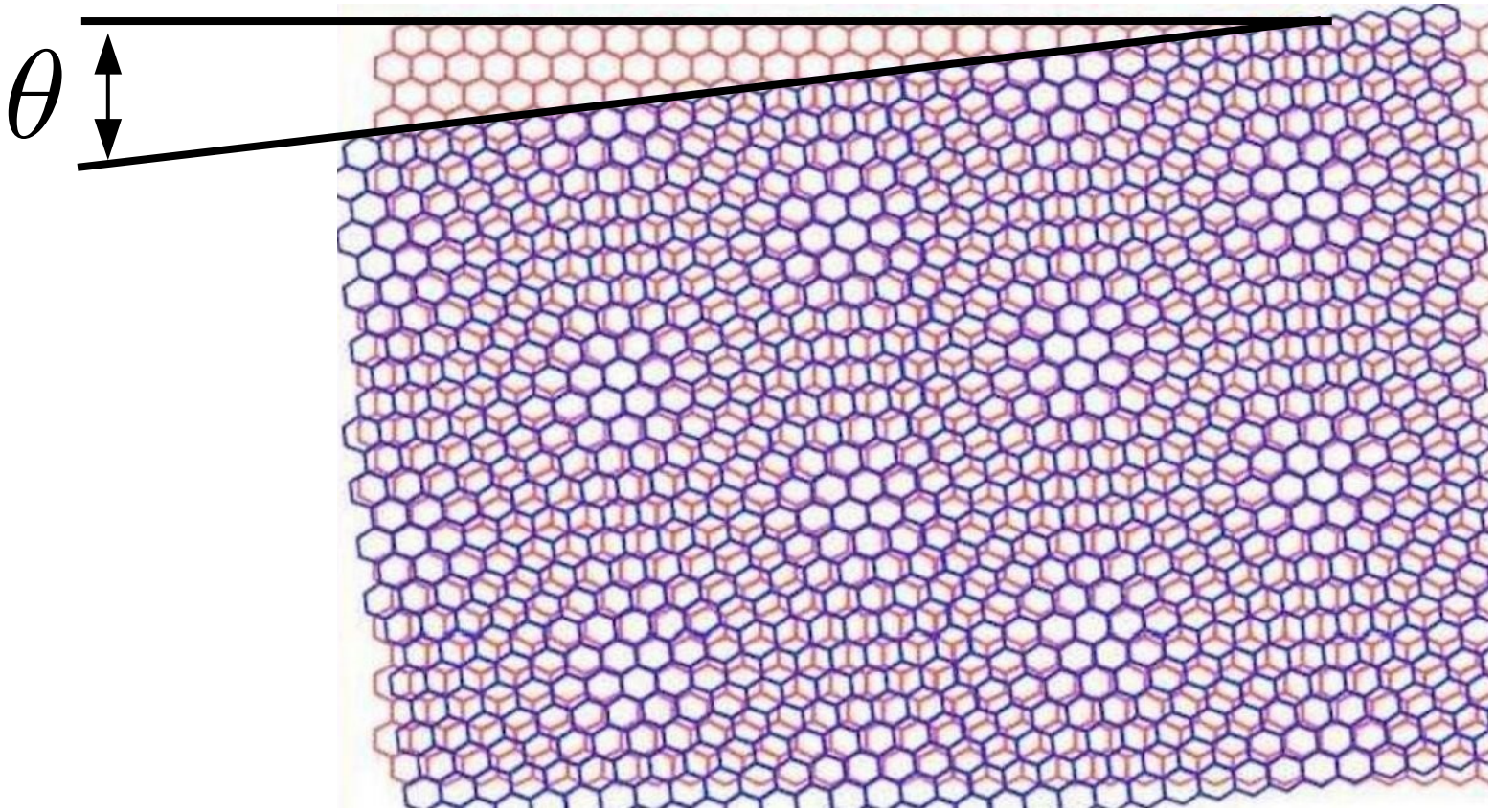
Broken-symmetry insulators: Applications to magic-angle twisted bilayer graphene

Nick Bultinck

MagLab Winter school 2023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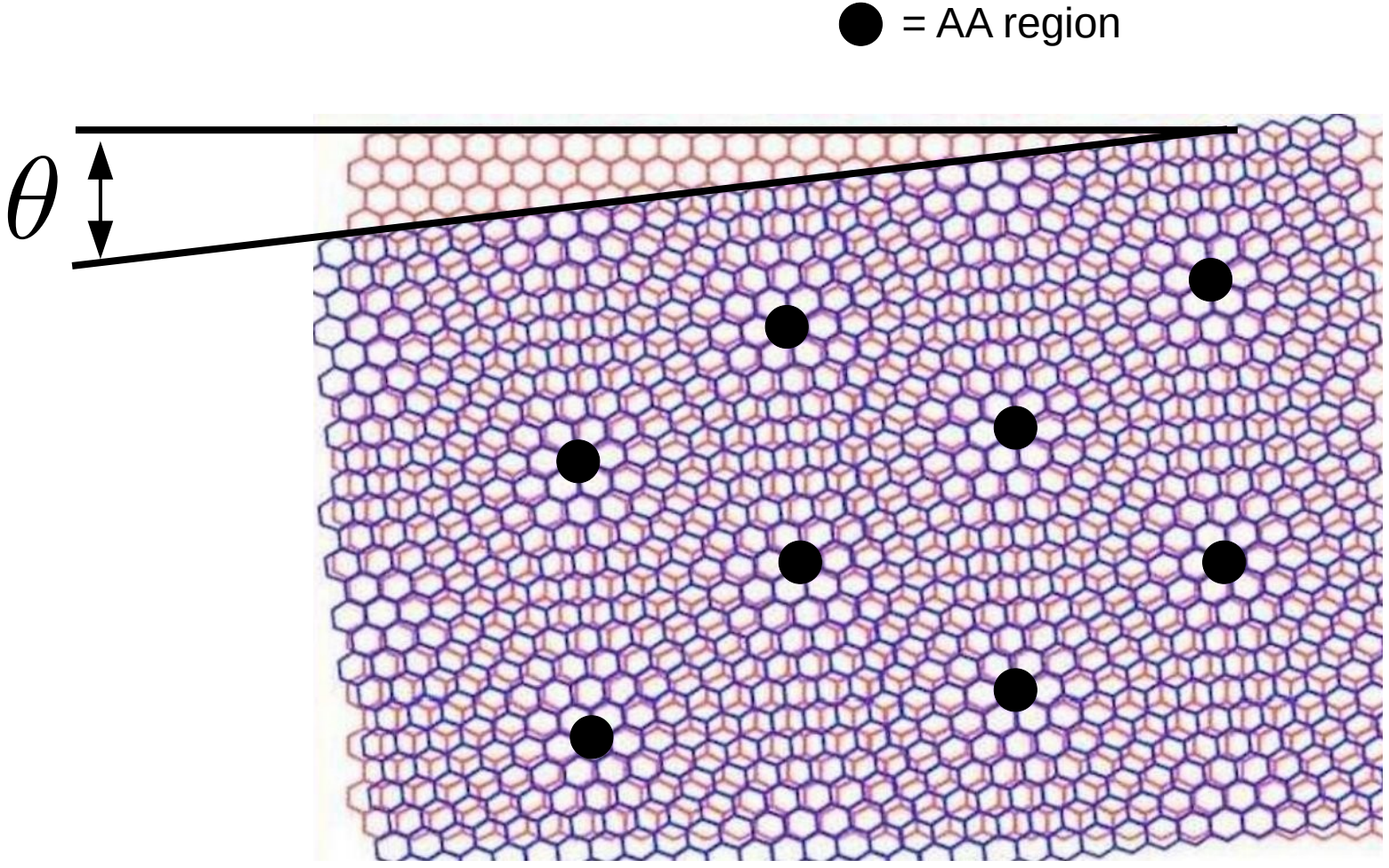
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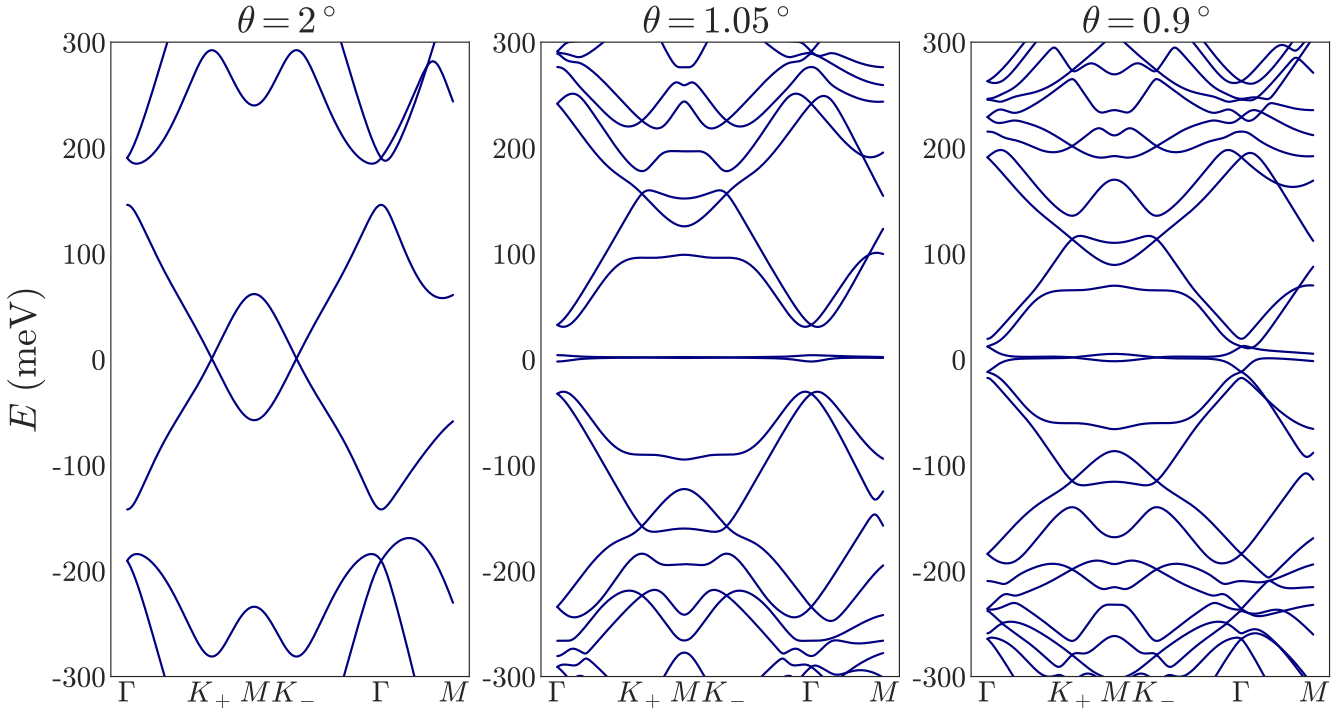
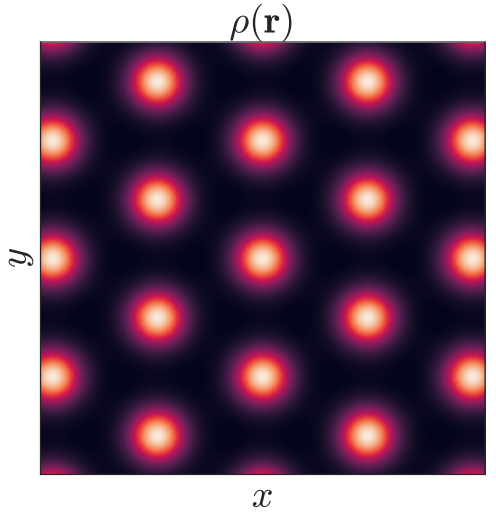
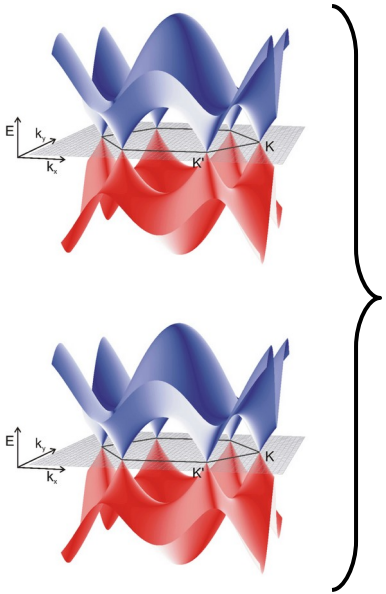
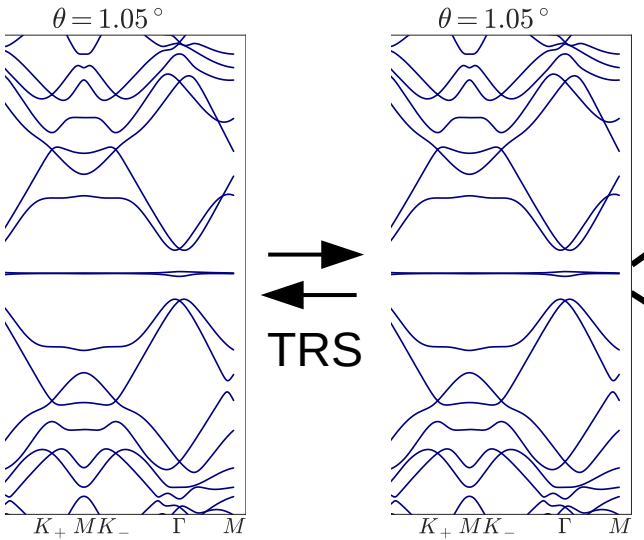




