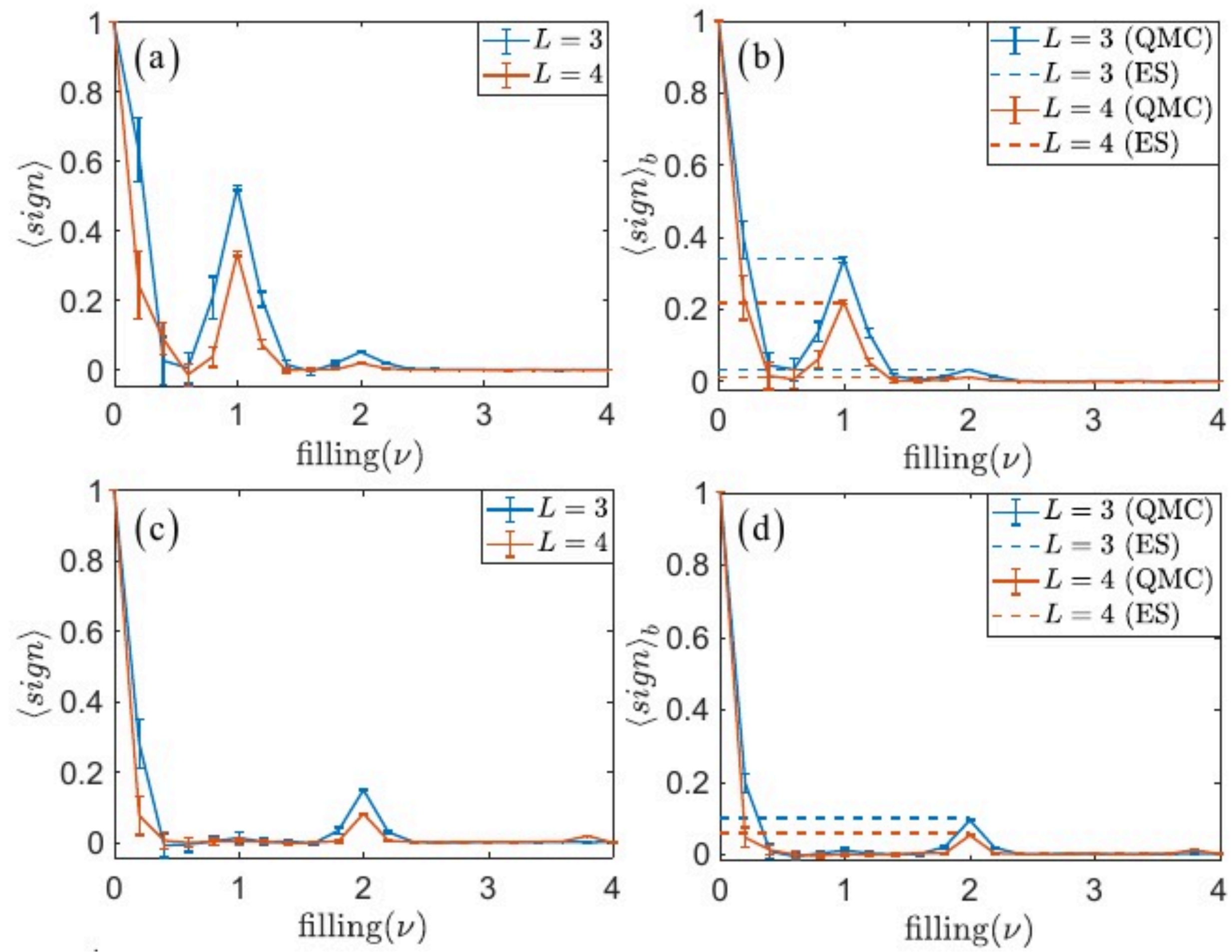
- Xu Zhang et al., Fermion sign bounds theory in quantum Monte Carlo simulation, PRB 106, 035121 (2022)
- Xu Zhang et al., Polynomial sign problem and topological Mott insulator in twisted bilayer graphene, PRB 107, L241105 (2023)

Polynomial Sign Problem and Topological Mott Insulator emerging in Twisted Bilayer Graphene

Xu Zhang,[1] Gaopei Pan,[2,3] Bin-Bin Chen,[1] Heqiu Li,[4] Kai Sun,[5,*] and Zi Yang Meng[1,†]

Phys. Rev. B 107, L241105 (2023)

Filling(ν)	Chiral($\gamma = 0$)	Non-chiral($\gamma = 0$)	Chiral($\gamma > 0$)
0	1	1	1
± 1	N^{-1}	✗	✗
± 2	N^{-2}	N^{-1}	N^{-2}
± 3	N^{-5}	✗	✗
± 4	N^{-8}	N^{-4}	N^{-4}



$$\langle sign \rangle \geq \frac{g_{\nu=1}}{g_{\nu=0}} = \frac{\frac{(N+3)^2(N+2)^3(N+1)^2}{(3!)^2}}{\frac{(N+3)^2(N+2)^4(N+1)^2}{(3!)^2(2!)^2}} \sim \frac{N^7}{N^8} = N^{-1}$$

$$g_{\nu=1} = 2g_{C_+=3,C_-=0} + 2g_{C_+=2,C_-=1} = \frac{(N+3)(N+2)(N+1)}{3} + \frac{(N+3)^2(N+2)^3(N+1)^2}{(3!)^2}$$

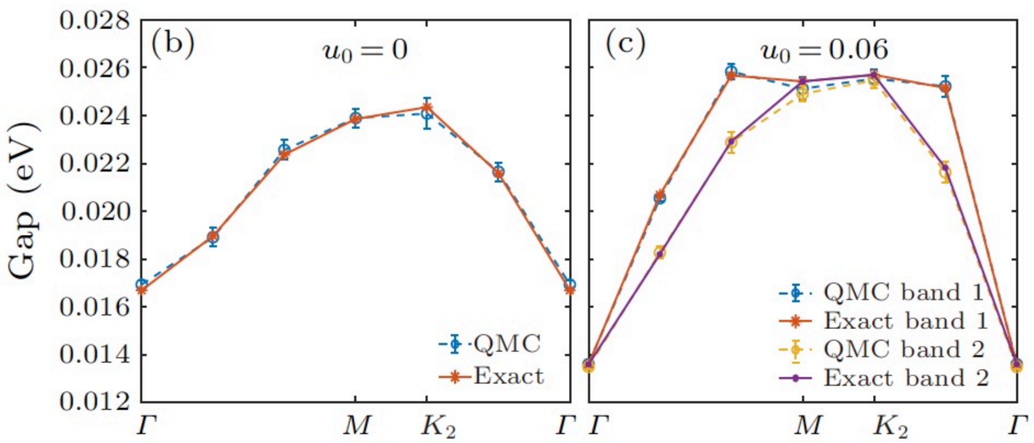
$$g_{\nu=0} = 2g_{C_+=4,C_-=0} + 2g_{C_+=3,C_-=1} + g_{C_+=2,C_-=2} = 2 + \frac{(N+3)^2(N+2)^2(N+1)^2}{(3!)^2} + \frac{(N+3)^2(N+2)^4(N+1)^2}{(3!)^2(2!)^2}$$

Dynamical properties of collective excitations in twisted bilayer graphene

Gaopei Pan,[1,2] Xu Zhang,[3] Heqiu Li,[4,5] Kai Sun,[4,*] and Zi Yang Meng[3,†]

