Insulating phases in twisted bilayer graphene

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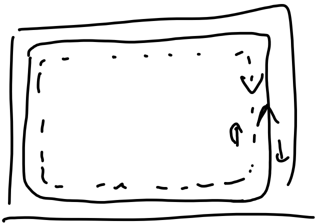
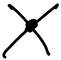


Kane and Mele (2005)

Not protected unless you have time reversal symmetry.

($T^2 = -1$ )

$\Rightarrow \mathbb{Z}_2$ TI

How do Chern insulators react in an external B field?

Magnetic length $l_B = \sqrt{\frac{\hbar}{eB}} \simeq \frac{26\ \text{nm}}{B^{1/2}\,[T]}$.

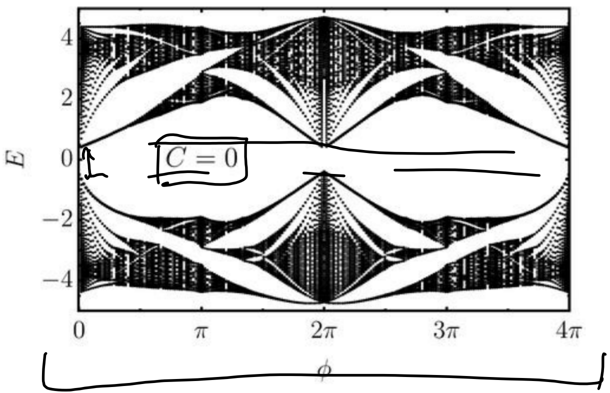
when $l_B \simeq$ atomic scale / lattice spacing

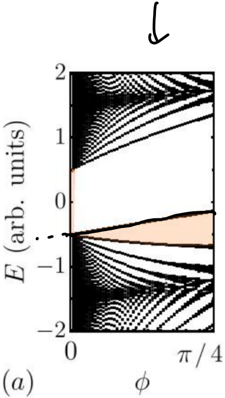
$\longrightarrow$ Hofstadter butterfly.

pure graphene $a \simeq 0.142\ \text{nm} \longrightarrow B \sim 10^4 T$

moiré $l \simeq 13\ \text{nm} \longrightarrow B \sim$ a few teslas.

Hofstadter and topology





What about a Chern insulator?

Středa formula: the filling factor of the band at non-zero flux depends on the Chern number C.

$$\sigma_{xy} = \frac{\partial n}{\partial B}.$$

Chern insulator $\sigma_{xy} = \frac{Ce^2}{h}.$

$\delta n \propto C \; \delta B$ $\quad \hookrightarrow$ magnetic field

variation of density

$$\delta\nu = C \frac{\Phi}{\Phi_0}$$

flux quantum h/e.

Back to TBG

* $C_{2z}T$ sym leads to fragile topology.

* P leads strong topology $\mathbb{Z}_2$ TI.

→ Chiral symmetry is helpful.

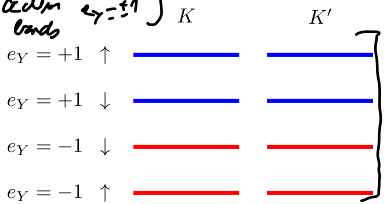
$C_{2z}T$ describes you two active bands using wavefunctions with opposite chern number $e_Y = \pm 1$.

(is not eigenstate of H).

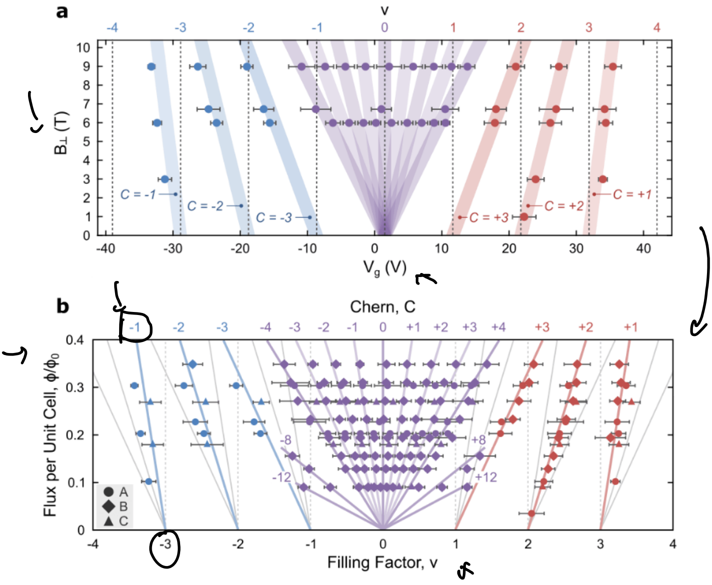
+ Chiral symmetry each e_Y is an eigenstate of C

$$\underset{\text{spin}}{2} \times \underset{\text{valley}}{2} \times \underset{\text{active bands } e_Y = \pm 1}{2} = 8 \text{ bands.}$$

- Filling factor $\nu = -4, \dots, 4$.
- Charge neutrality at $\nu = 0$.
- Chiral limit, each band has its own Chern,spin,valley quantum numbers.



