Topology, correlations and superconductivity in magic angle graphene II

Ashvin Vishwanath
Harvard University

Harvard

Eslam Khalaf

Shang Liu

Ground State and Hidden Symmetry of Magic Angle Graphene at Even Integer Filling

Nick Bultinck,[1,*] Eslam Khalaf,[2,*] Shang Liu,[2] Shubhayu Chatterjee,[1] Ashvin Vishwanath,[2] and Michael P. Zaletel[1,†]

arXiv:1911.02045

Berkeley

Nick Bultinck

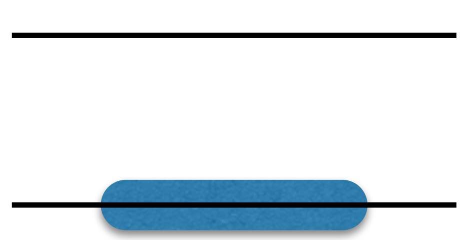
Shubhayu Chatterjee

Mike Zaletel

Two Paradigms for Correlated Electrons

- Interactions energy exceeds kinetic energy (U>t)

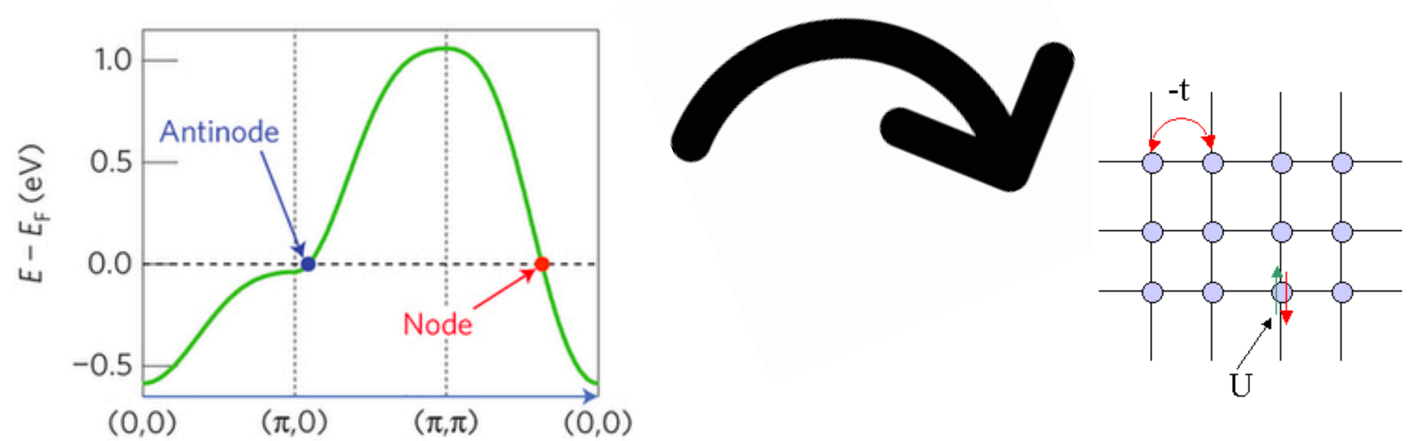
Quantum Hall



Landau Levels

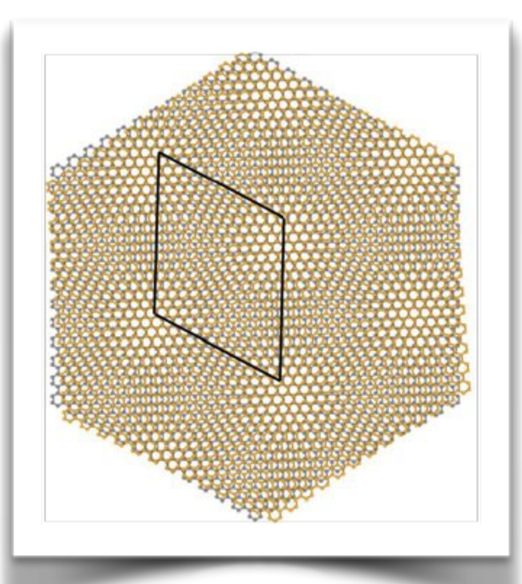
$$\psi_n = z^n e^{-\frac{|z|^2}{4}}$$

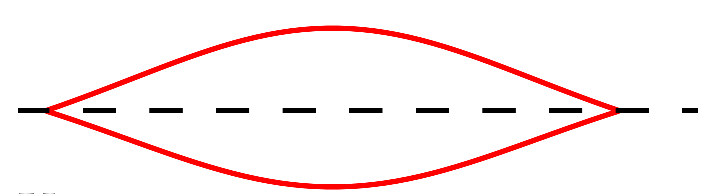
Correlated Solids eg. Cuprates



Wannier Functions

Hubbard Model





Magic angle graphene?

Topology:

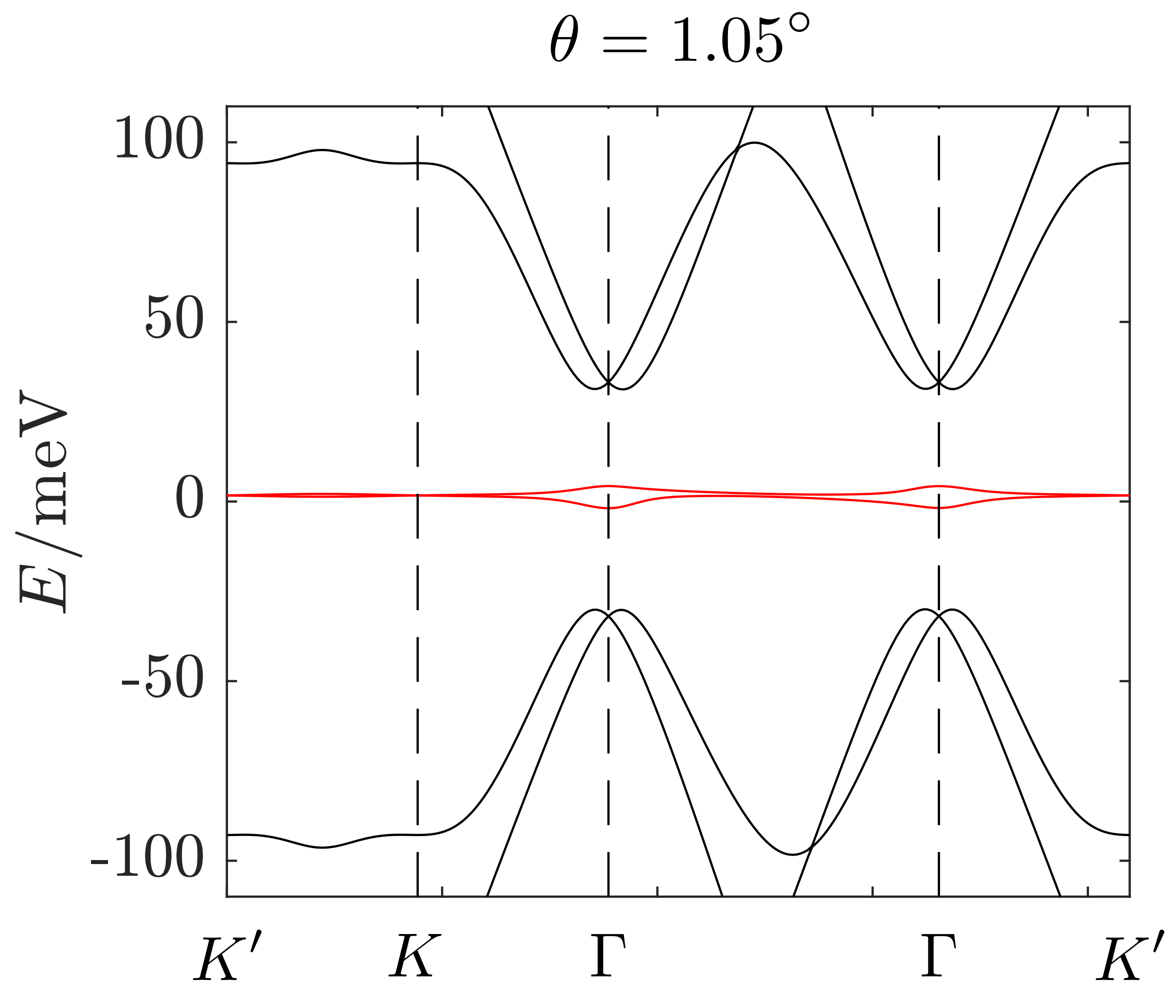
(i) Same chirality nodes

(ii) Landau **+** uɐpuɐ˥

BUT

admits an extended Hubbard model

Magic Angle Twisted Bilayer Graphene @ CNP



Eslam Khalaf

Shang Liu

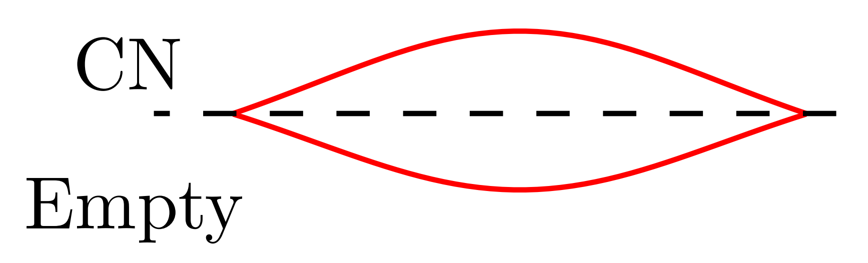
Liu, Khalaf, Lee, AV, 2019.

Bultinick, Khalaf, Liu, Chatterjee, AV, Zaletel
arXiv:1911.02045

- The C_2T symmetry protects the band touching.