Flat band electron density

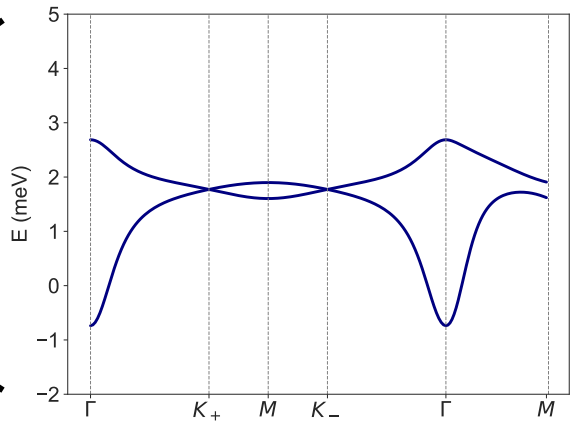


Dirac dispersion of two graphene layers



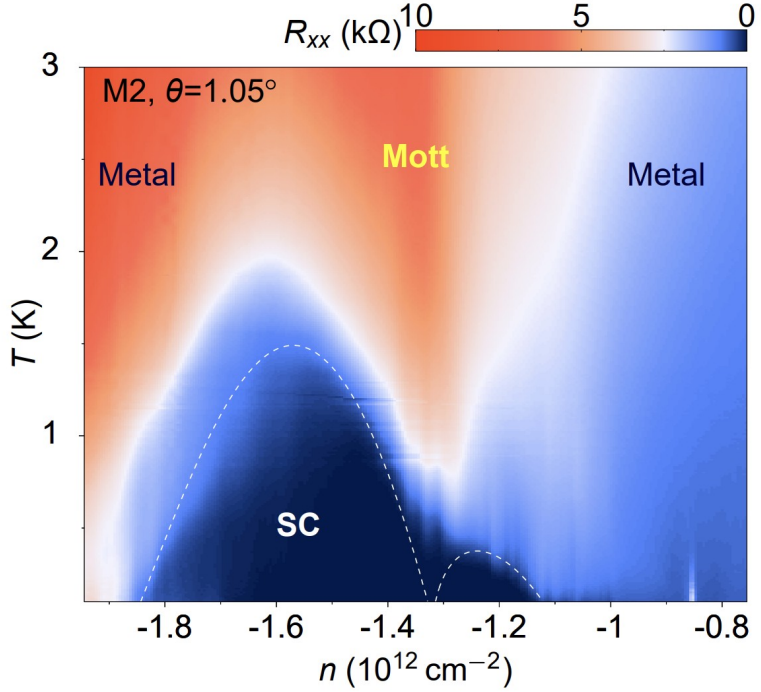
Valley K Valley K'

Emergent valley U(1) symmetry
+ independent spin rotations in both valleys.
Total (continous) symmetry group is
U(2)xU(2).

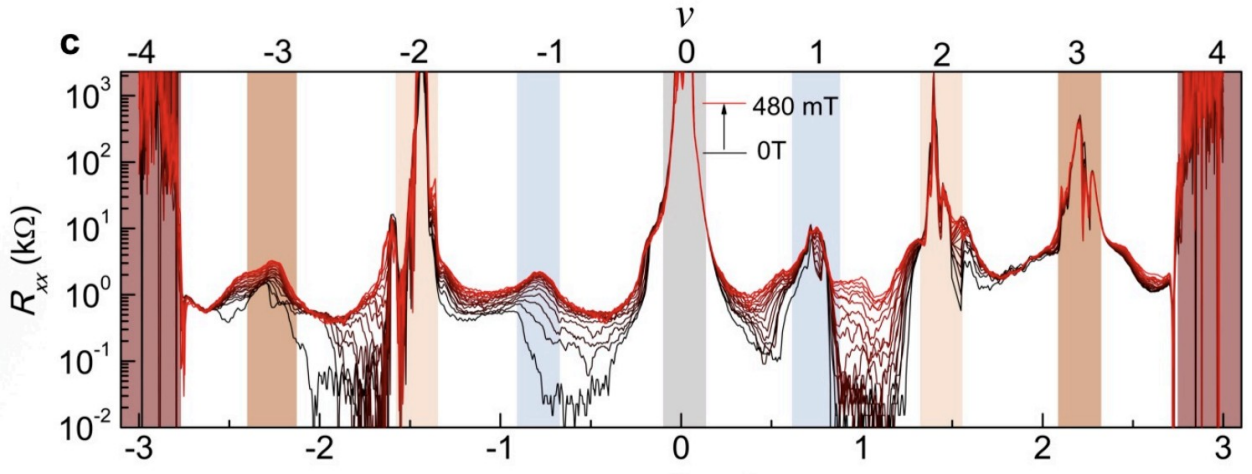


Band insulators at electron densities $\nu = \pm 4$

(4 electrons or holes per superlattice unit cell)