Quantized magnetic-field response in TBG



Nuckolls et al., Nature (2020)

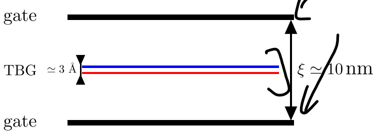
TBG: Turning on the interaction

Coulomb interaction

Screened Coulomb:

$$V(\mathrm{q}) = \pi\xi^2 U_\xi \frac{\tanh(\xi q/2)}{\xi q/2}$$

with $U_\xi = e^2/(\epsilon\xi) \simeq 25\mathrm{meV}.$
Same interaction for the intralayer and interlayer.



Interaction Hamiltonian:

$$\hat{H}_I = \frac{1}{2\Omega_{\mathrm{tot}}} \sum_{\mathbf{G}\in\mathcal{Q}_0} \sum_{\mathbf{q}\in\mathrm{MBZ}} V(\mathbf{q}+\mathbf{G})\delta\rho_{-\mathbf{q}-\mathbf{G}}\delta\rho_{\mathbf{q}+\mathbf{G}}$$

$\delta\rho_{\mathbf{q}+\mathbf{G}}$ Fourier transform of the electron density shifted at charge neutrality.

Total Hamiltonian: $\hat{H} = \hat{H}_0 + \hat{H}_I.$

Projecting the interaction

- Near the first magic angle, focus on the $2 \times 2 \times 2$ active bands.
- Simplify by projecting $\hat{H}$

sum only over the active bands

$$H_0 = \sum_{n=\pm 1} \sum_{\eta, s} \sum_{\mathbf{k} \in \mathrm{MBZ}} \epsilon_{n,\eta}(\mathbf{k}) c^\dagger_{\mathbf{k}n\eta s} c_{\mathbf{k}n\eta s}, \quad H_I = \frac{1}{2\Omega_{\mathrm{tot}}} \sum_{\mathbf{q} \in \mathrm{MBZ}} \sum_{\mathbf{G} \in \mathcal{Q}_0} O_{-\mathbf{q},-\mathbf{G}} O_{\mathbf{q},\mathbf{G}}$$

- $n = \pm 1$ TBG band index, $\eta = \pm$ valley index, $s = \uparrow, \downarrow$ spin index.
- $c^\dagger_{\mathbf{k}n\eta s} \leftrightarrow$ eigenstates of the one-body problem.
- H_I is *positive semi-definite* $O^\dagger_{\mathbf{q},\mathbf{G}} = O_{-\mathbf{q},-\mathbf{G}}$

$$O_{\mathbf{q},\mathbf{G}} = \sum_{\mathbf{k}\eta s} \sum_{m,n=\pm 1} \sqrt{V(\mathbf{q}+\mathbf{G})} M^{(\eta)}_{m,n}(\mathbf{k}, \mathbf{q}+\mathbf{G}) \left(c^\dagger_{\mathbf{k}+\mathbf{q},m,\eta,s} c_{\mathbf{k},n,\eta,s} - \frac{1}{2}\delta_{\mathbf{q},\mathbf{0}}\delta_{m,n} \right)$$

Kang-Vafek (2019), Huber(2017), TGB III

form factor.

Form factor and FMC

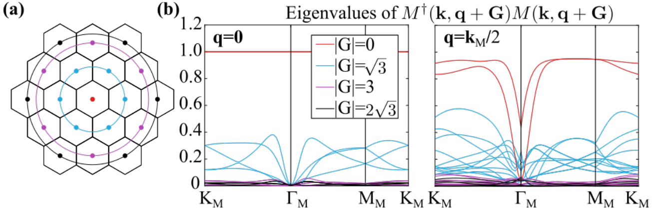
Form factor:

$$M_{m,n}^{(\eta)}(\mathbf{k},\mathbf{q}+\mathbf{G}) = \sum_{\alpha}\sum_{\mathbf{Q}\in\mathcal{Q}_\pm} u^*_{\mathbf{Q}-\mathbf{G},\alpha;m\eta}(\mathbf{k}+\mathbf{q})\, u_{\mathbf{Q},\alpha;n\eta}(\mathbf{k})$$

$u_{\mathbf{Q},\alpha;n\eta}$ eigenstates of the non-interacting Hamiltonian. Exponential convergence with $\mathbf{G}$.

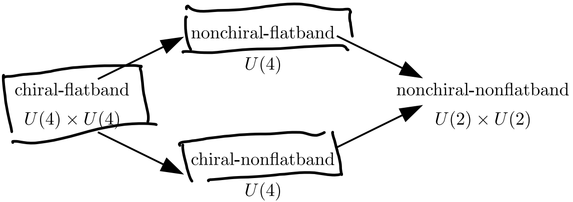
Flat Metric Condition (FMC):

$M_{m,n}^{(\eta)}(\mathbf{k},\mathbf{q}+\mathbf{G}) = \xi(\mathbf{q}+\mathbf{G})\,\delta_{m,n}$ i.e. the form factor does not depend on $\mathbf{k}$.
Is this a valid approximation? Worst case scenario picture $(w_0/w_1 = 0.8)$



Symmetries

- C_{3z}, C_{2z} and T. P is also a symmetry $\{P, H_0\} = 0$ but $[P, H_I] = 0$.
- $U(2) \times U(2)$ (one $U(2)$ spin+charge per valley).
- If we discard H_0 (flatband limit), $C_{2z}P$ becomes a symmetry and promotes $U(2) \times U(2)$ to $U(4)$.
- (1st) chiral symmetry acts differently: $\{C, H_0\} = 0$ but $[C, H_I] = 0$.
- $CC_{2z}P$ becomes a symmetry and promotes $U(2) \times U(2)$ to *another* $U(4)$.
- In the chiral-flatband, an extended $U(4) \times U(4)$ *(not the previous $U(4)$'s)*, one per e_Y.