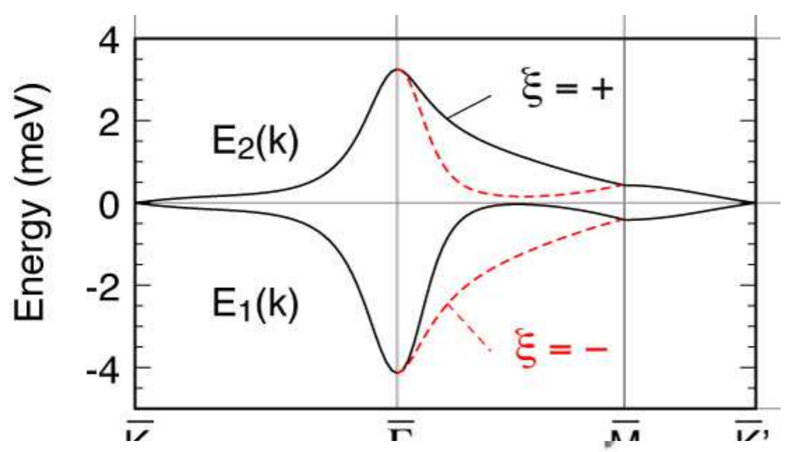
Po, Zou, AV, Senthil, 2018.

- Focus on the two flat bands at CNP. Experiments - insulator/



Brief Review of Experiment

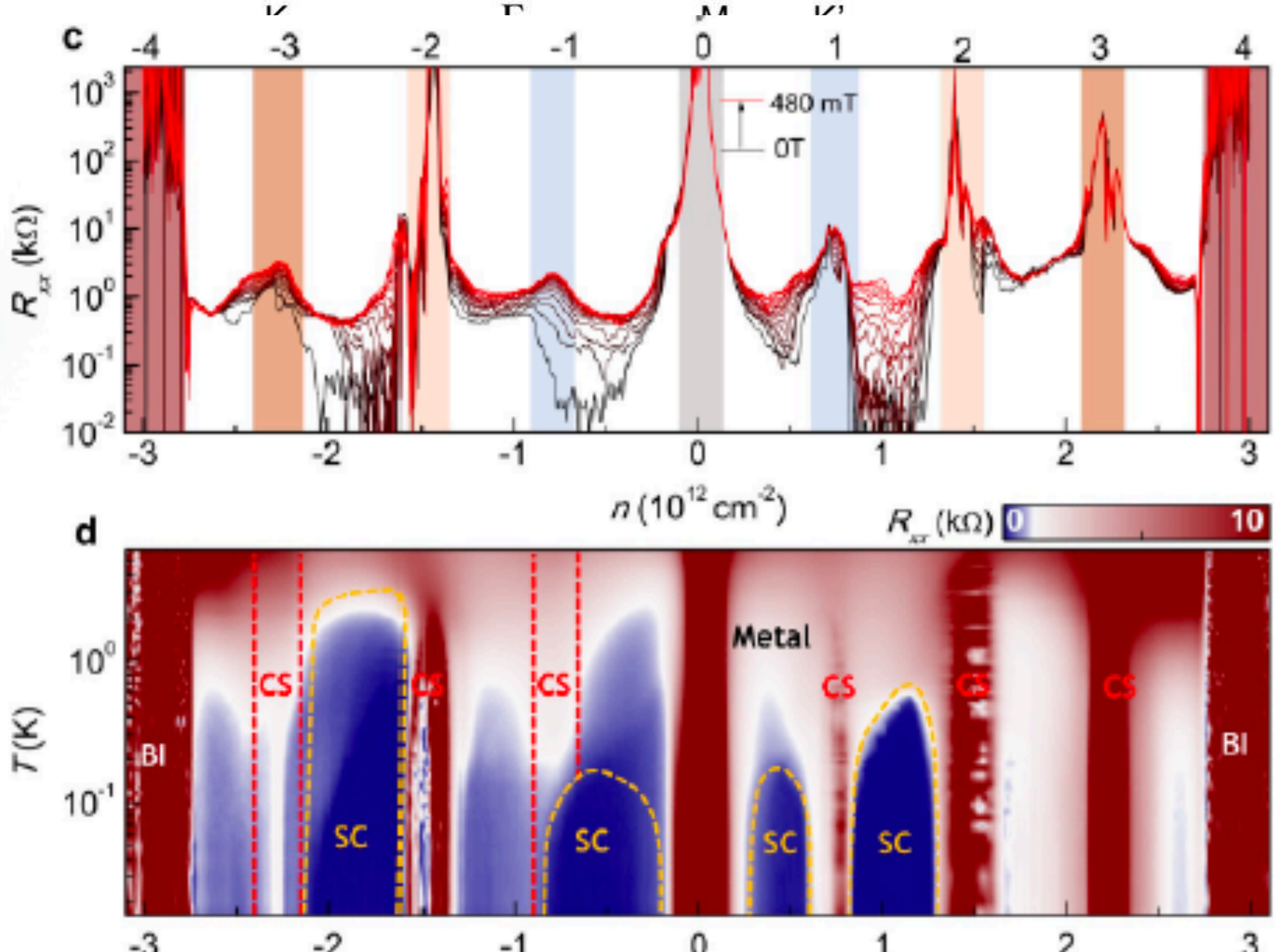
- More uniform samples: Lu *et al.* Nature 574, 653–657 (2019), Stepanos *et al.* arxiv:1911.09198 (2019)