[Cao, Fatemi, …, Jarillo-Herrero (2018)]



[Lu, Stepanov, …, Efetov (2019)]

Outline:

- The frozen remote band model
- Broken-symmetry insulators in pristine MATBG
- The importance of strain

The frozen remote band model

Bistritzer-MacDonald Hamiltonian in momentum space:

$$[H_{BM}(\mathbf{k})]_{\mathbf{g}_i,\mathbf{g}_j} = \begin{pmatrix} h(R_{-\theta/2}(\mathbf{k}+\mathbf{g}_i+\mathbf{\Gamma}_m))\delta_{\mathbf{g}_i,\mathbf{g}_j} & \sum_{m=0}^{2} T_m \delta_{\mathbf{g}_i+\tilde{\mathbf{g}}_m,\mathbf{g}_j} \\ \sum_{m=0}^{2} T_m \delta_{\mathbf{g}_i,\mathbf{g}_j+\tilde{\mathbf{g}}_m} & h(R_{\theta/2}(\mathbf{k}+\mathbf{g}_i+\mathbf{\Gamma}_m))\delta_{\mathbf{g}_i,\mathbf{g}_j} \end{pmatrix}$$

$\mathbf{g}_i = (R_{\theta/2} - R_{-\theta/2})\mathbf{G}_i$ moiré reciprocal lattice vectors

$\mathbf{\Gamma}_m$ mBZ Gamma point

R_θ 2x2 rotation matrix over angle θ

$\tilde{\mathbf{g}}_0 = 0$

$h(\mathbf{k})$ mono-layer graphene tight-binding Hamiltonian

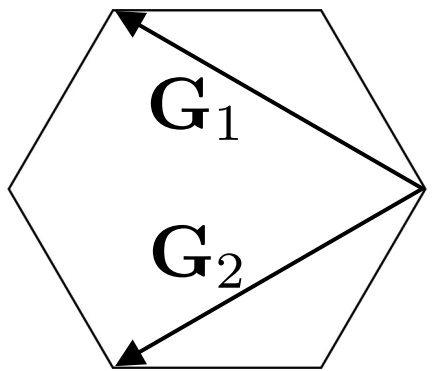
$\tilde{\mathbf{g}}_{1,2} = \mathbf{g}_{1,2}$

$$T_0 = w \begin{pmatrix} \kappa & 1 \\ 1 & \kappa \end{pmatrix}$$

$$T_1 = T_2^* = w \begin{pmatrix} \kappa & e^{-2\pi i/3} \\ e^{2\pi i/3} & \kappa \end{pmatrix}$$

$w = 110 \text{ meV}$

$\kappa \sim 0.5 - 0.8$



Bistritzer-MacDonald Hamiltonian in momentum space:

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Note that under shifts by moiré reciprocal lattice vectors the BM Hamiltonian transforms as

$$[H_{BM}(\mathbf{k}+\mathbf{g})]_{\mathbf{g}_i,\mathbf{g}_j} = [H_{BM}(\mathbf{k})]_{\mathbf{g}_i+\mathbf{g},\mathbf{g}_j+\mathbf{g}}$$

As a result, the BM eigenvectors satisfy

$$u_{m,\tau;\alpha,\mathbf{g}_i}(\mathbf{k}+\mathbf{g}) = u_{m,\tau;\alpha,\mathbf{g}_i+\mathbf{g}}(\mathbf{k})$$

BM band label

Valley

Layer/sublattice index

Let us now add the Coulomb interaction and go to momentum space:

$$\hat{H}_C = \frac{1}{2}\int \mathrm{d}\boldsymbol{r}\int \mathrm{d}\boldsymbol{r}'\, V(\boldsymbol{r}-\boldsymbol{r}')\psi^\dagger_\alpha(\boldsymbol{r})\psi^\dagger_\beta(\boldsymbol{r}')\psi_\beta(\boldsymbol{r}')\psi_\alpha(\boldsymbol{r})$$
$$= \frac{1}{2A}\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} V_{\boldsymbol{q}}\,\psi^\dagger_{\alpha,\boldsymbol{k}+\boldsymbol{q}}\psi^\dagger_{\beta,\boldsymbol{k}'-\boldsymbol{q}}\psi_{\beta,\boldsymbol{k}'}\psi_{\alpha,\boldsymbol{k}}\,,$$

with $\{\psi^\dagger_{\alpha,\boldsymbol{k}},\psi_{\beta,\boldsymbol{k}'}\} = \delta_{\alpha,\beta}\delta_{\boldsymbol{k},\boldsymbol{k}'}$

Next we rewrite the momentum sums as $\sum_{\mathbf{k}} \to \sum_{\tau}\sum_{\mathbf{k}\in \mathrm{mBZ}}\sum_{\mathbf{g}}$, and obtain

$$\hat{H}_C \approx \frac{1}{2A}\sum_{\tau,\tau'}\sum_{\mathbf{q}}\sum_{\mathbf{k},\mathbf{k}'\in \mathrm{mBZ}}\sum_{\mathbf{g},\mathbf{g}'} V_{\mathbf{q}}\psi^\dagger_{\alpha,\tau,\mathbf{g}}(\mathbf{k}+\mathbf{q})\psi^\dagger_{\beta,\tau',\mathbf{g}'}(\mathbf{k}'-\mathbf{q})\psi_{\beta,\tau',\mathbf{g}'}(\mathbf{k})\psi_{\alpha,\tau,\mathbf{g}}(\mathbf{k})$$

Note that here we have ignored inter-valley scattering V_q decays with q

Now we do a basis transformation and we go to the BM band basis by defining

$$f^{\dagger}_{m,\tau,\mathbf{k}} = \sum_{\alpha,\mathbf{g}} u_{m,\tau;\alpha,\mathbf{g}}(\mathbf{k}) \psi^{\dagger}_{\alpha,\tau,\mathbf{g}}(\mathbf{k})$$

Importantly, the f operators are periodic: $f^{\dagger}_{m,\tau,\mathbf{k}+\mathbf{g}} = f^{\dagger}_{m,\tau,\mathbf{k}}$

In the BM band basis, the Coulomb interaction becomes

$$\hat{H}_C = \frac{1}{2A} \sum_{\tau,\tau'} \sum_{\boldsymbol{q}} \sum_{\boldsymbol{k},\boldsymbol{k}' \in \mathrm{mBZ}} V_{\boldsymbol{q}} \left[\Lambda^{\tau}_{\boldsymbol{q}}(\boldsymbol{k})\right]_{mn} \left[\Lambda^{\tau'}_{-\boldsymbol{q}}(\boldsymbol{k}')\right]_{m'n'}$$
$$\times f^{\dagger}_{m,\tau,\boldsymbol{k}+\boldsymbol{q}} f^{\dagger}_{m',\tau',\boldsymbol{k}'-\boldsymbol{q}} f_{n',\tau',\boldsymbol{k}'} f_{n,\tau,\boldsymbol{k}} \,,$$

where we have defined the form factors as

$$\left[\Lambda^{\tau}_{\mathbf{q}}(\mathbf{k})\right]_{mn} = \sum_{\alpha,\mathbf{g}} u^{*}_{m,\tau;\alpha,\mathbf{g}}(\mathbf{k}+\mathbf{q}) u_{n,\tau;\alpha,\mathbf{g}}(\mathbf{k})$$

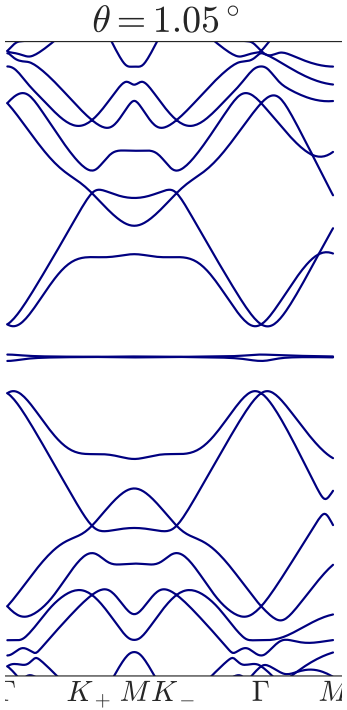
Exact Coulomb interaction **(up to inter-valley scattering)** in BM band basis:

$$\hat{H}_C = \frac{1}{2A}\sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{q}} : \left[\boldsymbol{f}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}}\Lambda_{\boldsymbol{q}}(\boldsymbol{k})\boldsymbol{f}_{\boldsymbol{k}}\right]\left[\boldsymbol{f}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q}}\Lambda_{-\boldsymbol{q}}(\boldsymbol{k}')\boldsymbol{f}_{\boldsymbol{k}'}\right] :$$

$$\Lambda_{\mathbf{q}}(\mathbf{k}) = \Lambda^{+}_{\mathbf{q}}(\mathbf{k}) \oplus \Lambda^{-}_{\mathbf{q}}(\mathbf{k})$$

This interaction preserves the U(2)xU(2) symmetry.

