



Competing phases of interacting electrons in twisted bilayer graphene and related moiré heterostructures

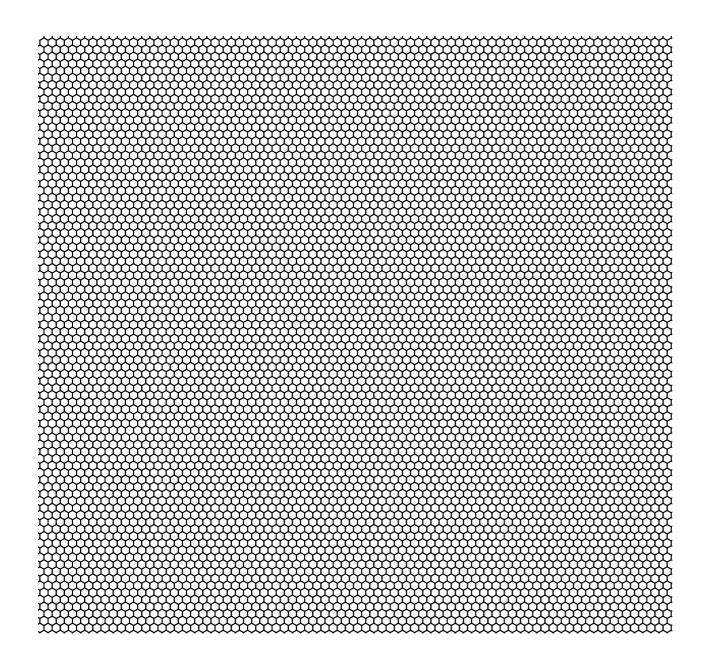
Michael M. Scherer

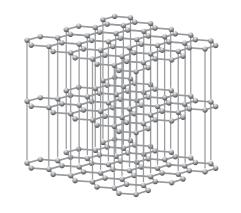
Institute for Theoretical Physics, Cologne University

June 26, 2019 @ Gießen University

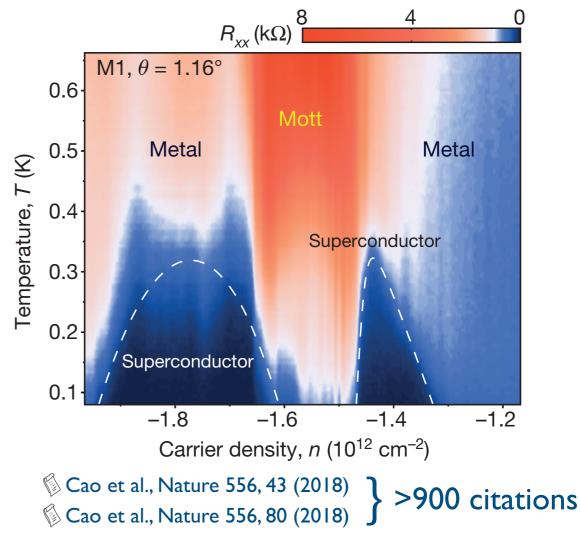
Magic-angle twisted bilayer graphene

- two graphene layers with small rotational mismatch $\boldsymbol{\theta}$
 - long-wavelength moiré pattern
 - @ $\theta_M \approx 1.05^\circ$, 1.16°: ~10,000 atoms per moiré cell





correlated insulator and superconductivity





Outline

• Introduction & motivation

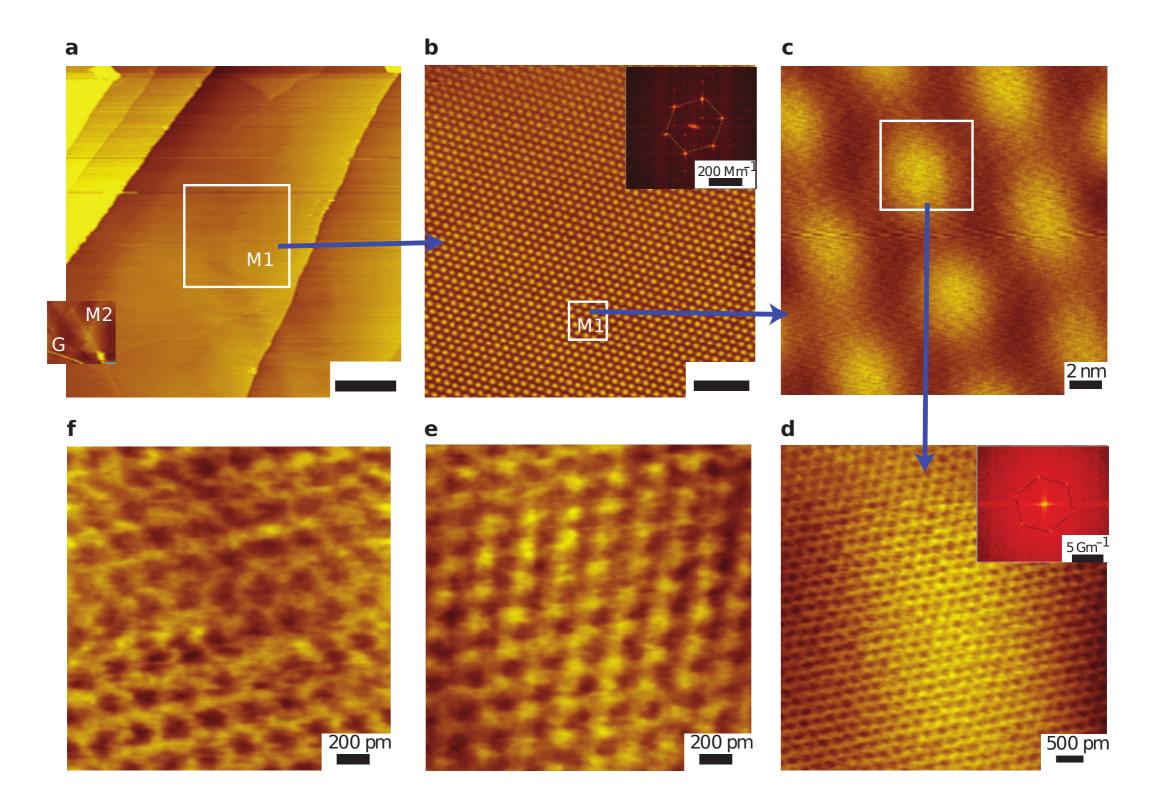
- twisted bilayer graphene basics & experiments
- related moiré heterostructures
- twisted bilayer graphene models

