Mottness and Topology in Haldane and KM/BHZ models

EFRC: DOE

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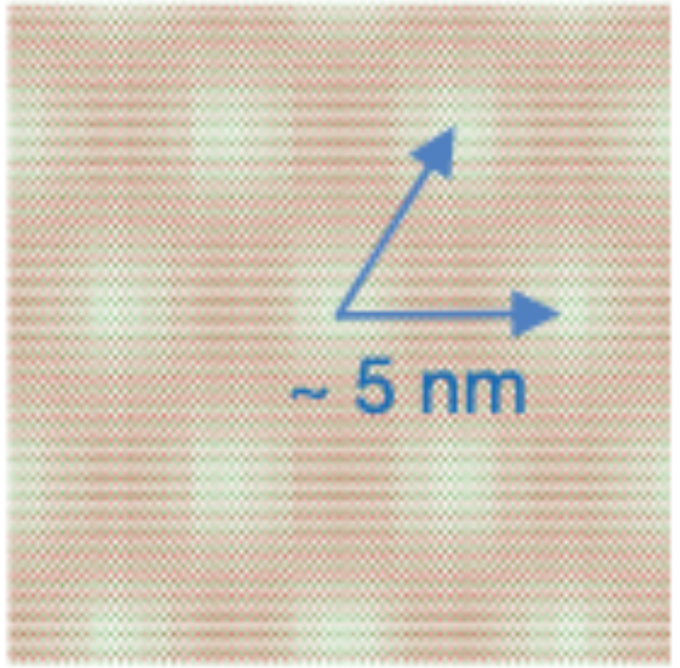

AA-stacking
0 twist angle

Article

Continuous Mott transition in semiconductor moiré superlattices

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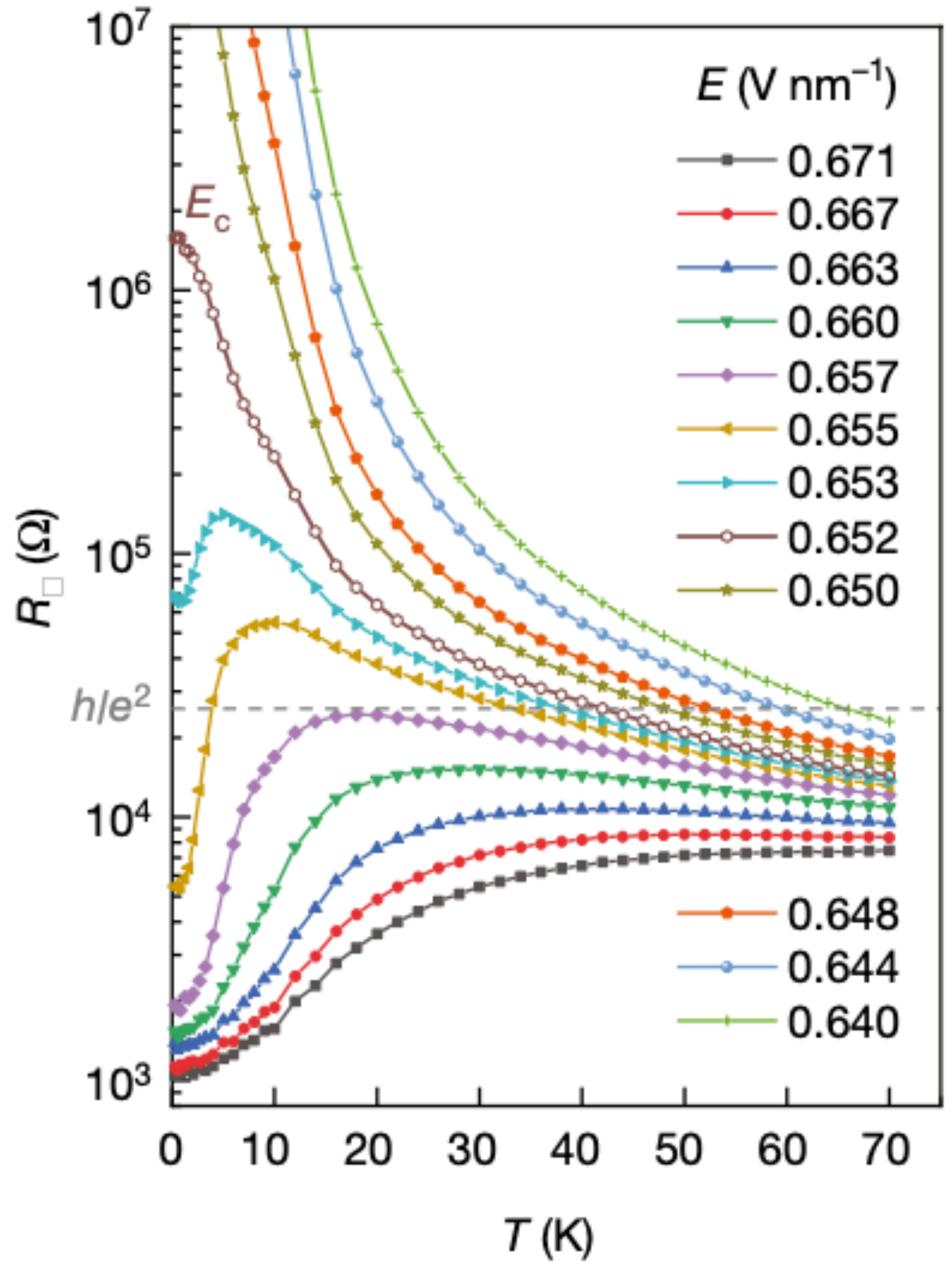

no topology

Article

Quantum anomalous Hall effect from intertwined moiré bands

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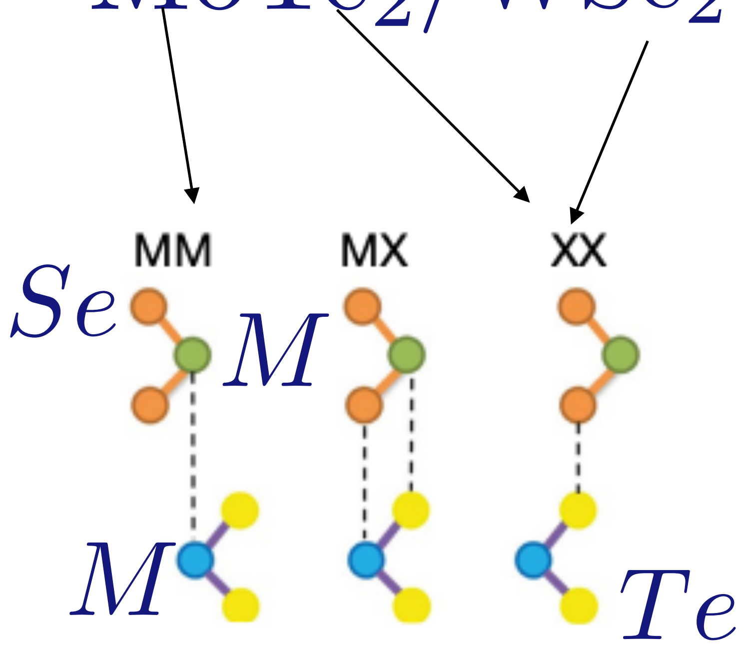
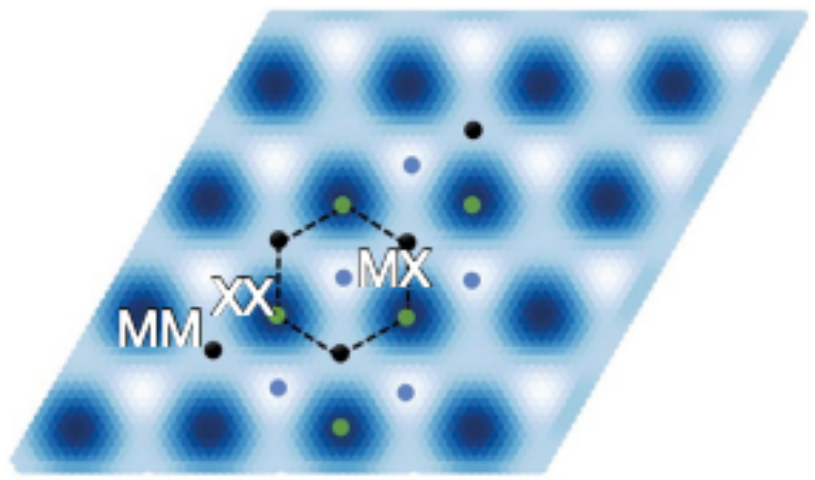
Tingxin Li[1,2,6], Shengwei Jiang[1,2,6], Bowen Shen[1,6], Yang Zhang[3,6], Lizhong Li[1], Zui Tao[1], Trithep Devakul[3], Kenji Watanabe[4], Takashi Taniguchi[4], Liang Fu[3], Jie Shan[1,5]✉ & Kin Fai Mak[1,5]✉

$MoTe_2/WSe_2$

triangular moir\'e superlattice





AB-stacking

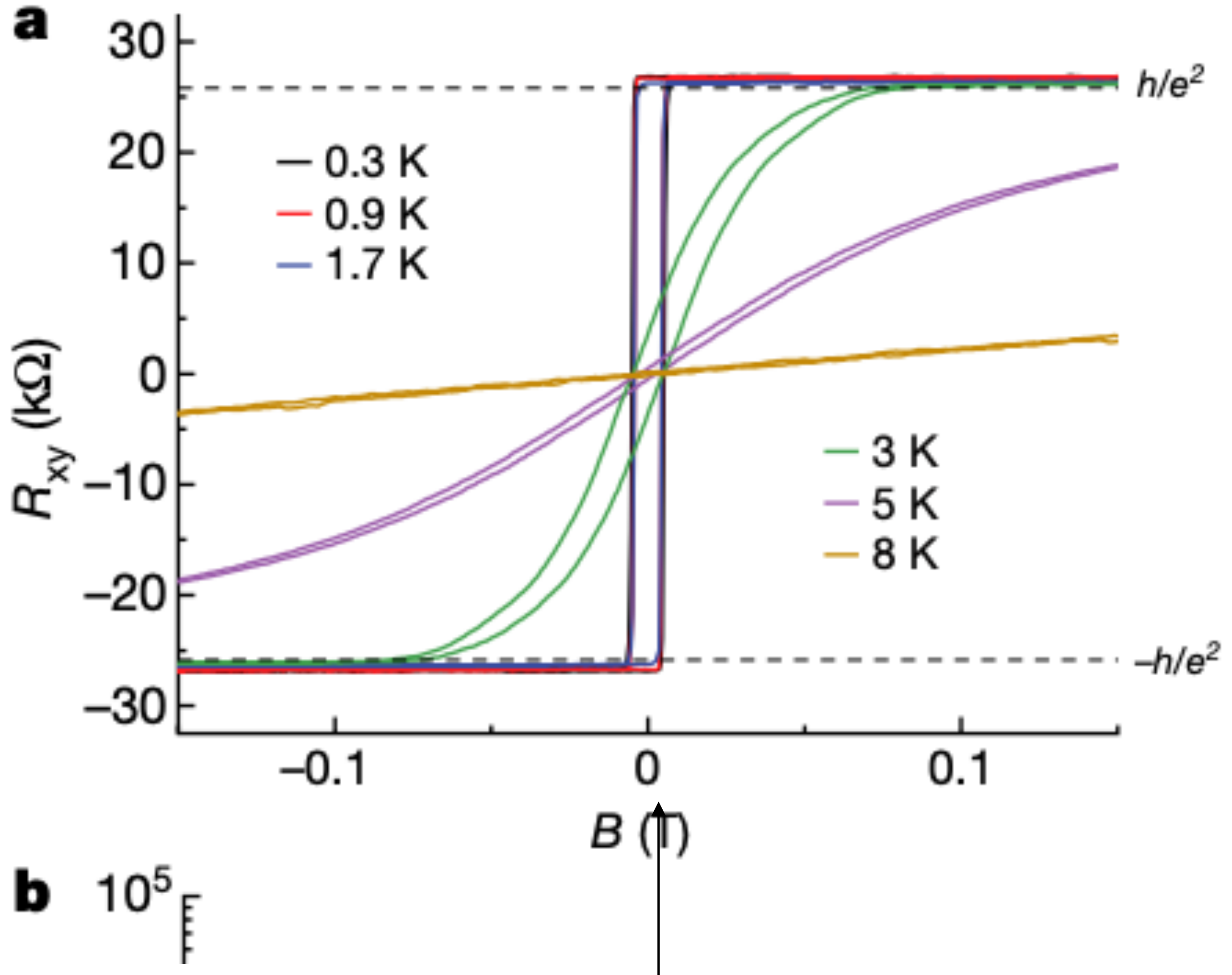
$$\lambda_M = 5nm$$

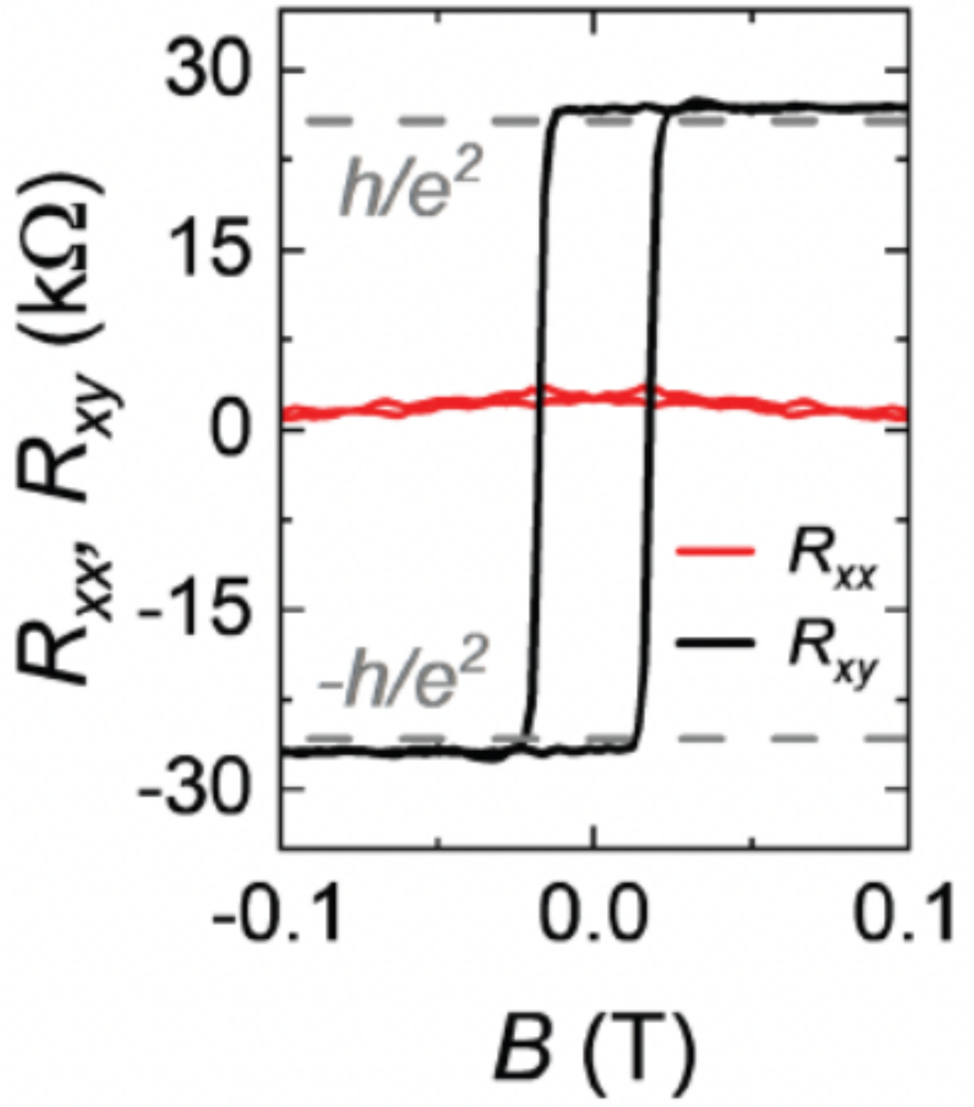
$$n_M = 5 \times 10^{12} cm^{-2}$$

$$\nu = \frac{n_e}{n_M}$$

$R_{\rm xy} \neq 0$

is this just
Haldane physics?



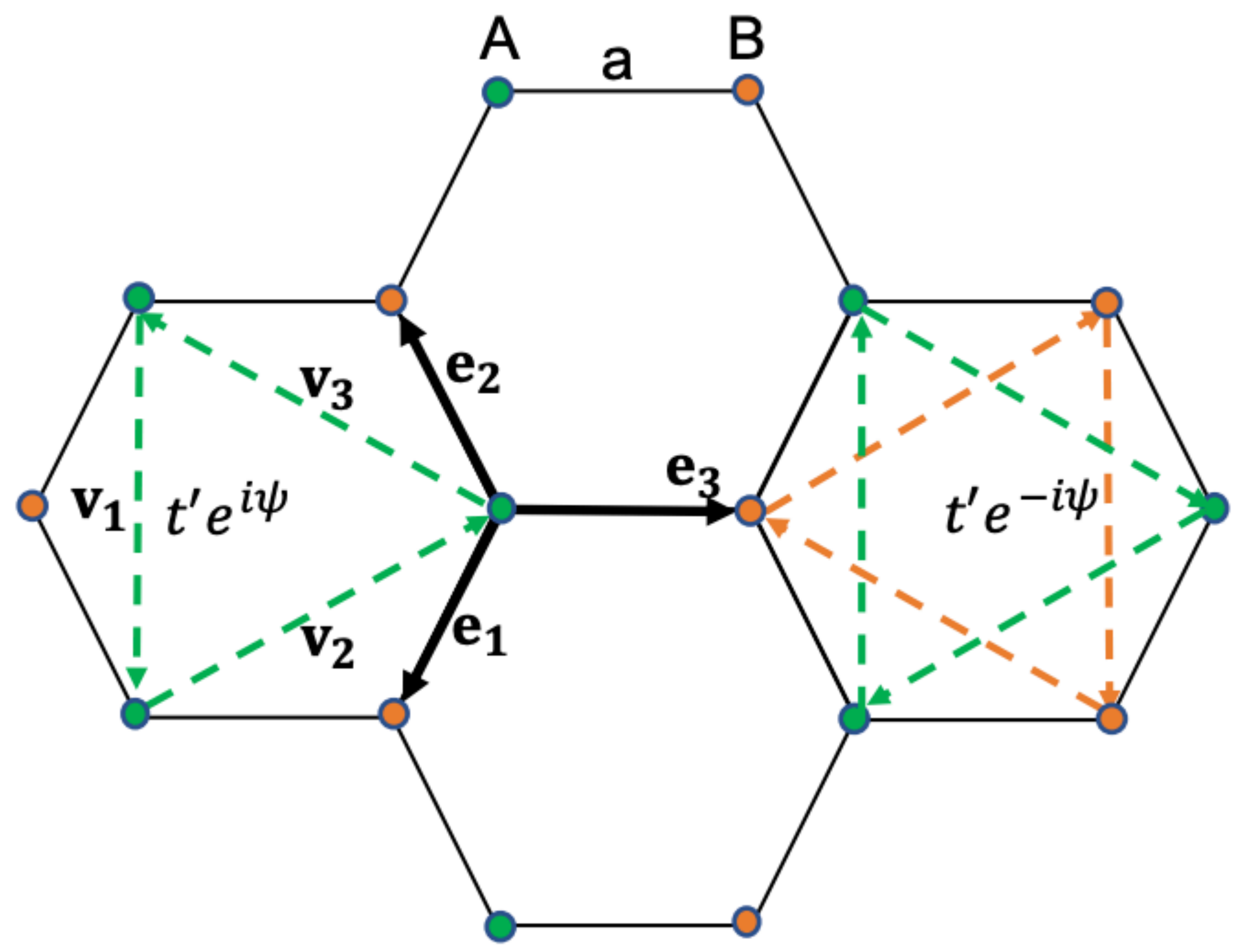


$B = 0$

$R_{\rm xx} \approx 0$

QAH

Haldane model



QHE without Landau levels

topology without net magnetic field!