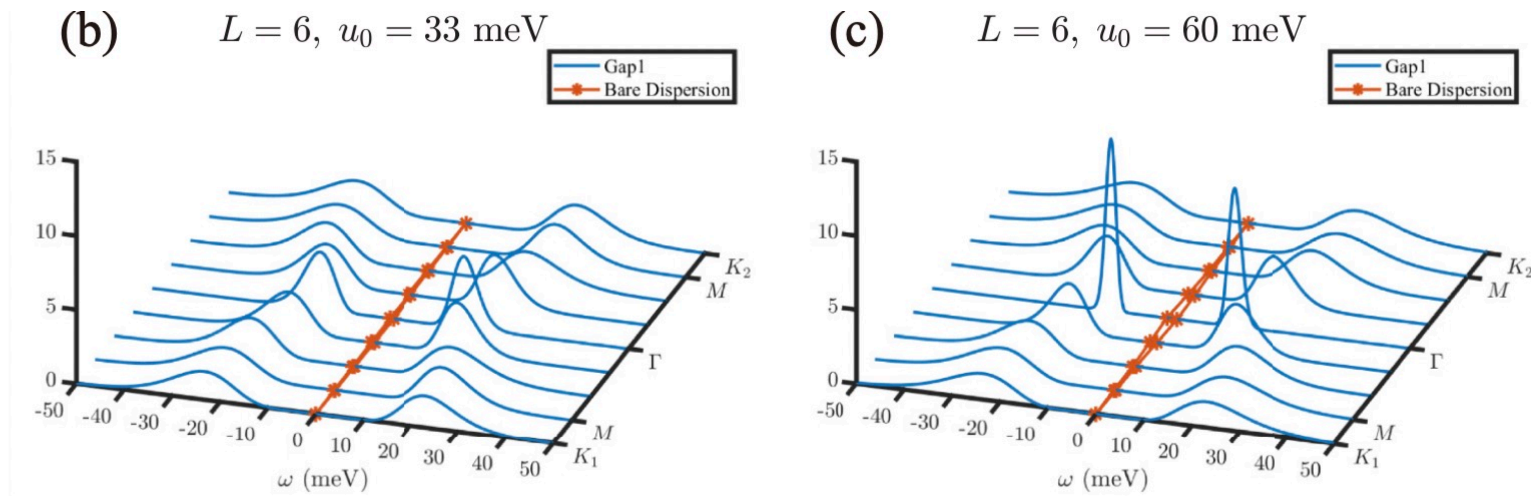
CPL 38, 077305 (2021) Express Letter

PRB 105, L121110 (2022)



single-particle excitations

$T = 0.667$ meV



$$\mathcal{O}_a(\boldsymbol{q},\tau) \equiv \sum_{\boldsymbol{k}} d^\dagger_{\boldsymbol{k}+\boldsymbol{q}}(\tau) M_a d_{\boldsymbol{k}}(\tau)$$