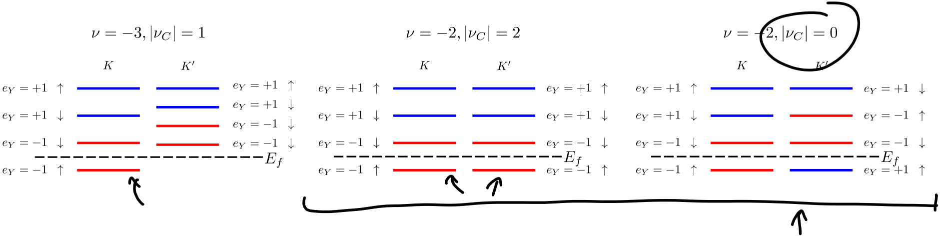


TBG III (2020), Vafek and Kang (2019), Bultinck et al. (2020)

Exact low energy states

Exact low energy states

- Flat band limit, H is positive semi-definite
- $O_{\mathbf{q},\mathbf{G}} |\Psi\rangle = 0$ for any q, G, then $|\Psi\rangle$ is a groundstate (not unique in principle).
- Additional hypotheses:
    - Chiral-flatband limit.
    - Flat metric condition or $\nu = 0$.
- For the different integer ν, the filled bands (i.e., product states) are *exact ground states*, "ferromagnetic" $U(4) \times U(4)$.



Exact low energy states: insulating phases

- At fixed ν, GS are *degenerate with different Chern numbers* $\nu_c = 4 - |\nu|, 2 - |\nu|, ..., |\nu| - 4$.
- Away from the FMC, we can only prove they are eigenstates.
- $\nu_c = 0$ are still exact GS in in the nonchiral-flat $U(4)$.

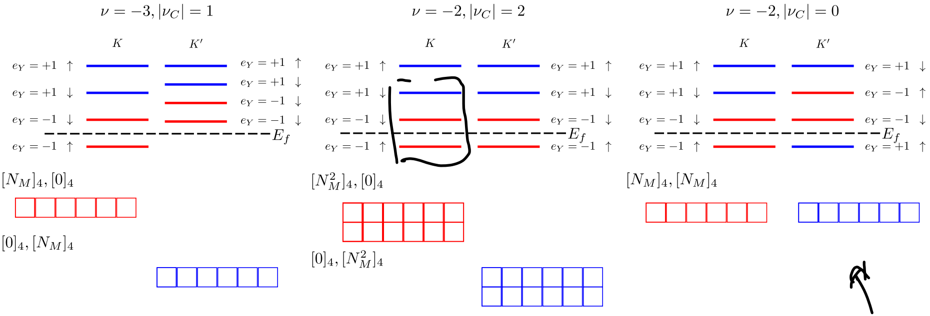
The whole gallery:

filling ν	Chern number ν_C	nonchiral-flat $U(4)$	chiral-flat $U(4) \times U(4)$	exact under	if nonchiral-flat GS
-3	± 1	$[N_M]_4$	$([N_M]_4, [0]_4)$	U(4)×U(4)	yes (perturbative)
-2	0	$[2N_M]_4$	$([N_M]_4, [N_M]_4)$	U(4)	yes (exact)
-2	± 2	$[N_M^2]_4$	$([N_M^2]_4, [0]_4)$	U(4)×U(4)	no
-1	± 1	$[2N_M, N_M]_4$	$([N_M^2]_4, [N_M]_4)$	U(4)×U(4)	yes (perturbative)
-1	± 3	$[N_M^3]_4$	$([N_M^3]_4, [0]_4)$	U(4)×U(4)	no
0	0	$[(2N_M)^2]_4$	$([N_M^2]_4, [N_M^2]_4)$	U(4)	yes (exact)
0	± 2	$[2N_M, N_M, N_M]_4$	$([N_M^3]_4, [N_M]_4)$	U(4)×U(4)	no
0	± 4	$[0]_4$	$([0]_4, [0]_4)$	U(4)×U(4)	no

Chiral-Flatband limit, $\nu = -3, -2$

filling ν	Chern number ν_C	chiral-flat $U(4) \times U(4)$	exact under
-3	± 1	$([N_M]_4, [0]_4)$	U(4)× U(4)
-2	0	$([N_M]_4, [N_M]_4)$	U(4)
-2	± 2	$([N_M^2]_4, [0]_4)$	U(4)×U(4)

- N_M number of moiré unit cells, number of electrons $N = (4 + \nu) N_M$.
- U(4)× U(4) irreps appearing by pairs $[a]_4, [b]_4$ and $[b]_4, [a]_4$ due to $C_{2z}T$ symmetry (if $[a]_4 \neq [b]_4$).



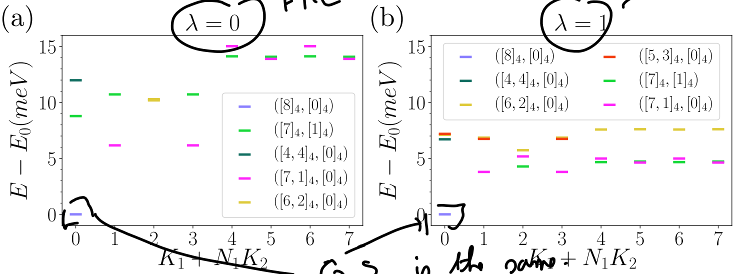
TBG: Away from the perfect world

Chiral-Flatband limit: how good is the FMC?