$$\varepsilon_{\pm,\mathbf{k}} = h_0(\mathbf{k}) \pm \sqrt{h_x^2(\mathbf{k}) + h_y^2(\mathbf{k}) + h_z^2(\mathbf{k})}$$

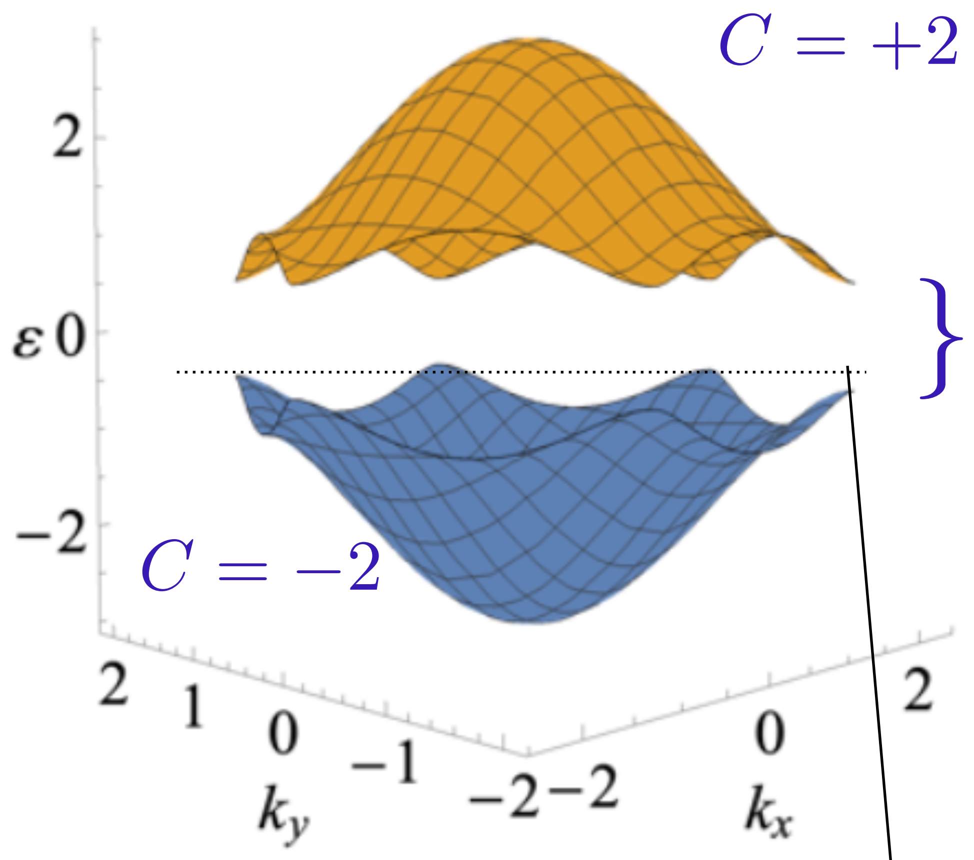
$$h_0(\mathbf{k}) = -2t' \cos\psi[\sum_{i=1}^{3} \cos(\mathbf{k}\cdot\mathbf{v}_i)],$$

$$h_x(\mathbf{k}) = -t[\sum_{i=1}^{3} \cos(\mathbf{k}\cdot\mathbf{e}_i)],$$

$$h_y(\mathbf{k}) = -t[\sum_{i=1}^{3} \sin(\mathbf{k}\cdot\mathbf{e}_i)],$$

$$h_z(\mathbf{k}) = M - 2t' \sin\psi[\sum_{i=1}^{3} \sin(\mathbf{k}\cdot\mathbf{v}_i)],$$

Semenoff mass



$$\Delta = \min(2\Delta_0, 2)$$

$$\Delta_0 = 3\sqrt{3}|t' \sin\psi|$$

$|M| > \Delta_0$ → $C = 0$

topologically trivial

AA-TMD

$|M| < \Delta_0$ → $C = \pm 2$

topologically non-trivial

AB-TMD

half-filling or $\nu = 2$

$$A_i = -i \sum_{\text{occupied}} \langle k, \alpha | \partial_{k_i} | k, \alpha \rangle$$