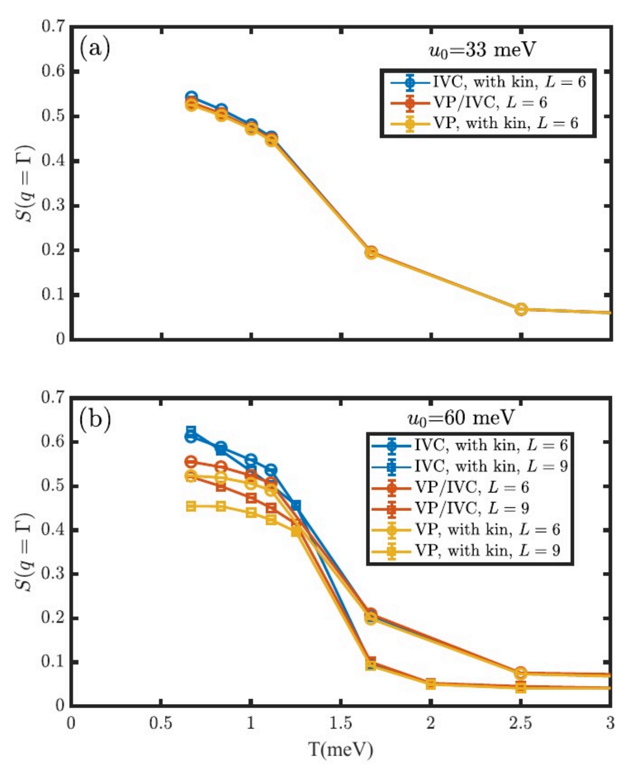
$$M_a = \tau_z \eta_0$$

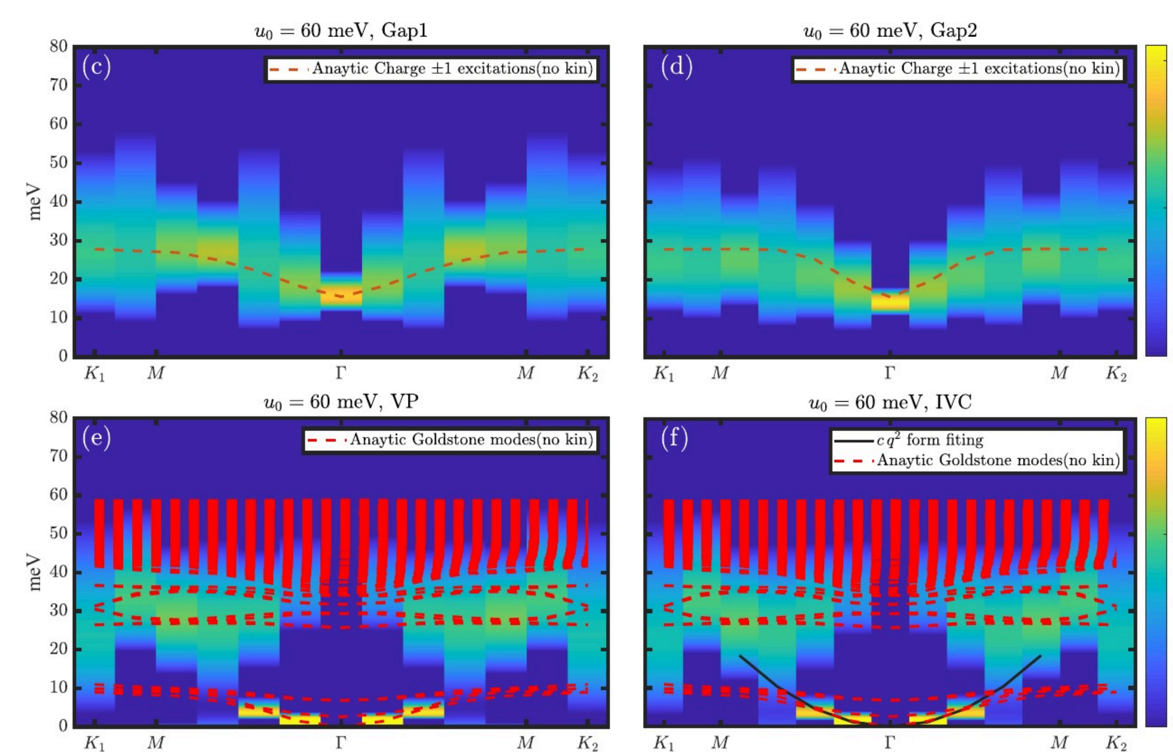
for valley polarized state

$$M_a = \tau_x \eta_y \ \text{ or } \ \tau_y \eta_y$$

for intervalley coherent state

Bosonic collective excitations

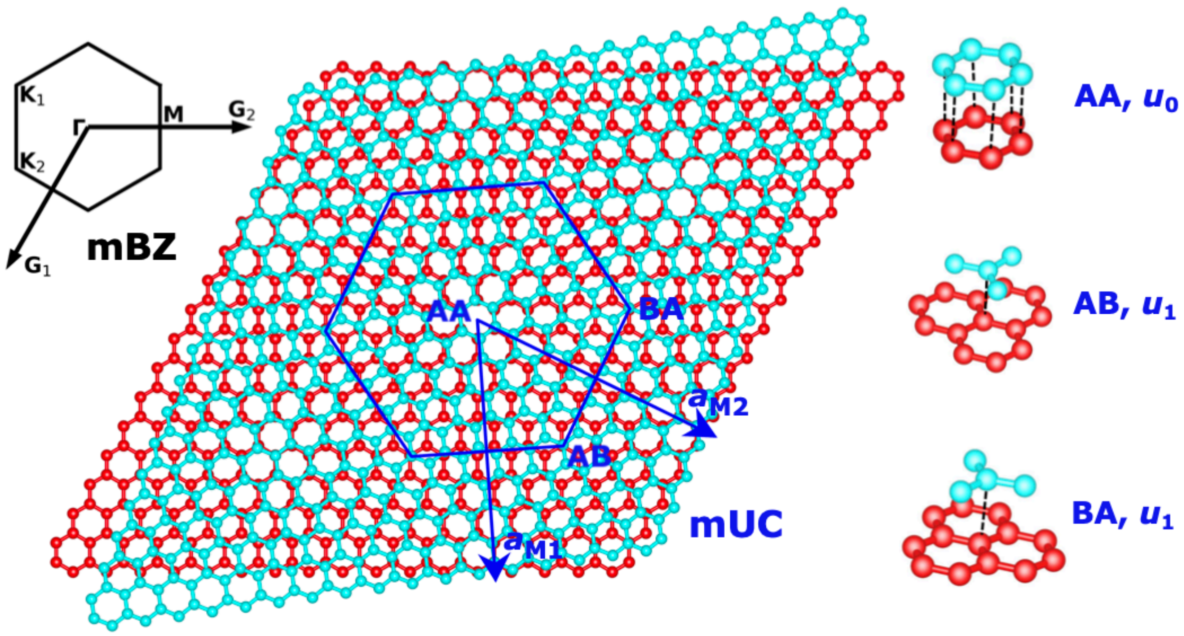


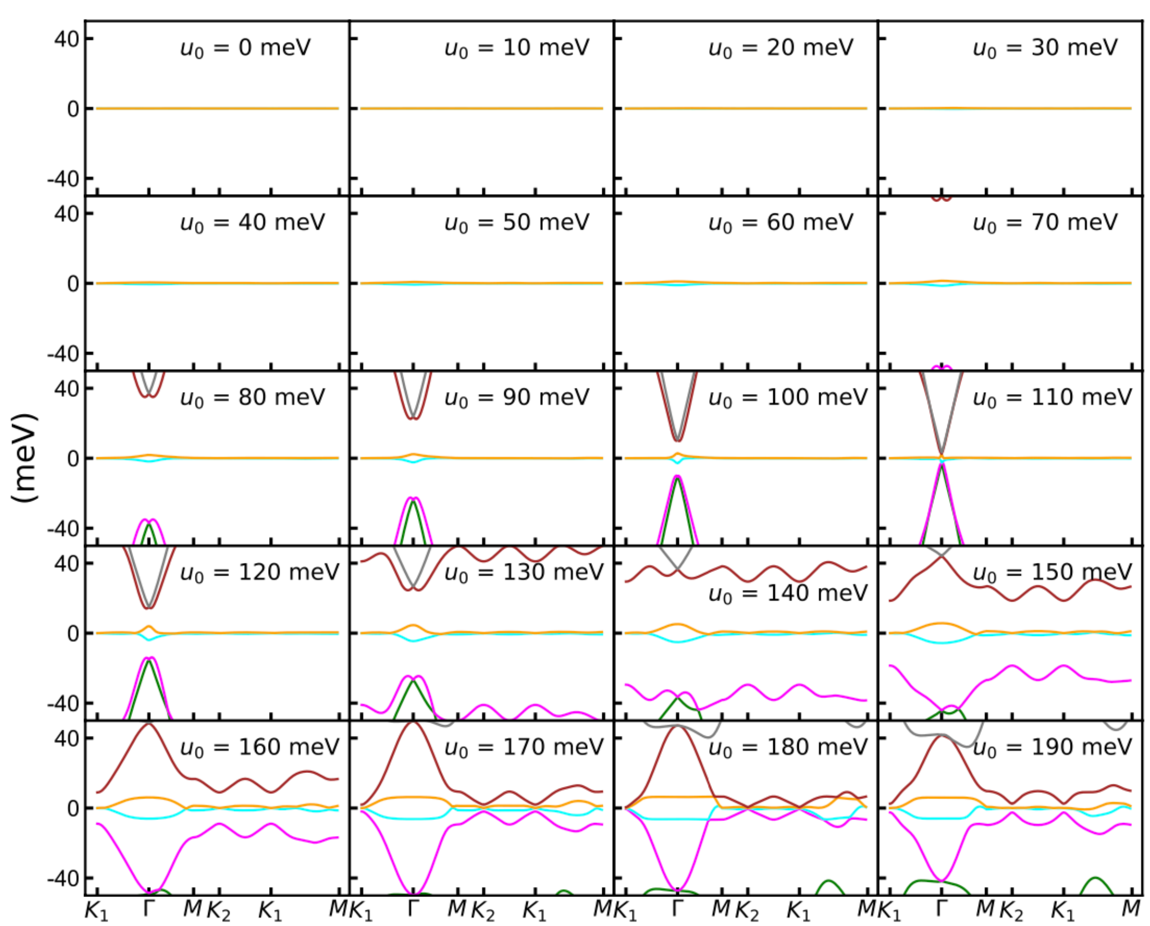


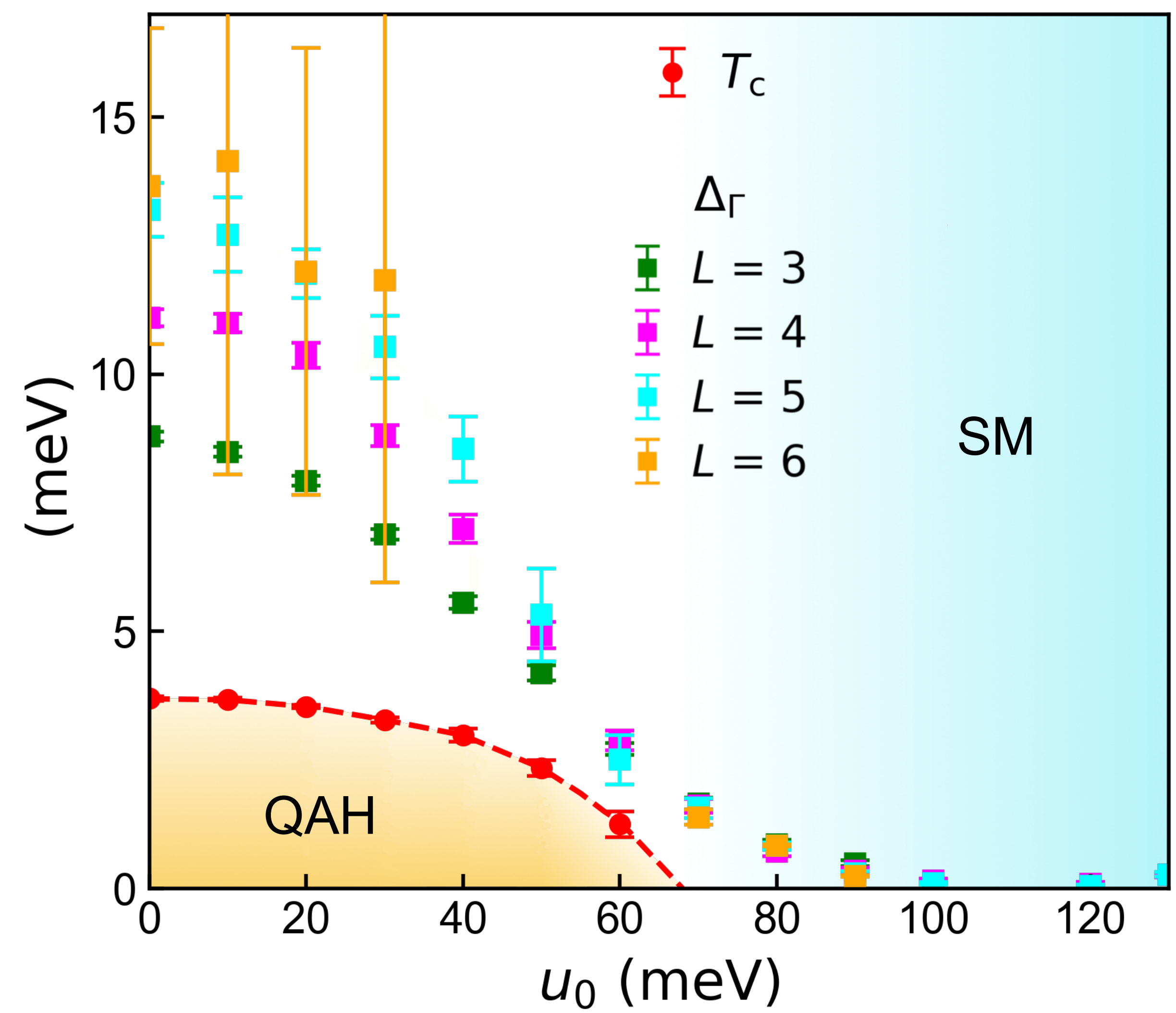