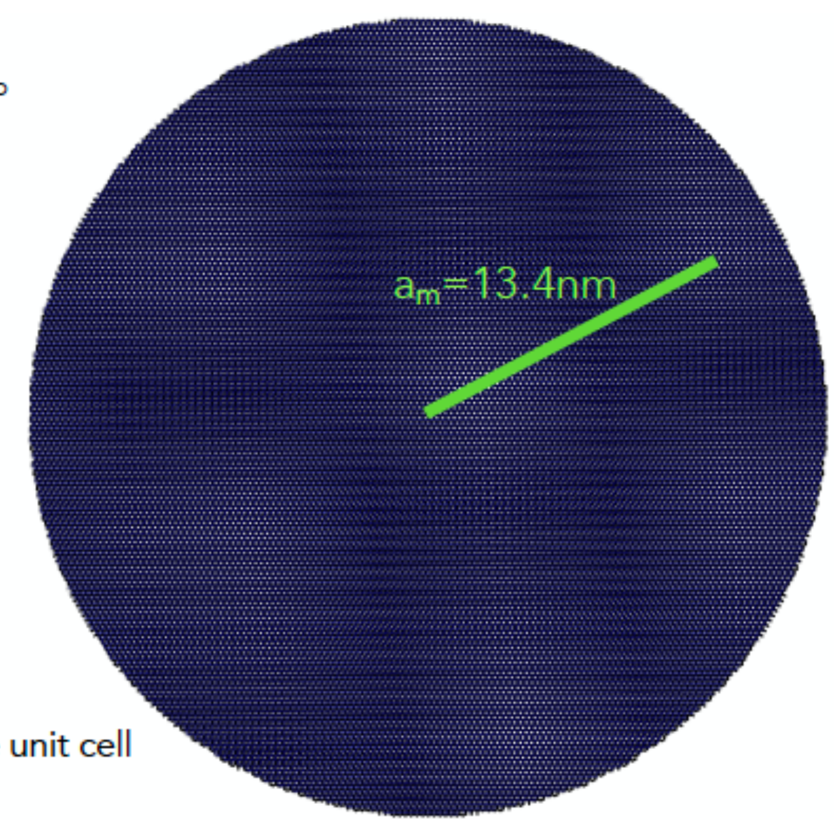
$\nu = +4$

Charge Neutrality

$\nu = -4$

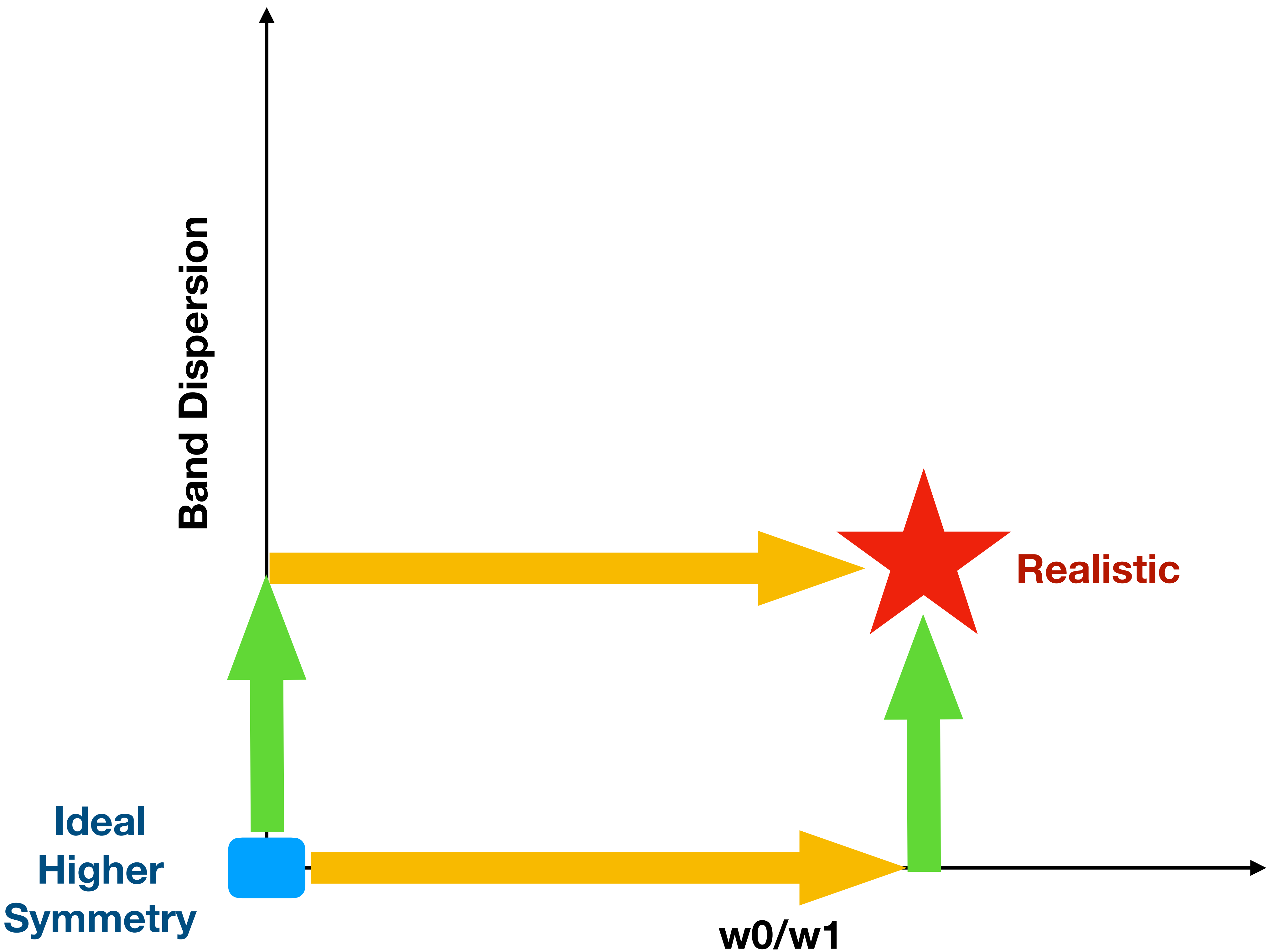


1°

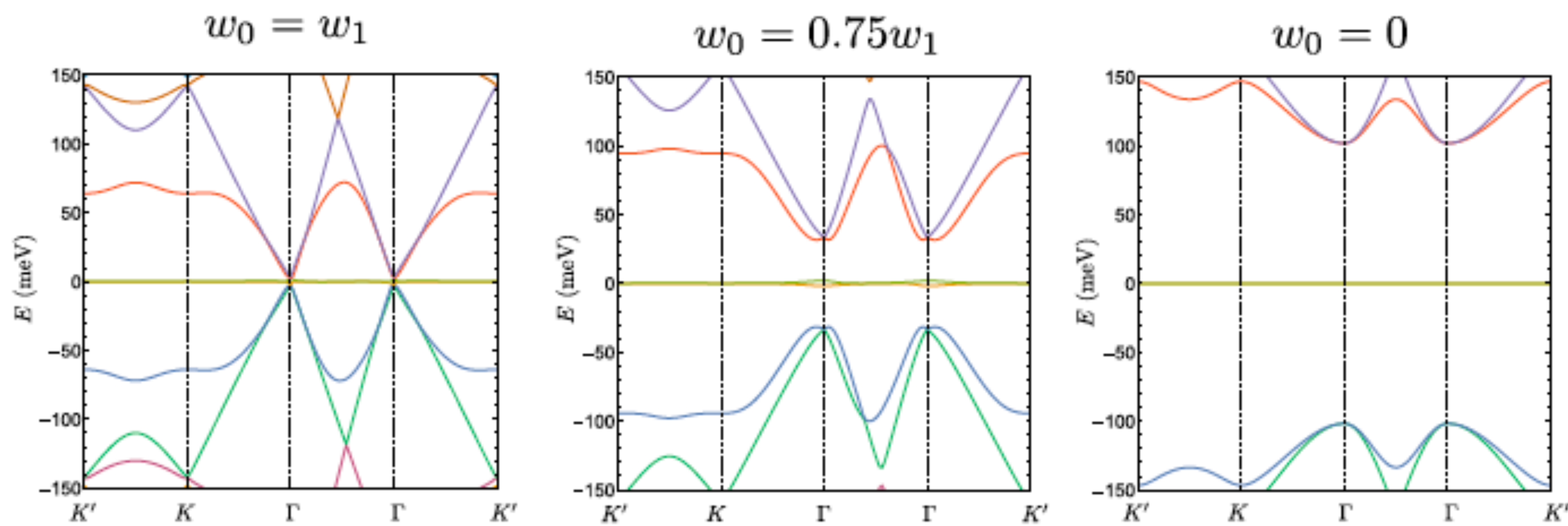


huge unit cell

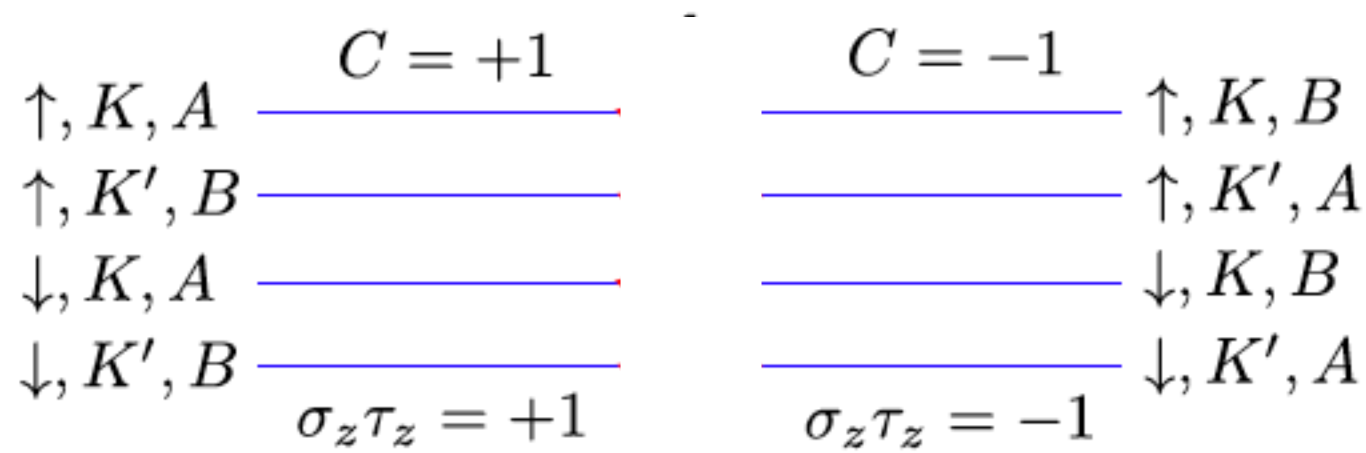
Including Interactions



Simplified Model:
Chiral Model, Flat Band @ Charge Neutrality



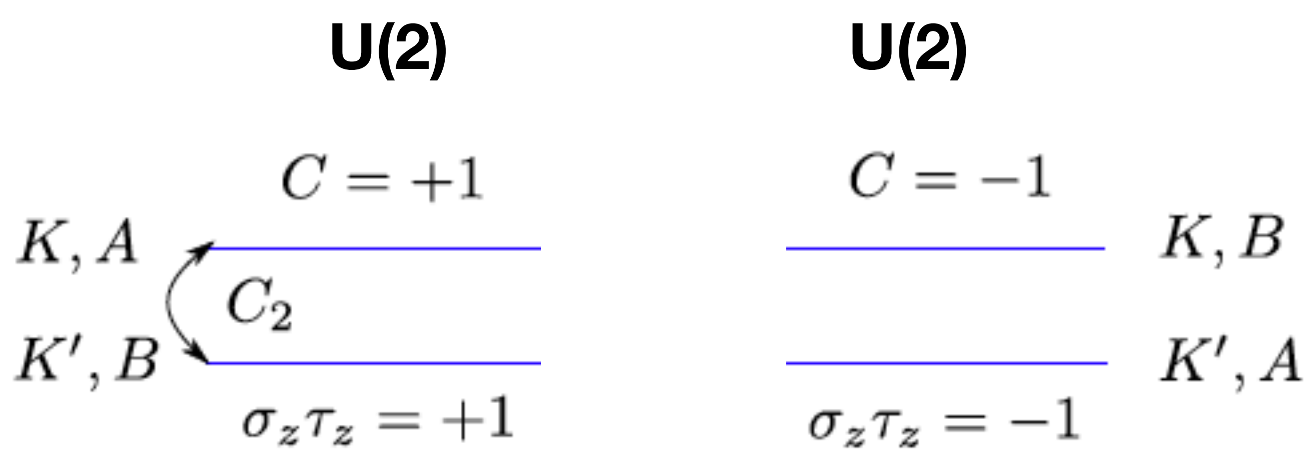
Valley	K	K’	Chern Number
Sublattice	A	B	C=+1
Sublattice	B	A	C=-1



U(4) **U(4)**

Interactions have U(4) x U(4) symmetry
“Generalized Ferromagnet”
Fill four of the eight states -but which four?

Simplified Model:
Chiral Model, Flat Band, Spinless



Fill two of the four states

A catalog of Slater det. states:

Q = ± 1; Filled (Empty) states

$$Q_{\alpha\beta} = \left\langle \Psi \,|\, \left[c_\alpha , c_\beta \right] \,|\, \Psi \right\rangle$$