- Testing the model with exact diagonalizations.
- Using the $U(4) \times U(4)$ symmetry to label eigenstates with their irrep.
- Discretize the MBZ: $N_1 \times N_2$ lattice points.
- $\lambda = 0$ with FMC, $\lambda = 1$ without FMC.
- Testing $\nu = -3$ on a $N_1 \times N_2 = 4 \times 2$ (irreps appear in pairs related by $C_{2z}T$, switching the 2 $U(4)$'s).

FMC

without FMC.

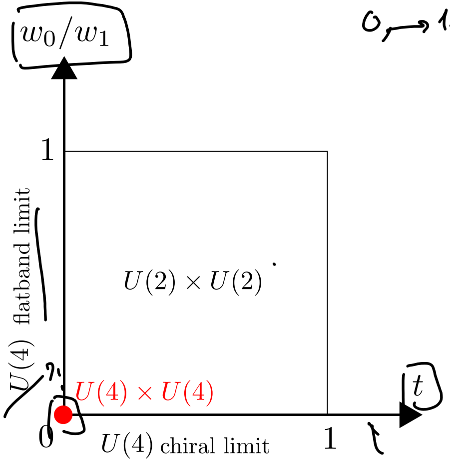


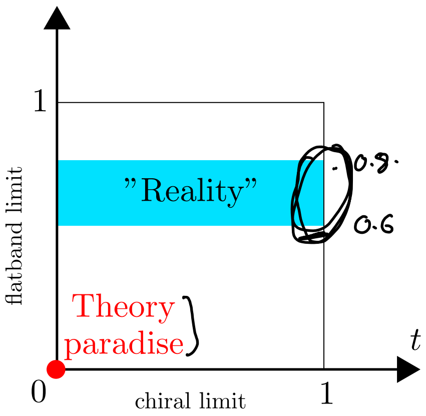
GS in the same

Reality check

$H = t\, H_0 + H_I$ ← interaction.

$0 \to 1$. non interacting

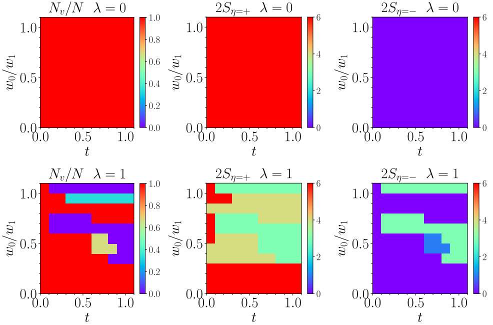




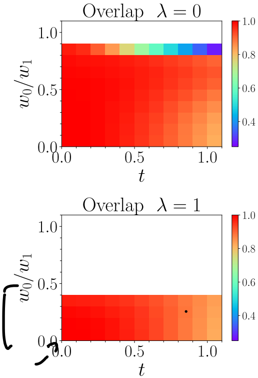
$\nu = -3$: away from the chiral-flatband limit

- Tune w_0/w_1 and t (0 flatband, 1 full model).
- Groundstate Chern state $\nu_c = \pm 1$ for $w_0/w_1 < 0.9$ (with FMC) and $w_0/w_1 < 0.4$ (w/o FMC).
- Large w_0/w_1. Transition to (nematic) metal or CDW at K_M , M_M, see DMRG, Kang, Vafek (2020), Zaletel (2020).

unpolarized:

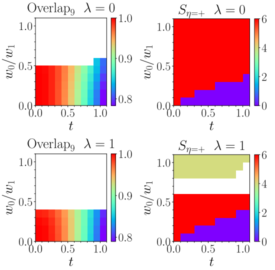


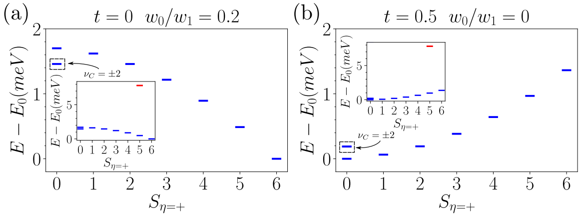
fully polarized:



$\nu = -2$: away from the chiral-flatband limit

- Two competing states: $\nu_c = 0$ and $\nu_c = 2$.
- ED for the valley polarized system ($N_1 \times N_2 = 3 \times 2$).
- *Nonchiral-flat*: spin FM favored (see (a)), lowest Chern number favored.
- *Chiral-nonflat*: spin singlet favored (see (b)), lowest Chern number favored.
- Without FMC, no longer spin FM when $w_0/w_1 > 0.6$ (in valley polarized sector, not ground state).



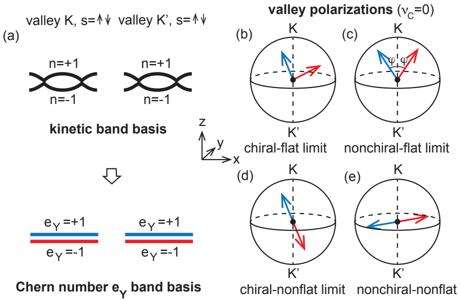


Perturbation theory (2nd order)

- $|\nu_C| = 0$ are still exact GS (with FMC) in the nonchiral-flat limit.
- For any ν, the smallest $|\nu_C|$ is favored.

nonchiral-nonflat:

- Chern number $\nu_C = 0$: fully intervalley coherent ($\phi_\uparrow = \phi_\downarrow = \pi/2$).
- Chern number $\nu_C < 4 - |\nu|$: partially intervalley coherent ($\phi_\uparrow = \pi/2, \phi_\downarrow = 0$).
- Highest Chern number $\nu_C = 4 - |\nu|$: valley polarized ($\phi_\uparrow = \phi_\downarrow = 0$, < 0.005 meV/electron gain).