Now we ‘freeze’ the remote bands:



Completely empty

Fully occupied

Freezing remote bands = projecting in the subspace with completely filled (empty) remote valence (conduction) bands.

$$f^{\dagger}_{m,\tau,\mathbf{k}} f_{n,\tau',\mathbf{k}} \rightarrow \langle f^{\dagger}_{m,\tau,\mathbf{k}} f_{n,\tau',\mathbf{k}} \rangle \big|_{BM}$$

if m,n are remote bands

Terms with an odd number of remote-band fermion operators vanish under the projection.

We find the following frozen remote band Hamiltonian acting in the flat-band subspace:

$$\hat{H}_{FRB} = \sum_{\mathbf{k}} \sum_{\alpha \in FB} \sum_{\tau,s} \varepsilon^{BM}_{\tau,\alpha,\mathbf{k}} f^{\dagger}_{\alpha,\tau,\mathbf{k}} f_{\alpha,\tau,\mathbf{k}} + \hat{H}_h[P_r(\mathbf{k})] + \hat{H}_f[P_r(\mathbf{k})]$$
$$+ \frac{1}{2A} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\lambda,\sigma \in FB} V_{\mathbf{q}} : f^{\dagger}_{\alpha,\mathbf{k}+\mathbf{q}} \left[\Lambda_{\mathbf{q}}(\mathbf{k})\right]_{\alpha\beta} f_{\beta,\mathbf{k}} f^{\dagger}_{\lambda,\mathbf{k}'-\mathbf{q}} \left[\Lambda_{-\mathbf{q}}(\mathbf{k}')\right]_{\lambda\sigma} f_{\sigma,\mathbf{k}'}$$

Here we have defined the Hartree and Fock potentials constructed from

$$\langle f^{\dagger}_{m,\tau,\mathbf{k}} f_{n,\tau,\mathbf{k}'} \rangle = [P(\mathbf{k})]_{(n,\tau'),(m,\tau)} \sum_{\mathbf{g}} \delta_{\mathbf{k},\mathbf{k}'+\mathbf{g}}$$

as

$$\hat{H}_h[P(\mathbf{k})] = \frac{V_0}{A} \sum_{\mathbf{g}} \left[\sum_{\mathbf{k}'} \mathrm{tr}\left(P(\mathbf{k}')\Lambda_{\mathbf{g}}(\mathbf{k}')\right) \right] \sum_{\mathbf{k}} f^{\dagger}_{\mathbf{k}} \Lambda_{-\mathbf{g}} f_{\mathbf{k}}$$

$$\hat{H}_f[P(\mathbf{k})] = -\frac{1}{A} \sum_{\mathbf{k},\mathbf{q}} V_{\mathbf{q}} f^{\dagger}_{\mathbf{k}} \Lambda_{\mathbf{q}}(\mathbf{k}-\mathbf{q}) P(\mathbf{k}-\mathbf{q}) \Lambda_{-\mathbf{q}}(\mathbf{k}) f_{\mathbf{k}}$$

and we have also defined

$[P_r(\mathbf{k})]_{(m,\tau),(n,\tau')} = \delta_{mn}\delta_{\tau\tau'}[P_r]_n$ where $[P_r]_n = 1$ if n is a remote valence band, and zero otherwise

There is an (important ?) subtlety which we have swept under the rug until now:

The BM Hamiltonian takes input from ab initio methods such as DFT, which already take into account some interaction effects. We have now added back the complete Coulomb interaction – this means that we are double counting some interaction effects.

How do we fix this? There seems to be no general consensus….

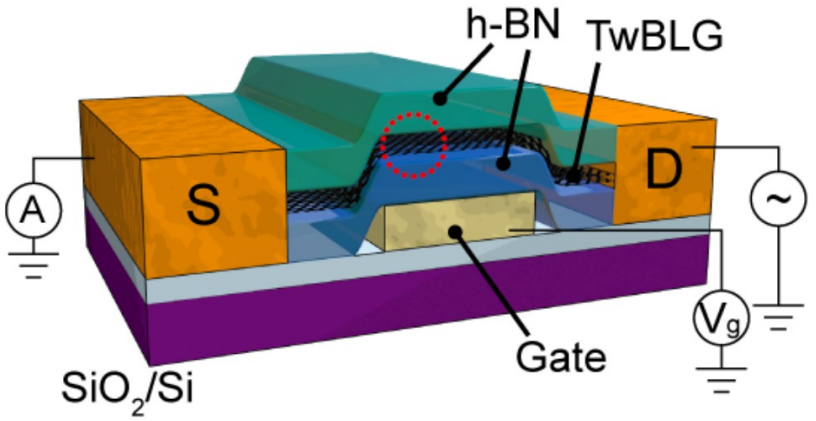
One example: Require the BM band structure at charge neutrality to be a solution to the Hartree-Fock self-consistency equation. This is true for the following Hamiltonian:

$$H = \underbrace{H_{BM}}_{\text{BM Hamiltonian}} + \underbrace{H_C}_{\text{Coulomb int}} - \underbrace{H_h[P_{BM}] - H_f[P_{BM}]}_{\text{‘Subtraction term’}}$$

Hartree and Fock potentials of the BM band structure at charge neutrality

Other subtraction schemes are also being used in the literature.

The effects of screening on the Coulomb potential:



[Cao, Fatemi, …, Jarillo-Herrero (MIT)]

Single-gate screening:

$$V_{\mathbf{q}}^{SG} = \frac{e^2}{2\epsilon_r \epsilon_0 q}(1 - e^{-2Dq})$$

Dual-gate screening:

$$V_{\mathbf{q}}^{DG} = \frac{e^2}{2\epsilon_r \epsilon_0 q}\tanh(Dq)$$

The relative dielectric constant of hBN is $\epsilon_r \sim 4 - 6$. Often larger values are used (~ 10 – 15) to take screening by the filled remote bands into account.

Broken-symmetry insulators in pristine MATBG

Symmetries of the BM model:

- U(2)xU(2) – spin/charge in each valley (valley-U(1) = $e^{i\theta\tau^z}$)
- Time-reversal $\mathcal{T} = \tau^x\mathcal{K}$
- Inversion $C_{2z} = \sigma^x\tau^x$ (interchanges sublattices)

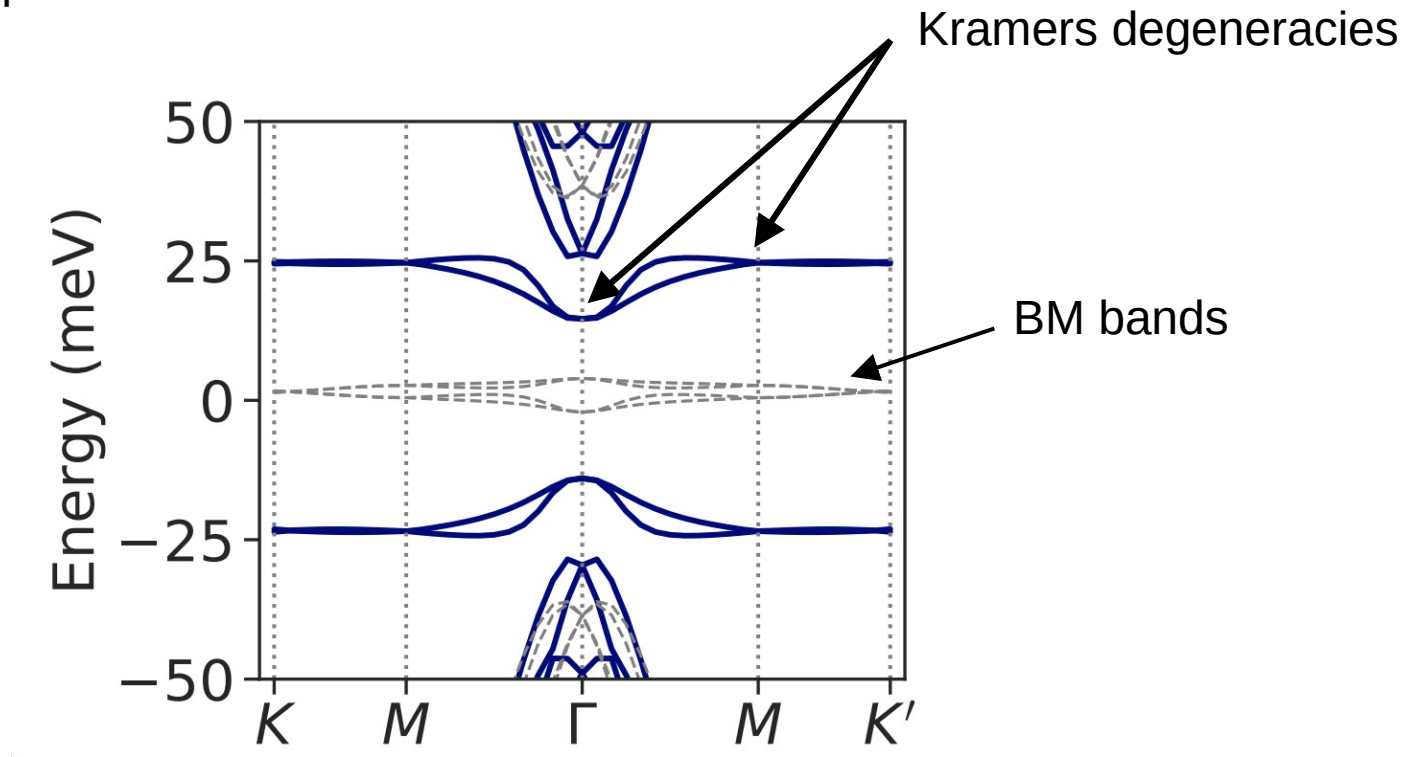
} $C_{2z}\mathcal{T}$ protects Dirac points