Sublattice (A/B) σ^z

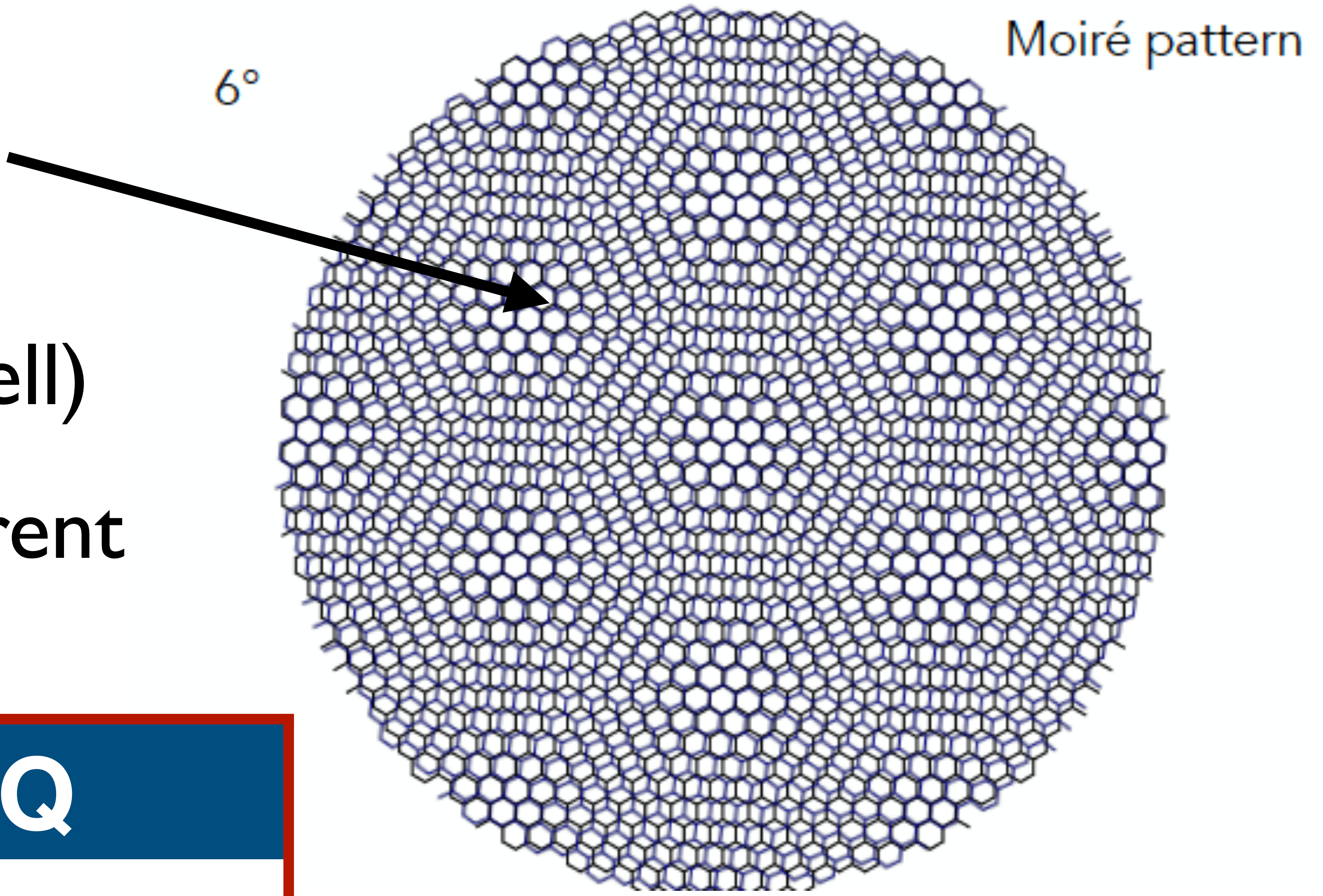
Valley (K/K') τ^z

State	Q
Valley Polarized (K or K')	$Q = \tau^z$
Sublattice Polarized/Valley Hall Induced by hBN substrate	$Q = \sigma^z$
Quantum Hall (C=2)	$Q = \sigma^z \tau^z$
Inter Valley Coherence	$Q \propto \tau_x , \tau_y$

Intervalley Coherence Order

- Breaks translation symmetry at the carbon atom scale (Triples the unit cell)
- But can have different form factors eg

IVC State	Q
Charge density wave	$Q = \Delta_R \tau_x + \Delta_I \tau_y$
Bond density wave (Kekule)	$Q = \sigma_x \left(\Delta_R \tau_x + \Delta_I \tau_y \right)$
Modulated Hopping Phase (breaks T)	$Q = \sigma_y \left(\Delta_R \tau_x + \Delta_I \tau_y \right)$



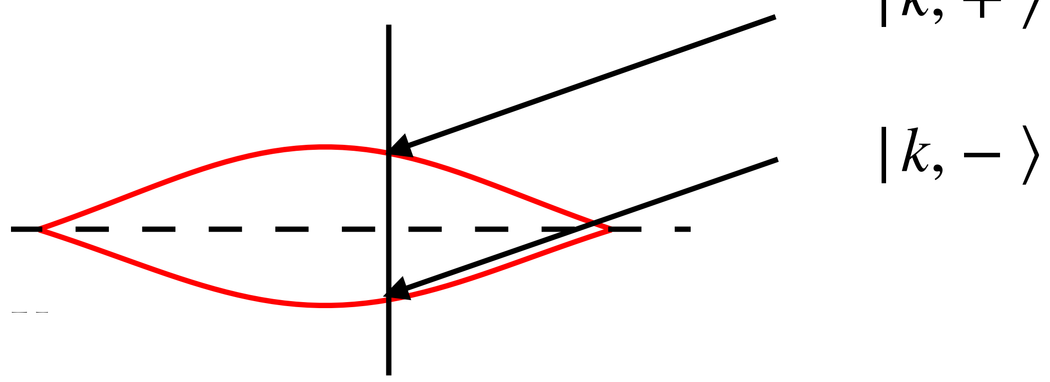
Energetics

$$\mathcal{H}_{\text{int}} = \frac{1}{2A} \sum_{q} V_{q} \delta\rho_{q} \delta\rho_{-q}, \quad \delta\rho_{q} = \rho_{q} - \bar{\rho}_{q}$$

Screened Coulomb

Density projected into the two bands:

$$\rho(q) = \sum_{k \in BZ} c_k^\dagger \Lambda_q(k) c_{k+q}$$



$$\Lambda_q^{\alpha\beta}(k) = \langle k, \alpha | e^{iq\cdot r} | k+q, \beta \rangle$$

Form factor plays a key role

In the Chiral Model
Very simple Form Factor:

$$\Lambda = F e^{i\phi \sigma_z \tau_z}$$

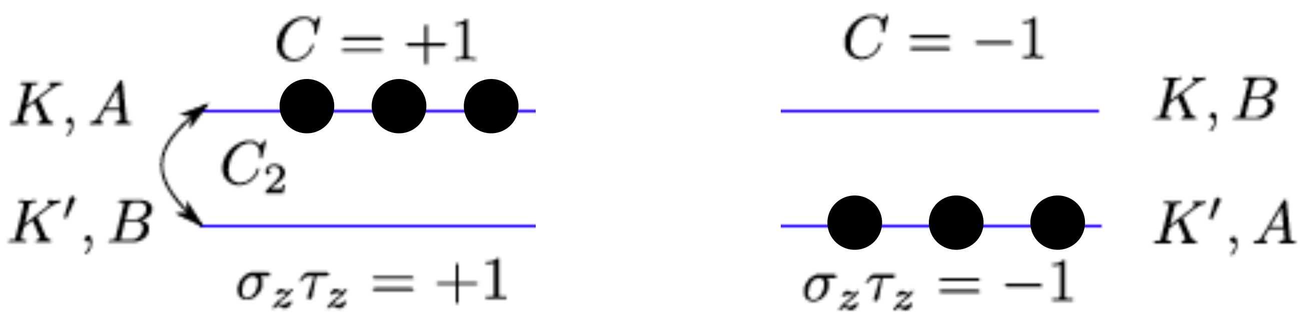
Ground State of Chiral Model-Generalized Ferromagnet

- Family of exact ground states - generalized ferromagnets. $[Q, \Lambda] = 0$

$$\mathcal{H}_{\text{int}} = \frac{1}{2A} \sum_{q} V_q \delta\rho_q \delta\rho_{-q},$$

Argument:

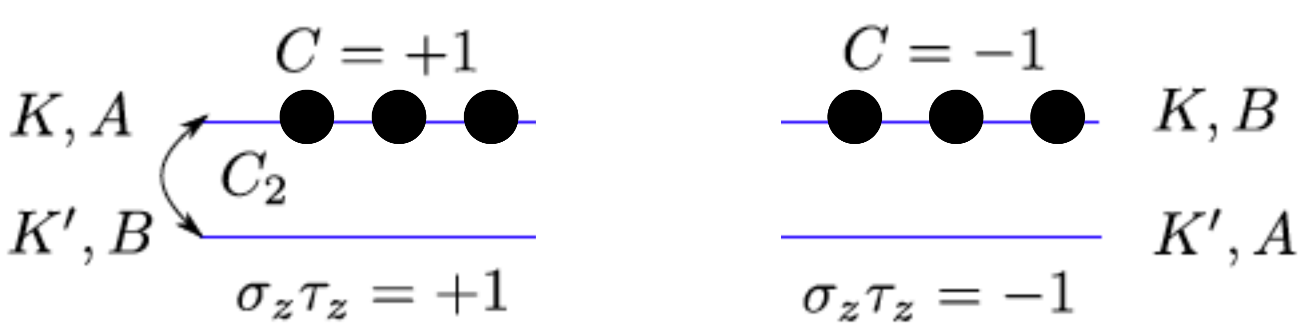
$V_q \geq 0$ and $\delta\rho_q |\Psi\rangle = 0$



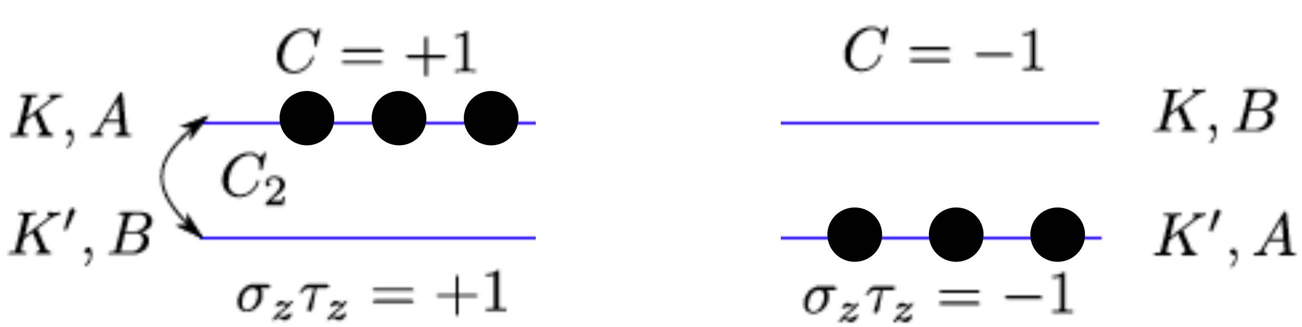
Ground State of Chiral Model- Generalized Ferromagnet