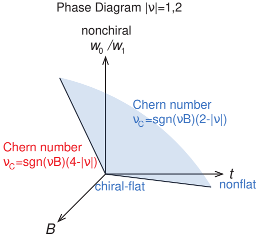


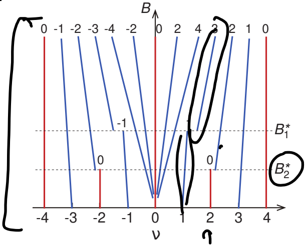
In-Field Transition and Experimental Consequence

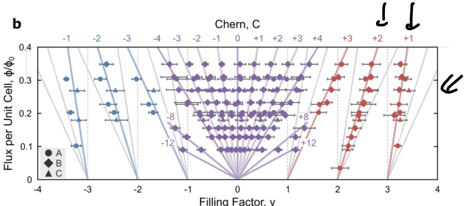
- For $|\nu| = 1, 2$, a 1st order phase transition from $\nu_C = \mathrm{sgn}(\nu B)(2 - |\nu|)$ to $\nu_C = \mathrm{sgn}(\nu B)(4 - |\nu|)$ (e.g. for $\nu = 2$, from $|\nu_C| = 0$ to $|\nu_C| = 2$).
- Transition field B^*_ν (from perturbation theory)

$$B^*_\nu = \frac{U_1 - \nu^2 U_2}{|\nu| U_0} \frac{h}{e\Omega_M}$$

- For $w_0/w_1 = 0.8$: $B^*_1 = 0.5\,T$ and $B^*_2 = 0.2\,T$
- In agreement with STM/transport experimental observations of states with Chern number $\nu_C = \mathrm{sgn}(\nu B)(4 - |\nu|)$ in magnetic field.



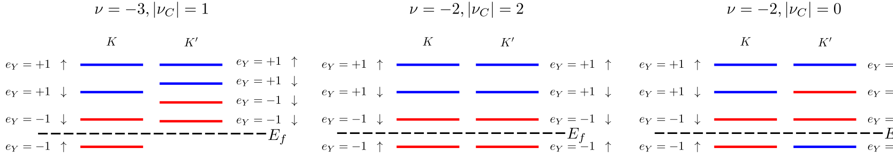




Scanning tunneling microscope:
Identifying insulators

A zoo of correlated insulators

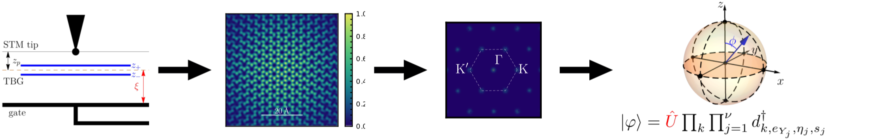
- For a given filling ν, you can choose how to occupy the Chern band basis



- Each Slater determinant ground state can be rotated ($\hat{U}$):

$$|\varphi\rangle = \hat{U} \prod_{\mathbf{k}} \prod_{j=1}^{4+\nu} \hat{d}^{\dagger}_{\mathbf{k},e_{Y_j},\eta_j,s_j} |0\rangle \, .$$

Lian *et al.*, 2021



Probing the TBG spectral function with STM

- Key quantity is the spectral function

$$A\left(\mathbf{r},\omega\right)=\sum_{\xi,s}\left[\left|\langle\xi|\hat{\psi}_s^{\dagger}\left(\mathbf{r}\right)|\varphi\rangle\right|^2\delta\left(\omega-E_{\xi}+E_{\varphi}\right)+\left|\langle\xi|\hat{\psi}_s\left(\mathbf{r}\right)|\varphi\rangle\right|^2\delta\left(\omega+E_{\xi}-E_{\varphi}\right)\right].$$

- In the case of the TBG insulators, this simplifies to

$$A\left(\mathbf{r},\omega\right)=\sum_{\mathbf{k}',\mathbf{k}\in\mathrm{MBZ}}\sum_{\substack{n,\eta\\n',\eta'}}\left[\mathcal{M}^{+}\left(\omega\right)+\mathcal{M}^{-}\left(\omega\right)\right]_{\mathbf{k}n\eta,\mathbf{k}'n'\eta'}\left[\mathcal{B}\left(\mathbf{r}\right)\right]_{\mathbf{k}n\eta,\mathbf{k}'n'\eta'}.$$

- Spectral function matrix elements depend on both the GS and its **charge-one excitations**

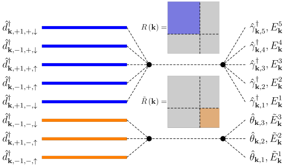
$$\left[\mathcal{M}^{+}\left(\omega\right)\right]_{\mathbf{k}n\eta,\mathbf{k}'n'\eta'}=\sum_{\xi,s}\langle\varphi|\hat{c}_{\mathbf{k}',n',\eta',s}|\xi\rangle\langle\xi|\hat{c}^{\dagger}_{\mathbf{k},n,\eta,s}|\varphi\rangle\delta\left(\omega-E_{\xi}+E_{\varphi}\right).$$

- Spatial factor $\mathcal{B}\left(\mathbf{r}\right)$ depends on the TBG active band wave-functions and graphene p_z orbitals.