Evolution from quantum anomalous Hall insulator to heavy-fermion semimetal in magic-angle twisted bilayer graphene

Cheng Huang,[1] Xu Zhang,[1] Gaopei Pan,[2,3] Heqiu Li,[4] Kai Sun,[5,*] Xi Dai,[6,†] and Zi Yang Meng[1,‡]

PRB 109, 125404 (2024)







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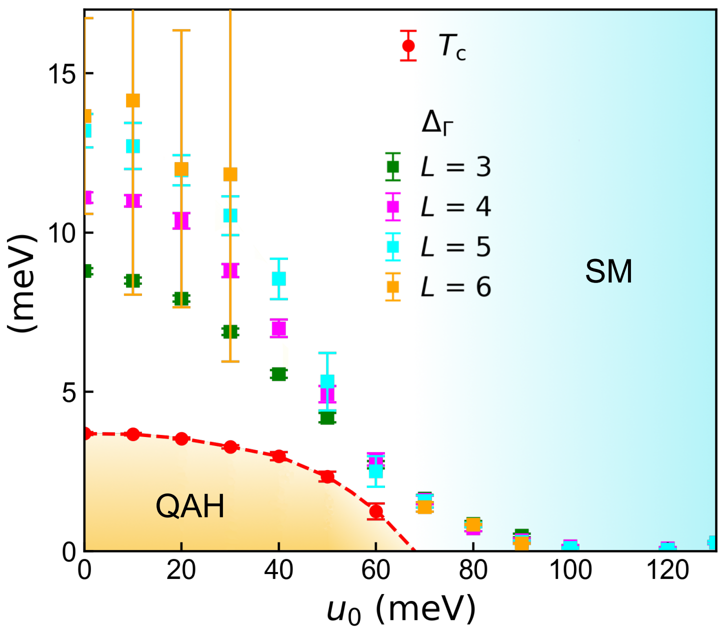
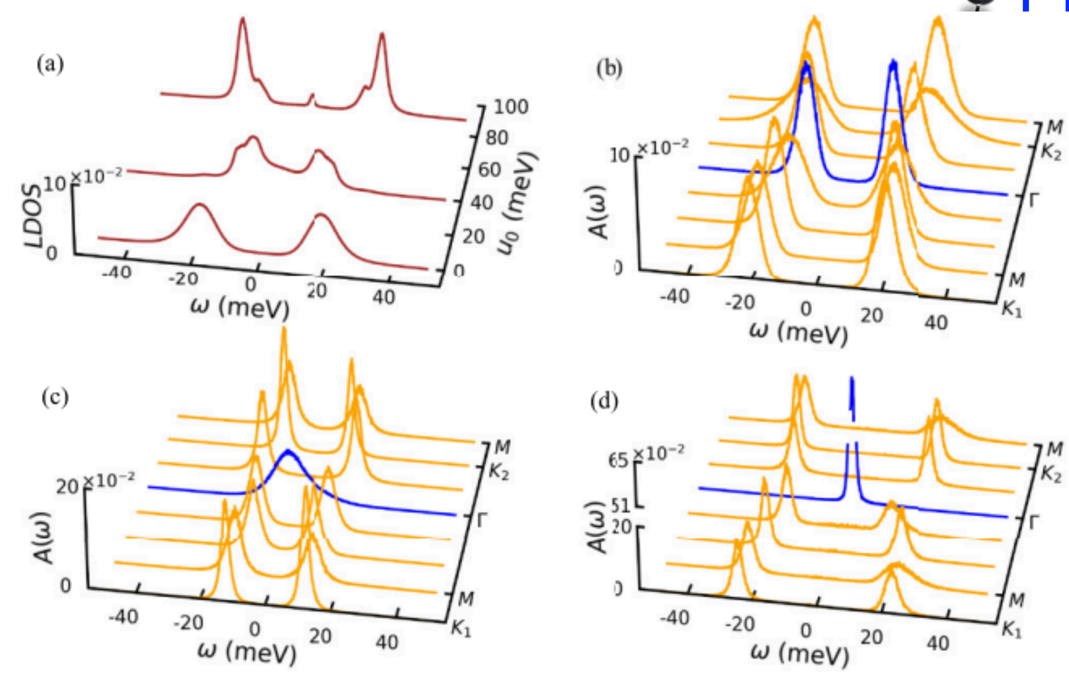
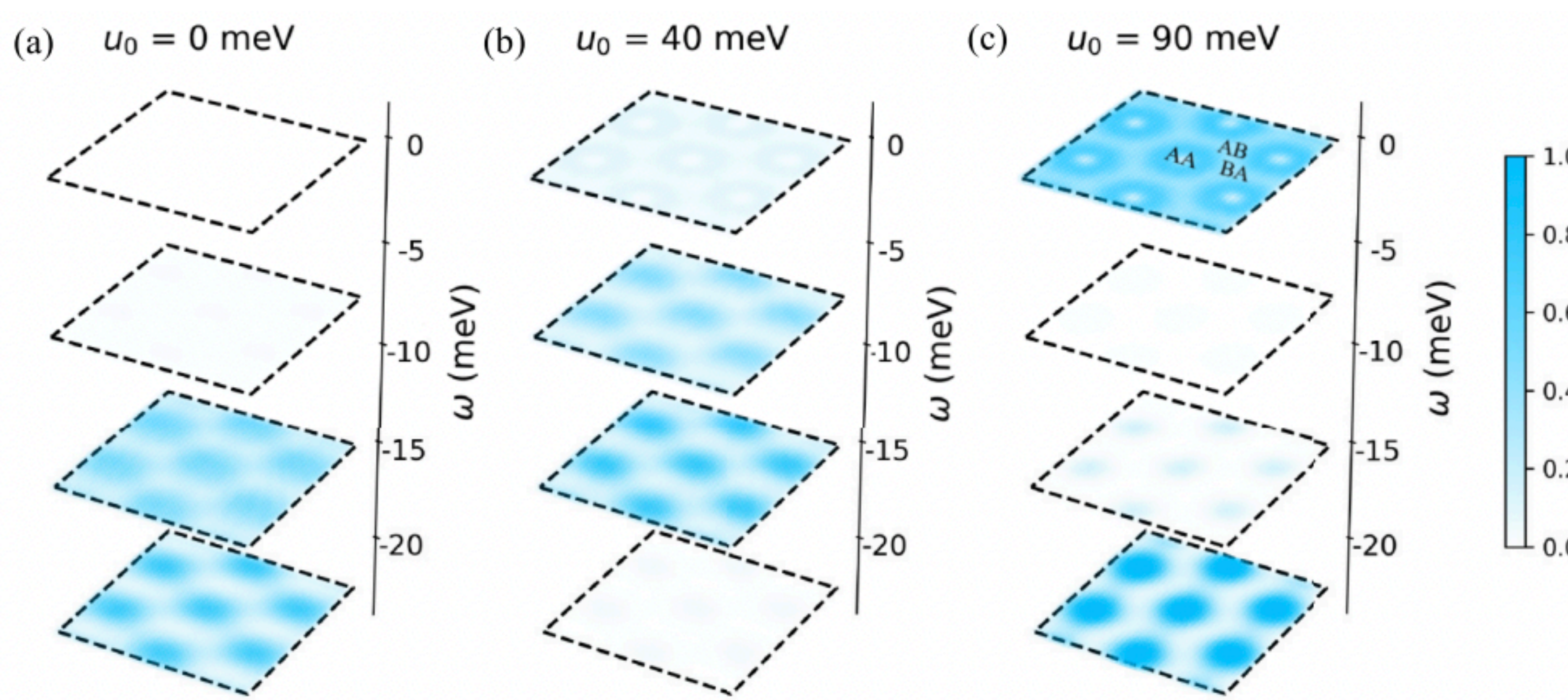
PRB 109, 125404 (2024)