(Note that inversion and valley-U(1) do not commute)

- In-plane and out-of-plane rotations: C_{3z}, C_{2x}
- Particle-hole symmetry $\mathcal{P}$

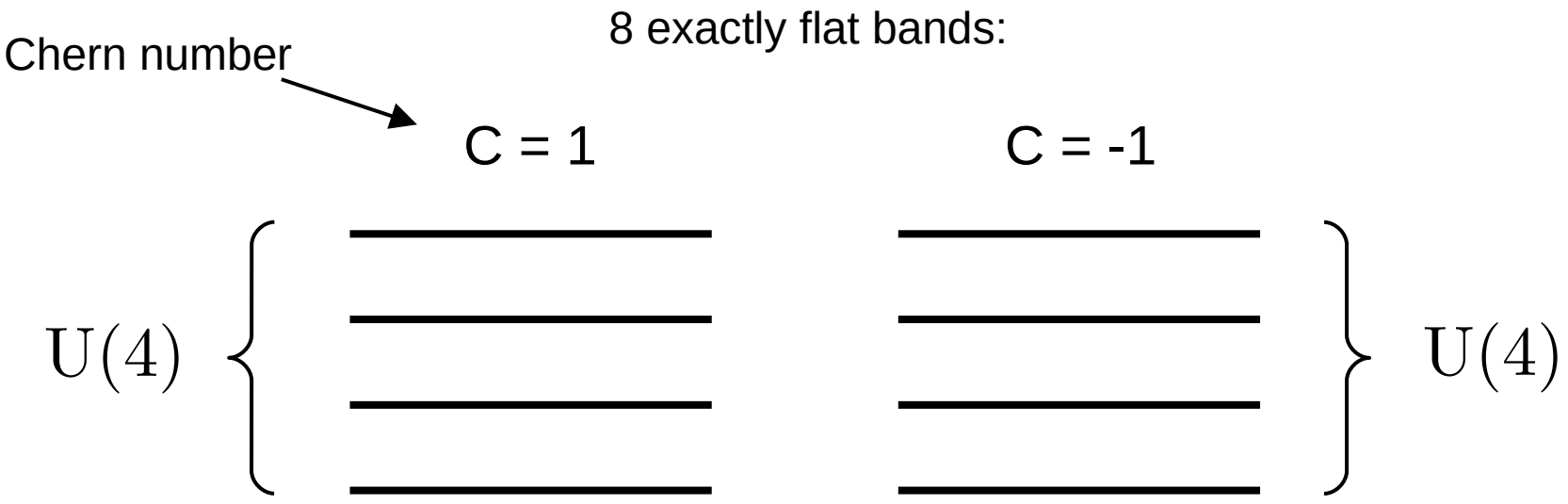
PH symmetry is broken in experiment. It can be broken explicitly by modifying the BM model with local (Kang,Vafek) or non-local (Carr, Kaxiras) inter-layer tunneling terms.

Mean-field band spectrum at $\nu = 0$:



This state breaks valley-U(1) and time-reversal. It preserves the product $\mathcal{T}' = \tau^y \mathcal{K}$, which is a Kramers time-reversal symmetry. Hence it is called the **K-IVC** state.
The order parameter takes the form $\Delta \sim \sigma^y \tau^x$.

The origin of the K-IVC state is naturally understood in the chiral limit $(\kappa = 0)$:



Combine U(2)xU(2), inversion, time reversal, particle-hole and chiral symmetry

➡ Coulomb interaction between electrons in the flat bands has a (approximate) $\mathrm{U}(4) \times \mathrm{U}(4)$ symmetry

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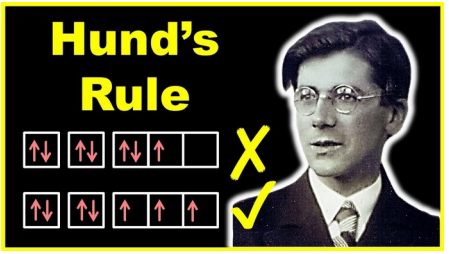
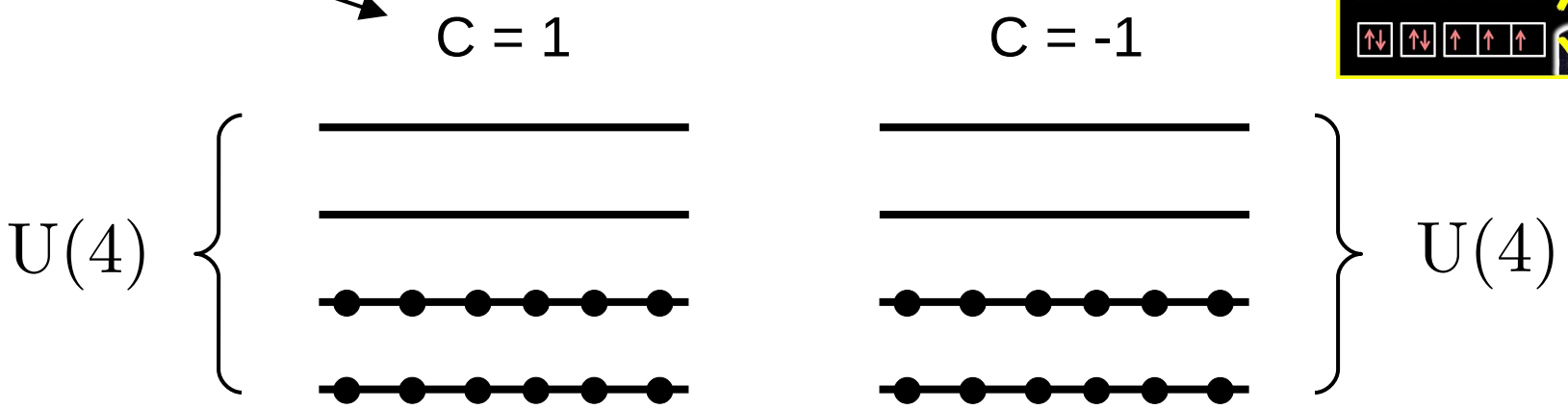


8 exactly flat bands:

Chern number



At integer fillings the exact ground states of the interaction term are $\mathrm{U}(4) \times \mathrm{U}(4)$ quantum Hall ferromagnets.

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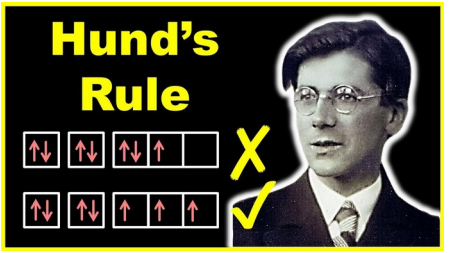