Charge-one excitation matrices

Spectral function shopping list

- GS wavefunction
- one particle excitation wf
- energy of the excitations



Vafek *et al.*, 2020; Bernevig *et al.*, 2021

- Because ground-state $|\varphi\rangle$ is **exact**, charge-one excitations are readily available:

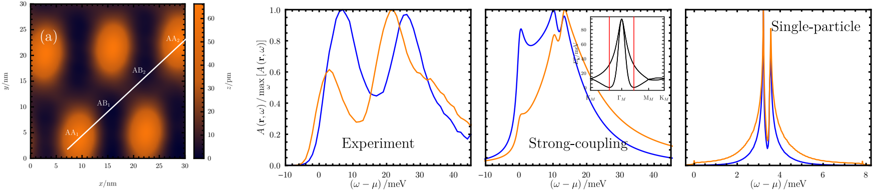
$$\left[H_I - \mu \hat{N}, \hat{c}^\dagger_{\mathbf{k},n,\eta,s}\right] |\varphi\rangle = \sum_m R^\eta_{mn}(\mathbf{k})\, \hat{c}^\dagger_{\mathbf{k},m,\eta,s} |\varphi\rangle ,$$

$$\left[H_I - \mu \hat{N}, \hat{c}_{\mathbf{k},n,\eta,s}\right] |\varphi\rangle = \sum_m \tilde{R}^\eta_{mn}(\mathbf{k})\, \hat{c}_{\mathbf{k},m,\eta,s} |\varphi\rangle .$$

- General trend for the TBG insulators: **exact** many-body n-particle excitations above $|\varphi\rangle$ can be computed as a $(n-1)$-body problem.
- Large system sizes can be achieved (*e.g.* 50×50 on a personal computer).

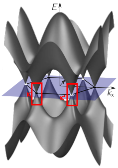
Warm-up: Evidence of strong correlations at $\nu = \pm 4$

- Validate strong-coupling approach by looking at the $\nu = -4$ **correlated band-insulator** (no ambiguity in the ground state wave-function).
- Inspect the signal at the AA and AB stacking centers

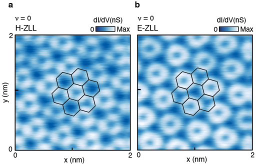


- Clear signatures of strong correlation:
  - Wide signal, due to the strong dispersion of the charge-one excitation bands.
  - Different peak structure.
  - The signal varies between the AA and AB stacking centers.

Kekulé distortion and intervalley-coherence

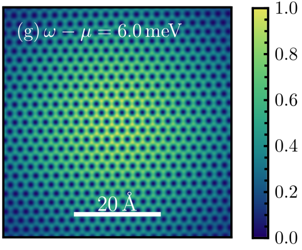


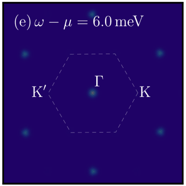
Intervalley coherence should lead to $3\times$ enlargement of the graphene unit cell ($\sqrt{3}\times\sqrt{3}$ ordering).



Graphene $+B$, Liu *et al.*, 2021

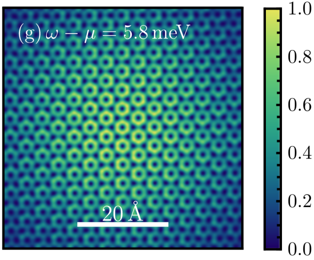
Without Kekulé

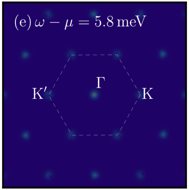




Graphene BZ

With Kekulé

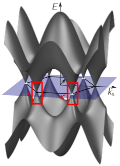




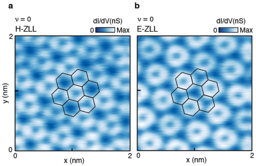
Graphene BZ

Graphene $a_0 = 2.46\mathring{A}$, Moiré unit cell $\simeq 13\mathrm{nm}$

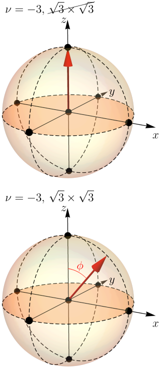
Kekulé distortion and intervalley-coherence

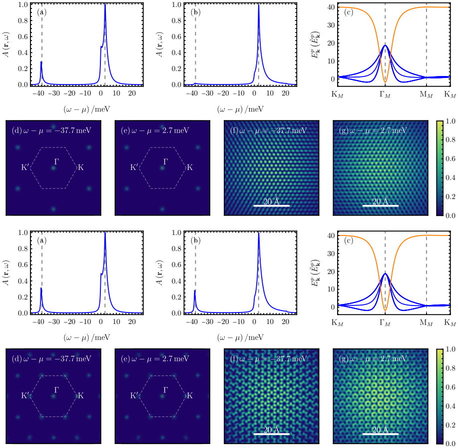


Intervalley coherence should lead to $3\times$ enlargement of the graphene unit cell ($\sqrt{3}\times\sqrt{3}$ ordering).