$$C_1 = \frac{1}{2\pi} \int \partial_{[x} A_{y]} d^2 k$$

A_i is singular

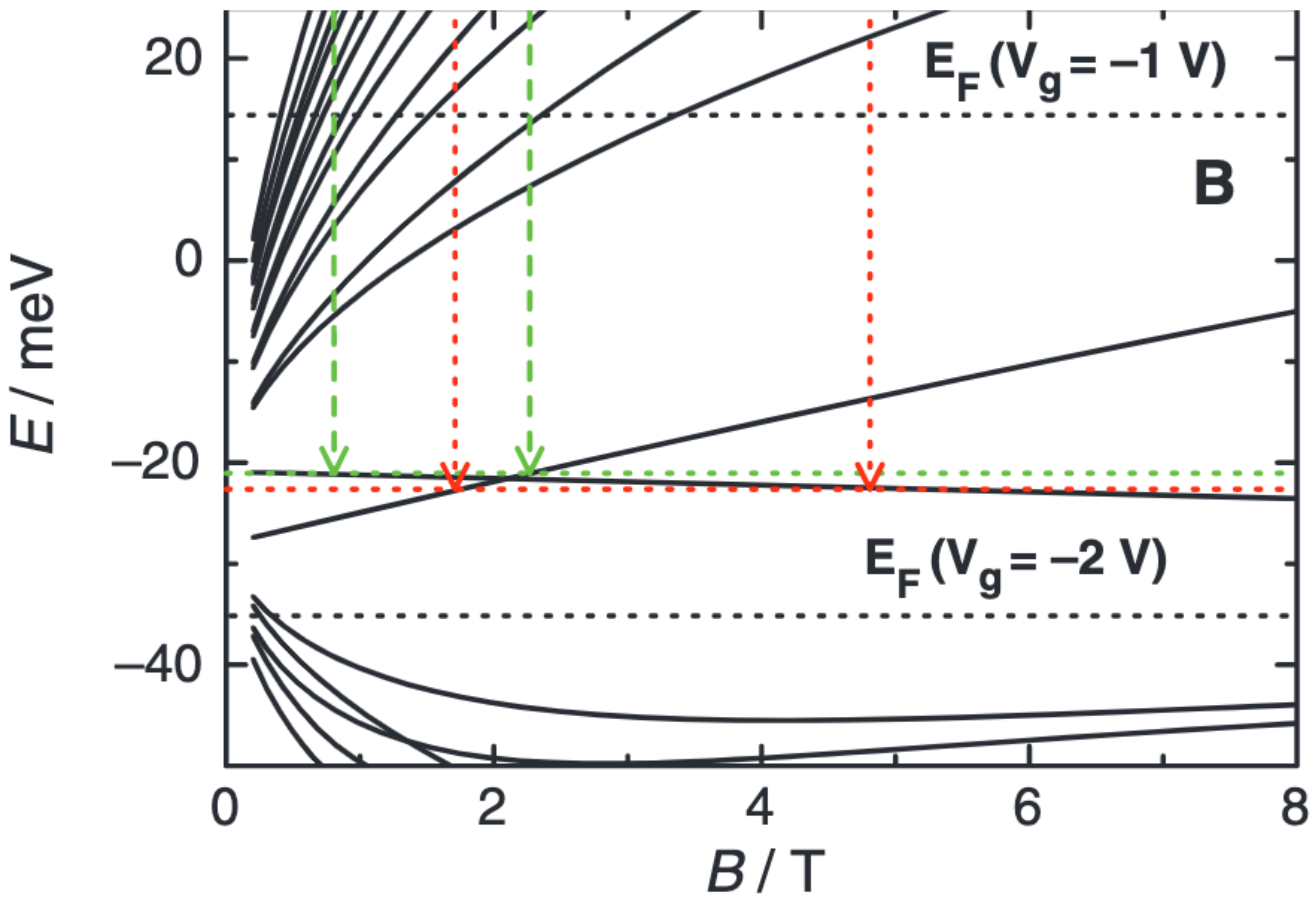
$$C_1 \neq 0$$

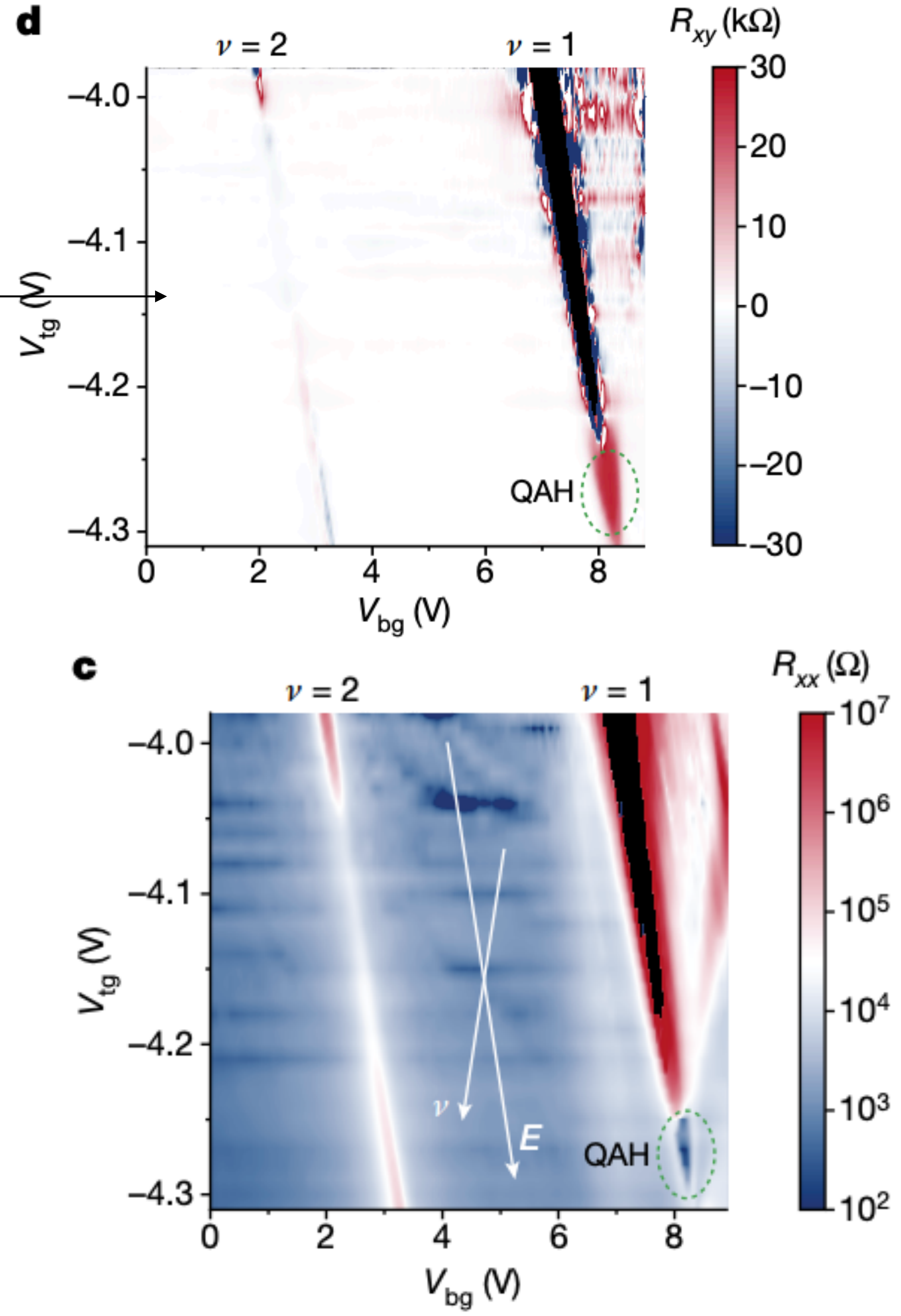
flux through 2-torus

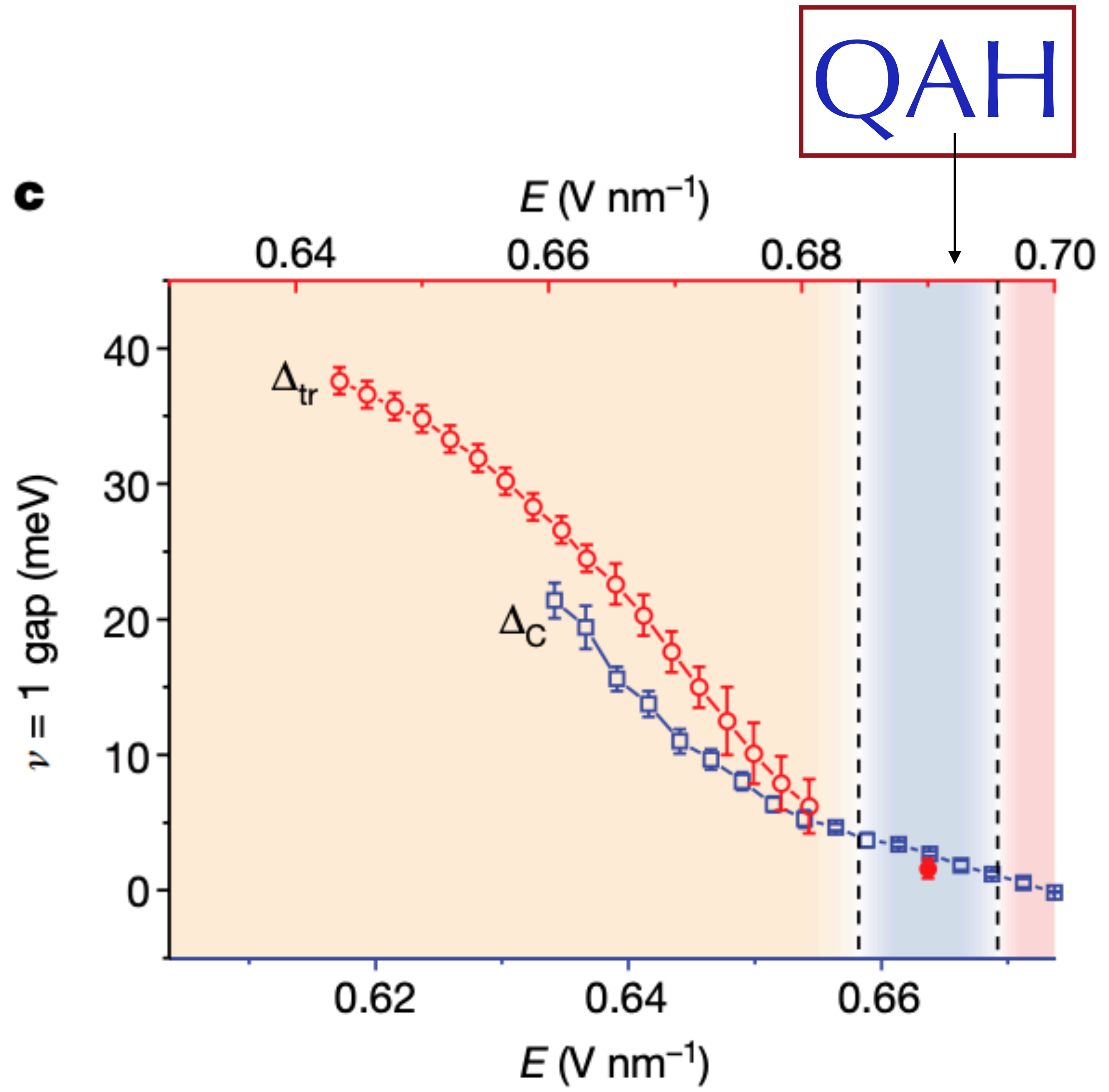
Experiment

$\nu = 1$

QSH effect





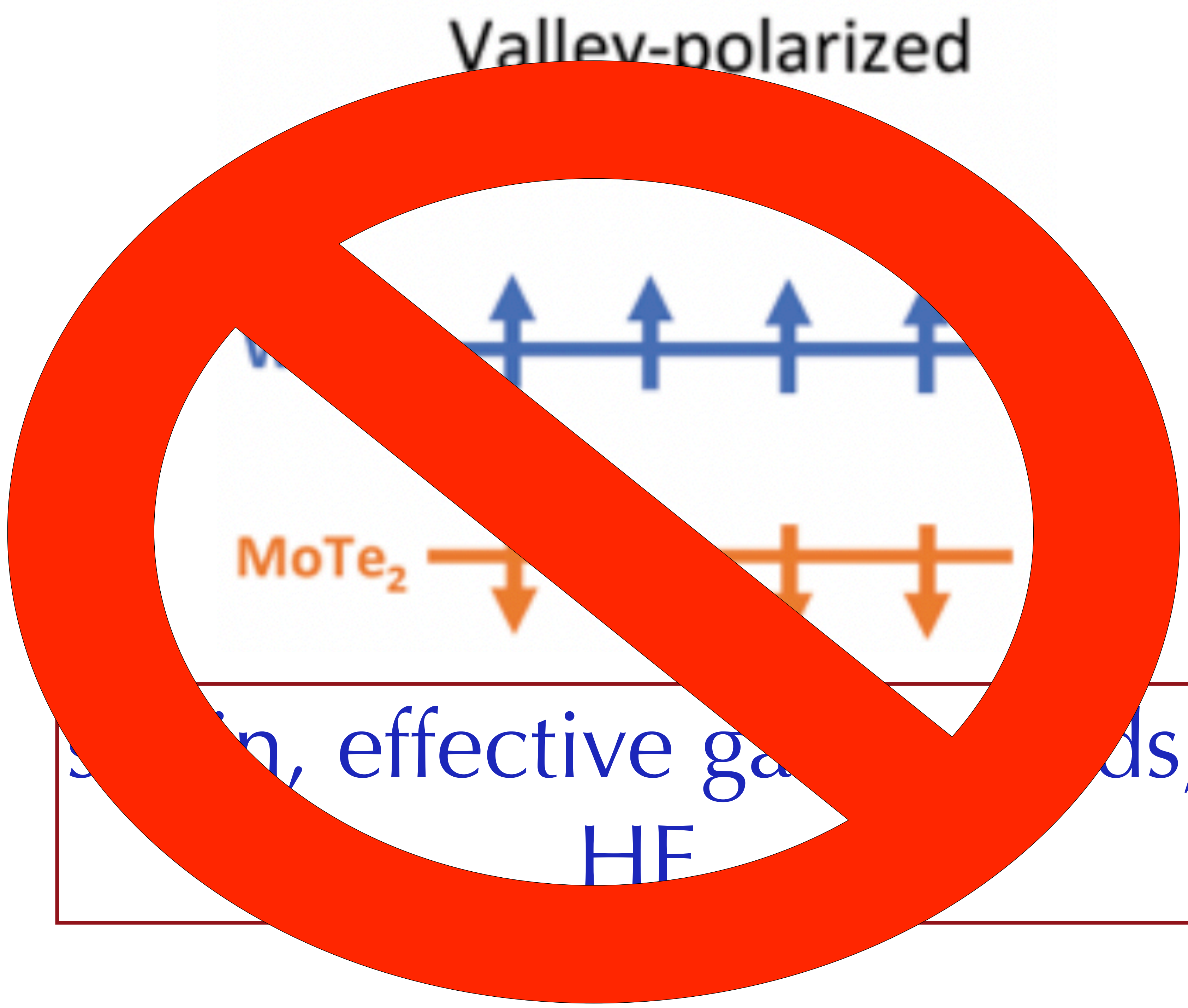


$$\nu = 2 \xrightarrow{\Delta \neq 0} \nu = 1$$

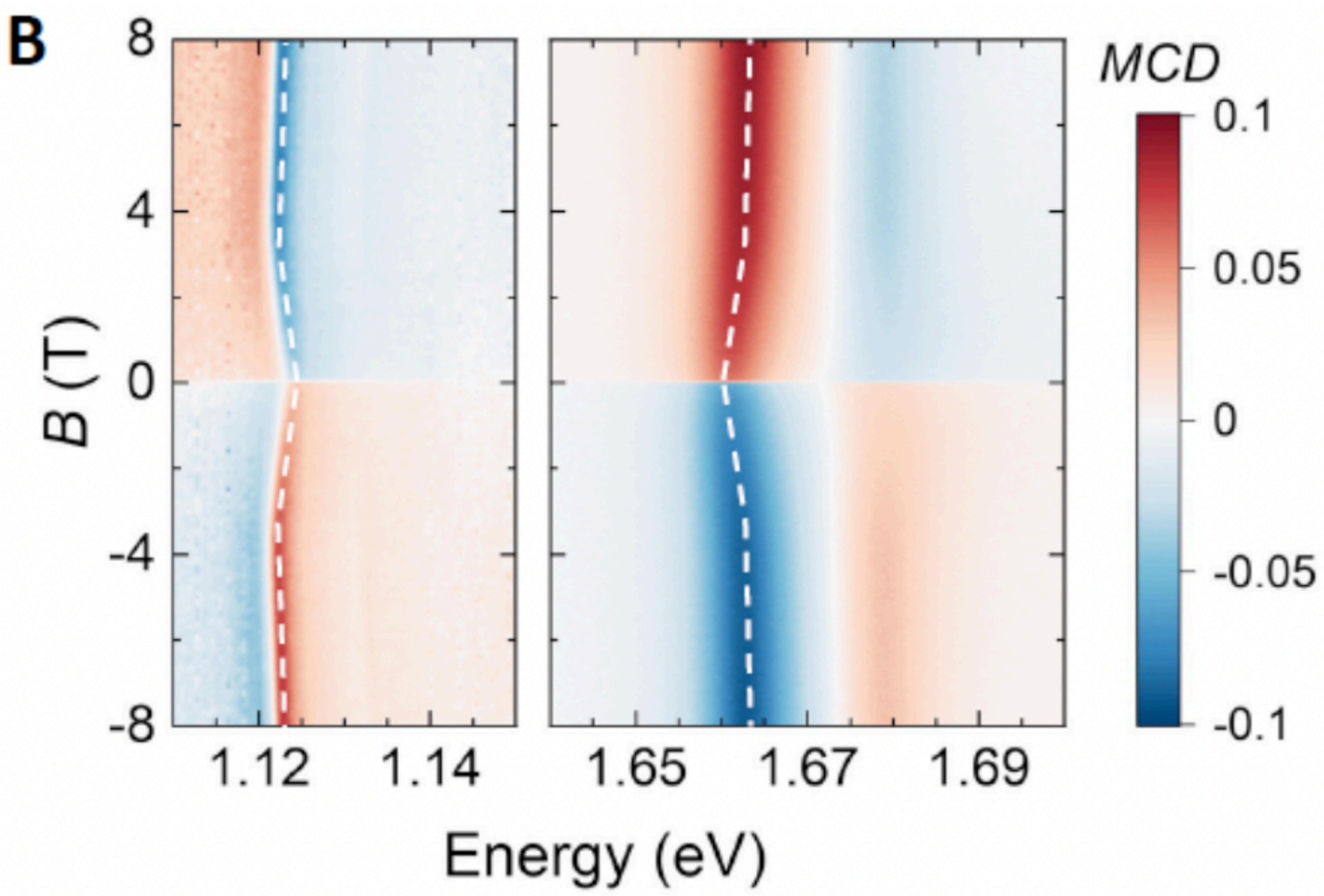
$$C_1 = 0 \qquad\qquad C_1 \neq 0$$

not just Haldane
non-interacting physics

arxiv-2208.07452

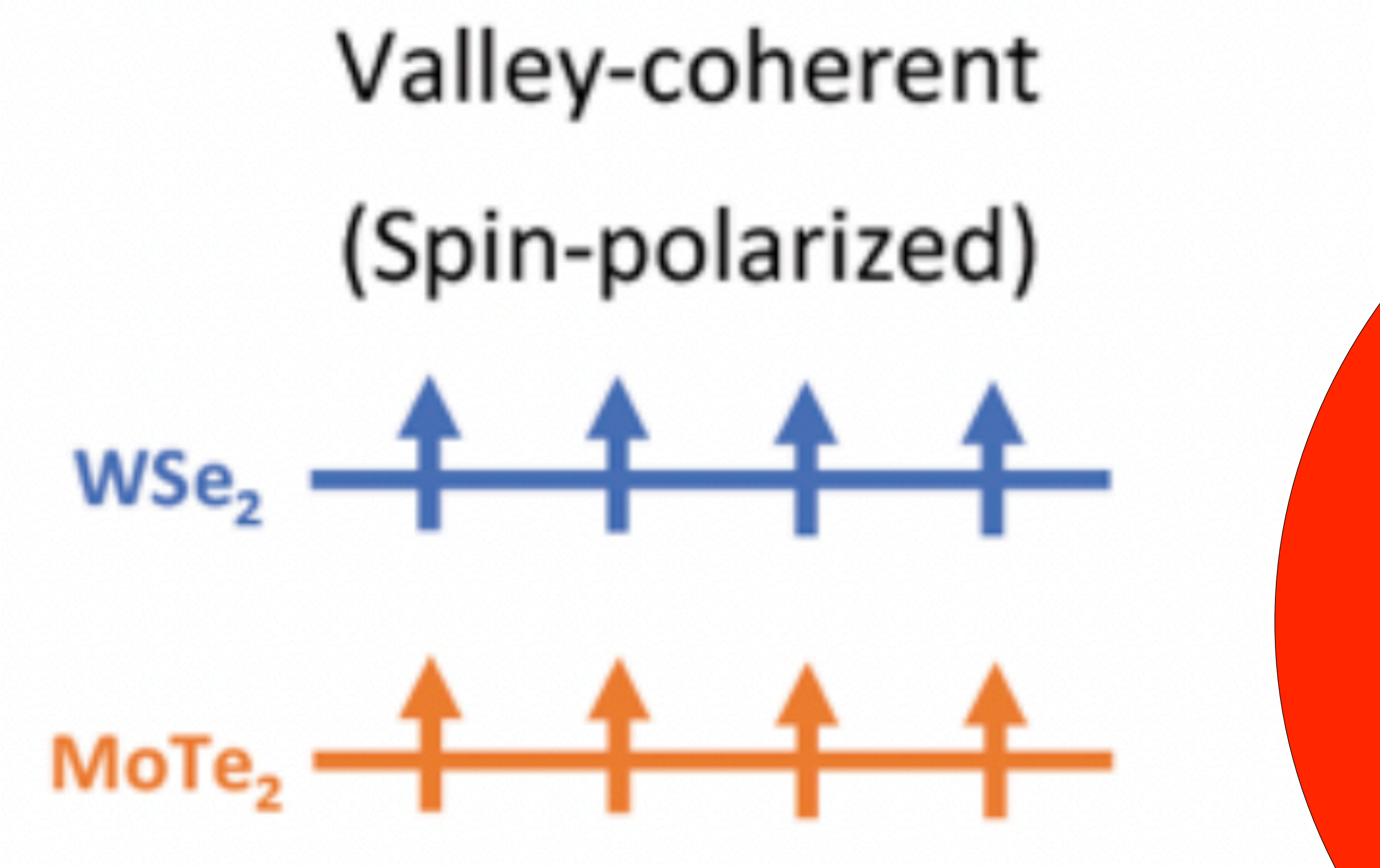


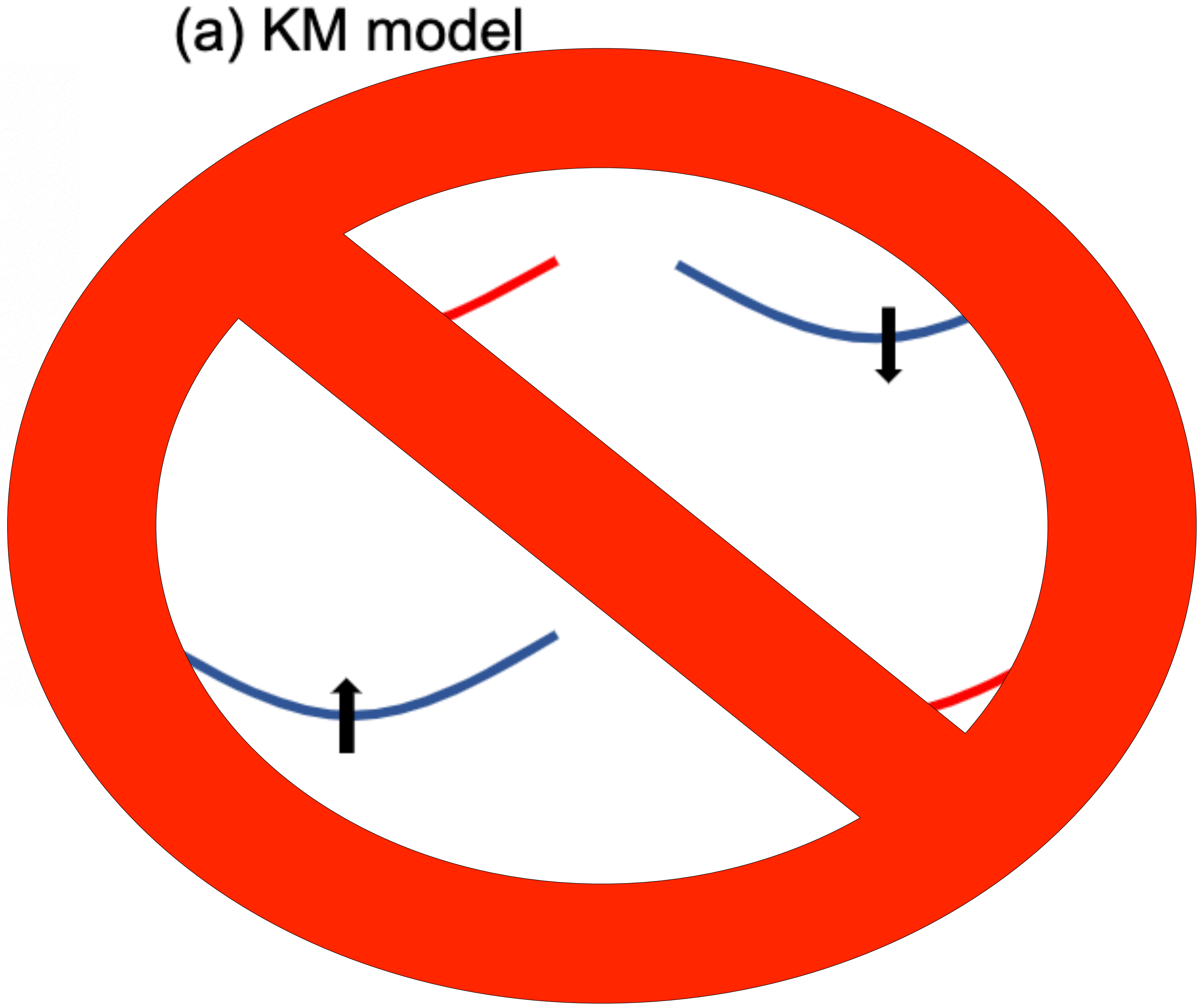
…n, effective ga… …ds,
HF



valleys contribute
equally

$C_1/\text{spin} \neq 0$





to explain

QSH+ QAH
in same sample

$$\nu = 2 \xrightarrow{\Delta \neq 0} \nu = 1$$

$C_1 = 0$ $\qquad$ $C_1 \neq 0$

beyond Haldane and
KM/BHZ models

are interactions important?

TABLE II. Wigner crystallization criteria for a nearly aligned HeMs at $\theta = 0.5^\circ$. Among the HeMs listed here, $MoSe_2/WSe_2$ and MoS_2/WS_2 seem to be the most susceptible to forming an electronic and hole GWC, respectively. At least one experimental study of the pertinent HeM is referenced here. The effective masses are adapted from Ref. [62]. The unit of density is $n_e = 10^{12}\,\mathrm{cm}^{-2}$. Asterisked values in the r_s row indicate values crossing the crystallization threshold.

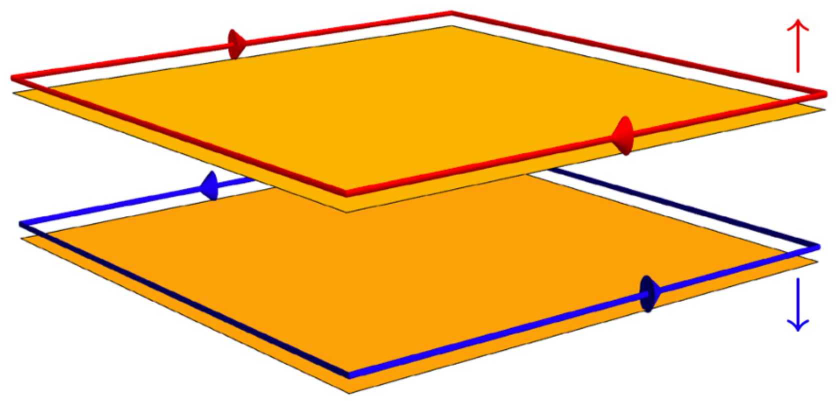
HeMs	WSe_2/WS_2	$MoSe_2/MoS_2$	$MoTe_2/MoSe_2$	$MoSe_2/WS_2$	$MoSe_2/WSe_2$	MoS_2/WS_2	$MoTe_2/WSe_2$
Refs.	[13,63]	[64]	[65,66]	[67]	[68,69]	[70]	[71]
$m^*_{e(h)}/m_0$	0.28 (0.46)	0.42 (0.71)	0.46 (1.37)	0.28 (0.71)	0.54 (0.44)	0.46 (1.70)	0.30 (1.33)
$2/(\epsilon_1^{-1}+\epsilon_2^{-1})$	2.9	3.35	4.08	3.29	3.29	2.95	3.5
λ_m (nm)	8.1	8.1	5.3	7.6	35.6	34.0	5.1
$U/W\|_{e(h)}$	3.0 (4.9)	3.9 (6.6)	2.3 (6.9)	2.5 (6.3)	22.4 (18.2)	20.3 (75.1)	1.7 (7.5)
$r_s^{e(h)}\|_{10^{12}\ \mathrm{cm}^{-2}}$	20.6 (33.8*)	26.7 (45.2*)	24.0 (71.6*)	18.2 (46.0*)	35.0* (28.5)	33.3* (122.9*)	18.3 (81.1*)
T_L (K)	7.1	6.1	7.6	6.7	1.4	1.7	9.3
$n^{\max}_{e(h)}$ (10^{12} cm^{-2})	0.5 (1.3)	0.8 (2.3)	0.7 (5.9)	0.4 (2.4)	1.4 (0.9)	1.3 (17.4)	0.4 (7.5)
$\nu^{e(h)}_{\max}$	0.28 (0.73)	0.46 (1.31)	0.17 (1.46)	0.2 (1.19)	15.56 (10.0)	13.0 (174.0)	0.09 (1.7)

Topology + Strong Correlations?

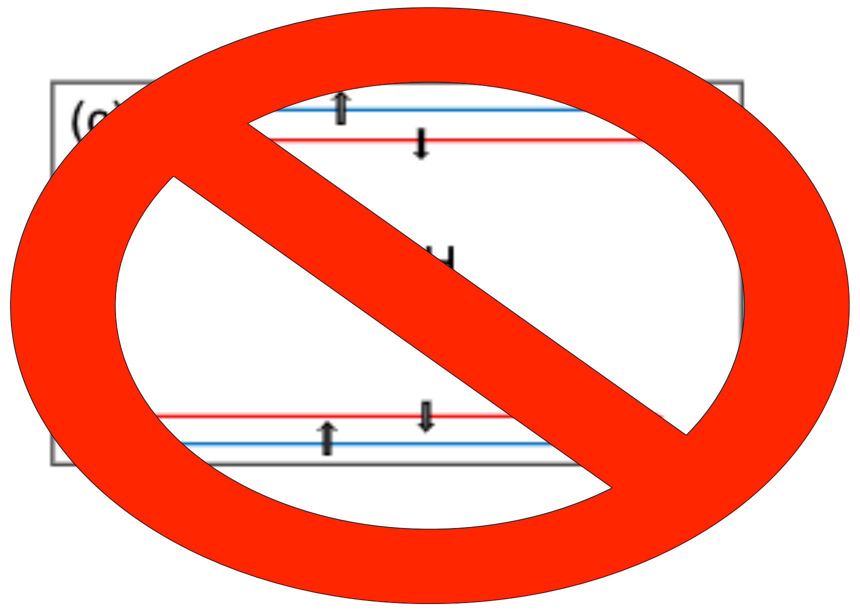
Are Exact Statements Possible?

yes

why is 1/4-filling important?



+ interactions → $E_k(\uparrow) \neq E_k(\uparrow\downarrow)$



only singly occupied state
can cross the chemical potential

edge state with bulk gap

$$1/2 \rightarrow 1/4$$

topology

interactions

k-space

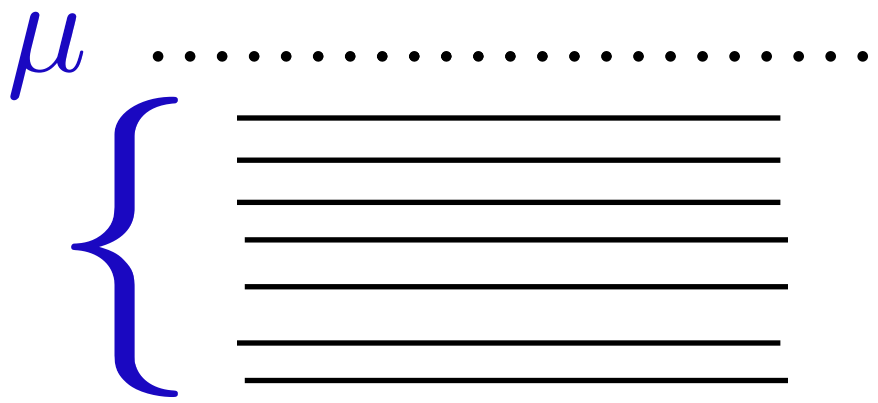
real space

how should they be combined?