- Family of exact ground states - generalized ferromagnets. $[Q, \Lambda] = 0$

Valley polarized



Valley Hall



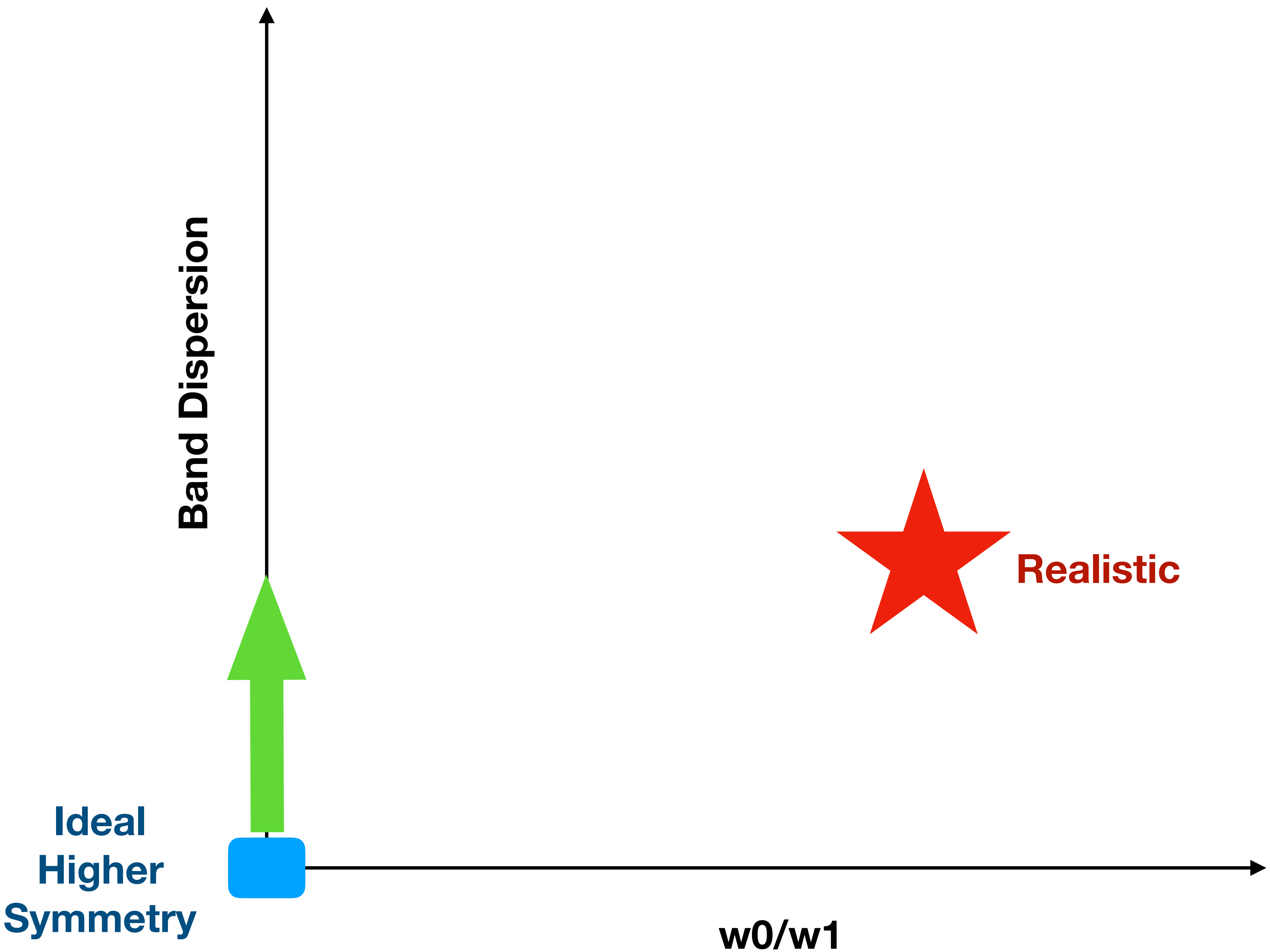
Ground State of Chiral Model- Generalized Ferromagnet

- Family of exact ground states - generalized ferromagnets. $[Q, \Lambda] = 0$

Some IVCs allowed and others ruled out

CDW	$Q = \Delta_R \tau_x + \Delta_I \tau_y$
T-IVC	$Q = \sigma_x \left(\Delta_R \tau_x + \Delta_I \tau_y \right)$
K-IVC	$Q = \sigma_y \left(\Delta_R \tau_x + \Delta_I \tau_y \right)$

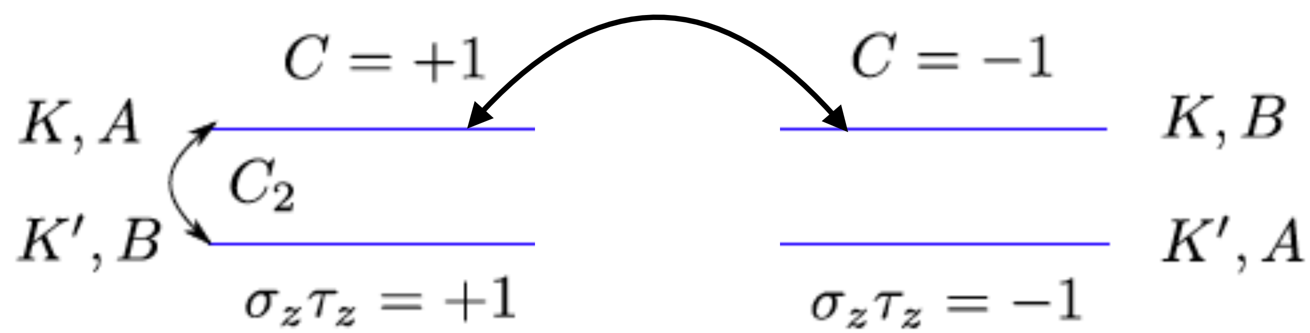
Including Interactions



Breaking the Degeneracy

Dispersion:

Favors states that can fluctuate.
(Retains a U(2) symmetry)



$$\{Q, \sigma_x\} = 0 \quad [Q, \Lambda] = 0$$

Quantum Hall $Q = \sigma_z \tau_z$ ✓

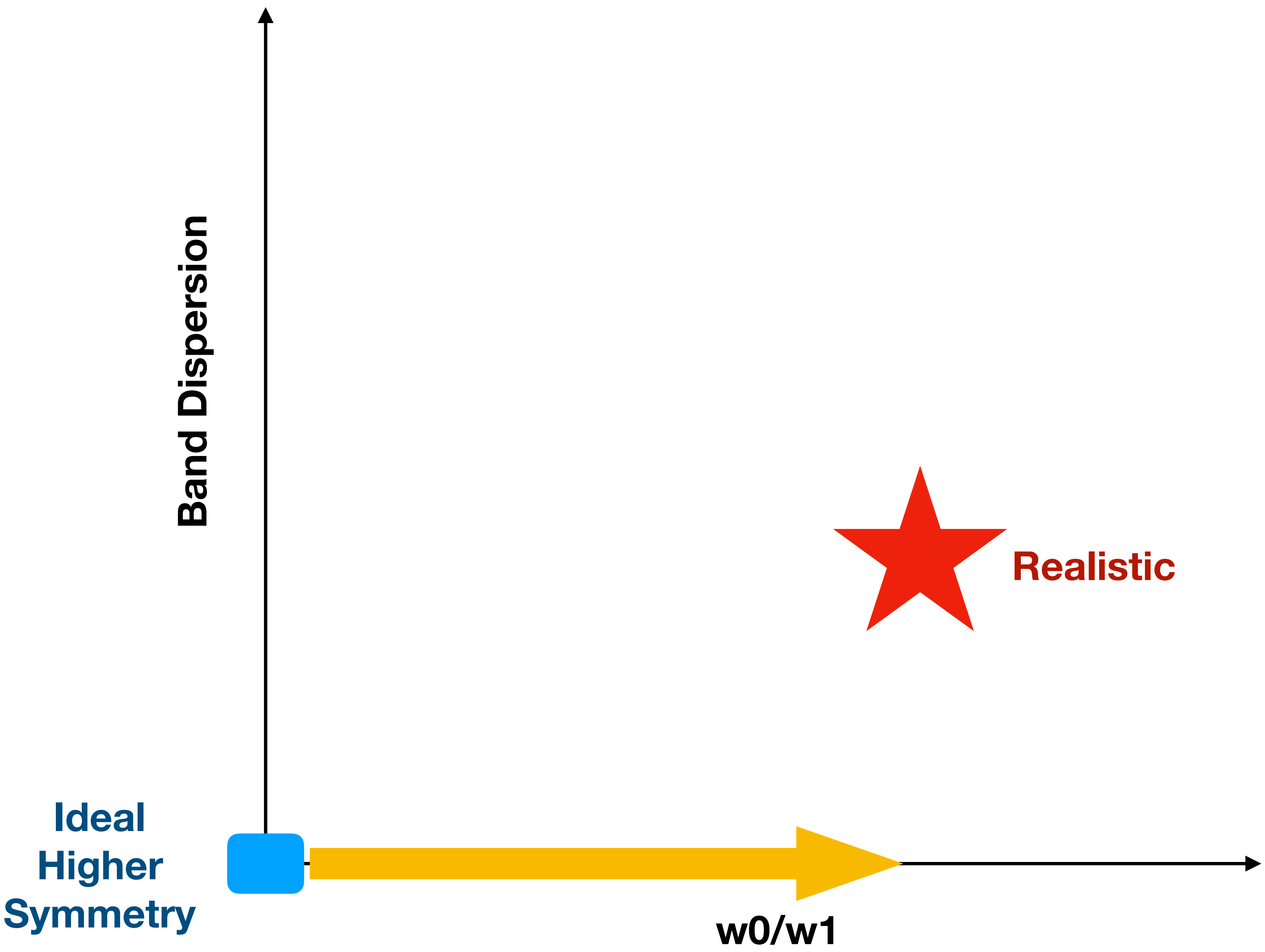
Valley Hall $Q = \sigma_z$ ✓

K-IVC $Q = \sigma_y \left(\Delta_R \tau_x + \Delta_I \tau_y \right)$ ✓

- "Antiferromagnetic" coupling $J \sim h^2/U \simeq 1\text{-}2$ meV

Mass terms for Dirac equation

Breaking the Degeneracy



Breaking the Degeneracy

Away from Chiral Limit:
(Retains a different U(2) symmetry)
Analysis appears to hold even if w0/w1 not small