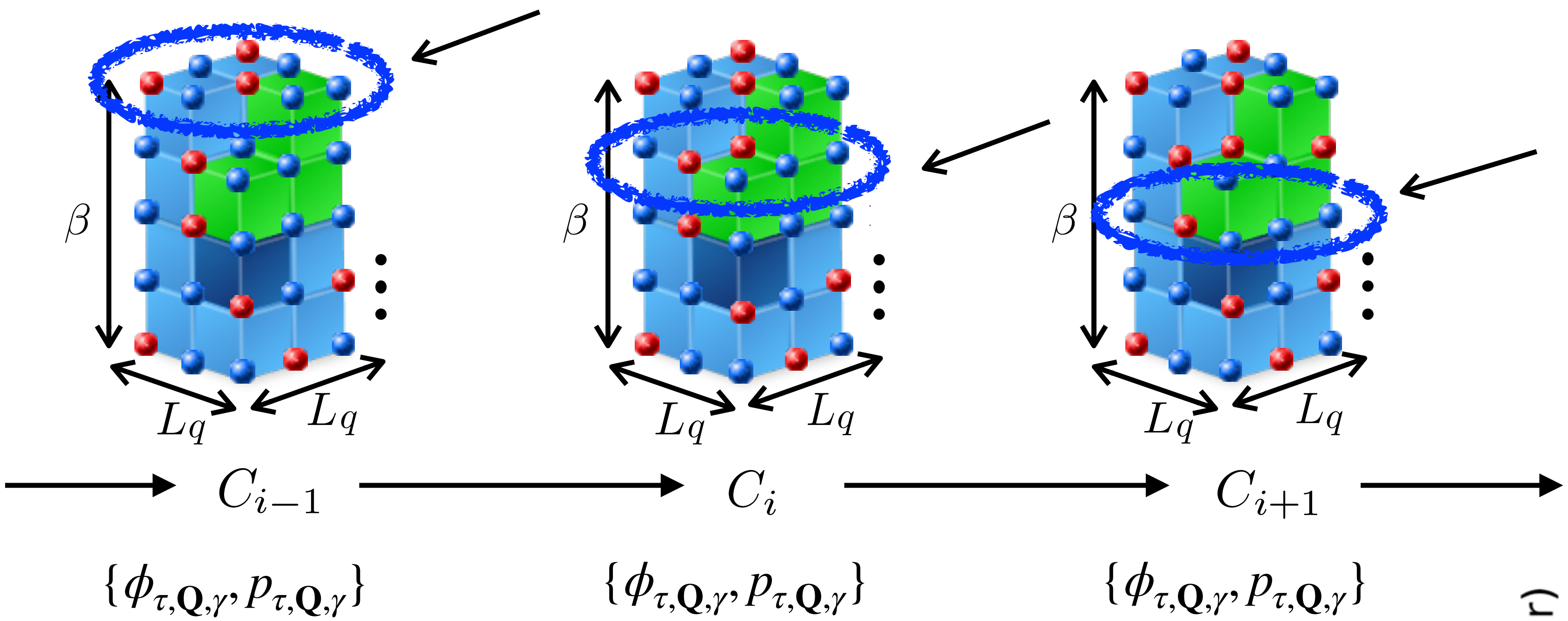
Continuous Field Momentum-Space QMC

Cheng Huang et al., arXiv: 2412.11382

$$Z = \int \prod_{\tau,\boldsymbol{Q}} d\phi_{\tau,\boldsymbol{Q},1} d\phi_{\tau,\boldsymbol{Q},2} e^{-\frac{1}{2}\sum_{\tau,Q}\left(\phi^2_{\tau,\boldsymbol{Q},1}+\phi^2_{\tau,\boldsymbol{Q},2}\right)} \times \mathrm{Tr}\left(\prod_{\tau} e^{-\Delta\tau H_0} e^{\mathrm{i}\sum_{\boldsymbol{Q}}\left(-\phi_{\tau,\boldsymbol{Q},1}\sqrt{\alpha_2(\boldsymbol{Q})}A_{\boldsymbol{Q}}+\mathrm{i}\phi_{\tau,\boldsymbol{Q},2}\sqrt{\alpha_2(\boldsymbol{Q})}B_{\boldsymbol{Q}}\right)}\right)$$

$$= \int \prod_{\tau,\mathbf{Q},\gamma} d\phi_{\tau,\mathbf{Q},\gamma}\, dp_{\tau,\mathbf{Q},\gamma}\ \exp\Big(-\underbrace{\big(\frac{1}{2}\sum_{\tau,\mathbf{Q},\gamma}(p^2_{\tau,\mathbf{Q},\gamma}+\phi^2_{\tau,\mathbf{Q},\gamma}) - \ln(\det(M)\big)}_{\mathscr{H}}\Big)$$

$$M = \begin{pmatrix} \mathbf{1} & 0 & 0 & \cdots & 0 & B_{N_\tau} \\ -B_1 & \mathbf{1} & 0 & \cdots & 0 & 0 \\ 0 & -B_2 & \mathbf{1} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \mathbf{1} & 0 \\ 0 & 0 & 0 & \cdots & -B_{N_\tau-1} & \mathbf{1} \end{pmatrix}$$