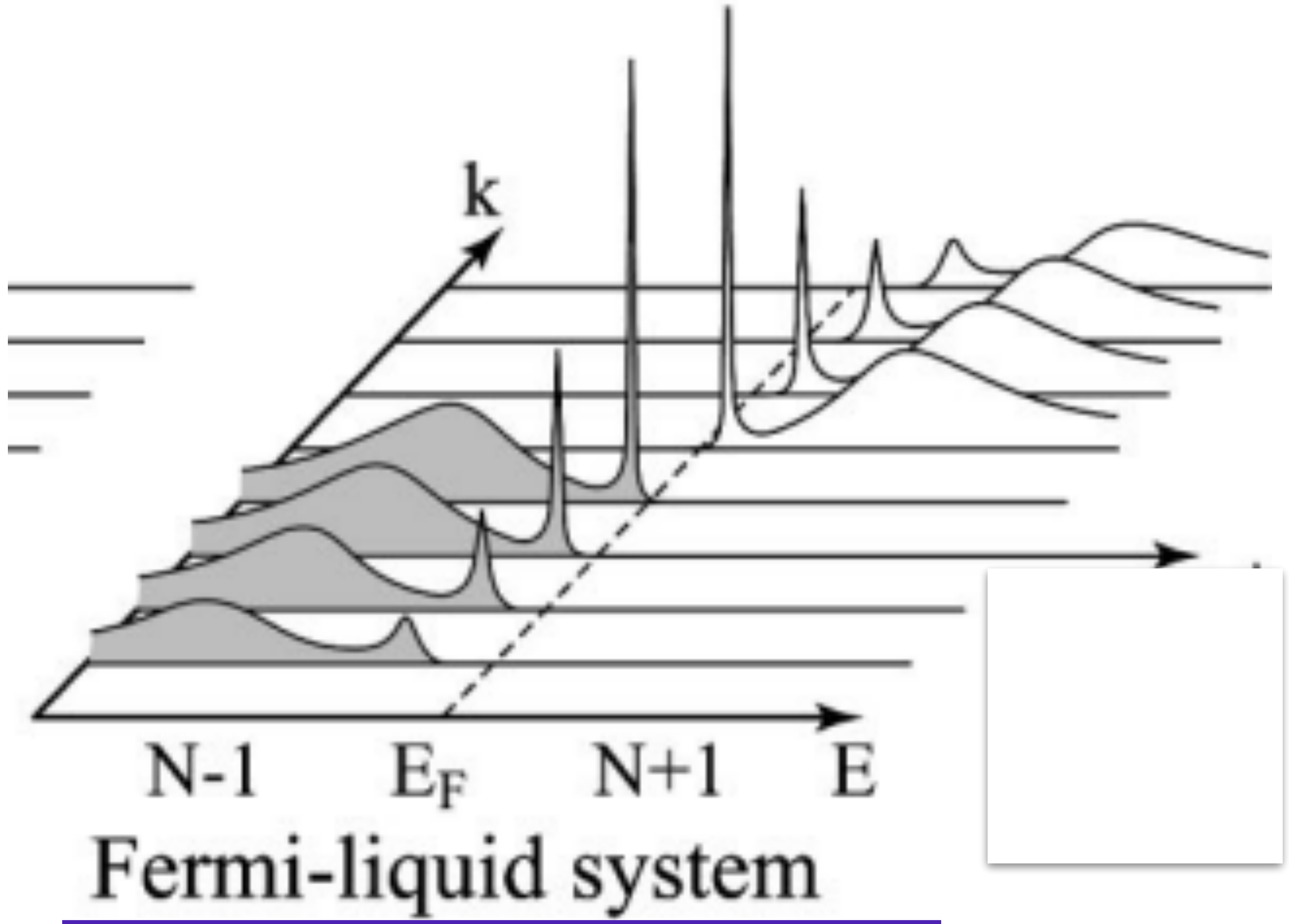
Fermi liquids

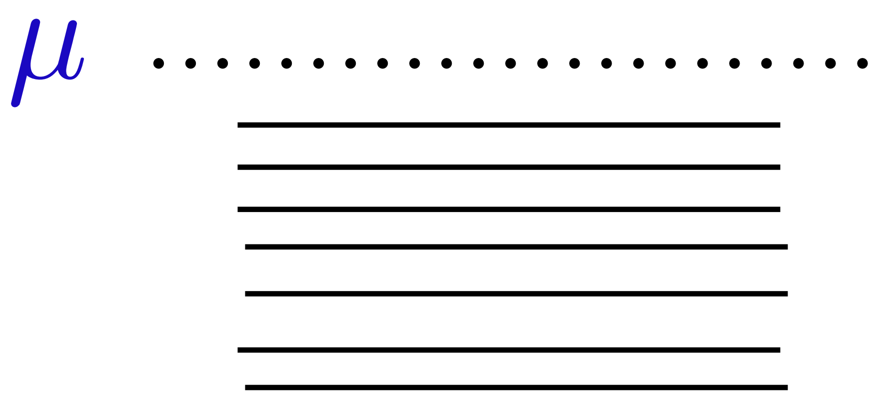
NFL

doubly occupied



Is single occupancy below chemical potential possible?





with time-reversal symmetry in tact?

p-h symmetry

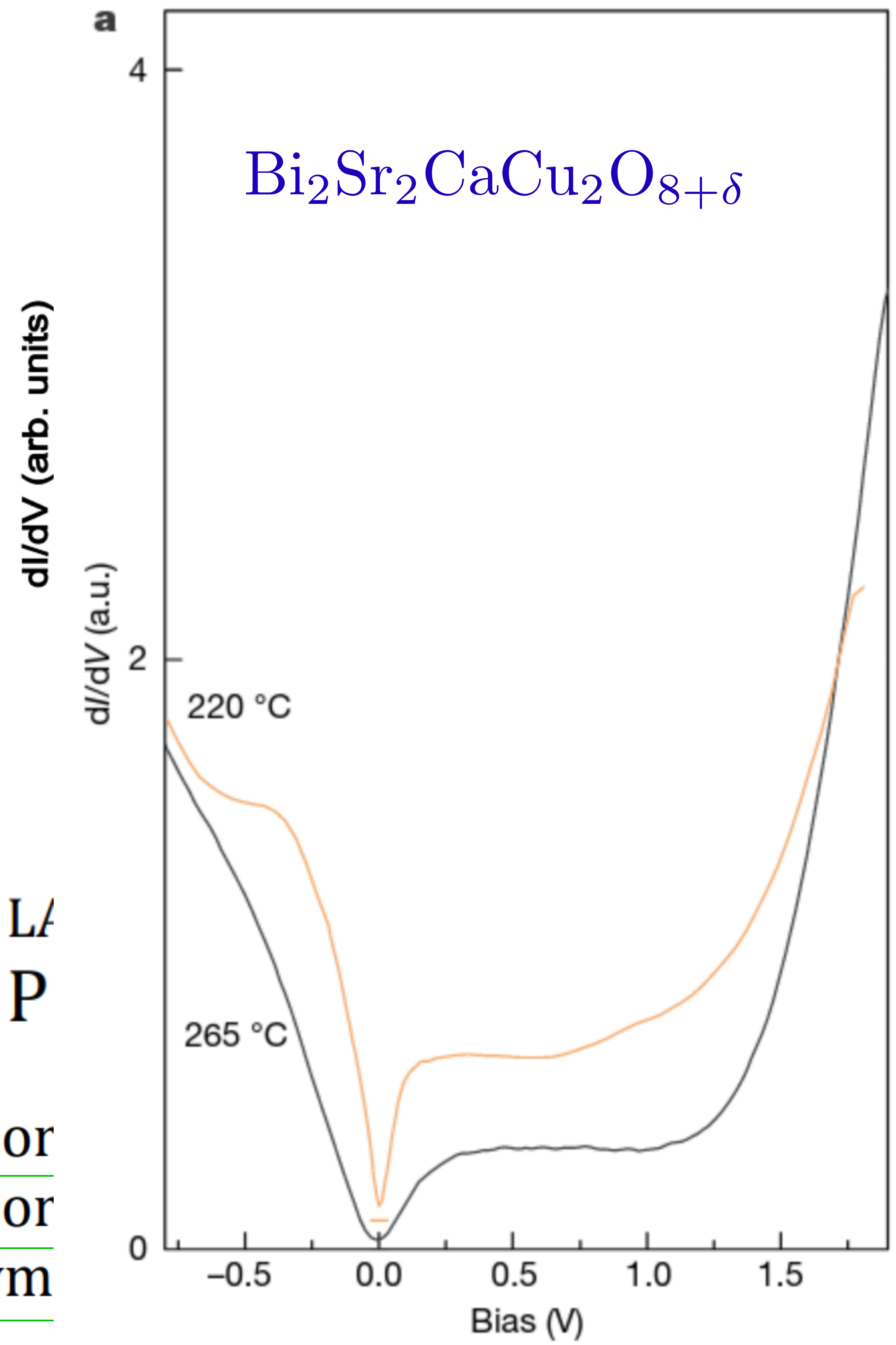
LA

P iversity

theor universal refusal of

theor f hole-particle

asym t the first step of any



single occupancy

?

particle-hole asymmetry

Anderson
Haldane
2000

3 citations

Fermi liquids

$$H = \sum_{p,\sigma} (\epsilon(p) - \epsilon_F)\, n_{p\sigma} + \cdots \quad \rightarrow 0$$

$(n_{p\uparrow}, n_{p\downarrow})$ conserved currents

$(c_{p\uparrow}, c_{p\downarrow}, \mathrm{h.c.})$ 4 objects

$O(4)$

$\mathrm{DetM} = 1$ → SO(4) proper rotations

$\mathrm{DetM} = -1$ → improper rotations

$$\mathrm{Det}\, M = \pm 1 \implies Z_2 = O(4) \div SO(4)$$

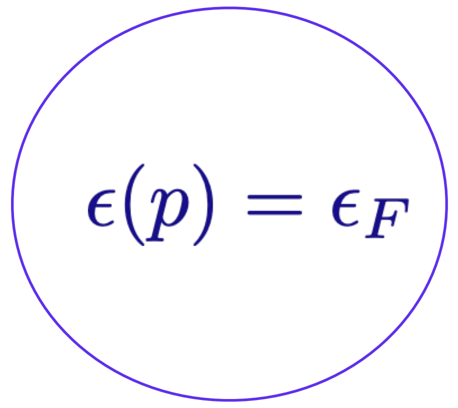
Improper Rotations

Majorana basis

$$\begin{pmatrix} c_{p\uparrow} \\ c^\dagger_{p\uparrow} \\ c_{p\downarrow} \\ c^\dagger_{p\downarrow} \end{pmatrix} \longrightarrow \begin{pmatrix} c_{p\uparrow} + c^\dagger_{p\uparrow} \\ i(c_{p\uparrow} - c^\dagger_{p\uparrow}) \\ c_{p\downarrow} + c^\dagger_{p\downarrow} \\ i(c_{p\downarrow} - c^\dagger_{p\downarrow}) \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} c_{p\uparrow} + c^\dagger_{p\uparrow} \\ i(c_{p\uparrow} - c^\dagger_{p\uparrow}) \\ c_{p\downarrow} + c^\dagger_{p\downarrow} \\ i(c_{p\downarrow} - c^\dagger_{p\downarrow}) \end{pmatrix} \Rightarrow c_{p\downarrow} \to c^\dagger_{p\downarrow}$$

p-h transformation



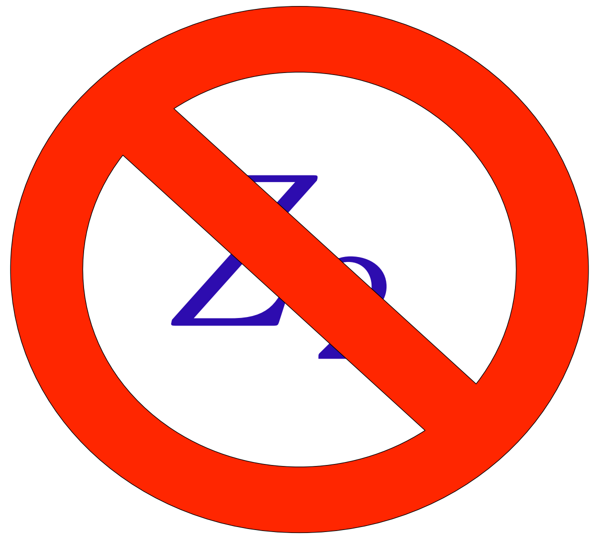
Fermi Surface

$$H = 0$$

$$\left.\begin{array}{r} n_{p\uparrow} \to 1 - n_{p\uparrow} \\ n_{p\downarrow} \to n_{p\downarrow} \end{array}\right\} Z_2$$

at Fermi surface only

How to destroy Fermi liquids?



$$H = \sum_{p,\sigma} (\epsilon(p) - \epsilon_F)\, n_{p\sigma} + U n_{p\uparrow} n_{p\downarrow}$$

odd under Z_2

New fixed point!

Hatsugai-Kohmoto or Baskaran model

scaling dimension

$[n_{p\uparrow} n_{p\downarrow}] = -2$

relevant interaction

Hubbard not necessary!

General HK Model

$$\sum_k (\xi_k (n_{k\uparrow} + n_{k\downarrow}) + U n_{k\uparrow} n_{k\downarrow}) \quad [\hat{U}_{\rm int}(k), \hat{T}] = 0$$

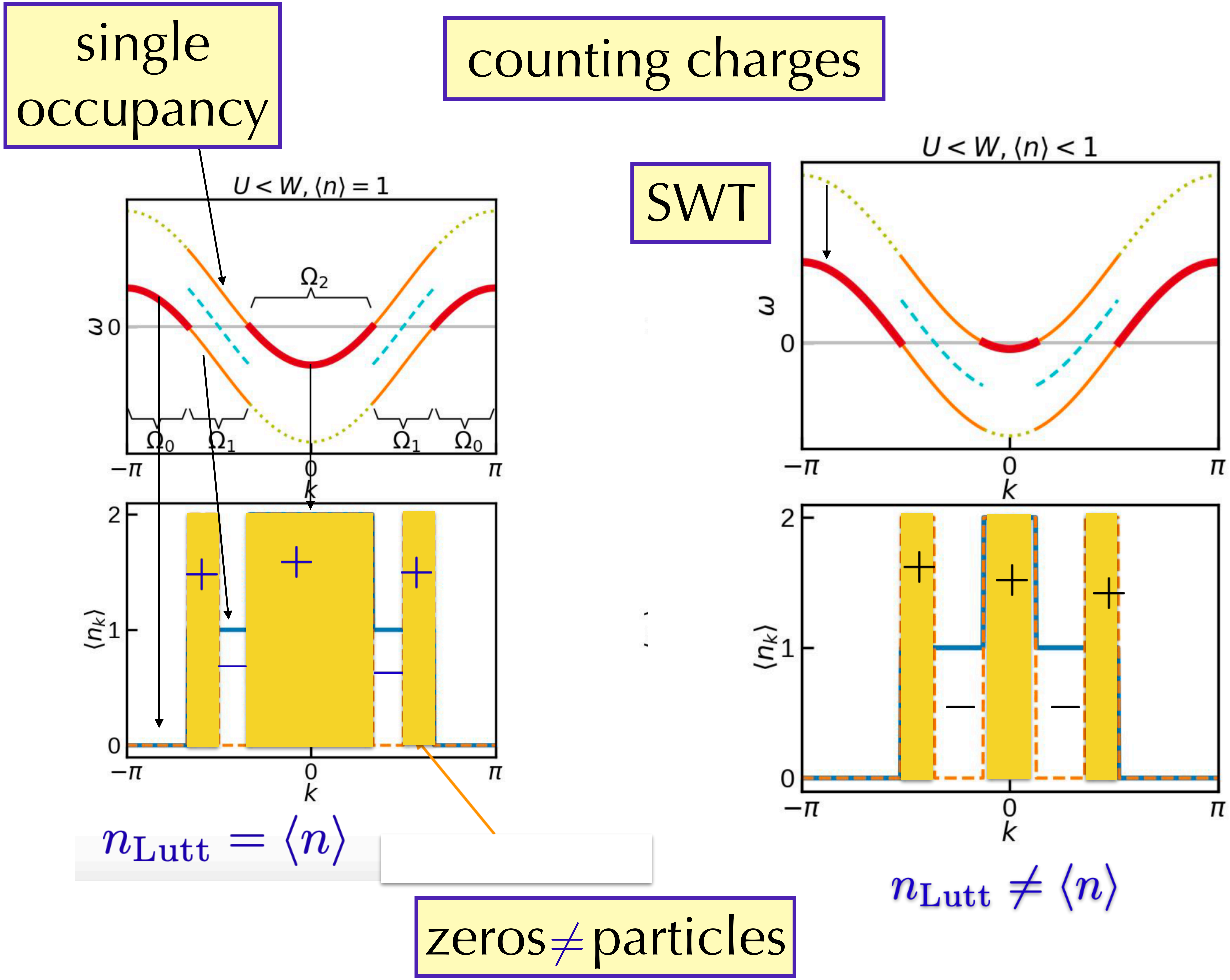
Solvable Mott transition:U>W

$$G_{k\sigma}(i\omega_n \to z) = \frac{1 - \langle n_{k\bar{\sigma}} \rangle}{z - \xi_k} + \frac{\langle n_{k\bar{\sigma}} \rangle}{z - (\xi_k + U)} \neq \frac{1}{z - \omega_k}$$

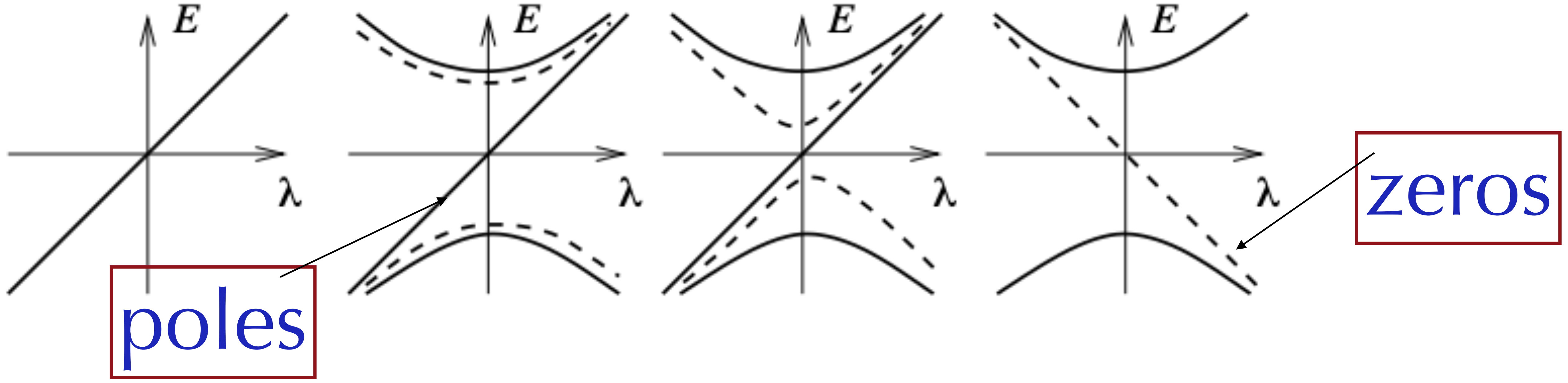
lower Hubbard band

upper Hubbard band

zeros



single occupancy
counting charges
SWT
U < W, ⟨n⟩ = 1
U < W, ⟨n⟩ < 1
Ω2
Ω0
Ω1
Ω1
Ω0
ω
0
−π
0
π
k
⟨nk⟩
2
1
0
+
−
$n_{\mathrm{Lutt}} = \langle n \rangle$
$n_{\mathrm{Lutt}} \neq \langle n \rangle$
zeros≠particles