$$\left[Q, \sigma_x \tau_z\right] = 0$$

$$\left[Q, \Lambda\right] = 0$$

Valley Hall $Q = \tau_z$

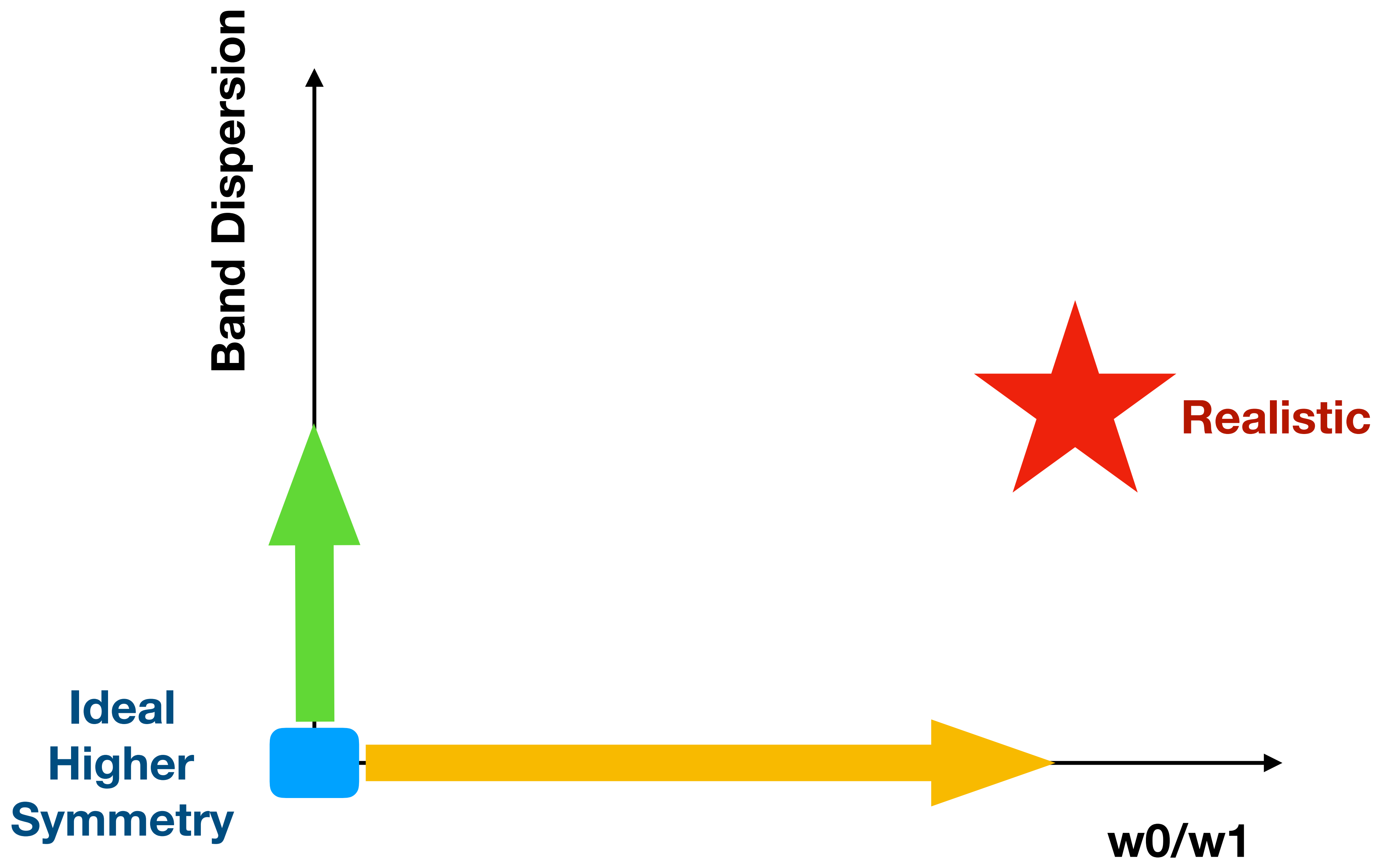
K-IVC $Q = \sigma_y \left(\Delta_R \tau_x + \Delta_I \tau_y \right)$

Ground State - Kramers IVC

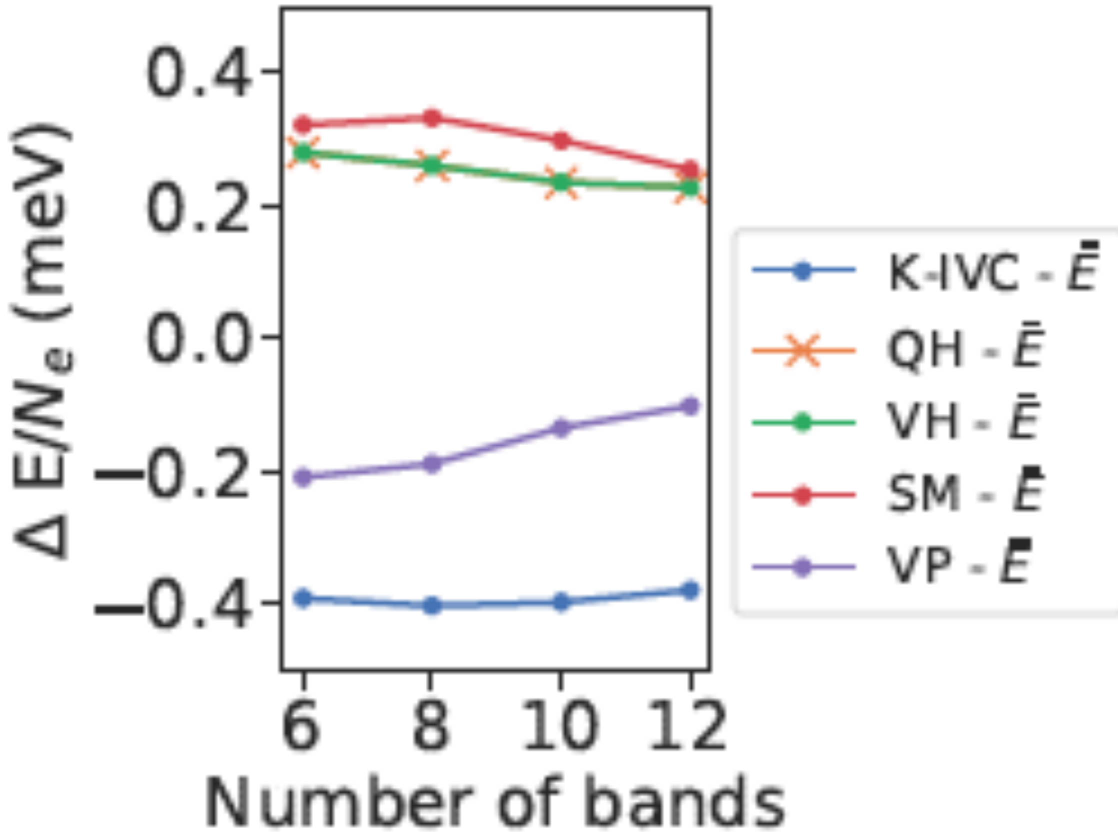
Both perturbations pick the same state
Unfrustrated -

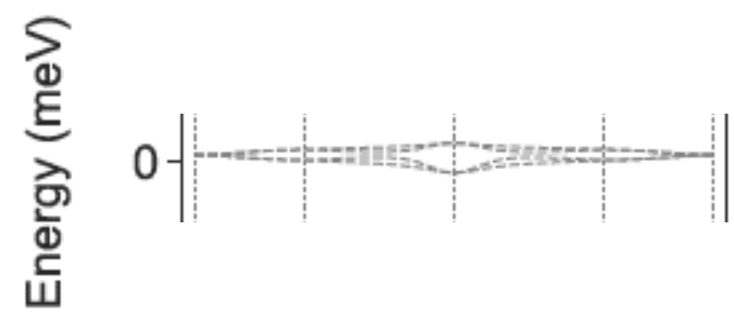
K-IVC

$$Q = \sigma_y \left(\Delta_R \tau_x + \Delta_I \tau_y \right)$$



Hartree Fock Numerics





Keeping remote bands (not important for CNP)