• Effective lattice models & many-body approaches

- functional renormalization group approach
- next-to-minimal model and tentative phase diagram
- conclusions & outlook

Twisted bilayer graphene - basics & experiments

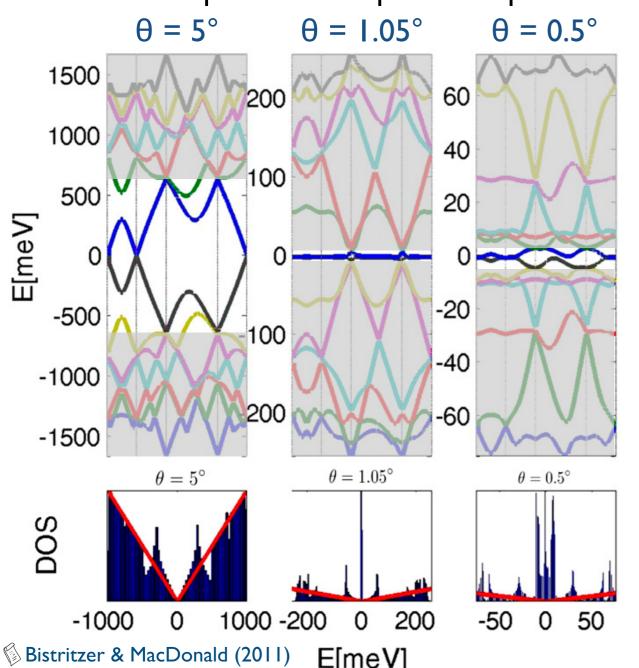
Moiré pattern in STM



Li et al., Nature Physics 6 (2010)

Correlated magic-angle **tBLG** - **basic mechanism**

- for small twist angles $\theta < 10^{\circ}$
 - moiré pattern \rightarrow superlattice potential \rightarrow reconstruction of low-energy band structure:



E[meV]

- flat band structure at magic angle $\theta \approx 1^\circ$:
 - $2 \times 2 \times 2 = 8$ nearly flat bands
 - 2 bands crossing at mini-Dirac points
 - spin (2 x)
 - singlelayer valley (2 x)
 - vary carrier concentration by gate voltage:
 - between $n = \pm 4n_0$