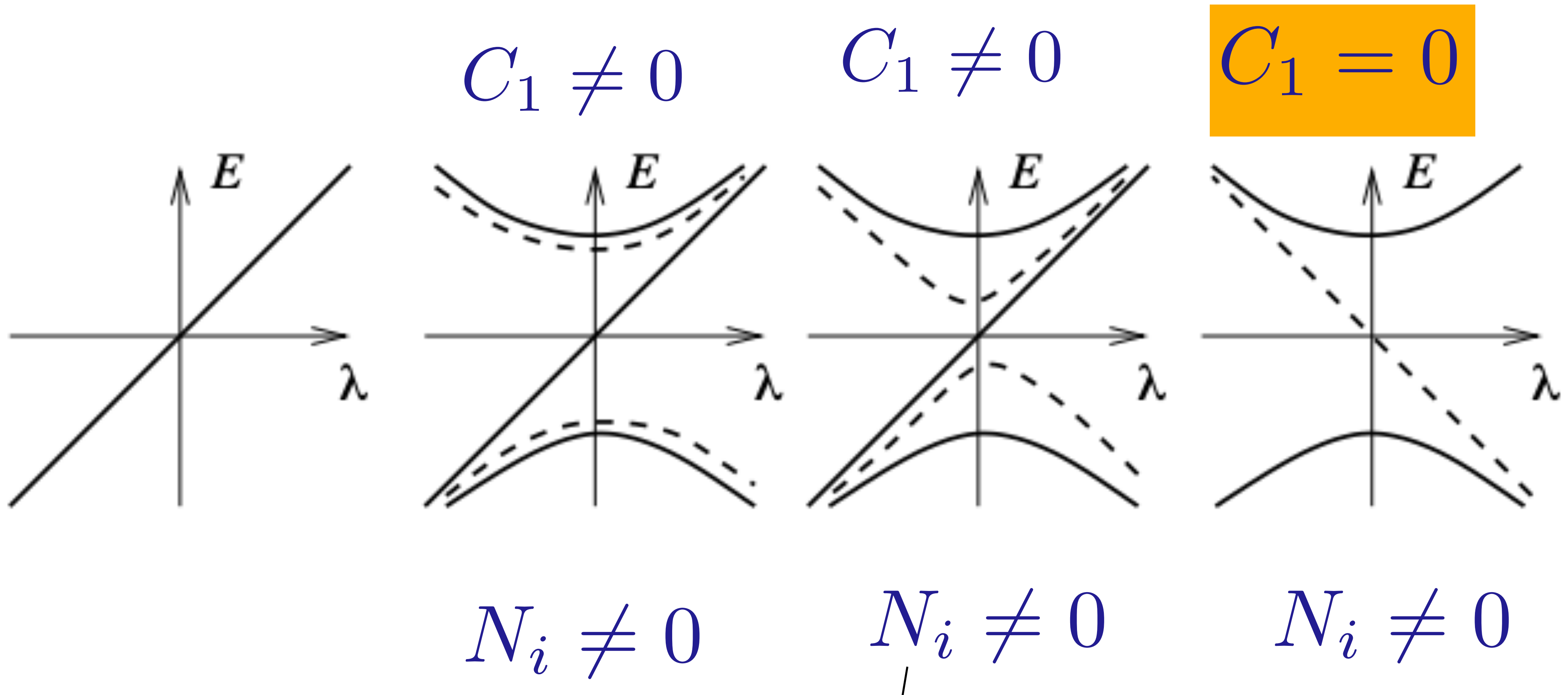


invariants

poles zeros

$$N_1 = \mathrm{Tr}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}G^{-1}\partial_\omega G = \sum_n \mathrm{sgn}(\epsilon_n) - \sum_s \mathrm{sgn}(r_s)$$

$$N_3 = \frac{\varepsilon_{\alpha\beta\delta}}{6}\mathrm{Tr}\int_{-\infty}^{\infty}d\omega\int_{\mathrm{BZ}}d^2k G^{-1}\partial_\alpha G G^{-1}\partial_\beta G G^{-1}\partial_\delta G$$



Luttinger count

$$n_e = \int_{\mathrm{DetReG}(\omega=0,\mathrm{k})>0} \frac{d^d k}{(2\pi)^d}$$

zeros+poles

same ambiguity

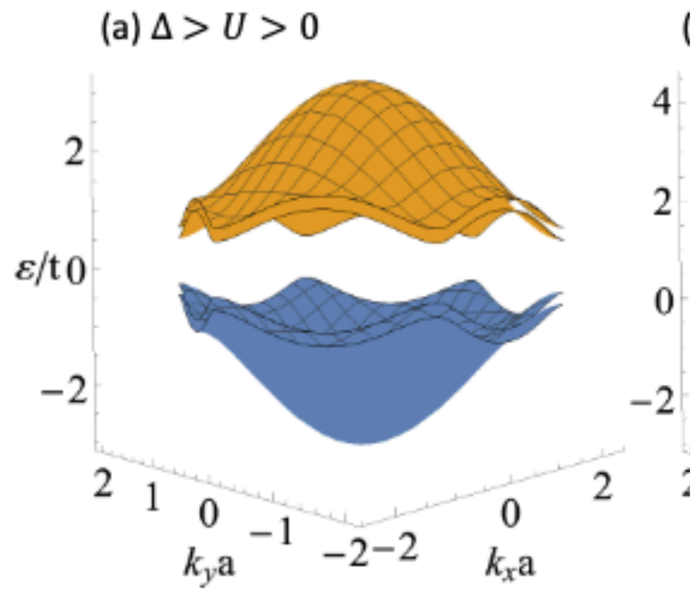
Haldane bands

$$H = \sum_{\mathbf{k},\sigma} \left[(\varepsilon_{+,\mathbf{k}} - \mu) n_{+,\mathbf{k}\sigma} + (\varepsilon_{-,\mathbf{k}} - \mu) n_{-,\mathbf{k}\sigma} \right]$$

$$+U \sum_{\mathbf{k}} (n_{+,\mathbf{k}\uparrow} n_{+,\mathbf{k}\downarrow} + n_{-,\mathbf{k}\uparrow} n_{-,\mathbf{k}\downarrow})$$

Hubbard in momentum space

generalisation $n_{+,-k\uparrow} n_{\pm,k\downarrow}$



TI

$\langle n \rangle = 2$

$C = -2$

1/4-filled MI

$\langle n \rangle = 1 \quad C = -1$

$\langle n \rangle = 2 \quad C = 0$

$\langle n \rangle = 3 \quad C = 1$

topological MI because Haldane gap is preserved

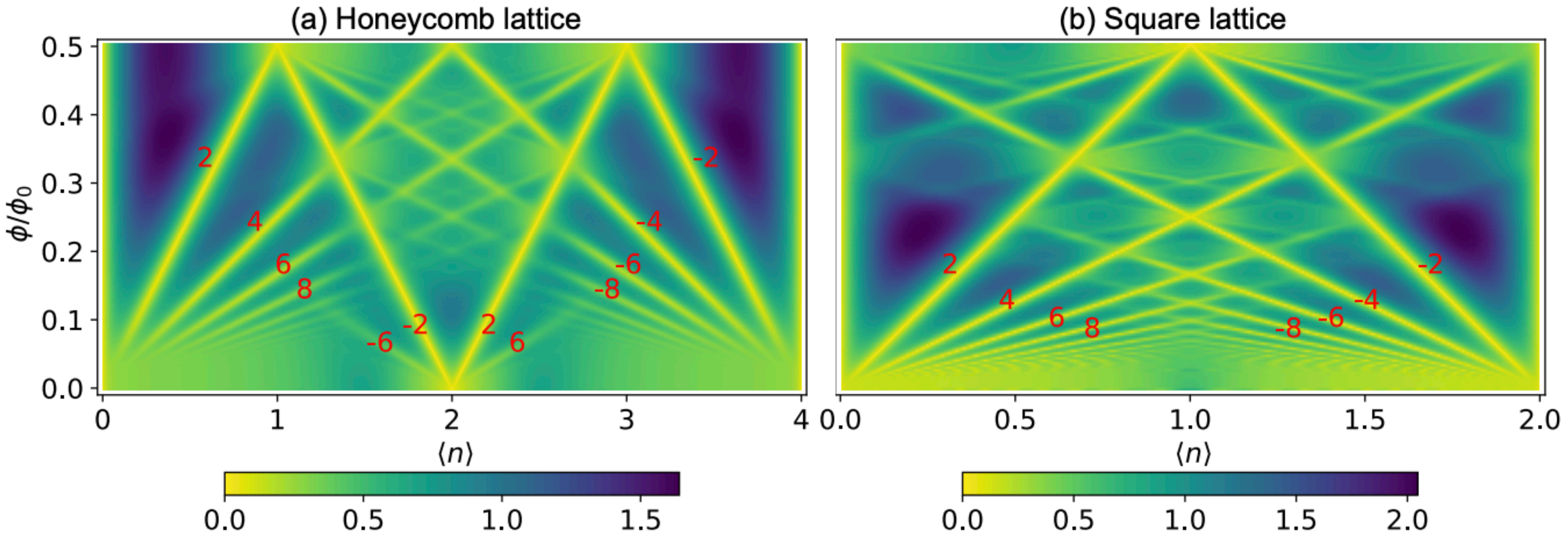
Haldane-Hubbard model?