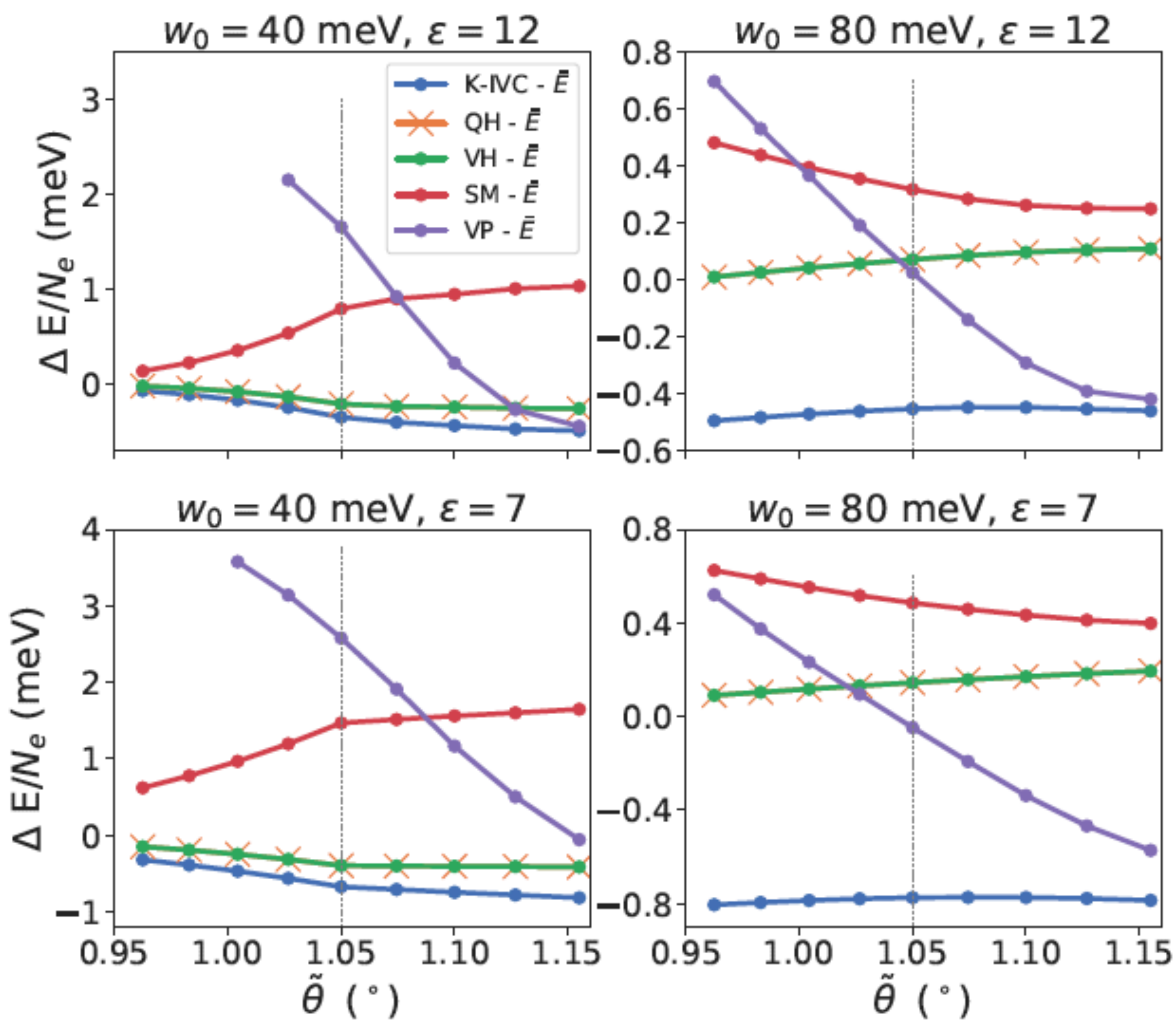
Ground state & Gap

K-IVC

$$Q = \sigma_y \left(\Delta_R \tau_x + \Delta_I \tau_y \right)$$

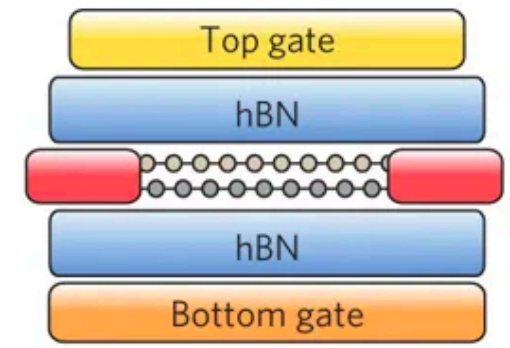
Hartree Fock Numerics

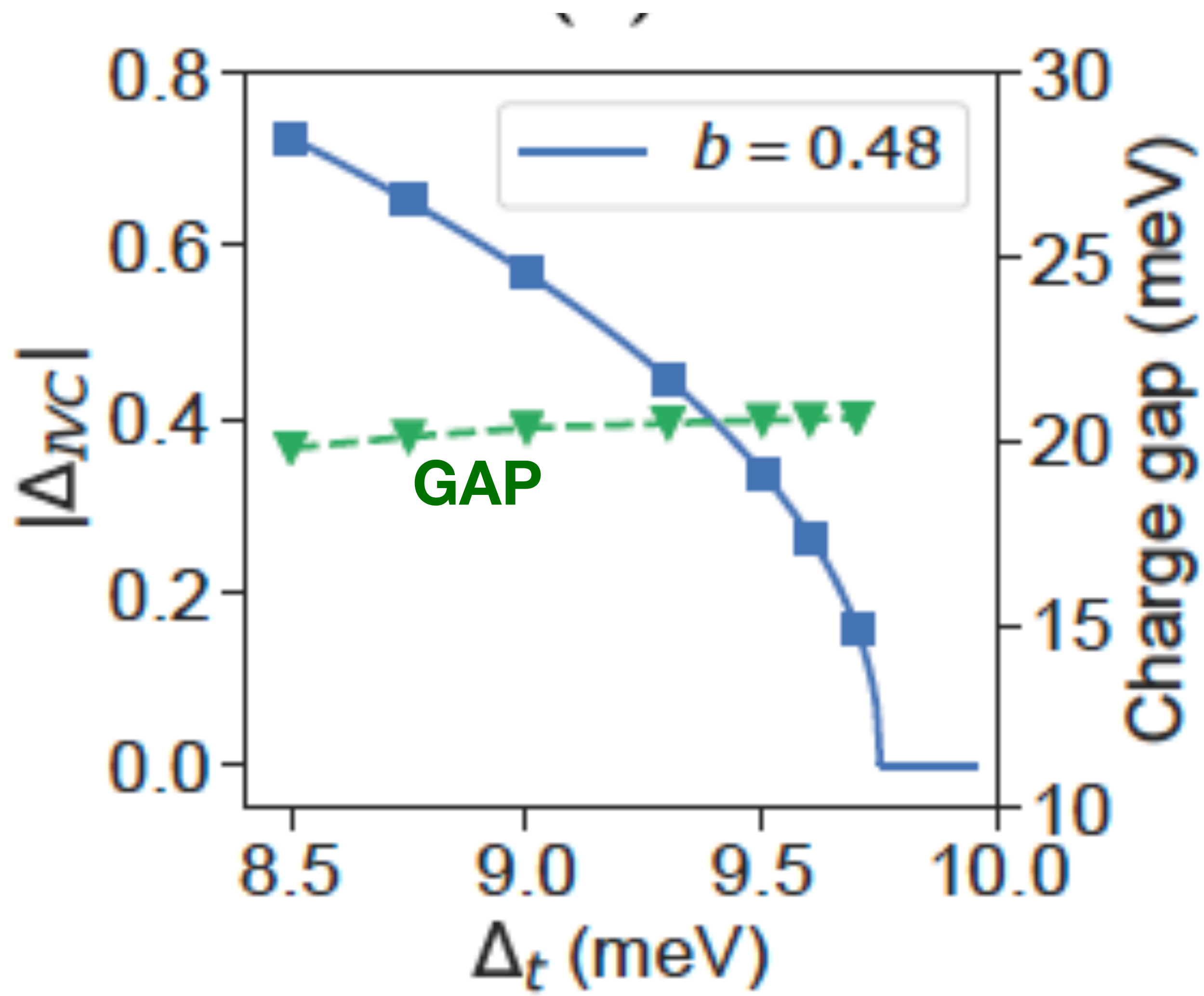
Ground state and low lying excited states

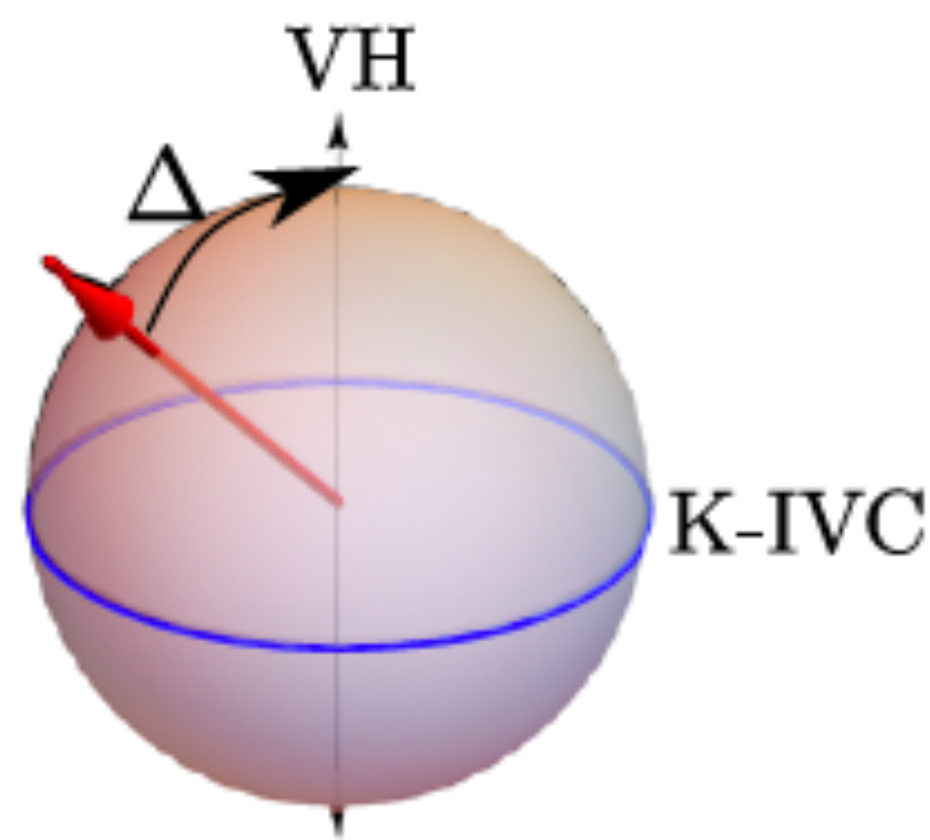


Quantum Phase Transition

Drive a quantum phase transition by hBN substrate which induces Valley Hall







Kramers IVC - Properties

Kramers time reversal and topological phase.

K-IVC

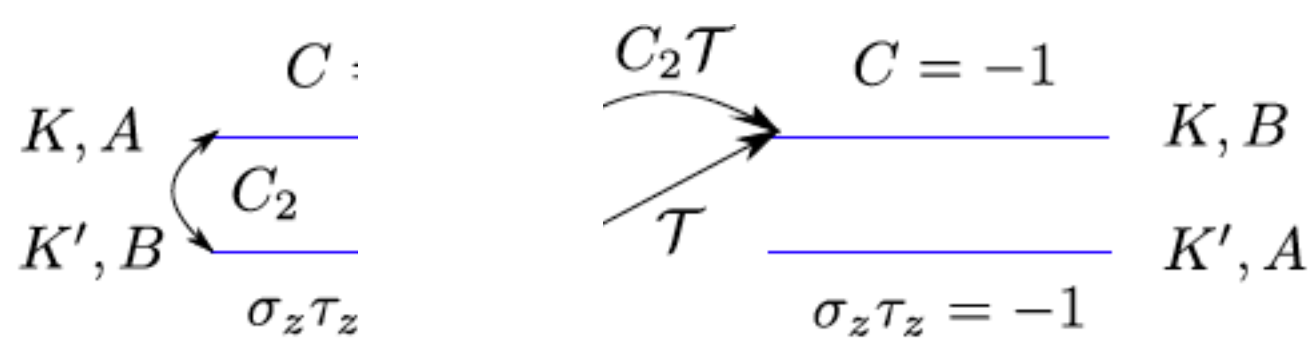
$$Q = \sigma_y \left(\Delta_R \tau_x + \Delta_I \tau_y \right)$$

$$U(1)_{\text{valley}}$$

- Spontanuously breaks $\mathcal{T}$, but preserves a combination of $\mathcal{T}$ and π valley rotation $\mathcal{T}' = \tau_z \mathcal{T} = \tau_y \mathcal{K}$.