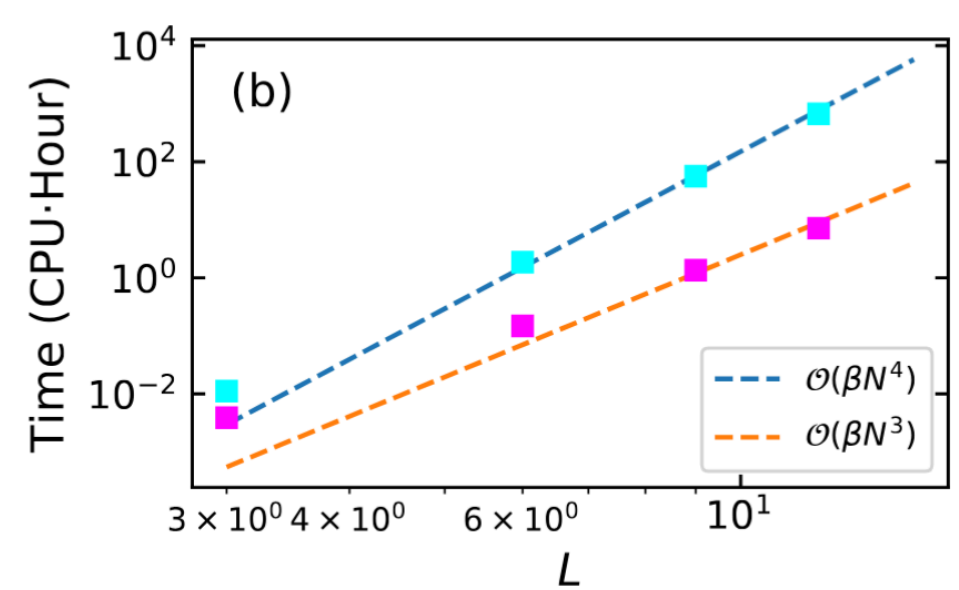


$$\begin{cases} \dfrac{dp_{\tau,\mathbf{Q},\gamma}}{dt} = -\dfrac{\partial\mathscr{H}}{\partial\phi_{\tau,\mathbf{Q},\gamma}} = -\phi_{\tau,\mathbf{Q},\gamma} + \mathrm{Tr}(M^{-1}\dfrac{\partial M}{\partial\phi_{\tau,\mathbf{Q},\gamma}}) \\ \dfrac{d\phi_{\tau,\mathbf{Q},\gamma}}{dt} = \dfrac{\partial\mathscr{H}}{\partial p_{\tau,\mathbf{Q},\gamma}} = p_{\tau,\mathbf{Q},\gamma} \end{cases}$$

sparse matrix
O(N^2)