Hofstadter Spectrum

$$\langle n \rangle = r\frac{\phi}{\phi_0} + s$$

$r \equiv C$

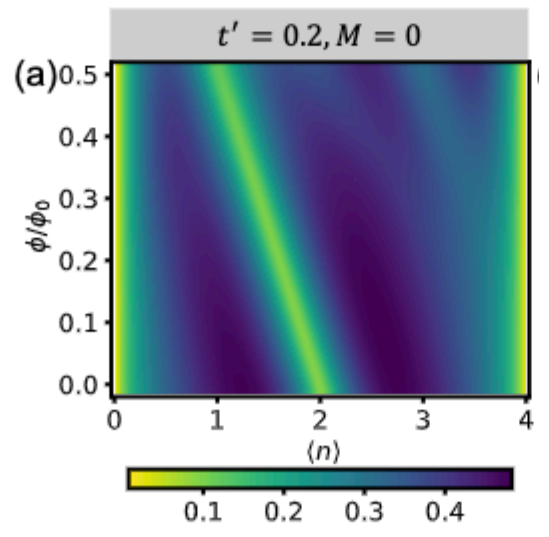
intercept



spin degeneracy=even Chern numbers

Hubbard-Haldane model

$U = 0$



M=1
topologically trivial

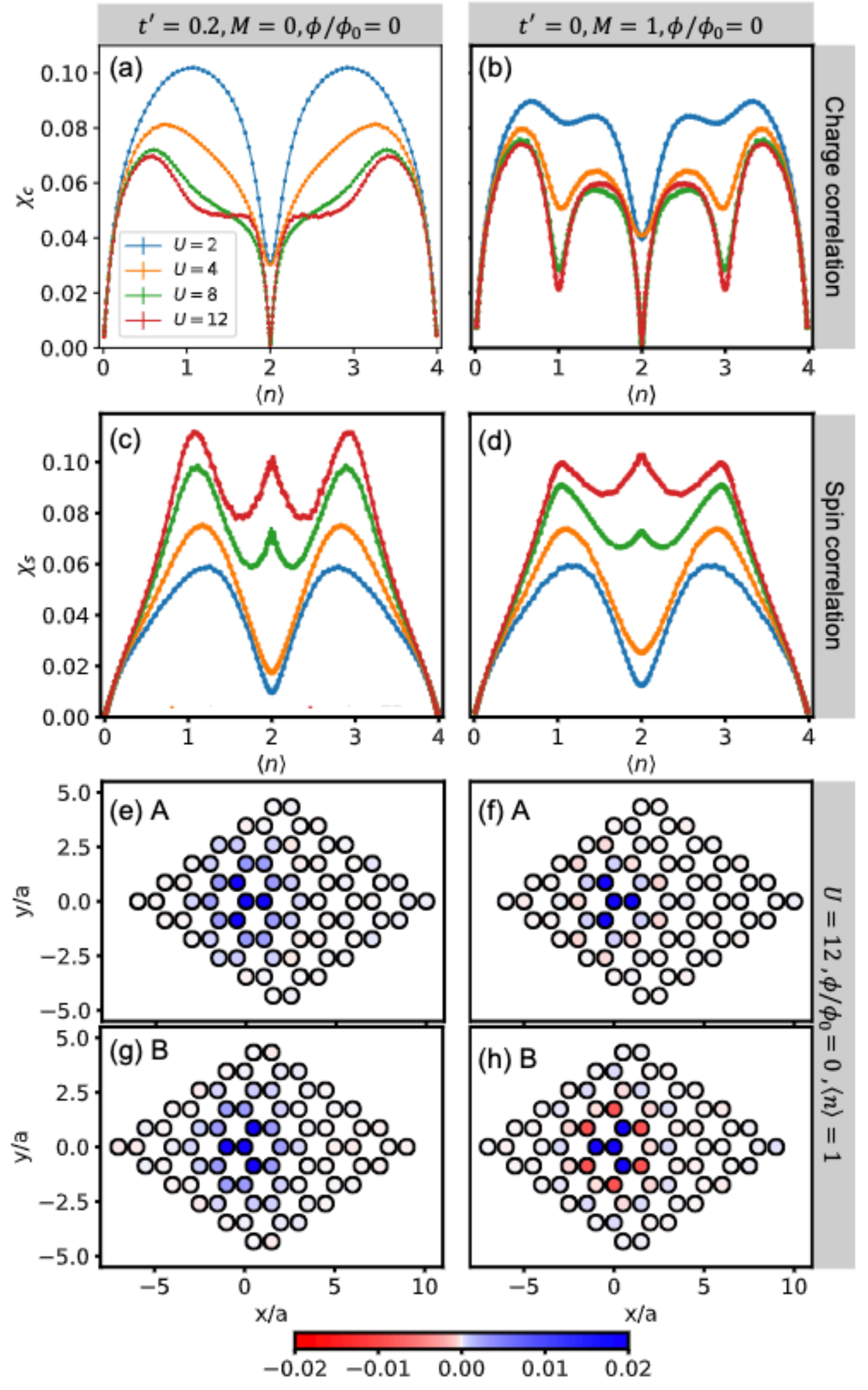
spin correlation

spin susceptibility

Chern number

same as in HK

$\langle n \rangle$ N_{site}



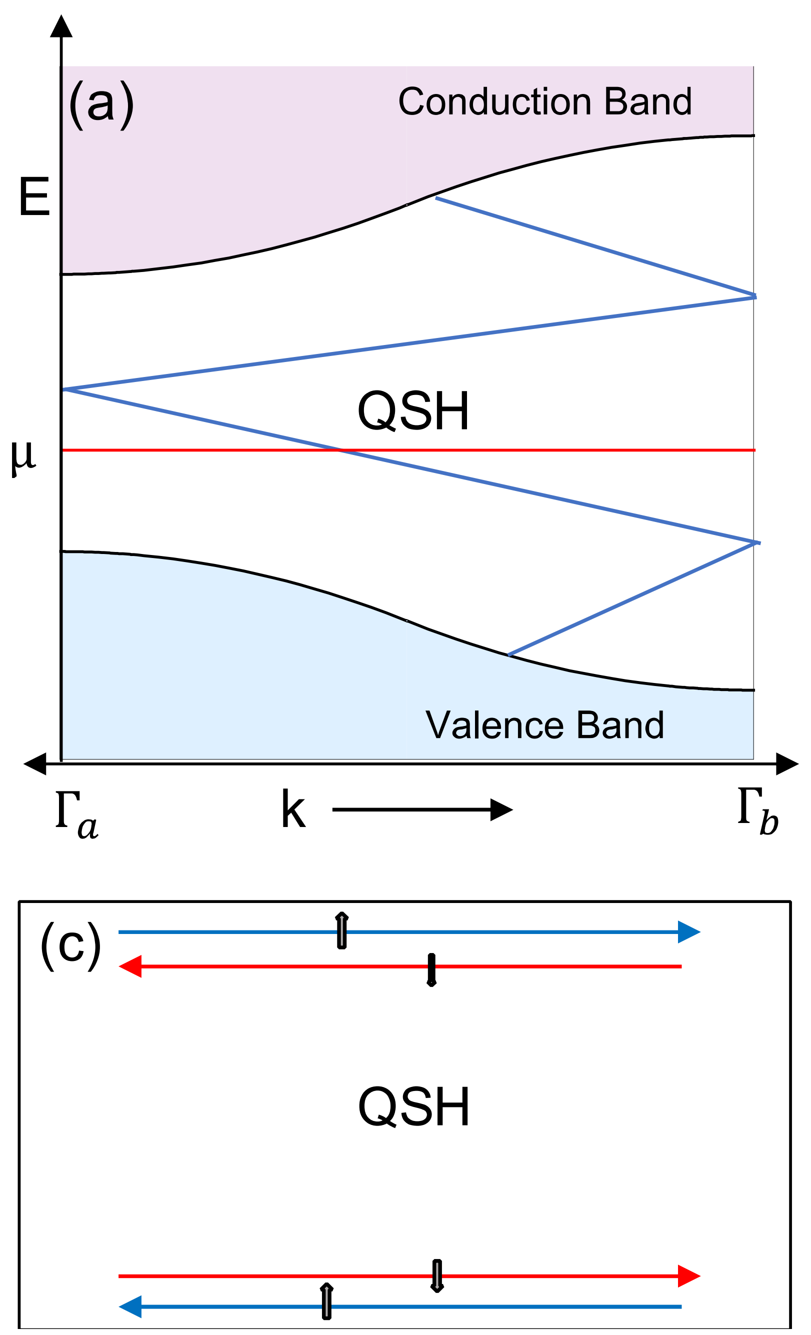
ferromagnetism in TMI

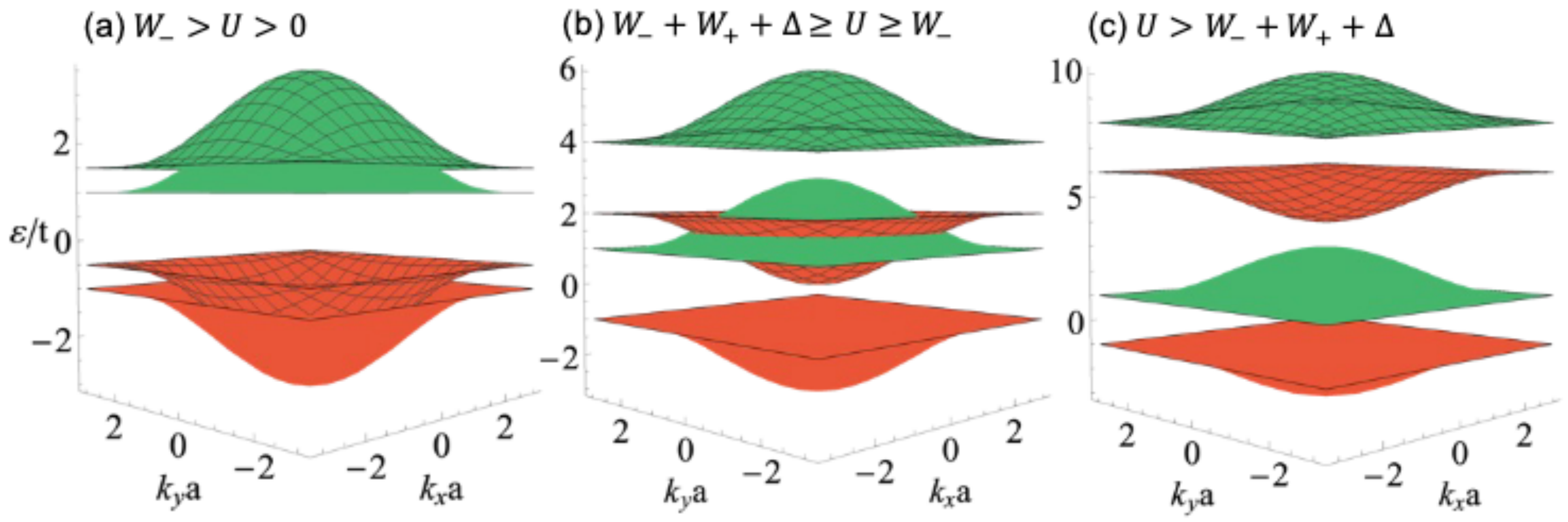
anti-ferromagnetism

Quantum spin Hall Effect

KM/BHZ models

Quantum spin Hall topological Mott Insulator





$$C_s = 2$$

$$C_{\uparrow 0} - C_{\downarrow 0} = 1 - (-1) = 2$$

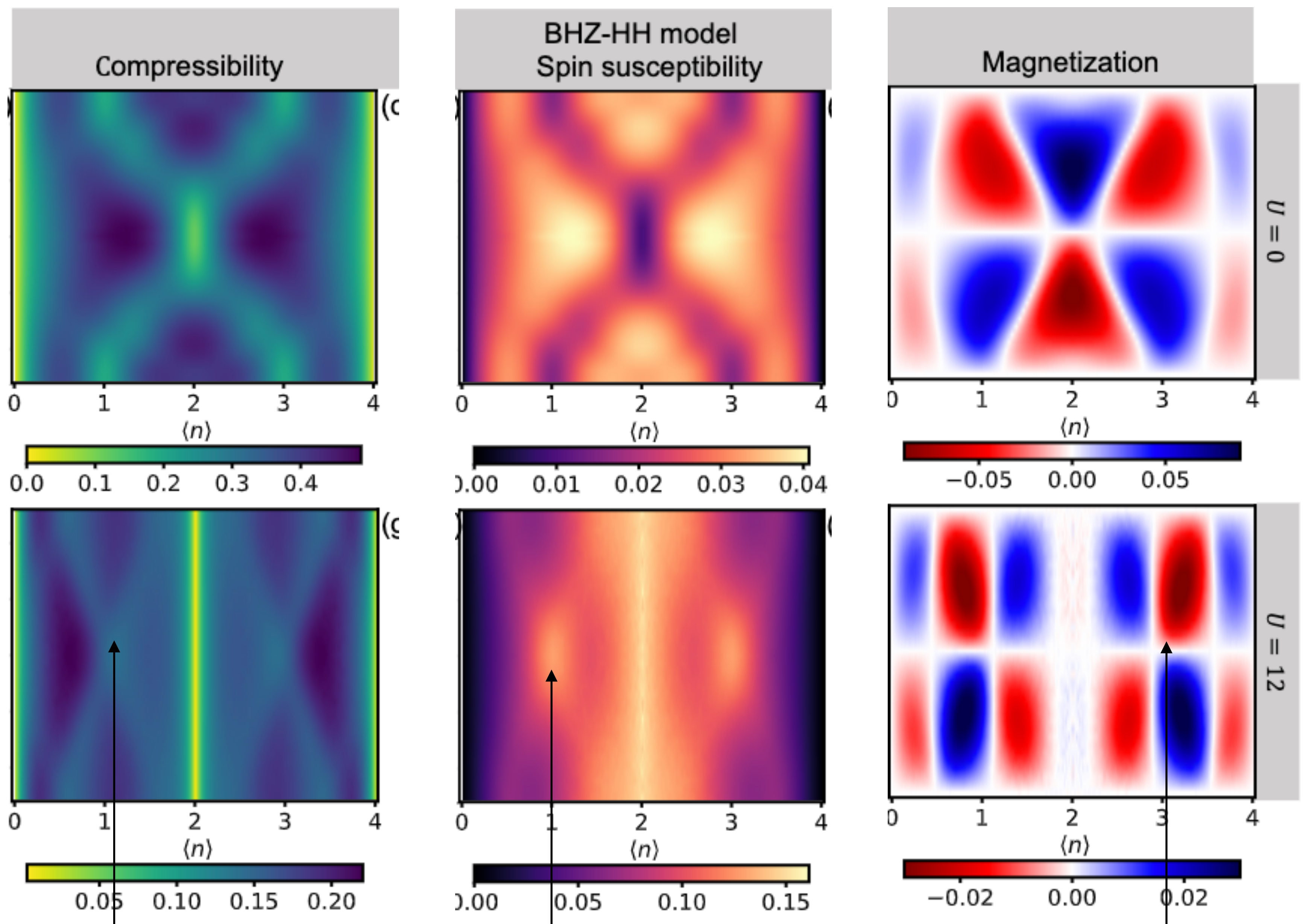
$$C_s = 1$$

$$\bar{C}_\uparrow = \frac{\sum_{N_\uparrow=1}^{N_c} \binom{N_c-1}{N_\uparrow-1}}{2^{N_c}} C_{0\uparrow} = C_{0\uparrow}/2$$