$$i\tau_z = e^{i\frac{\pi}{2}\tau_z}$$

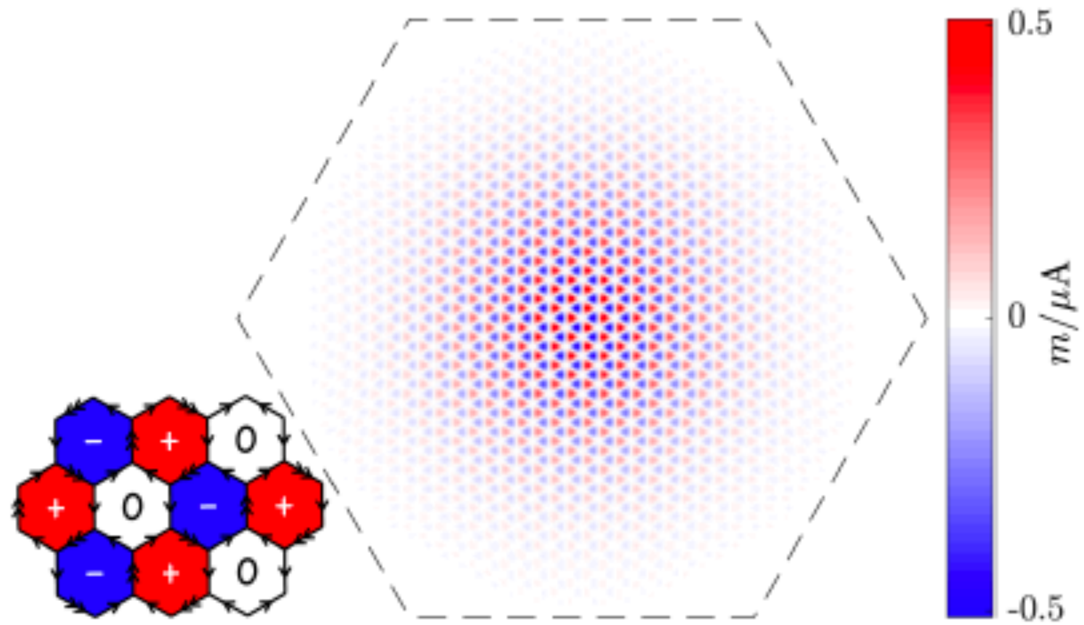
$$\mathcal{T}'^2 = -1$$



Same symmetries as topological insulator

Involves opposite Chern number band
Nontrivial Z2 topology!

Ground State- “Kramers” IVC



Spontaneous currents in the ground state
$U(1)_{valley}$ spontaneously broken - Goldstone modes
Edge states? Requires `smooth’ edge since we invoke $U(1)_{valley}$

Kramers IVC & Superconductivity

Kramers time reversal and Anderson theorem

Superconductivity coexisting with K-IVC?

In solids - Anderson’s theorem guarantees protection of Cooper pairs dues to Kramers Time reversal.

Here, effective Kramers time reversal implies **K_IVC + spin triplet superconductor** may be robust to small angle impurity scattering.

Interactions that lead to K_IVC also lead to superconductivity? Role of Phonons?

Reintroducing Spin

- $\nu = 0$: $\mathrm{U}(2)$ manifold of K-IVC states including spin-singlet $Q \propto s_0$ and spin-triplet $Q \propto \boldsymbol{n} \cdot \boldsymbol{s}$.
- $\nu = \pm 2$: spin-polarized K-IVC states spanning $\mathrm{U}(1) \times S^2 \times S^2$.

Locked by internally Hund's coupling (sign important)!

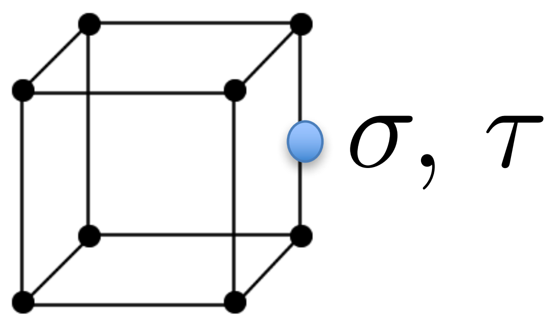
Conclusions

- 1 particle physics of twisted bilayer graphene is nontrivial, topology & symmetry important to model building.
  - Origin of flat bands - intriguing connection to topology.

- Nature of the Mott insulator and superconductor?
  - Opportunity to understand central questions in solid state physics - ferromagnetism vs anti ferromagnetism, novel superconductors …

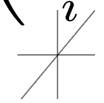
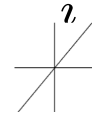
- The Kramers-IVC, a subtle symmetry breaking state with nontrivial topology appears to be the ground state in all our calculations on pristine TBLG. Relation to experiments?

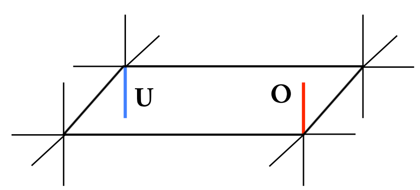
Surface Topological order in an Exactly Soluble Model



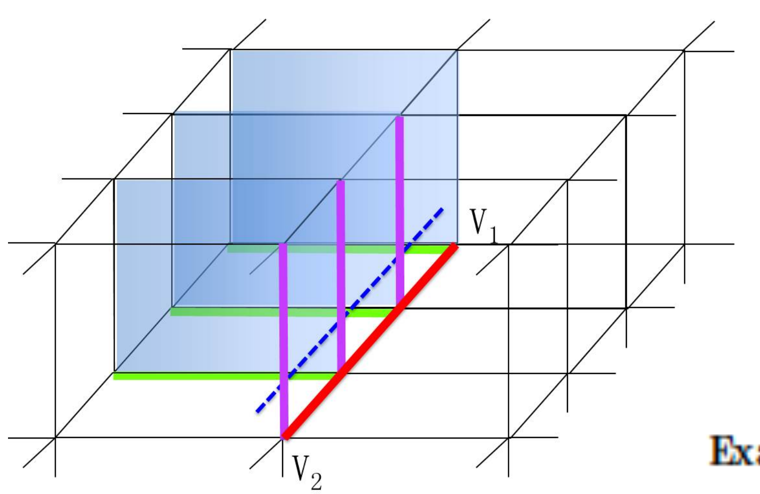
$$H = -\sum_V A_V - \sum_P B_P$$

$$A_V = \left(\prod_i \sigma_i^x + \prod_i \tau_i^x \right)$$



$$B_P = [\sigma^x]_{\mathrm{O}} \prod_{\square} \sigma^z [\sigma^x \tau^x]_{\mathrm{U}} + [\sigma^x \tau^x]_{\mathrm{O}} \prod_{\square} \tau^z [\tau^x]_{\mathrm{U}}$$



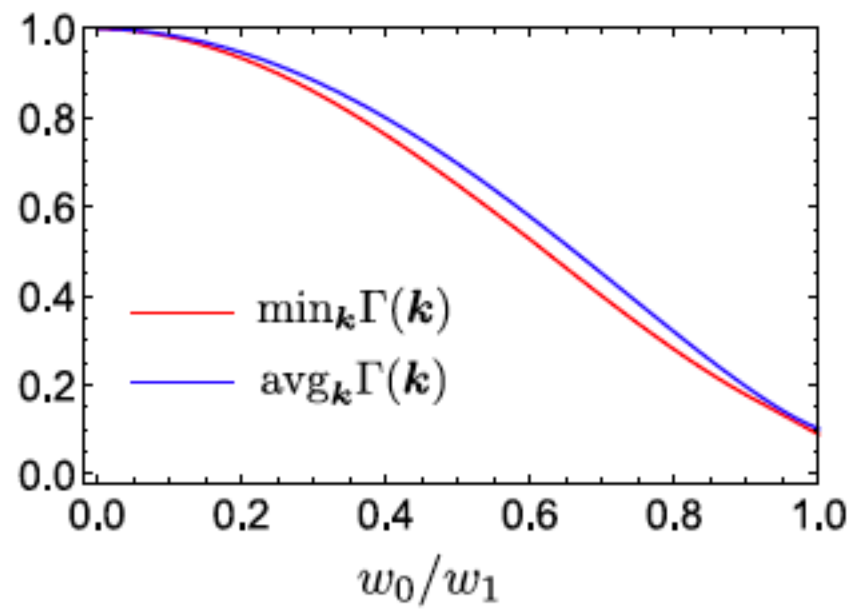
Point defects *confined* in the bulk but *deconfined* on surface.
3-fermion Z2 surface state is realized.

Exactly Soluble Model of a 3D Symmetry Protected Topological Phase of Bosons with Surface Topological Order

F. J. Burnell[1,2], Xie Chen[3,4], Lukasz Fidkowski[3,5], and Ashvin Vishwanath[3]

Away from the chiral limit

- $w_0 = 0.75 w_1$ not very small
- Sublattice polarization $\Gamma(\boldsymbol{k}) = \sqrt{\frac{1}{2}\,\mathrm{tr}\langle u_{\boldsymbol{k}}|\sigma_z|u_{\boldsymbol{k}}\rangle^2}$ remains finite
- Breaks $\mathrm{U}(4)\times\mathrm{U}(4)\to\mathrm{U}_{\mathcal{C}}(4)$ with the extra generator $\mathcal{C}$



- Intrasublattice form factor Λ^+ larger than intersublattice one Λ^-

$$\mathcal{H} = \mathcal{H}_+ + \mathcal{H}_-, \qquad U_-/U_+ \sim 0.2\text{-}0.3$$

- Projection onto the low-energy manifold $\mathcal{H}_- \sim U_-^2/U_+ \sim 1\text{-}2$ meV
- Minimize $\mathcal{H}_-$, $[Q,\sigma_y]=0$.
- Sublattice symmetry still holds approximately for dispersion $\{h,\sigma_z\}\approx 0$