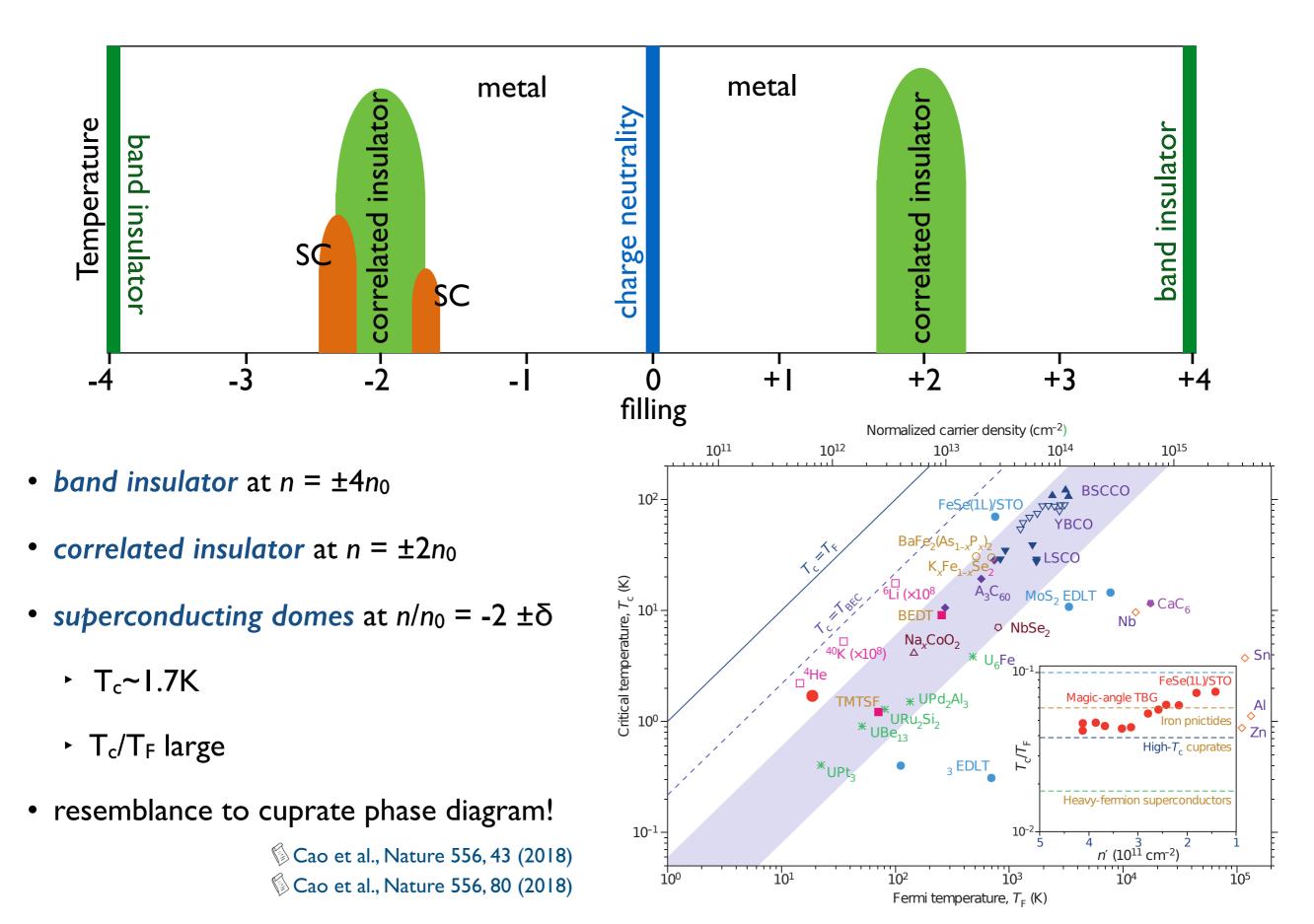
(relative to charge neutrality)

- $n_0 \triangleq I e^{-}$ per unit cell of superlattice

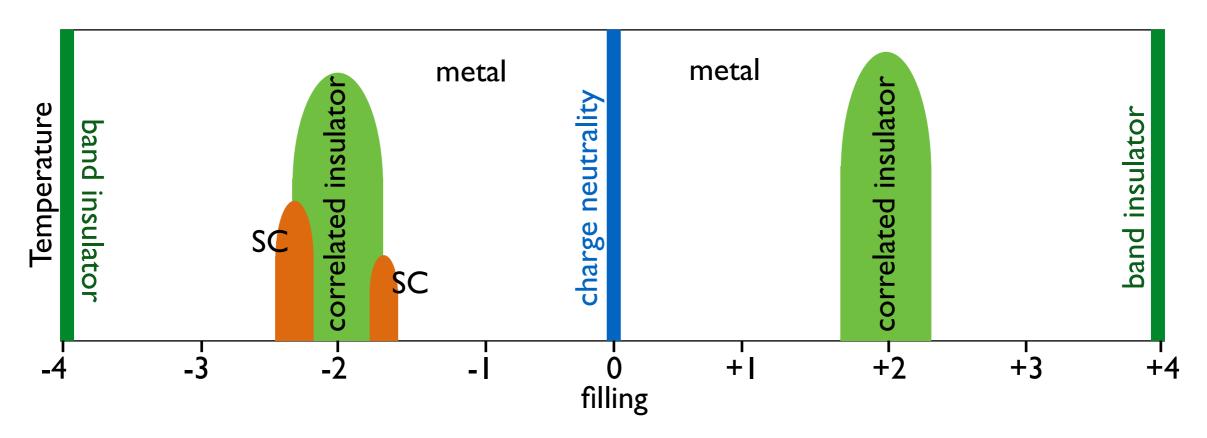
angle θ controls ratio bandwith/interaction: $t/U \sim |\theta - \theta_M|$

strongly-correlated states!