BHZ-Hubbard-Hofstadter model

$U = 0$

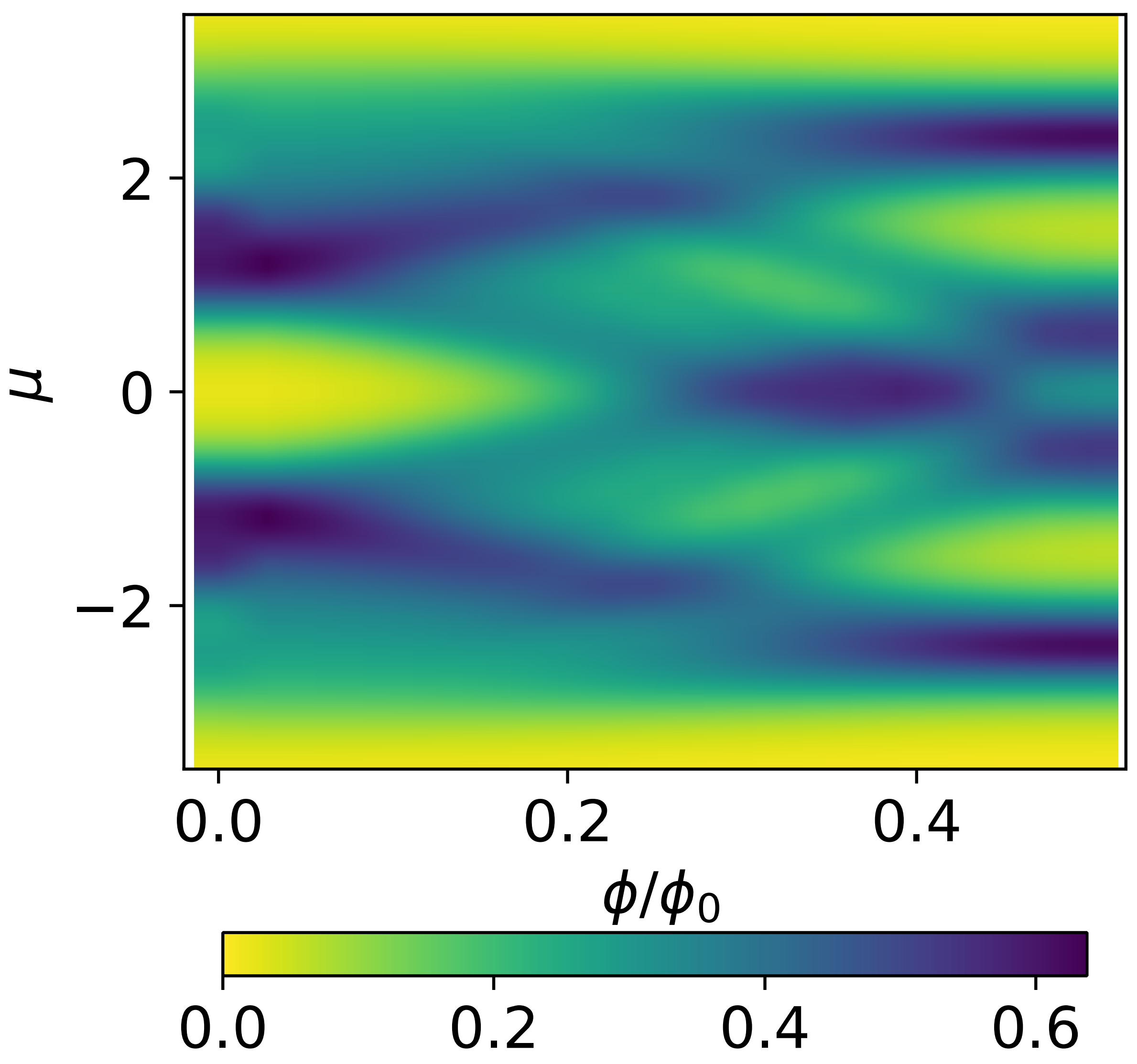
$U = 12$

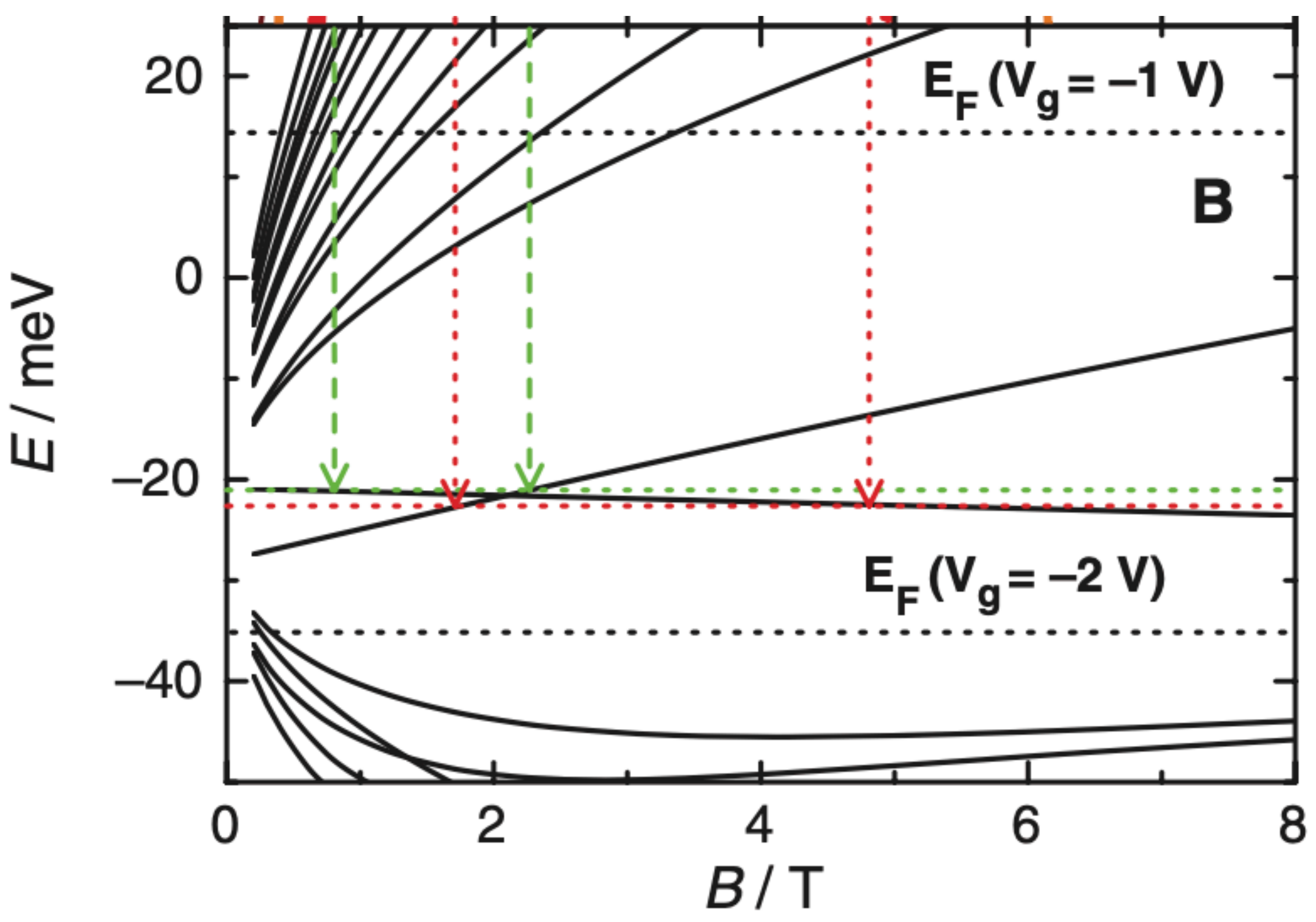


QSH: C=1

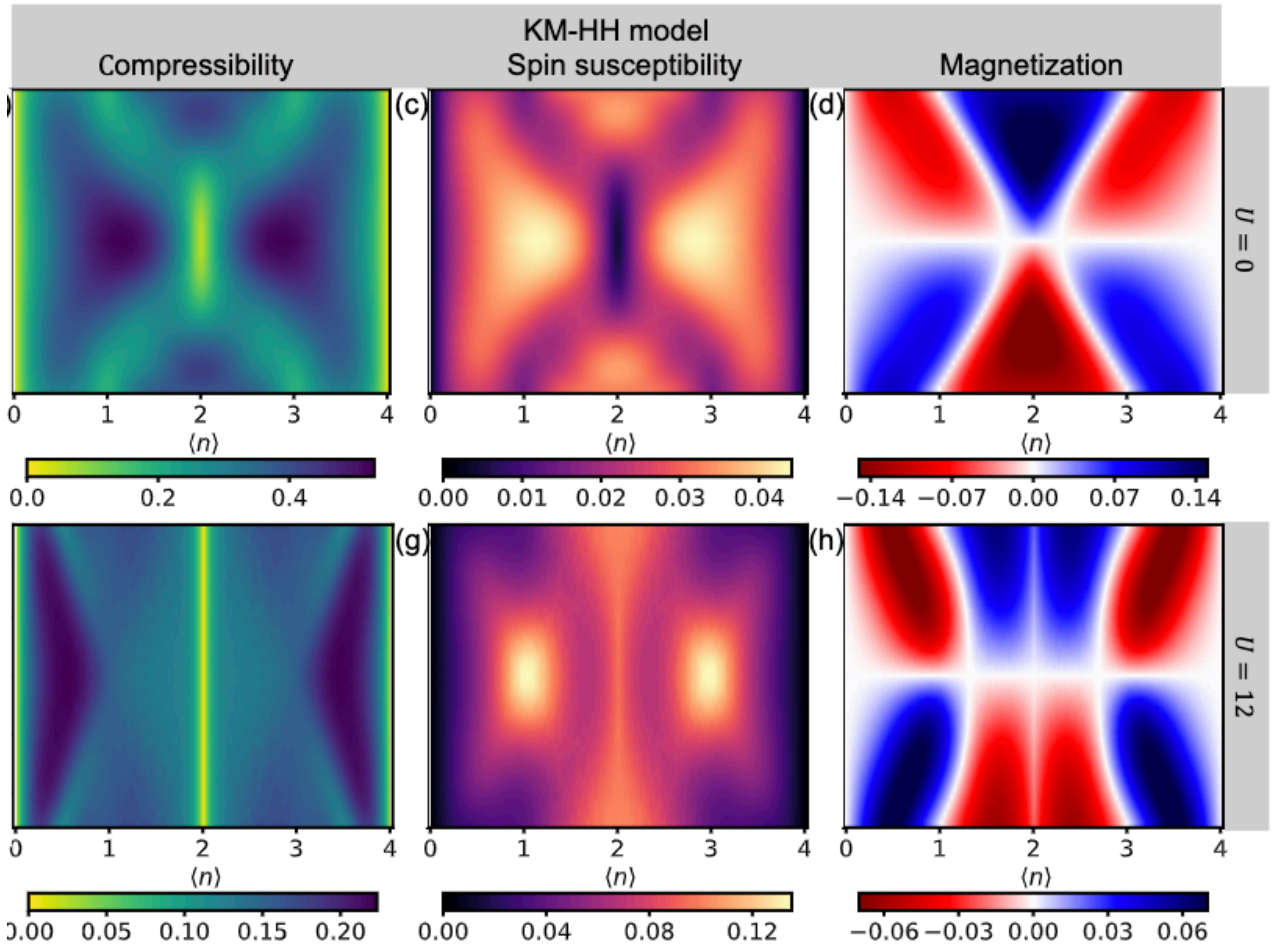
ferromagnetic correlations

M=0 at B=0


μ
2
0
−2
0.0
0.2
0.4
ϕ/ϕ0
0.0
0.2
0.4
0.6


E / meV
20
0
−20
−40
EF (Vg = −1 V)
B
EF (Vg = −2 V)
0
2
4
6
8
B / T

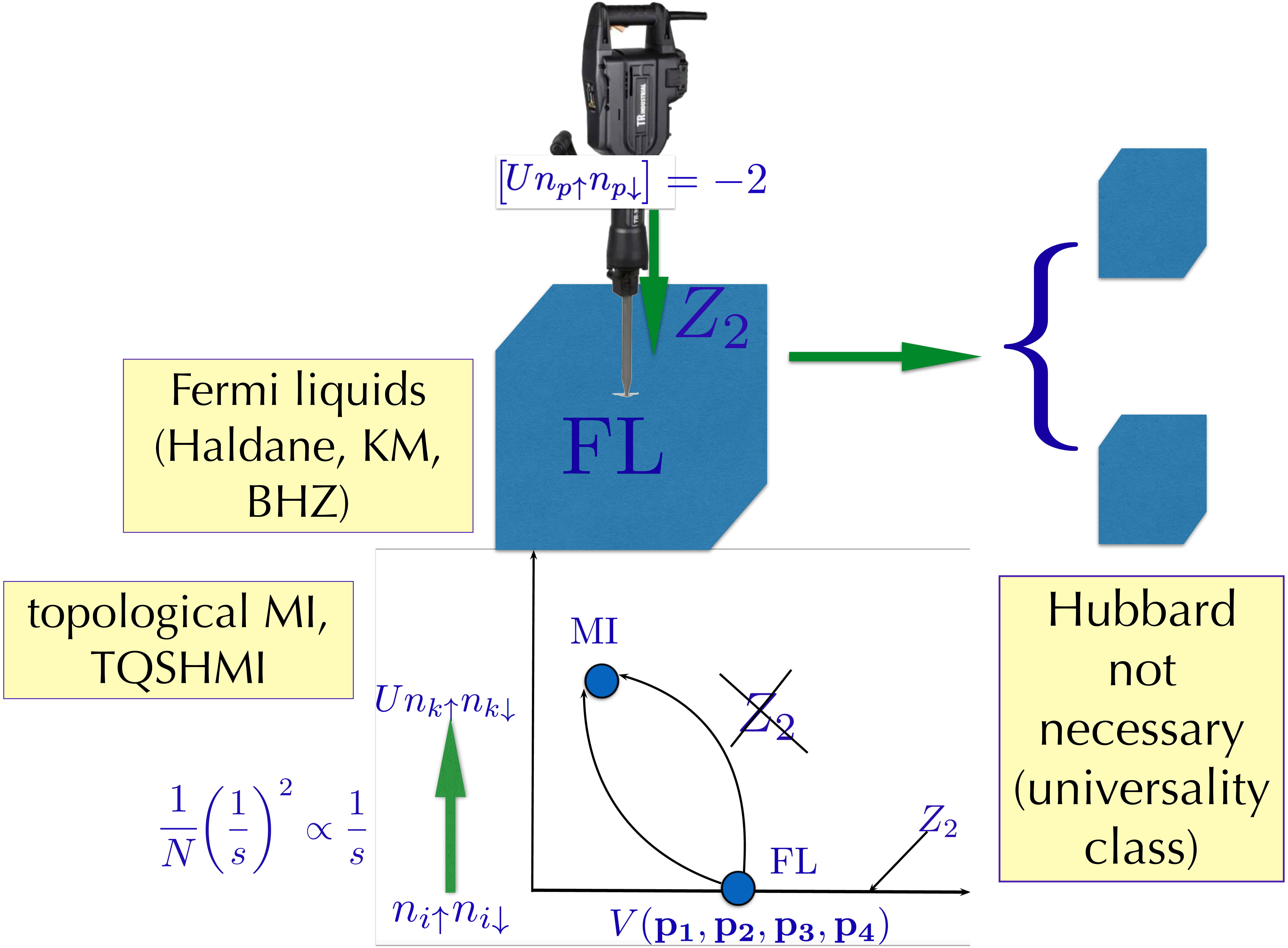
Kane-Mele (KM) model



real-space and momentum-space Hubbard models agree

1/4-filled Haldane (KM/BHZ) model is a topological Mott insulator (QSHMI) why?

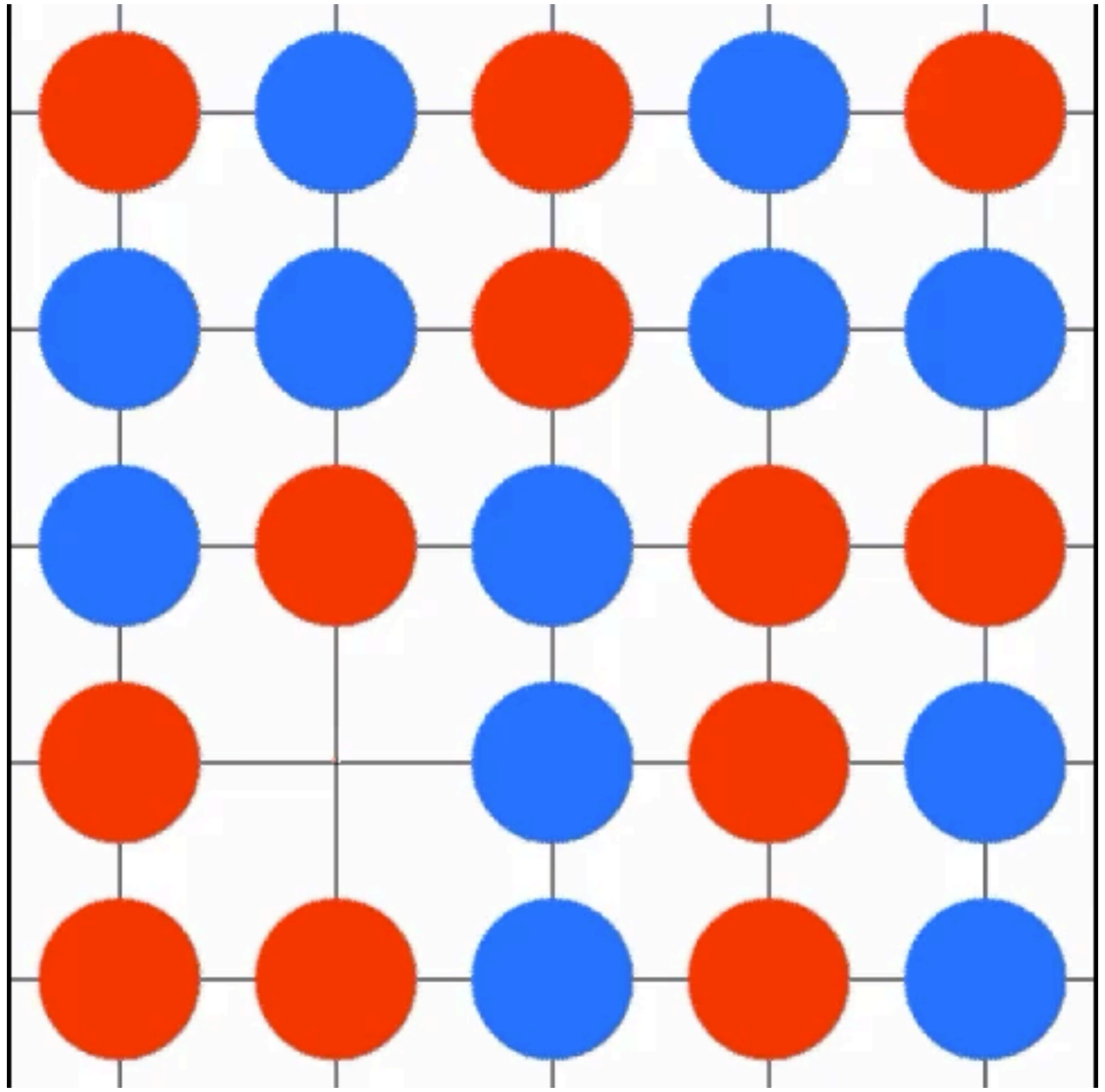
universality



$[U n_{p\uparrow} n_{p\downarrow}] = -2$
Z_2
FL
Fermi liquids (Haldane, KM, BHZ)
topological MI, TQSHMI
$U n_{k\uparrow} n_{k\downarrow}$
$n_{i\uparrow} n_{i\downarrow}$
$\frac{1}{N}\left(\frac{1}{s}\right)^2 \propto \frac{1}{s}$
MI
Z_2
FL
Z_2
$V(\mathbf{p_1}, \mathbf{p_2}, \mathbf{p_3}, \mathbf{p_4})$
Hubbard not necessary (universality class)

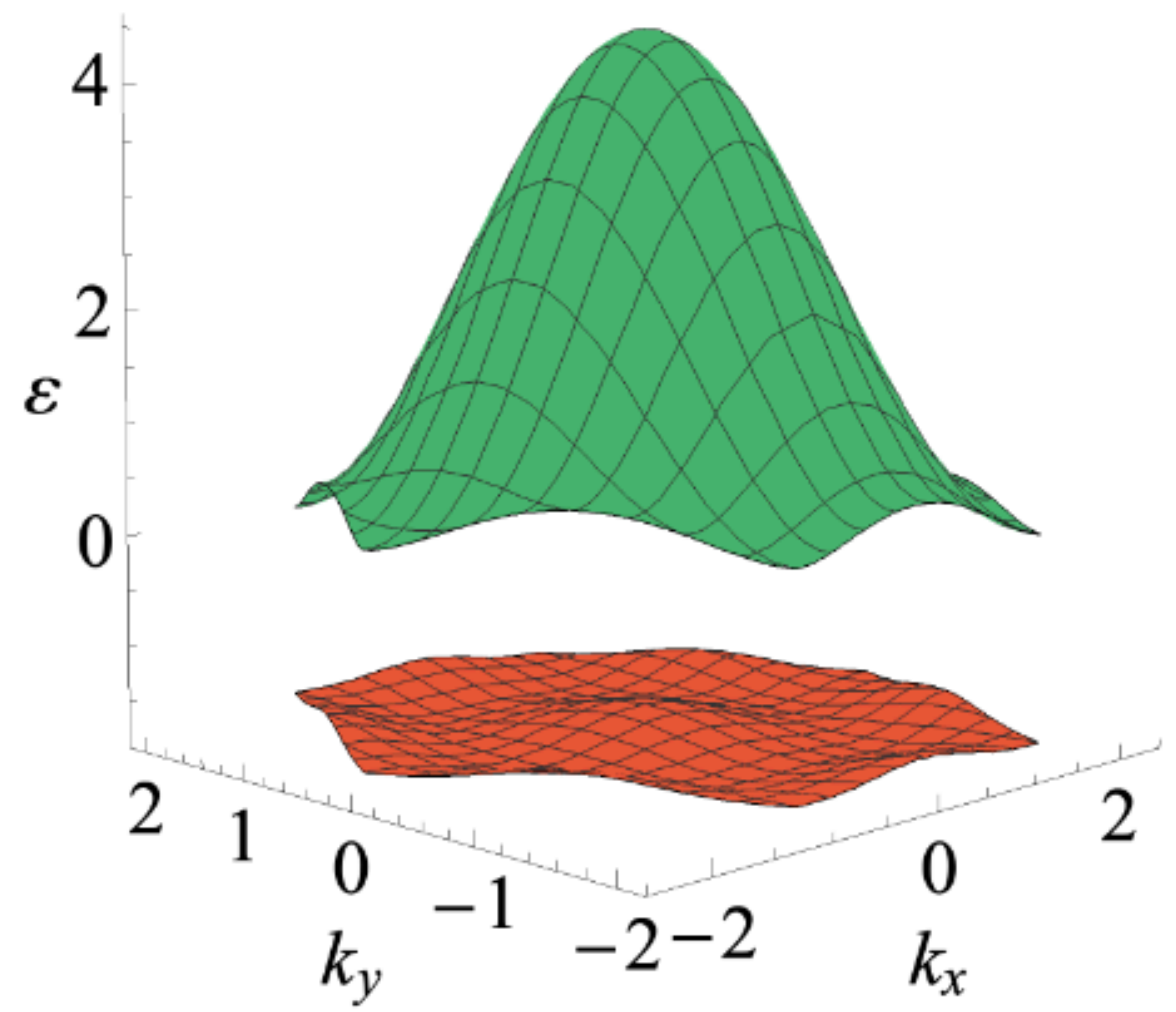
what does the HK model leave out??

$$[H_t, H_U] \neq 0$$



dynamical spectral weight transfer

flat-band limit



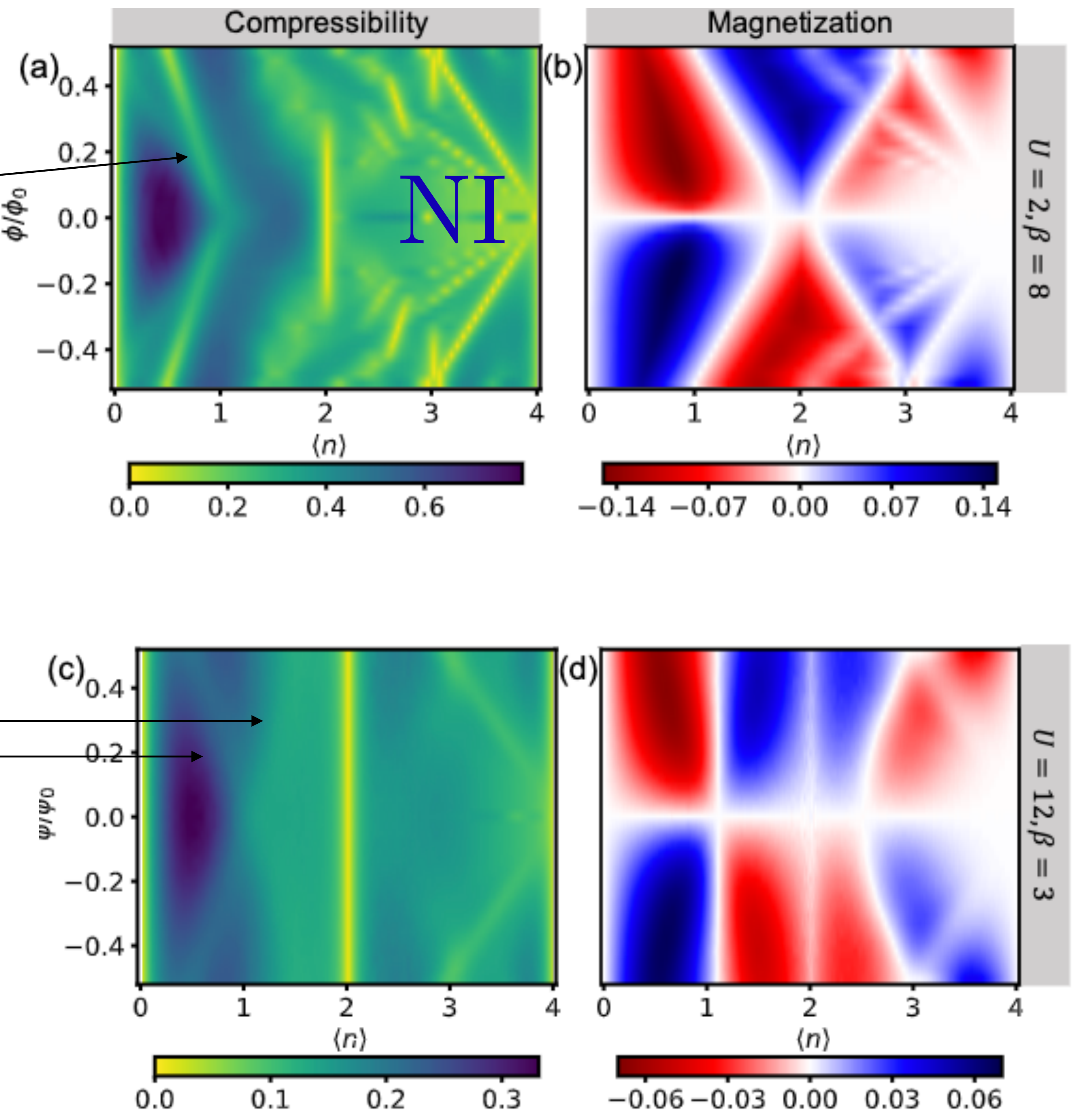
experiments:
QAH?