Update the entire time slice and update the Green's function

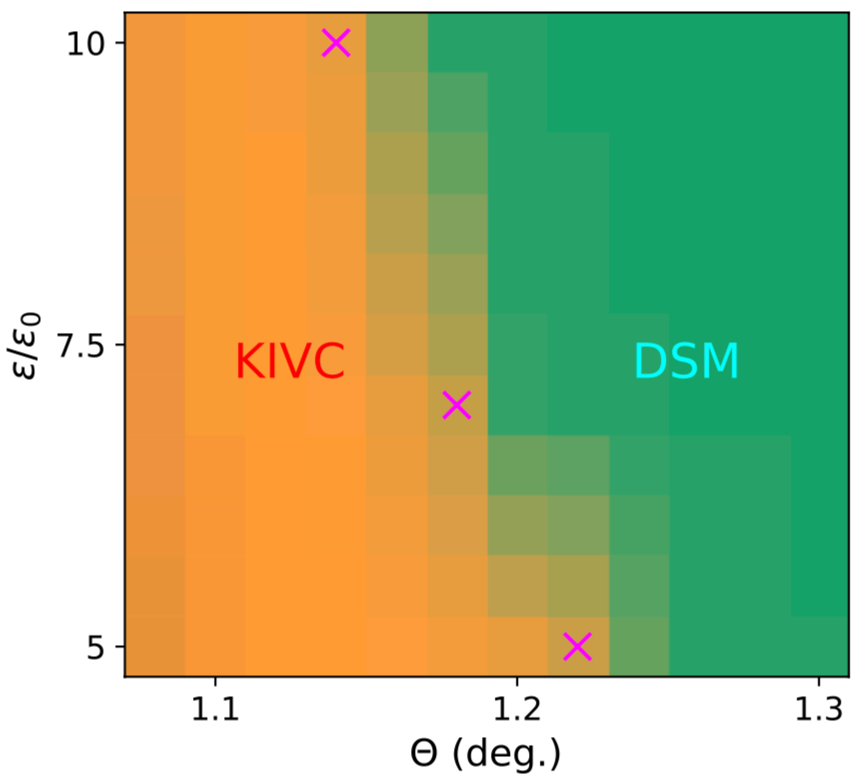
$O(N^2)$ $O(N^3)$

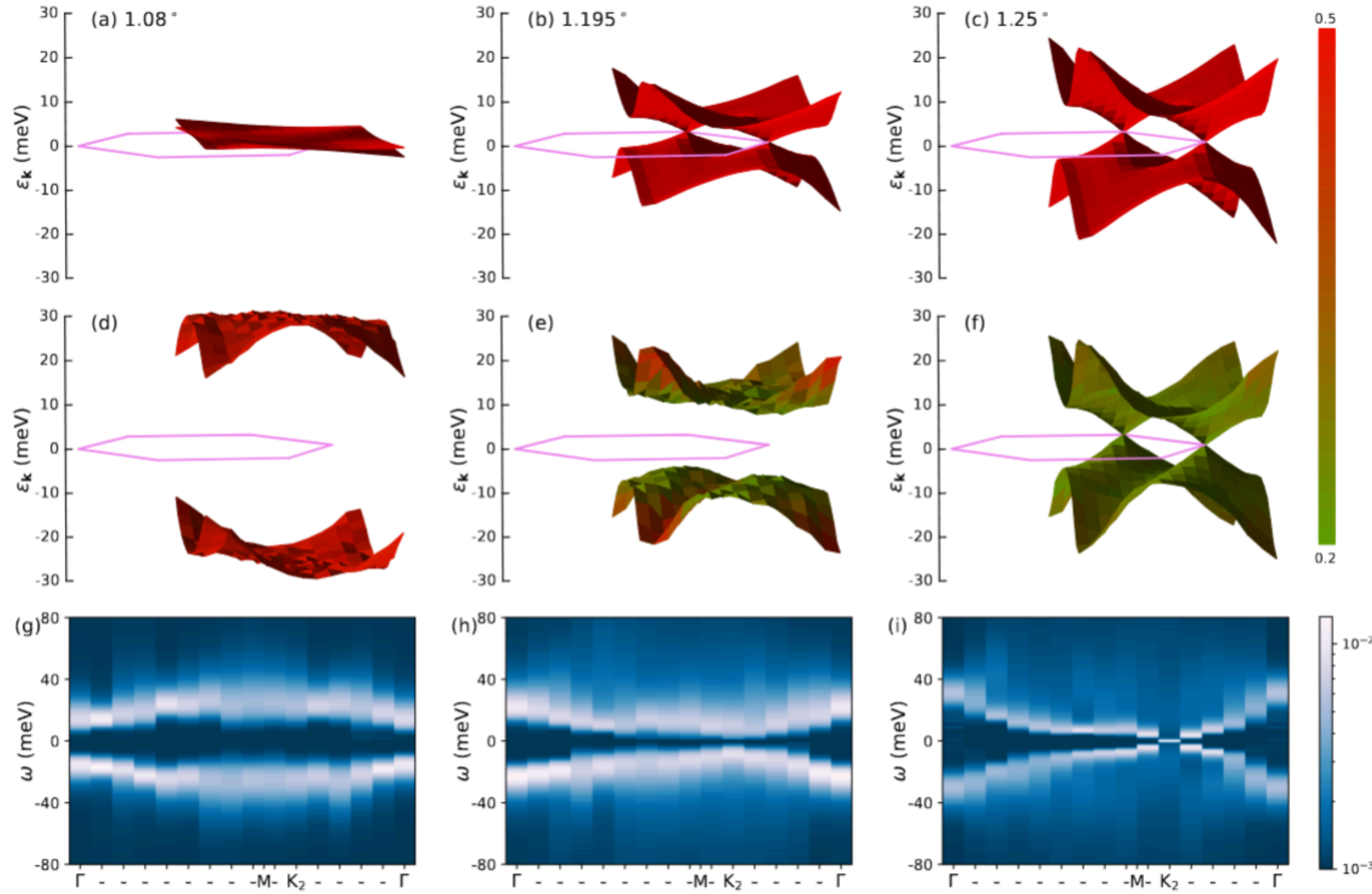


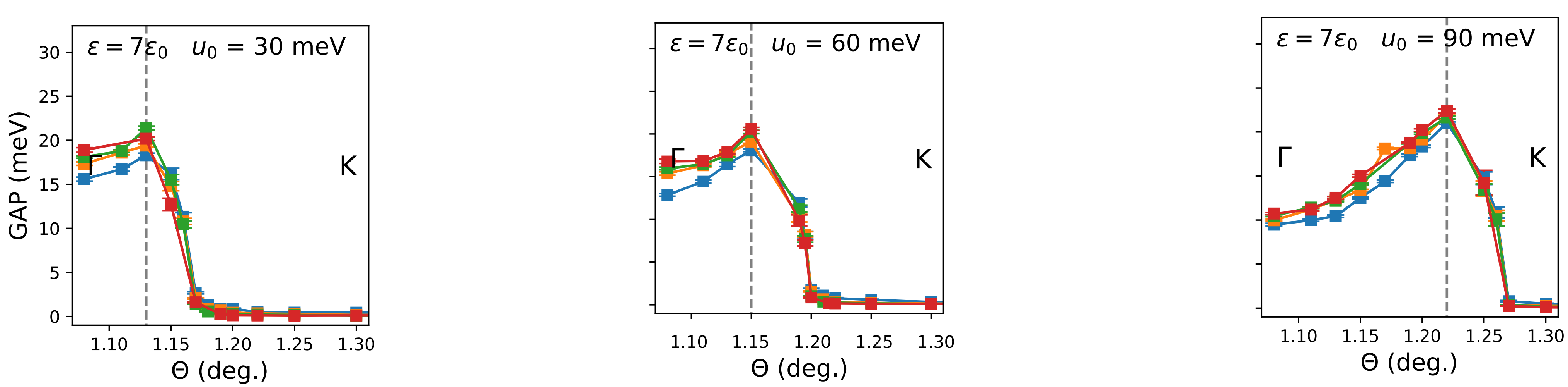
Angle-Tuned Gross-Neveu Quantum Criticality in Twisted Bilayer Graphene: A Quantum Monte Carlo Study

Cheng Huang,[1] Nikolaos Parthenios,[2,3] Maksim Ulybyshev,[4] Xu Zhang,[1,5] Fakher F. Assaad,[4,6] Laura Classen,[2,3,*] and Zi Yang Meng[1,†]