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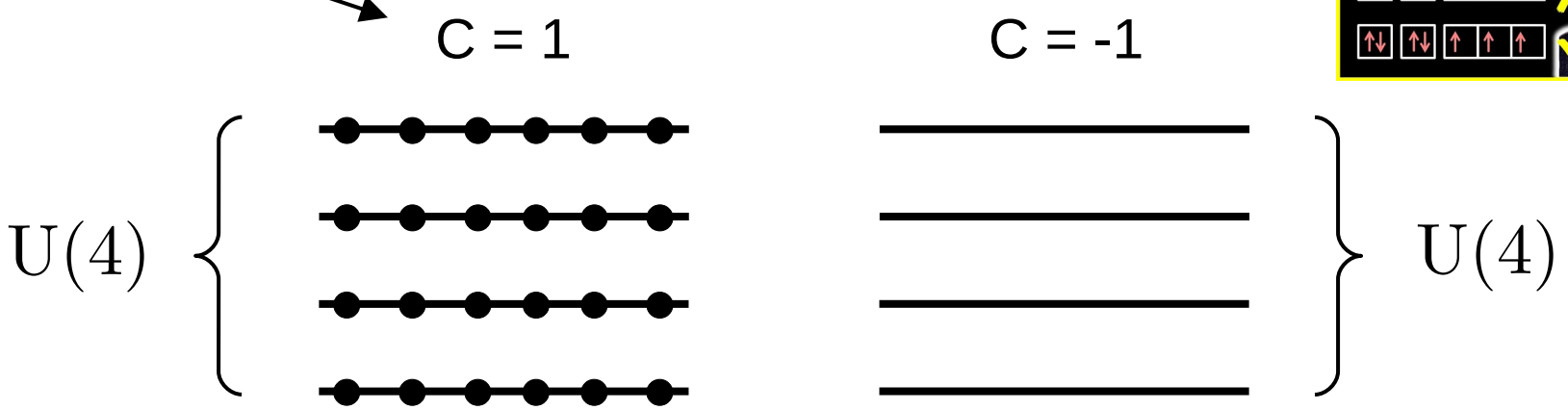
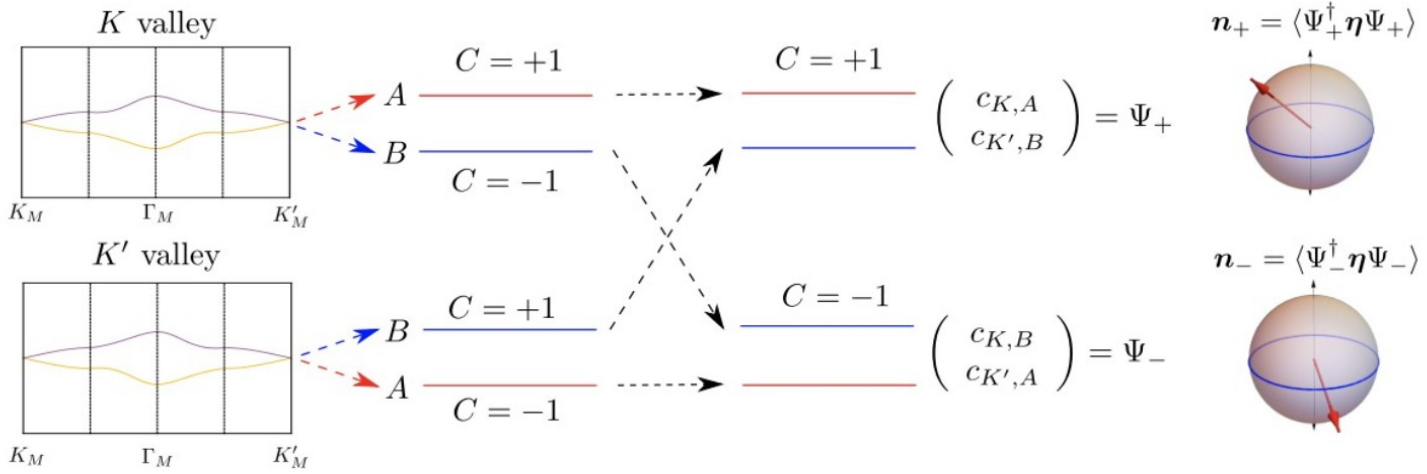


The large ground state degeneracy is lifted in perturbation theory by taking small deviations from the chiral limit into account. This given unique ***quantum Hall ferromagnetic*** ground states all integer fillings.

To understand how the K-IVC gets selected at neutrality we can consider a spinless model:

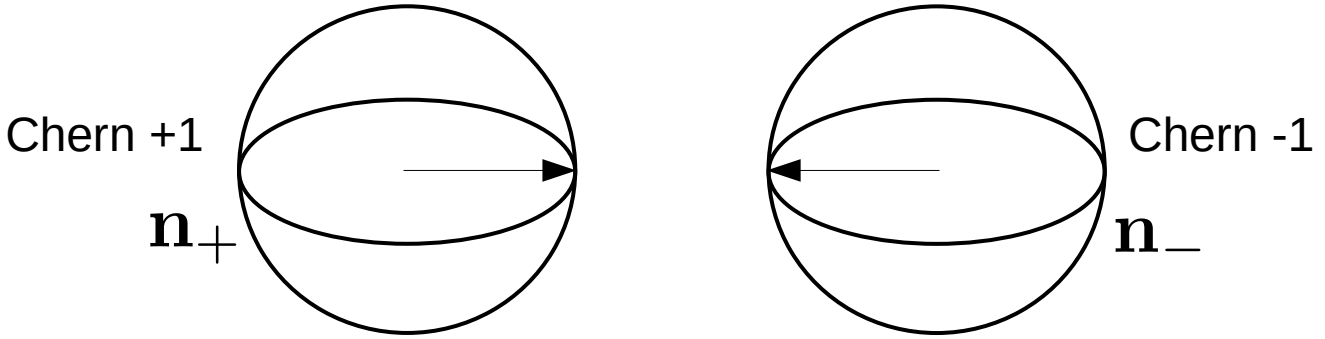


The low-energy theory of the QHFM is described by the following Lagrangian:

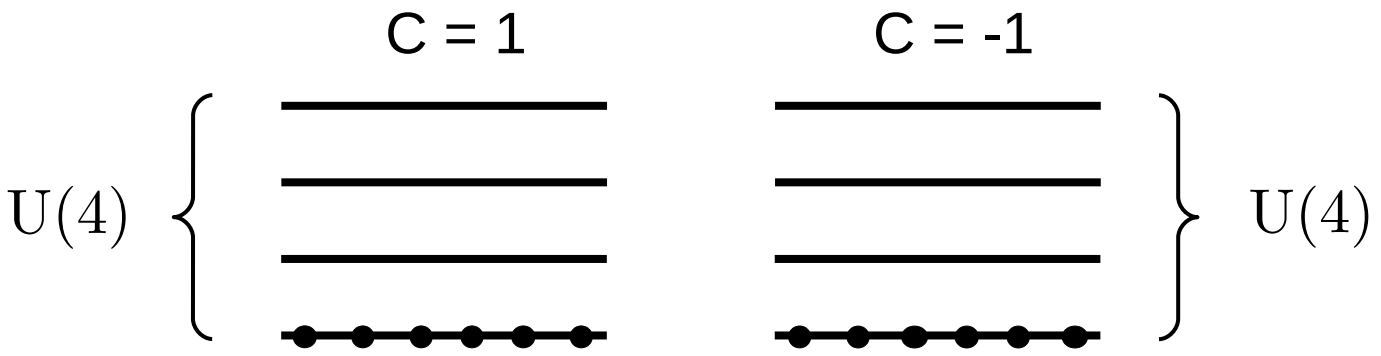
$$\mathcal{L} = \sum_{\gamma=\pm} \left(\frac{1}{2A_M} \mathcal{A}[\mathbf{n}_\gamma] \cdot i\partial_t \mathbf{n}_\gamma + \frac{\rho_s}{2} (\nabla \mathbf{n}_\gamma)^2 \right) + \underbrace{J\mathbf{n}_+ \cdot \mathbf{n}_-}_{\text{Dispersion}} + \underbrace{\lambda(\mathbf{n}_+^{xy} \cdot \mathbf{n}_-^{xy} - n_+^z n_-^z)}_{\text{Symmetry-breaking terms in the interaction}}$$

$$\mathcal{L} = \sum_{\gamma=\pm} \left(\frac{1}{2A_M} \mathcal{A}[\mathbf{n}_\gamma] \cdot i\partial_t \mathbf{n}_\gamma + \frac{\rho_s}{2} (\nabla \mathbf{n}_\gamma)^2 \right) + J\mathbf{n}_+ \cdot \mathbf{n}_- + \lambda(\mathbf{n}_+^{xy} \cdot \mathbf{n}_-^{xy} - n_+^z n_-^z)$$

Ground state = in-plane anti-ferromagnet = ‘K-IVC’ insulator



The QHFM formalism predicts insulators at all integer fillings



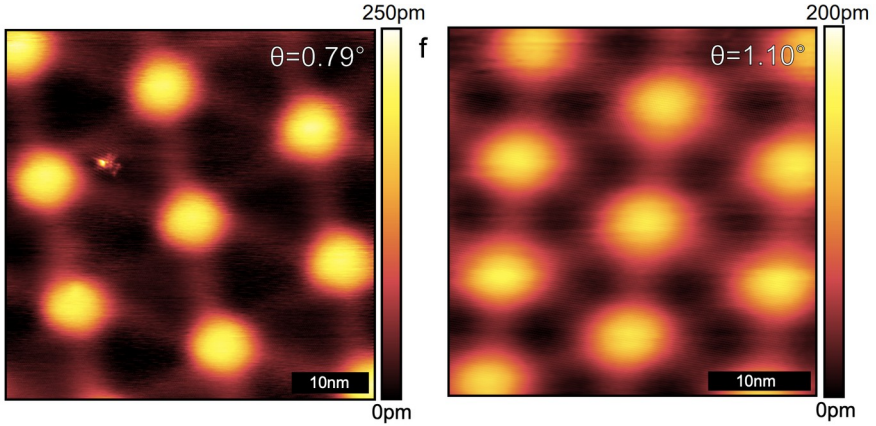
Numerical Hartree-Fock and DMRG simulations on the FRB model for pristine MATBG away from the chiral limit find ground states that agree with the QHFM predictions at $\nu = 0, \pm 1, \pm 2$

Moreover, DMRG shows that Hartree-Fock is extremely accurate.

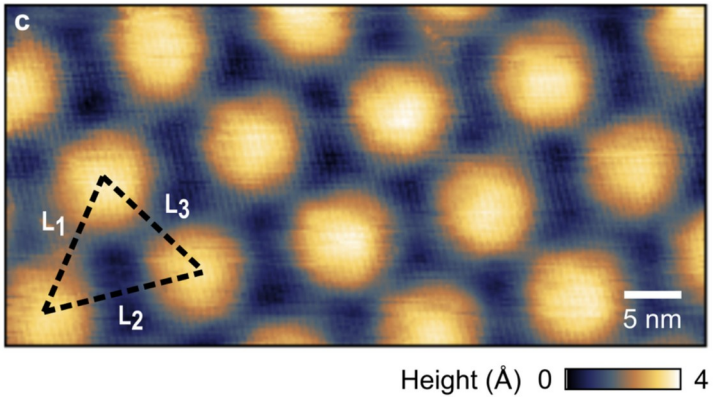
In the QHFM picture, $\nu + C = 0 \mod 2$ (c.f. Amir Yacoby's talk)

The importance of strain

[Kerelsky, McGilly, …. , Dean, Rubio, Pasupathy (2019)]



[Xie, Lian, … , Bernevig, Yazdani (2019)]



Heterostrain of magnitude $\epsilon \sim 0.1 - 0.7\%$ observed in STM.