Magic-angle tBLG - phase diagram 1.0 (2018)

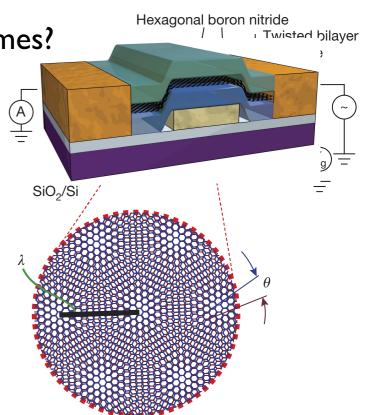


Questions

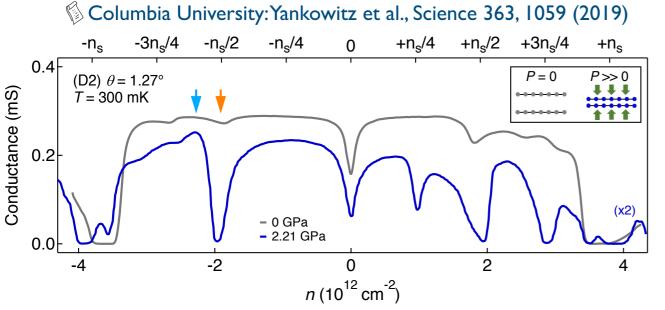


• Are the integer fillings $n/n_0 = \pm 2$ special?

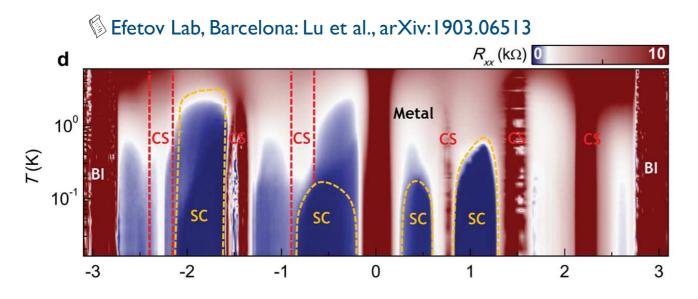
- Are there *further correlated states* in different parameter regimes?
- Which symmetries are broken/preserved in correlated states?
 - spin-rotation / time-reversal / ... ?
- What is the *pairing channel* of the superconducting state?
- What is the role of *electron-phonon interactions*?
- How does the phenomenology depend on the substrate?



2nd generation of tBLG experiments (2019)



- *apply* hydrostatic *pressure P* variation of interlayer tunneling w
 - \Box changes magic angle $\theta_{M} \sim w$
 - \Box in-situ control of $t/U \sim |\theta \theta_M|$
- pressure increases θ_M
 - reduce moiré lattice constant
 - increase energy scale: T_{c, SC} ~3K
- correlated insulator also at $n/n_0 = +3$, superconductor near $n/n_0 = \pm 2$



- very low twist-angle disorder
 - reduced modulations of θ across device
 - ∆θ < 0.02°
 - insulating gaps at n/n₀ = -3,-2,-1,0,+1,+2,+3
 - SC domes in between $(T_{c, SC} \sim 0.14 3K)$

new platform established for study of correlated electrons

✓ high control of twist angle, low level of disorder, pressure/gate tunable band widths/fillings

Related 2D van der Waals moiré heterostructures

- magic-angle twisted bilayer graphene ✓
- ABC trilayer graphene on hexagonal boron nitride
 - experiments: tunable insulating and SC behavior
 Chen et al., Nat. Phys. 15, 237 (2019)
- twisted double bilayer graphene
 - experiments: spin-polarized correlated insulating and SC behavior