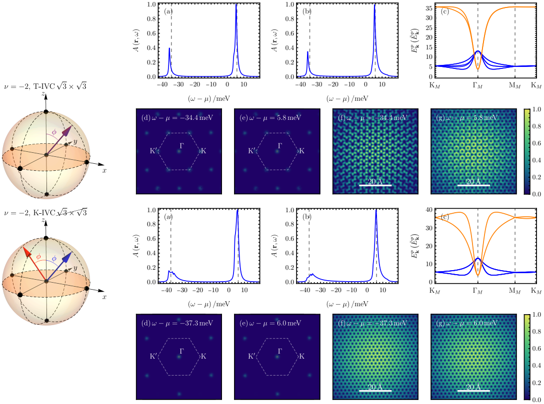


Graphene $+B$, Liu *et al.*, 2021





Does intervalley-coherence **always** lead to $\sqrt{3}\times\sqrt{3}$ ordering?



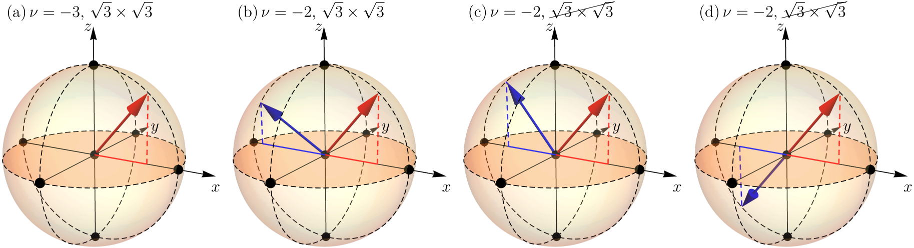
Breaking valley $\mathrm{U}(1)$ symmetry is a necessary, but not sufficient condition for observing Kekulé distortion

$$|\text{T-IVC}\rangle = \prod_{\substack{\mathbf{k}\\ e_Y=\pm 1}} \frac{\hat{d}^\dagger_{\mathbf{k},e_Y,+,\uparrow}+\hat{d}^\dagger_{\mathbf{k},e_Y,-,\uparrow}}{\sqrt{2}}\,|0\rangle$$

$$|\text{K-IVC}\rangle = \prod_{\substack{\mathbf{k}\\ e_Y=\pm 1}} \frac{\hat{d}^\dagger_{\mathbf{k},e_Y,+,\uparrow}+e_Y\hat{d}^\dagger_{\mathbf{k},e_Y,-,\uparrow}}{\sqrt{2}}\,|0\rangle$$

Discrete symmetries of TBG lead to an exact cancellation of the $\sqrt{3}\times\sqrt{3}$ signal

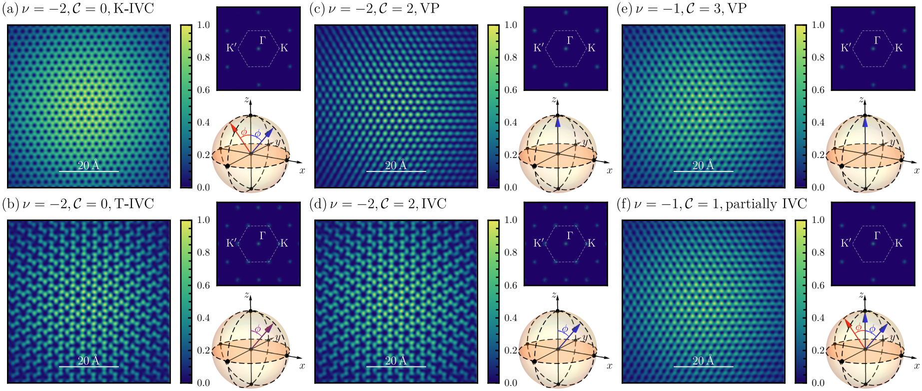
An intuitive picture for maximally spin-polarized insulators



1. Filling a single IVC Chern band will give rise to Kekulé distortion
2. An exact cancellation of the $\sqrt{3}\times\sqrt{3}$ signal occurs upon filling a pair of Chern bands with opposite Chern numbers whose valley polarization projections in the valley *xy* plane of the Bloch sphere are nonzero and cancel out.

Further differentiating between different insulators

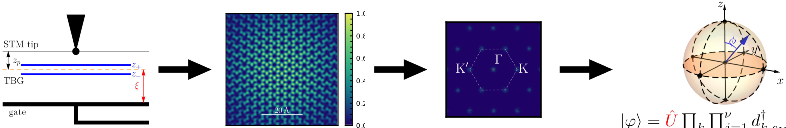
$\hat{d}^\dagger_{\mathbf{k},e_Y,\eta,s}$ located (primarily) on a single sublattice depending on $e_Y\eta = \pm 1$.