arXiv: 2412.11382







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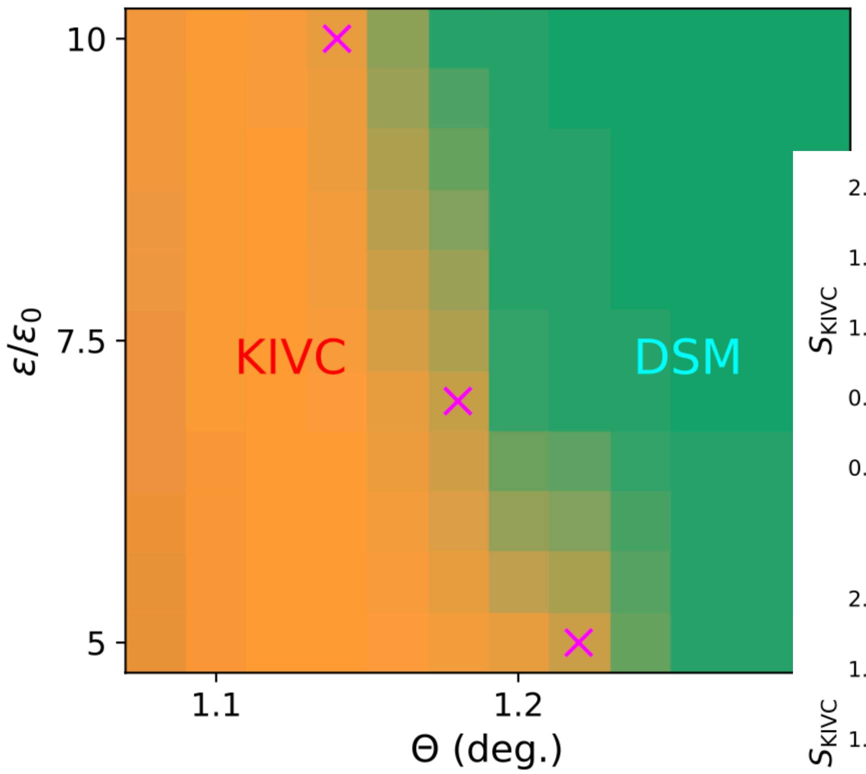
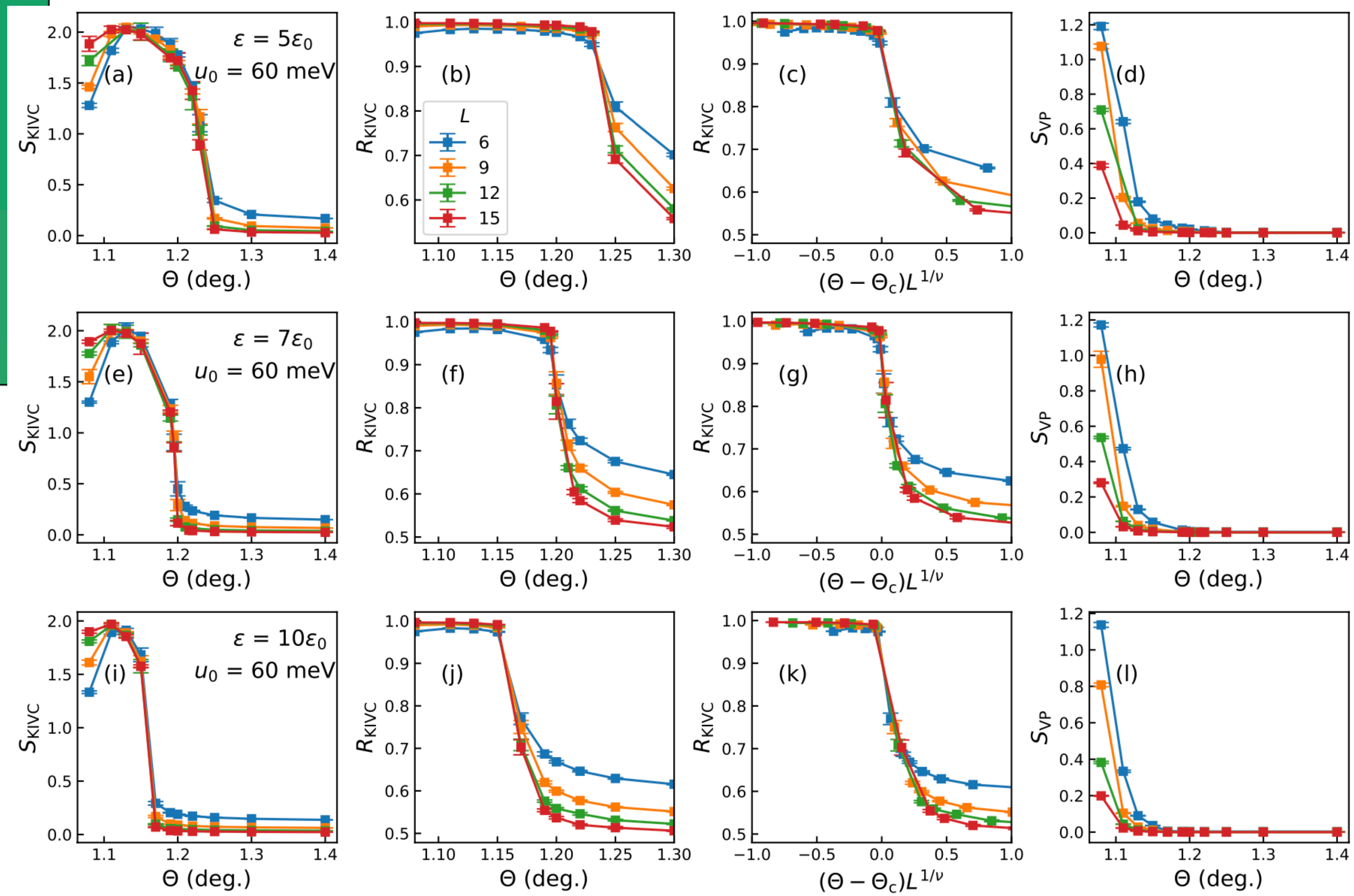
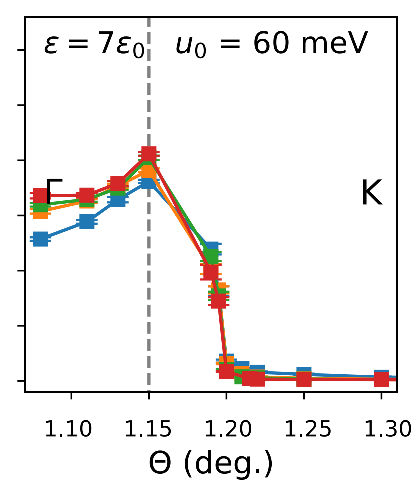
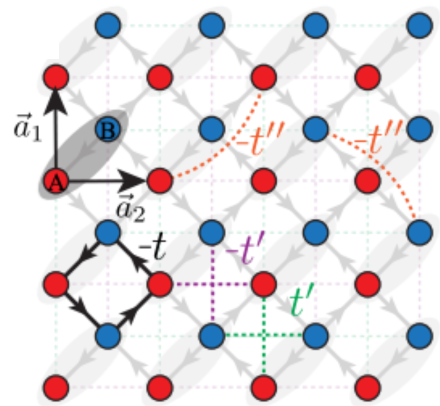
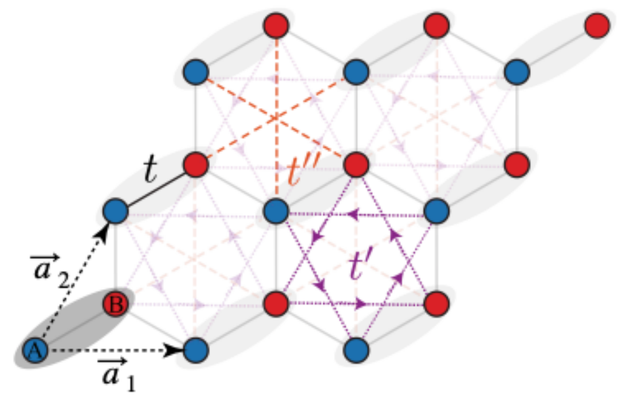


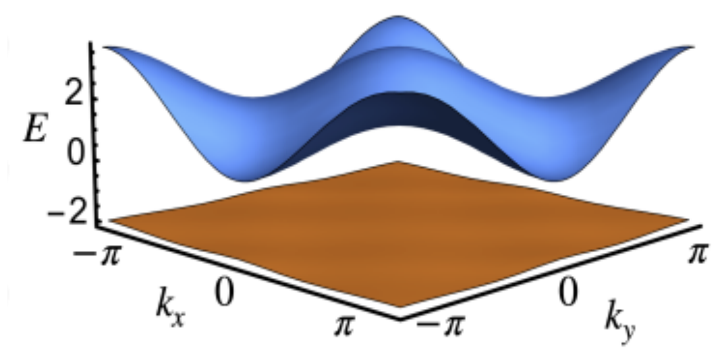




Fractional Chern Insulator



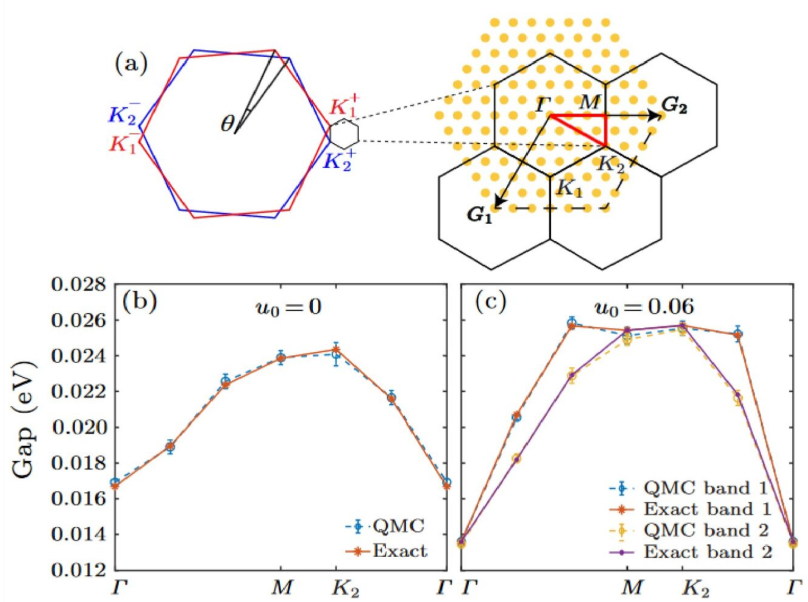




(thermal) tensor-network,
magnetorotons,
chiral gravitons,
…

- arXiv: 2505.04138
- Phys. Rev. Lett 134, 076601 (2025)
- arXiv: 2404.06745
- Phys. Rev. Lett 132, 236502 (2024)
- Rep. Prog. Phys 87, 108003 (2024)

Twisted Bilayer Graphene



Momentum-space QMC,
spectral functions,
KIVC-DSM transition
…

- arXiv: 2412.11382
- Phys. Rev. B 109, 125404 (2024)
- Phys. Rev. Lett 130, 016401 (2023)
- Chin. Phys. Lett 38, 077305 (2021)