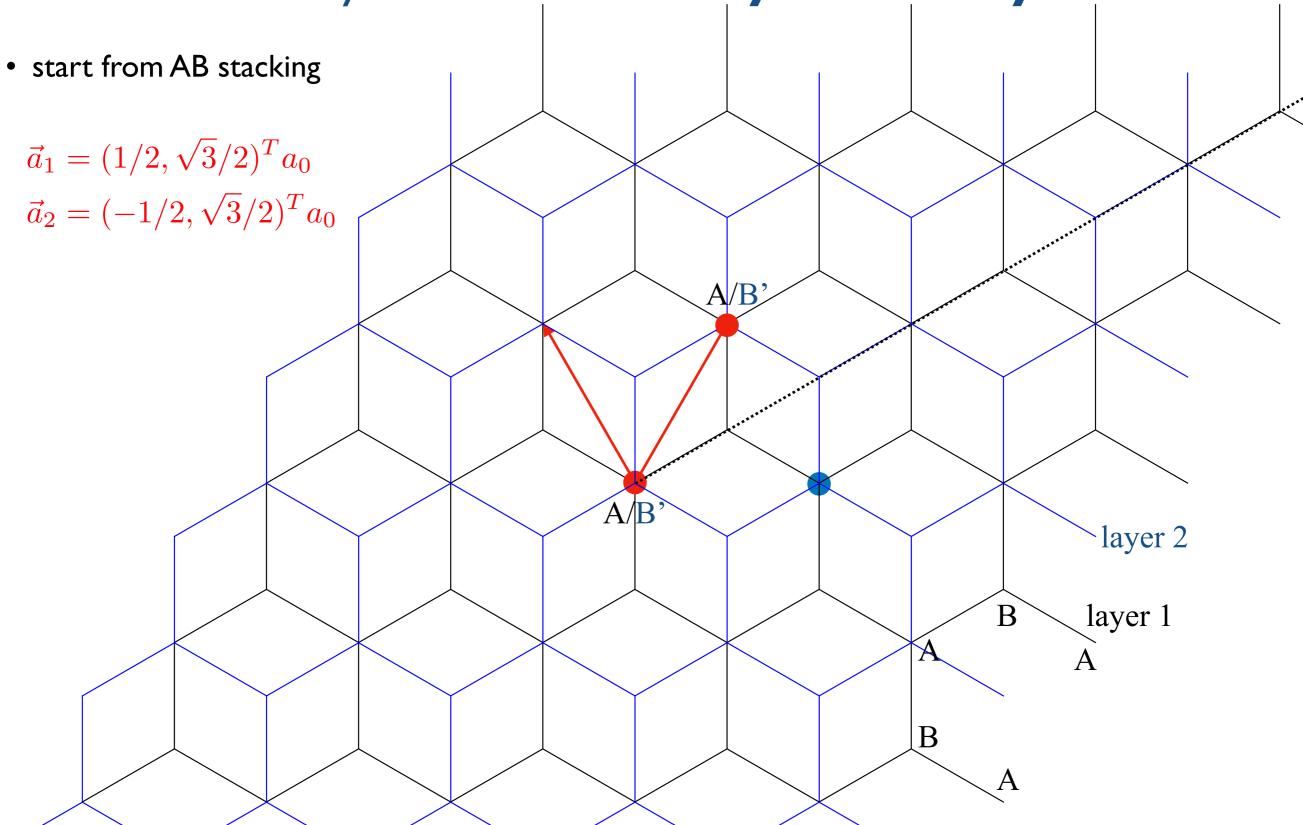
Liu et al., arXiv:1903.08130 (2019) Cao et al., arXiv:1903.08596 (2019)

© Chen et al., arXiv:1901.04621 (2019)

- twisted bilayer boron nitride
 - theoretical: multi-flat bands and strong correlations
 Xian et al., arXiv:1812.08097 (2018)
- transition metal dichalcogenides
 - theoretical: flat bands and strong correlations with and without twist...

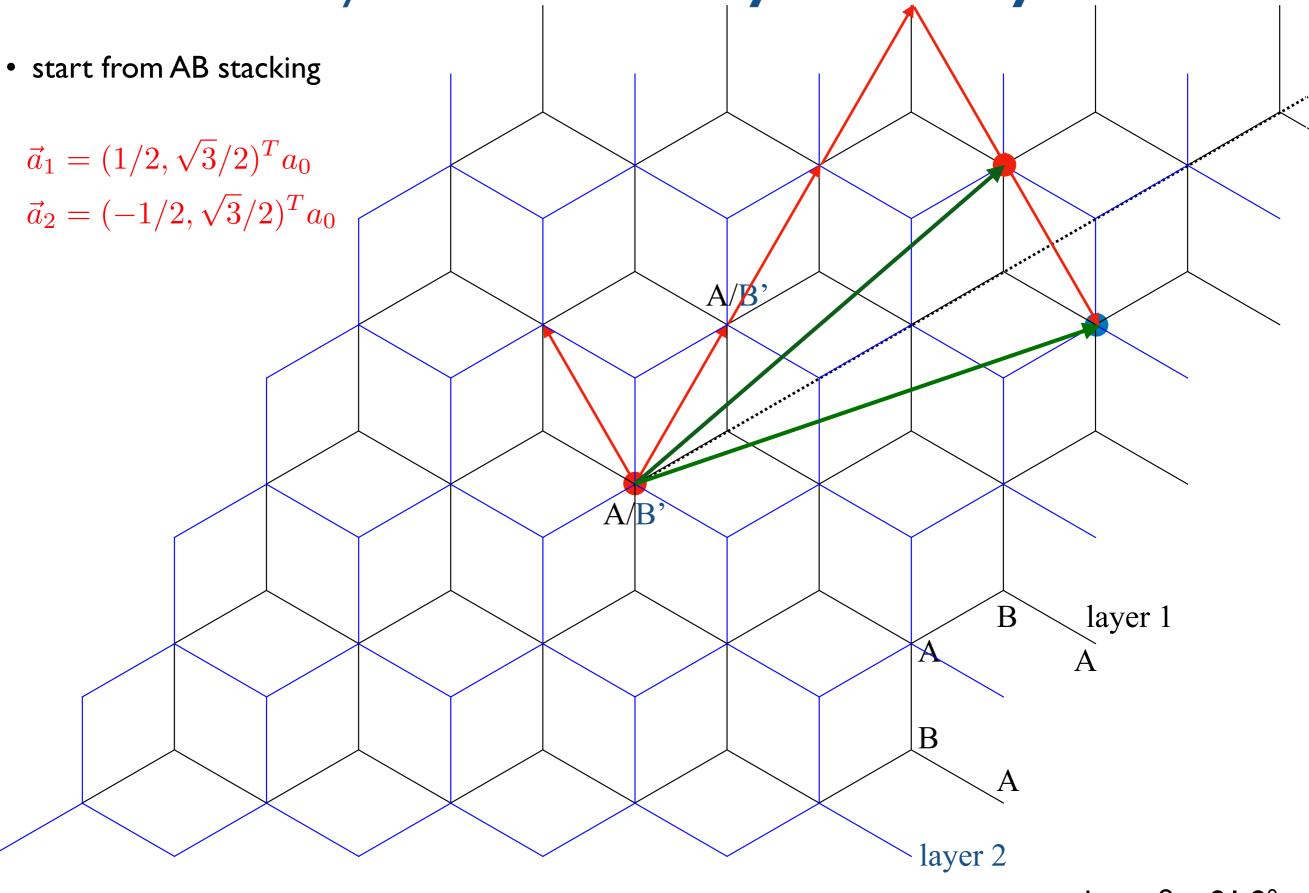
Wu et al., PRL 121, 026402 (2018)