This is small, but moiré patterns act like a magnifying glass for strain.

To lowest order, strain couples to mono-layer graphene as a vector potential.

$$h_D(\mathbf{k}) = \hbar v_F (M[\mathbf{k} - \mathbf{A}]) \cdot \boldsymbol{\sigma}$$

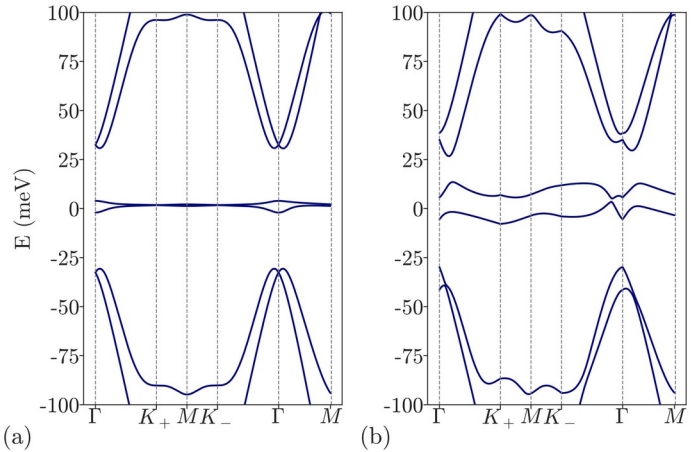
$$M = \begin{pmatrix} 1+\epsilon_{xx} & \epsilon_{xy} \\ \epsilon_{xy} & 1+\epsilon_{yy} \end{pmatrix}$$

[Suzuura, Ando (2002); Sasaki, Saito (2008)]

$$\boldsymbol{A} = \frac{\beta}{2a}(\epsilon_{xx} - \epsilon_{yy}, -2\epsilon_{xy})$$

Effect of strain on MATBG band spectrum (DPs in a single valley are no longer related by symmetry):

Without strain →

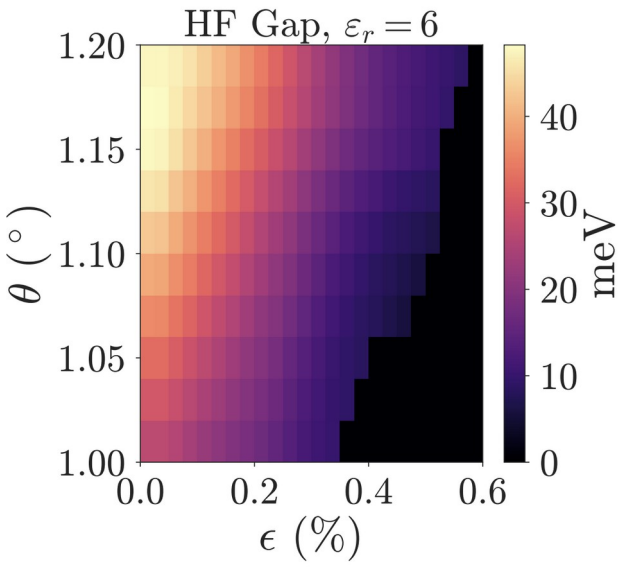


← With the experimentally observed strain

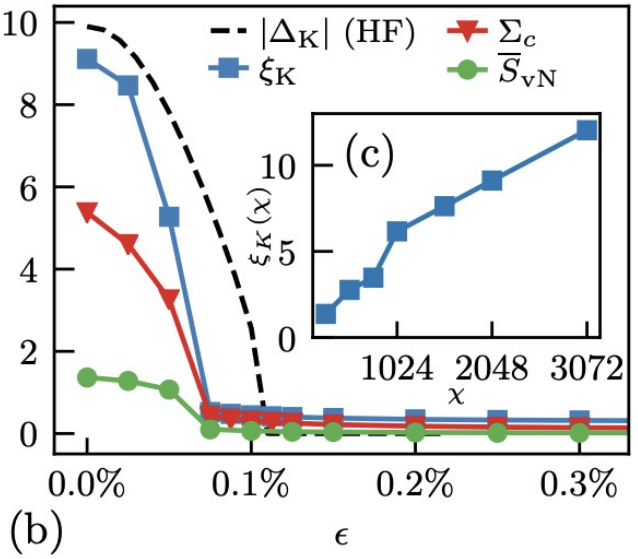
[Bi, Yuan, Fu (2019)]

Effect of strain on MATBG at neutrality: $(\nu = 0)$

Self-consistent Hartree-Fock



DMRG

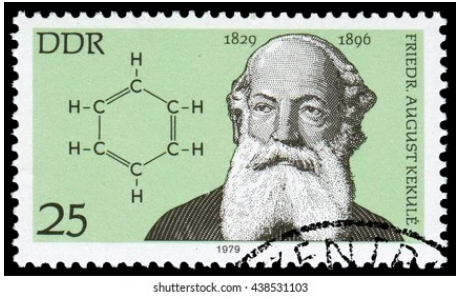


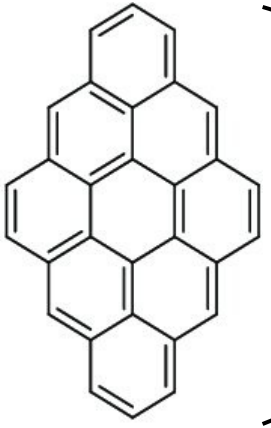
Experimentally-relevant strains make MATBG semi-metallic at neutrality.

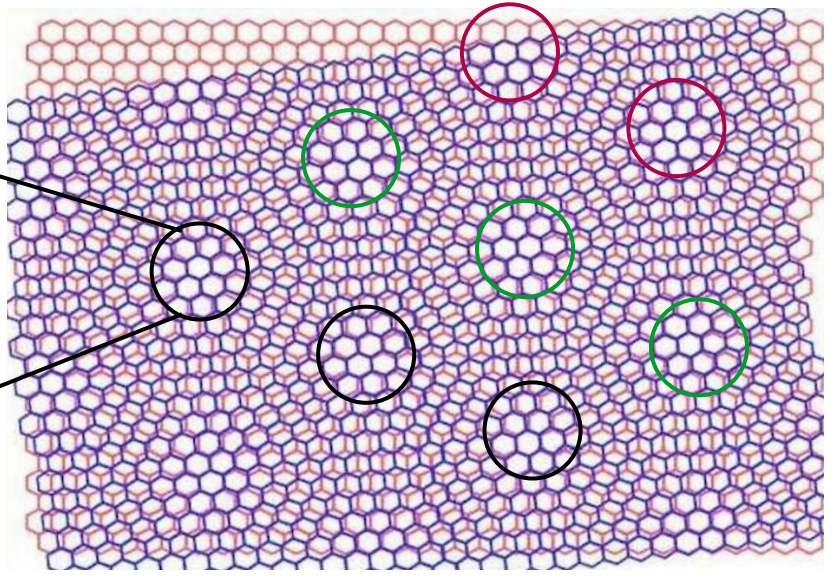
The effect of strain at non-zero integer fillings:

A new broken-symmetry order stabilized by strain: Incommensurate Kekulé Spiral (IKS) order

Kekulé pattern:







$\sqrt{3} \times \sqrt{3}$ Kekulé pattern is the result of a spontaneous breaking of the valley U(1) symmetry

The Kekulé pattern modulates on the superlattice scale with an incommensurate wavevector

The IKS order has a non-zero wavevector and thus breaks translation symmetry. However, it preserves a modified translation symmetry:

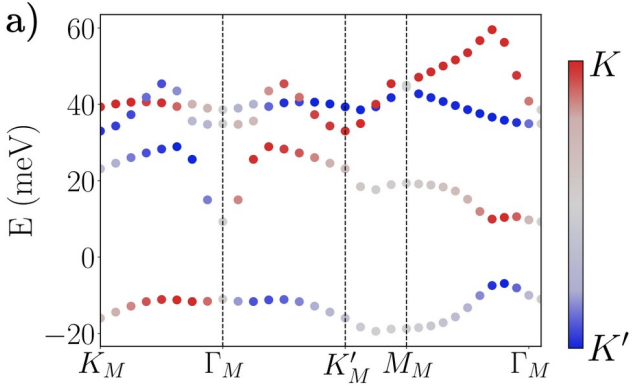
$$\hat{T}'_{\mathbf{a}_i} = \hat{T}_{\mathbf{a}_i} e^{i\mathbf{a}_i \cdot \mathbf{q}\tau^z}$$

This implies a generalized Bloch theorem:

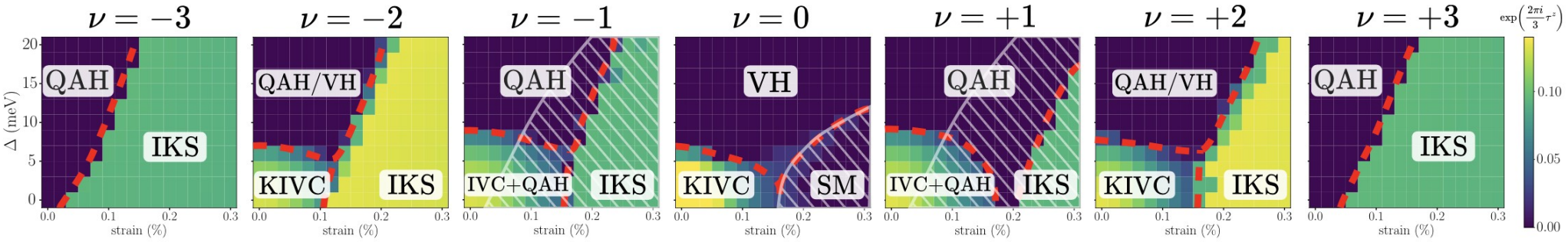
$$\psi_{\tilde{\mathbf{k}}}(\mathbf{r}) = e^{i\mathbf{r}\cdot(\tilde{\mathbf{k}} - \mathbf{q}\tau^z/2)} u_{\tilde{\mathbf{k}}}(\mathbf{r})$$

$$u_{\tilde{\mathbf{k}}}(\mathbf{r} + \mathbf{a}_i) = u_{\tilde{\mathbf{k}}}(\mathbf{r})$$

Mean-field IKS band structure at $\nu = -2$

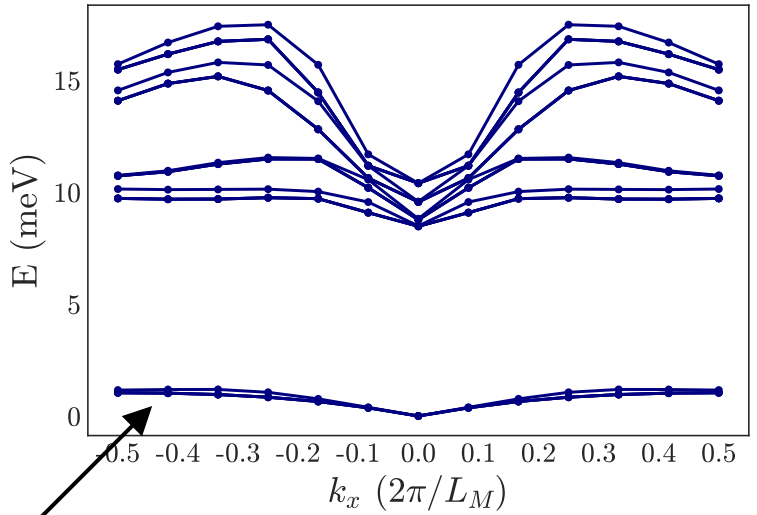


Beyond mean-field theory, the modified translation symmetry pins IKS insulators to integer superlattice fillings as the result of a generalized Lieb-Schultz-Mattis theorem



- IKS order at every integer filling except charge neutrality
- Strongest insulators at $\nu = \pm 2$
- No time-reversal symmetry breaking and QAH states

Collective modes of the IKS at $\nu = -2$:



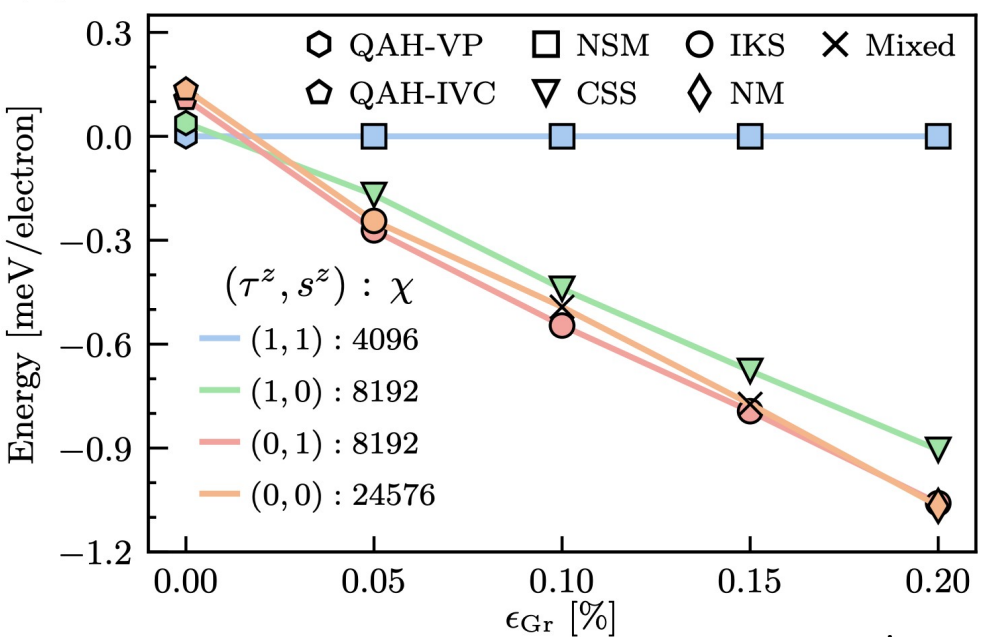
This state has zero spin polarization.

Four Goldstone modes! (one singlet, one triplet)

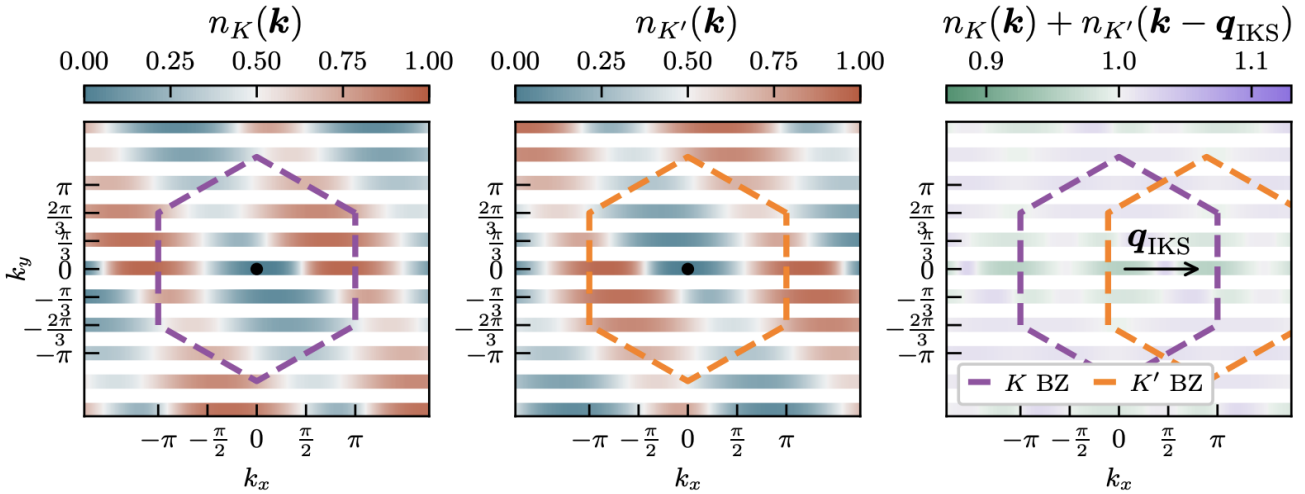
Broken symmetry generators: $\tau^z, s^x\tau^z, s^y\tau^z, s^z\tau^z$

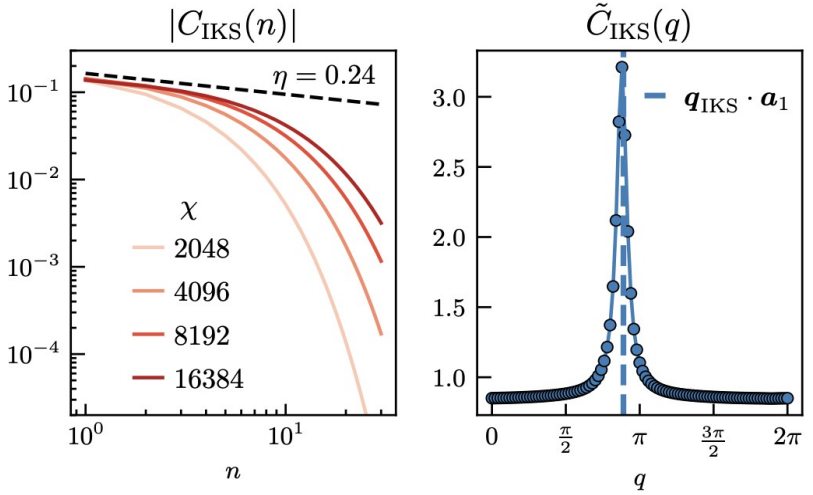
IVC states, spin polarized or unpolarized, always have Goldstone modes associated with spin fluctuations.

DMRG results at $\nu = -3$:



(For more details, see Tianle's poser today)





(For more details, see Tianle's poser today)

Thank you!