Experiment: flat-band limit

only left-moving state
QAH

intermediate interaction strength

AB/TMD

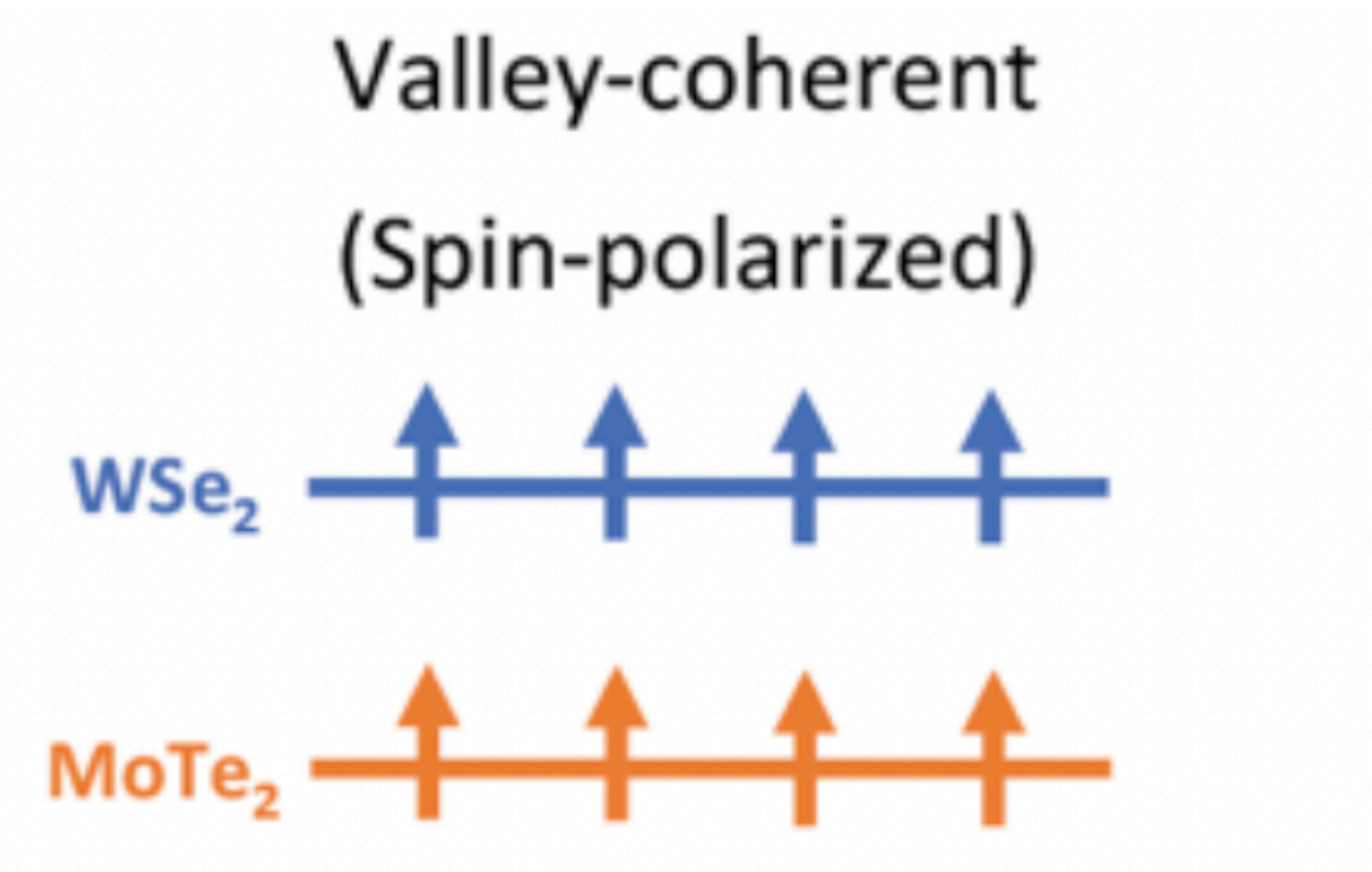


both Landau levels
QSH

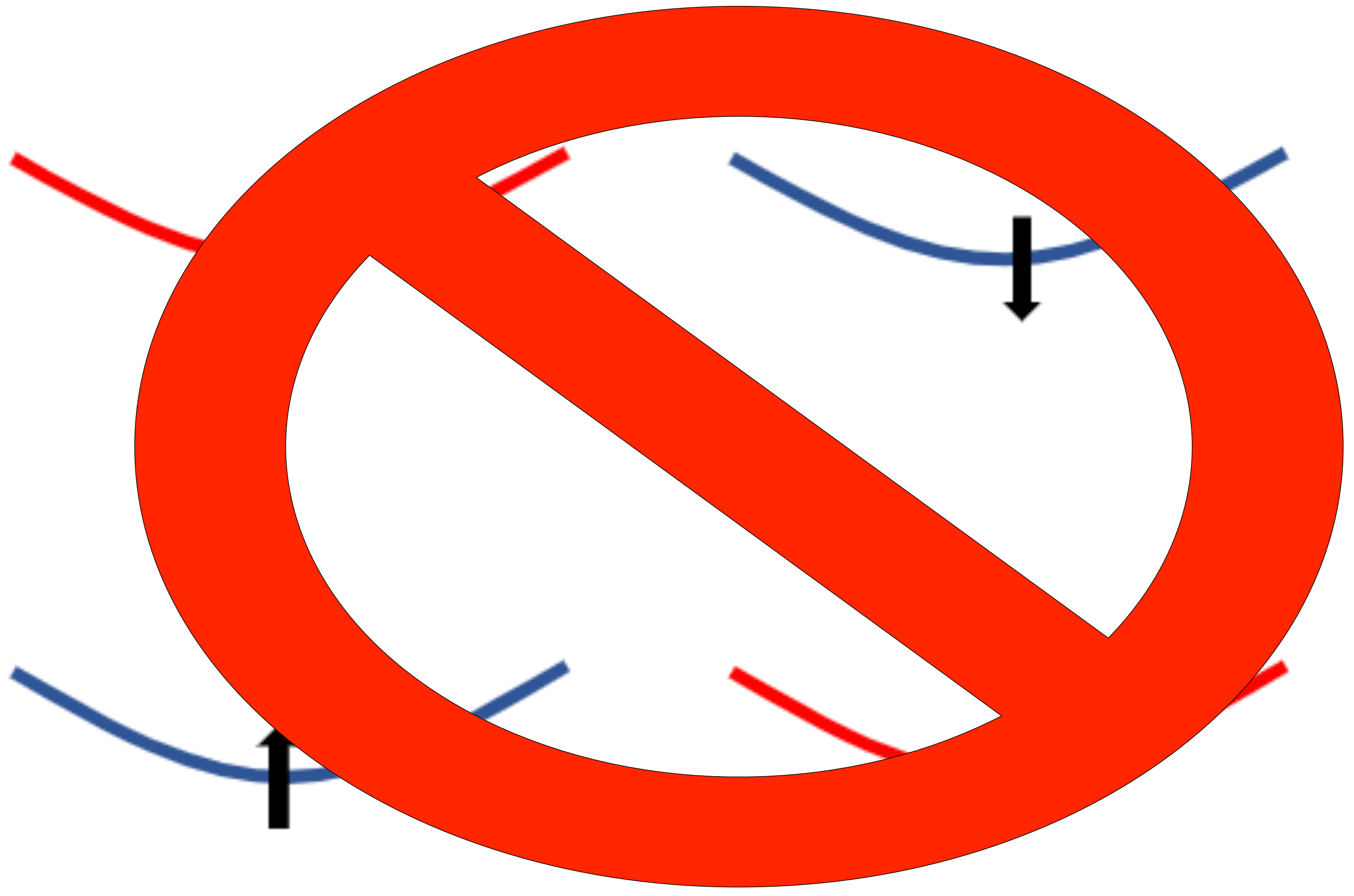
U>W

AA/TMD

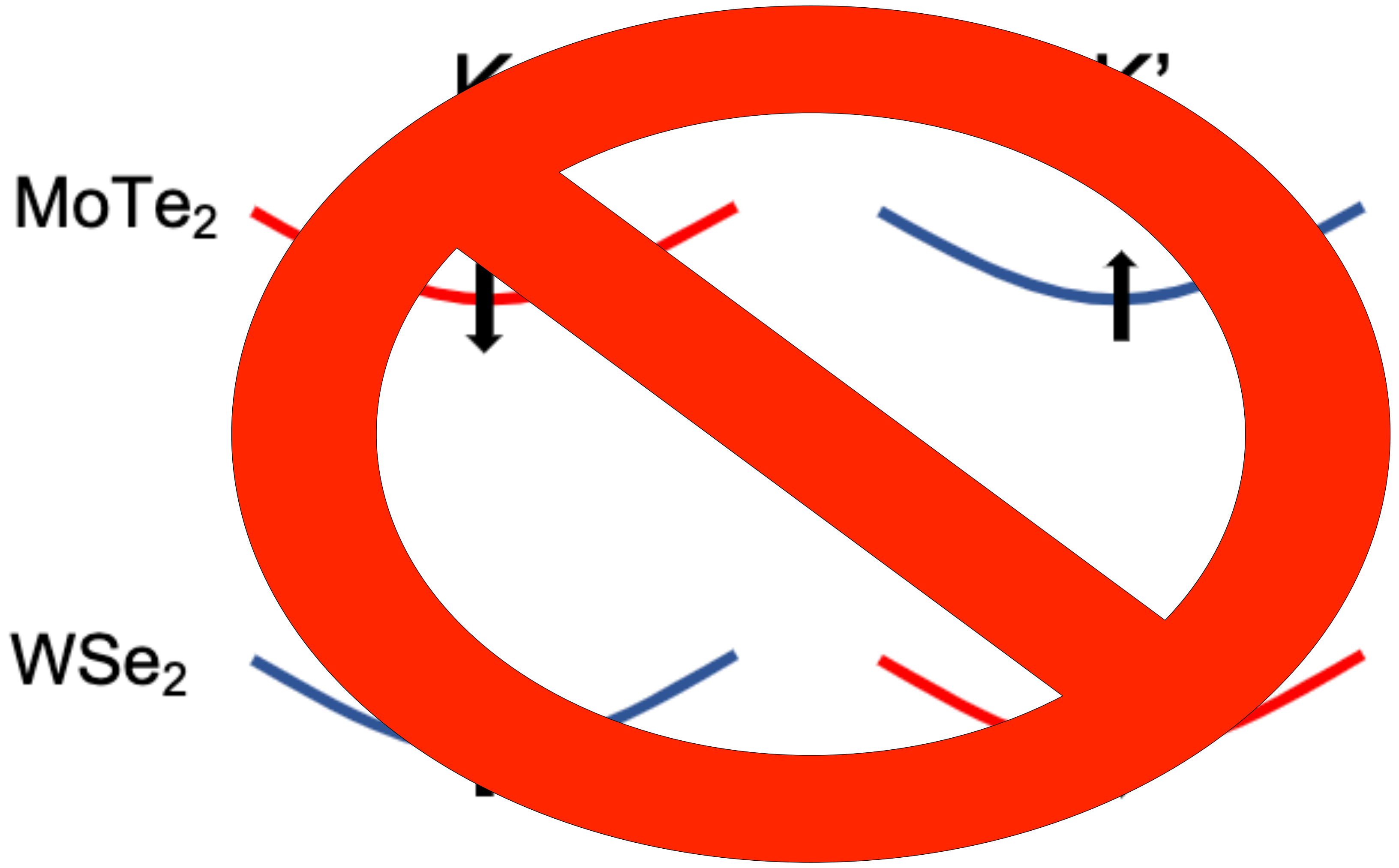
?


Valley-coherent
(Spin-polarized)
WSe2
MoTe2

(a) KM model



(b) AB stacked $MoTe_2/WSe_2$ heterobilayer



solution: two copies

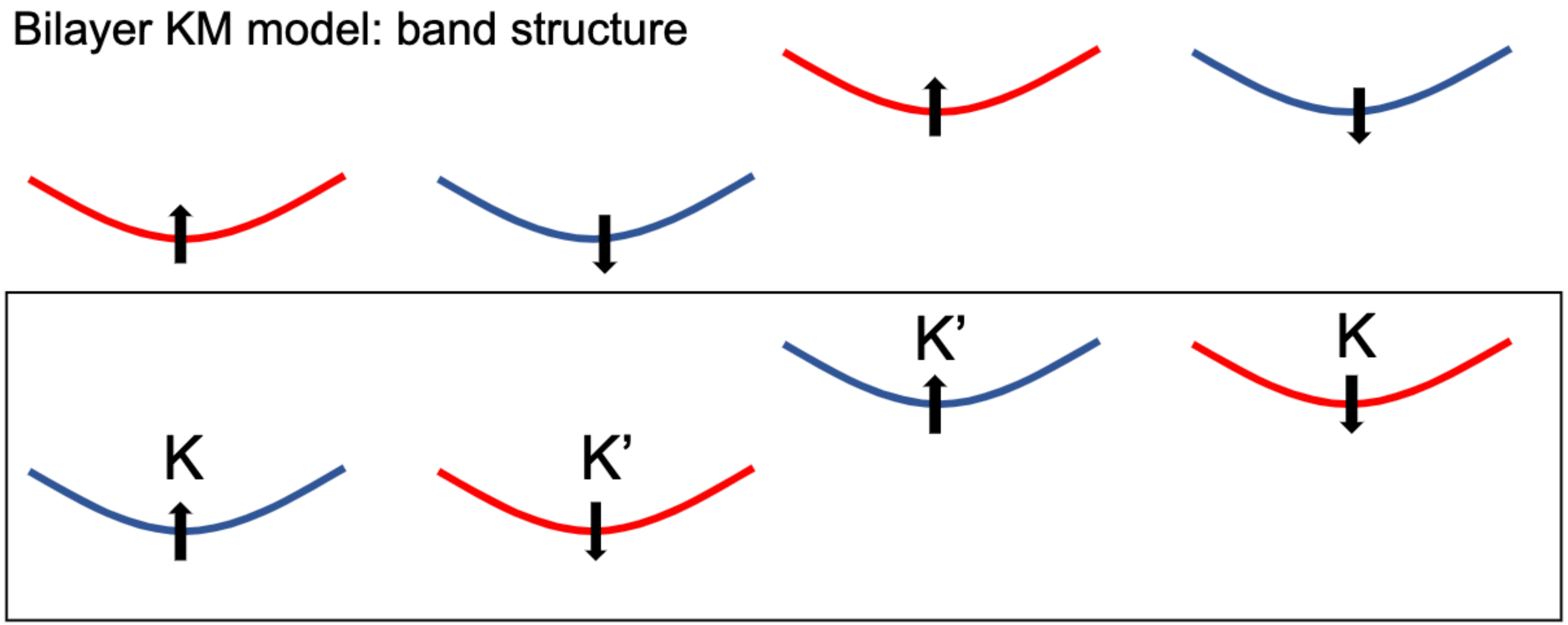
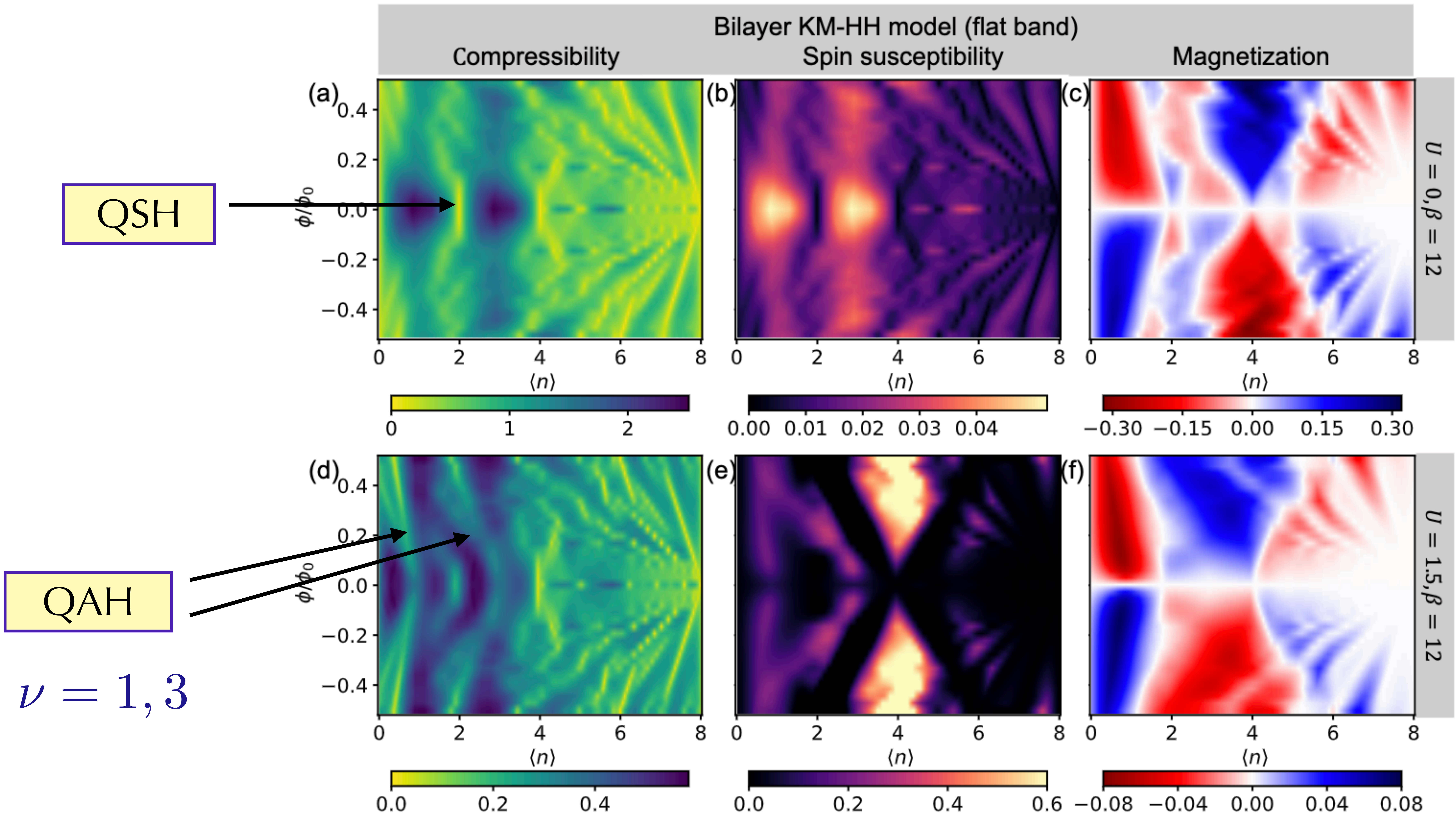


FIG. S13: The schematic band structure of the bilayer KM model. Blue and red colors represent Chen number $C = 1$ and -1 respectively.

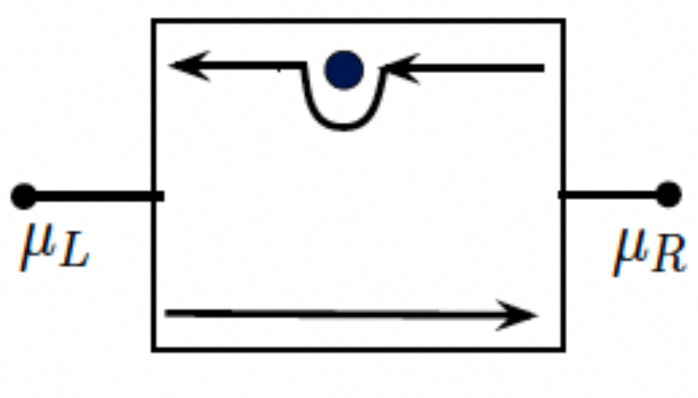


Bilayer KM-HH model (flat band)
Compressibility
Spin susceptibility
Magnetization
QSH
QAH
$\nu = 1, 3$
(a)
(b)
(c)
(d)
(e)
(f)
ϕ/ϕ_0
$\langle n \rangle$
$U = 0, \beta = 12$
$U = 1.5, \beta = 12$

Summary

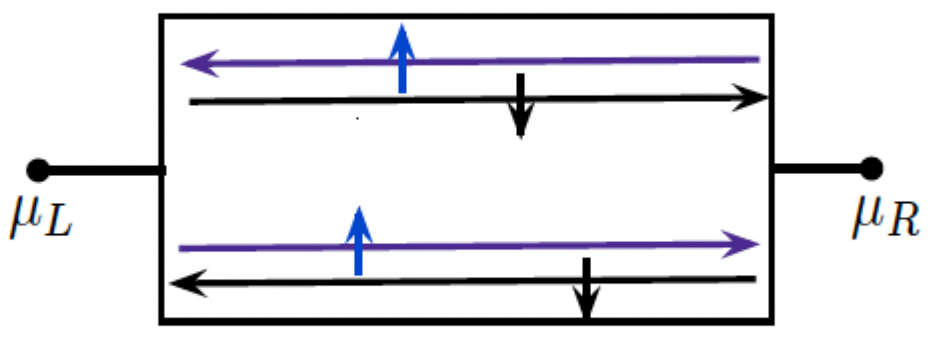
QH

$$2 = 1 + 1$$



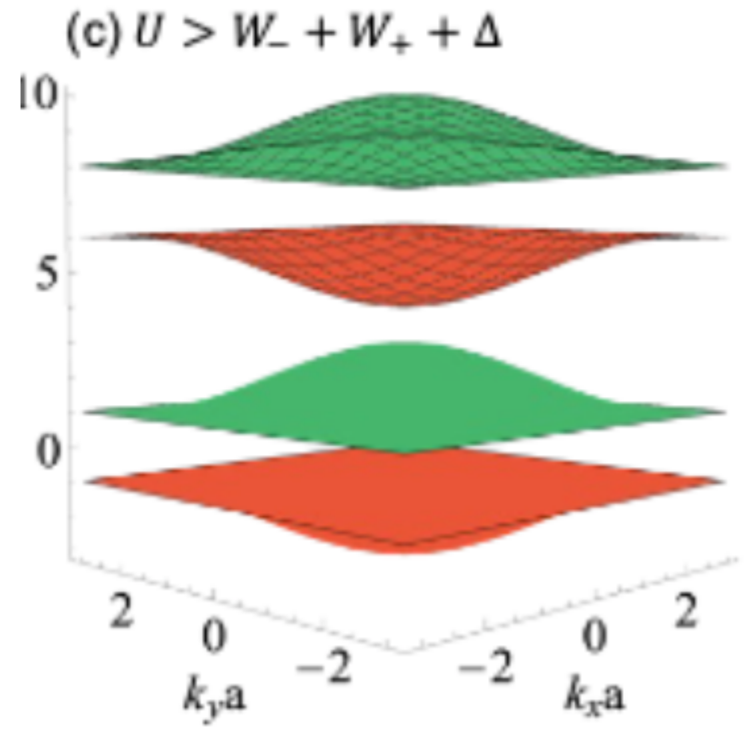
QSH

$$4 = 2 + 2$$



TMI/QSH 1/4-filling

$$4 = 1 + 1 + 1 + 1$$



QAH $\xrightarrow{U > W}$ QSH

$$AB \to AA$$