Twisted bilayer graphene - models



commensurate structure when B' rotated to site formely occupied by other B'

• 2D bilayer crystal only at discrete set of commensurate rotation angles

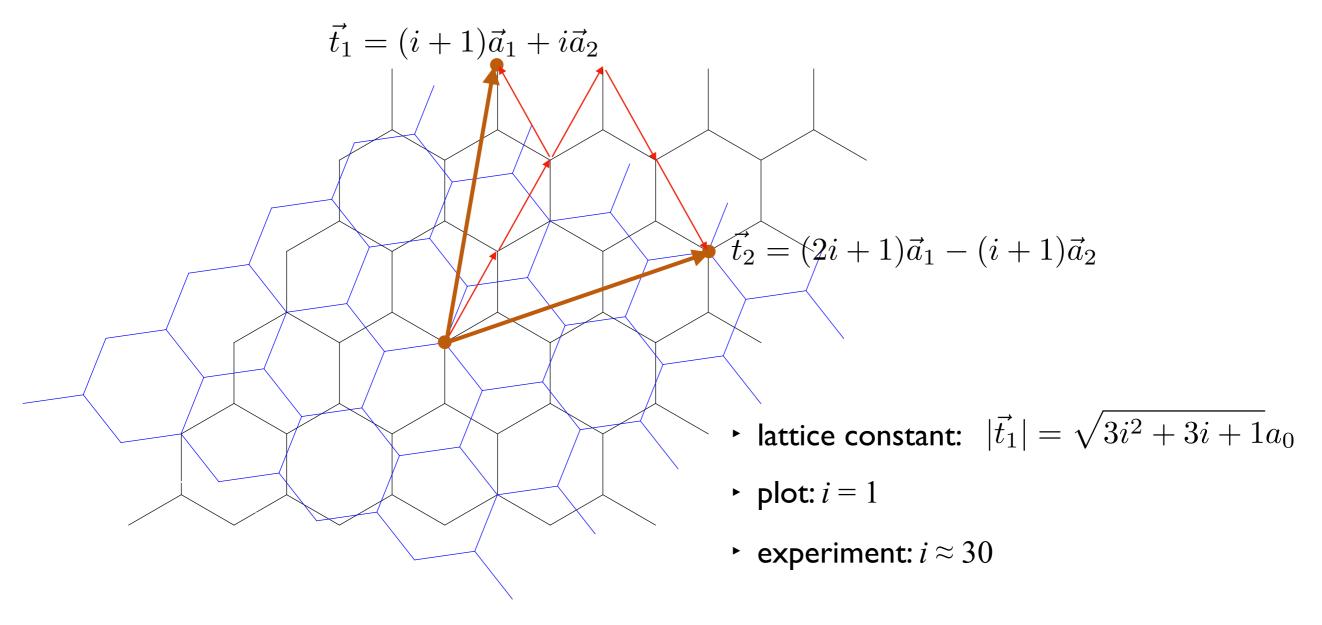


here: $\theta \approx 21.8^{\circ}$

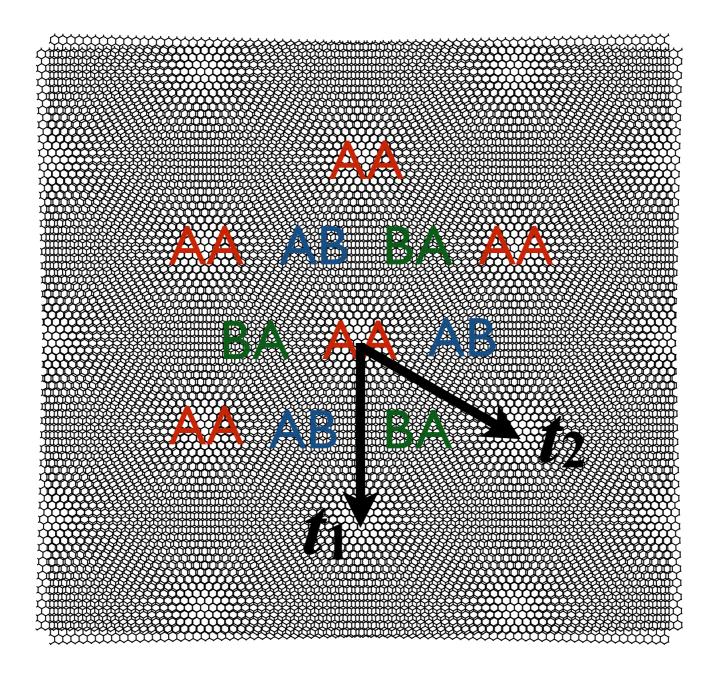