See also J.P. Hong et al. arXiv:2110.14674

Conclusion

- Combination of chiral and flat limits, the Coulomb interacting Hamiltonian exhibit enhanced $U(4)$ or $U(4) \times U(4)$ symmetries.
- Exact/perturbative (Chern) insulators are derived at integer fillings and confirmed in ED.
- Charge excitations can be exactly calculated.
- STM signal for the most promising correlated insulator candidates.
- STM signal of different correlated insulators contains distinctive features which can be seen "by eye".
- Breaking valley $\mathrm{U}(1)$ symmetry does not necessarily lead to $\sqrt{3} \times \sqrt{3}$ ordering.
- Reconstruct the GS using STM measurements, as was done recently for the zeroth Landau level of graphene.



$$|\varphi\rangle = \hat{U} \prod_k \prod_{j=1}^{\nu} d^\dagger_{k, e_{Y_j}, \eta_j, s_j}$$

Quantum many-body physics is a harsh problem

Look back at the interaction term

$$\hat{H}_I = \frac{1}{2\Omega_{\text{tot}}} \sum_{\mathbf{G}\in\mathcal{Q}_0} \sum_{\mathbf{q}\in\mathrm{MBZ}} V(\mathbf{q}+\mathbf{G})\delta\rho_{-\mathbf{q}-\mathbf{G}}\delta\rho_{\mathbf{q}+\mathbf{G}}$$

Electron density shifted at charge neutrality

$$\delta\rho_{\mathbf{q}+\mathbf{G}} = \sum_{\mathbf{k}\in\mathrm{MBZ}} \sum_{\eta,s} \sum_{\mathbf{Q}\in\mathcal{Q}_\pm} \sum_{\alpha} \left(c^\dagger_{\mathbf{k}+\mathbf{q},\mathbf{Q}-\mathbf{G},\alpha,\eta,s} c_{\mathbf{k},\mathbf{Q},\alpha,\eta,s} - \frac{1}{2}\delta_{\mathbf{q},0}\delta_{\mathbf{G},0} \right)$$

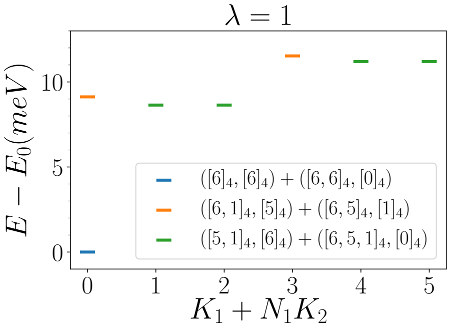
Using the one-body eigenstate basis

$$c^\dagger_{\mathbf{k},m,\eta,s} = \sum_{\mathbf{Q}\alpha} u_{\mathbf{Q}\alpha,m\eta}(\mathbf{k}) c^\dagger_{\mathbf{k},\mathbf{Q},\eta,\alpha,s}, \quad c^\dagger_{\mathbf{k},\mathbf{Q},\eta,\alpha,s} = \sum_m u^*_{\mathbf{Q},\alpha,m\eta}(\mathbf{k}) c^\dagger_{\mathbf{k},m,\eta,s}$$

$$\delta\rho_{\mathbf{q}+\mathbf{G}} = \sum_{\mathbf{k}\in\mathrm{MBZ}} \sum_{\eta,s} \sum_{m,n} \left(\sum_{\mathbf{Q}\in\mathcal{Q}_\pm} \sum_{\alpha} u^*_{\mathbf{Q}-\mathbf{G},\alpha m\eta}(\mathbf{k}+\mathbf{q}) u_{\mathbf{Q},\alpha n\eta}(\mathbf{k}) \right) \left(c^\dagger_{\mathbf{k}+\mathbf{q},m,\eta,s} c_{\mathbf{k},n,\eta,s} - \frac{1}{2}\delta_{\mathbf{q},0}\delta_{m,n} \right)$$

Chiral-Flatband limit: how good is the FMC?

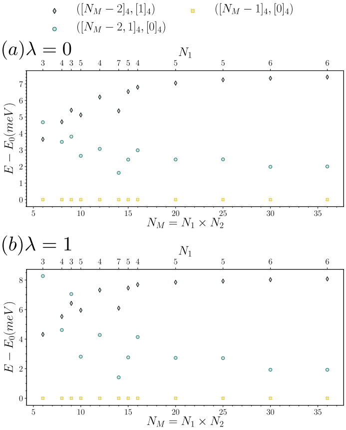
- Testing the model with exact diagonalizations.
- Using the $U(4) \times U(4)$ symmetry to label eigenstates with their irrep.
- Discretize the MBZ: $N_1 \times N_2$ lattice points.
- $\lambda = 0$ with FMC, $\lambda = 1$ without FMC.
- Testing $\nu = -2$ on a $N_1 \times N_2 = 3 \times 2$ (irreps appear in pairs related by $C_{2z}T$, switching the 2 $U(4)$'s).



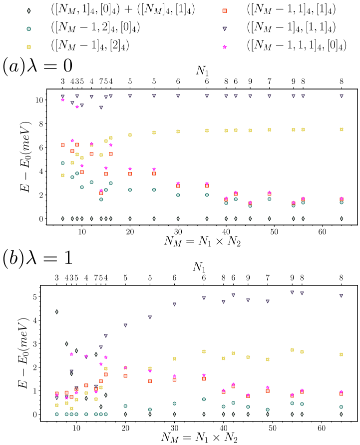
Charged excitations, size effects

- Charge ± 1 at $\nu = -3$ (see TBG VI for other ν's).
- Focus on irreps close to the $U(4) \times U(4)$ ferromagnet.

charge -1:



charge $+1$:



To :: or not to :: ?

- No normal ordering in H_I. Does not matter before projection.
- Difference normal/no normal ΔH_I is the "Hartree-Fock" contribution from the filled passive bands.
- Restore the PH symmetry $\nu \leftrightarrow -\nu$. Focus on $\nu < 0$.
- Like fractional Chern insulator (trivial in Landau level).
- Could wash away insulating phases, e.g., at $\nu = 0$