• 2D bilayer crystal only at discrete set of commensurate rotation angles

$$\cos(\theta_i) = \frac{3i^2 + 3i + 1/2}{3i^2 + 3i + 1}, \quad i \in \mathbb{N}_0$$

• emergent moiré superlattice spanned by real space lattice vectors t_1 and t_2

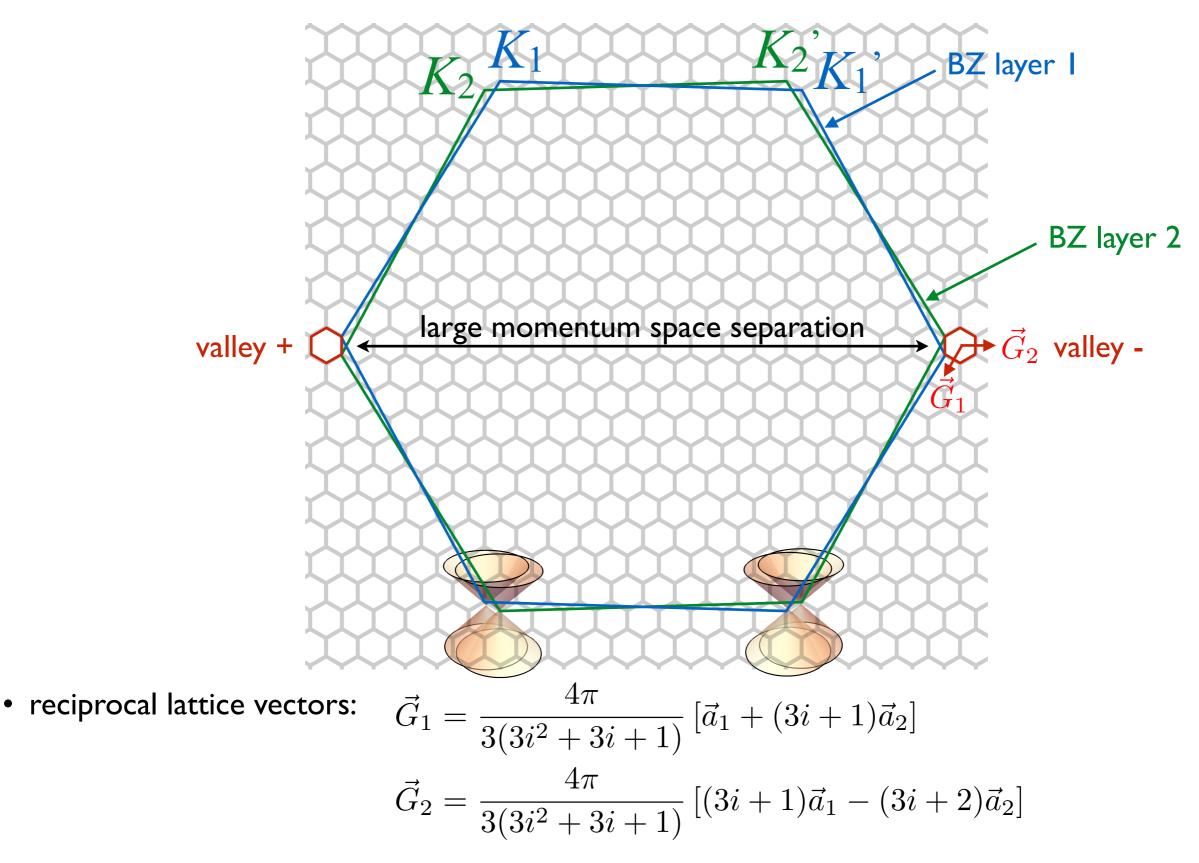


• example: $\theta \approx 2.6^{\circ}$ (*i* = 12)



- Iocal AA, AB and BA stacking regions
- moiré superlattice vectors t₁ and t₂

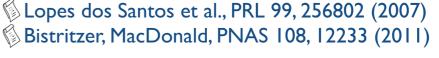
Mini Brillouin zone

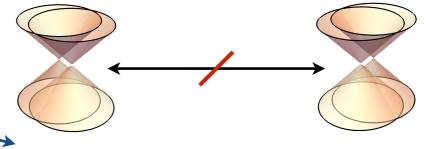


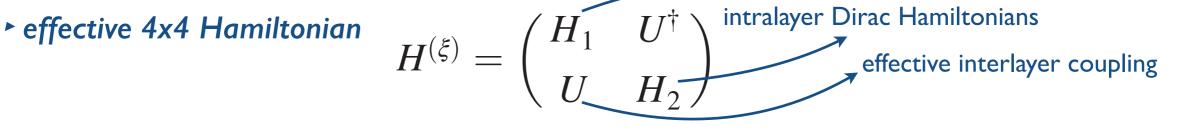
• Dirac points of single-layer graphene layers: $K_{1,}K_{1,}K_{2,}K_{2}$

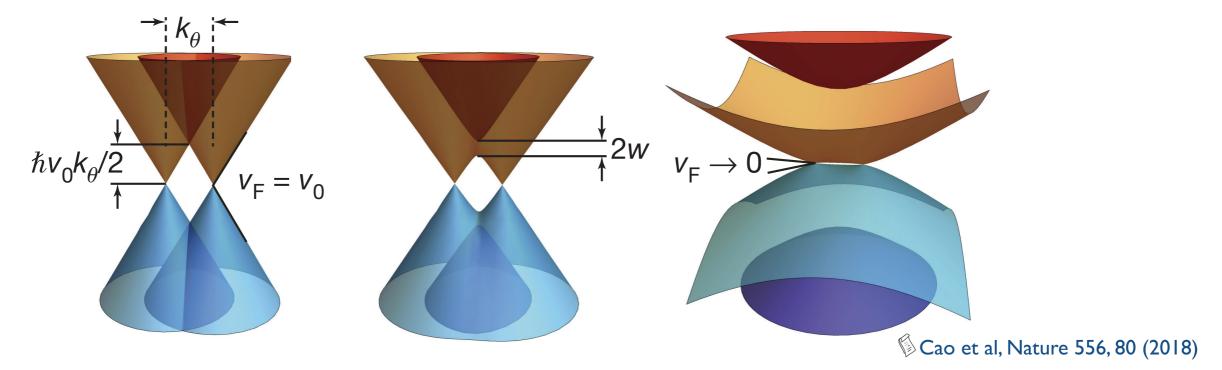
Effective continuum model

- moiré period much larger than atomic scale → continuum model
 © Lopes dos Santos et al., PRL 99, 256802 (2007)
- neglect intervalley mixing (large momentum space separation)
 - independent calculation for each valley $\xi \in \pm$
 - I Dirac cone from each layer: interlayer hybridization





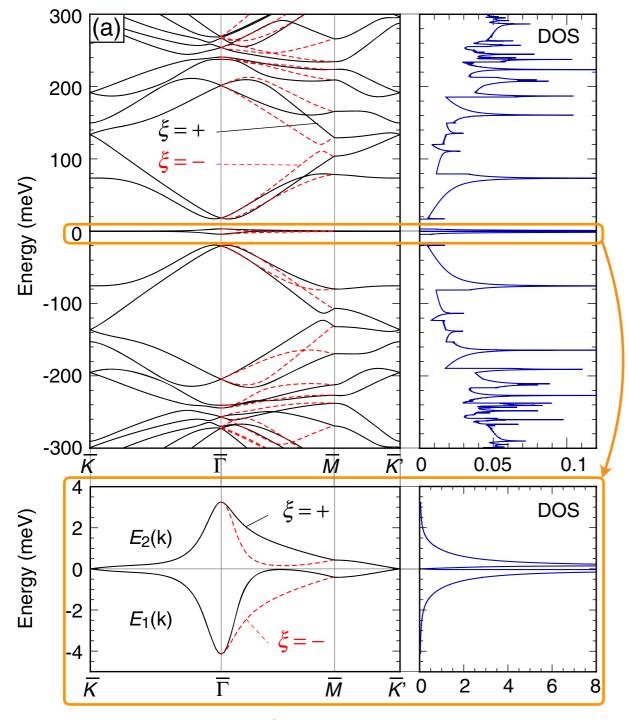




- Dirac cones become nearly flat for magic angles
- dependence on modelling of interlayer coupling (lattice relaxation, corrugation,...)

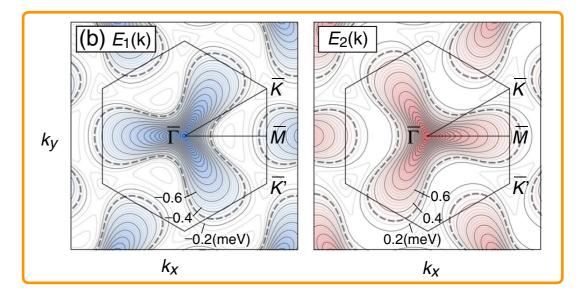
Effective continuum model

• full calculation of band dispersion in continuum model



Koshino et al, PRX 8, 031087 (2018)

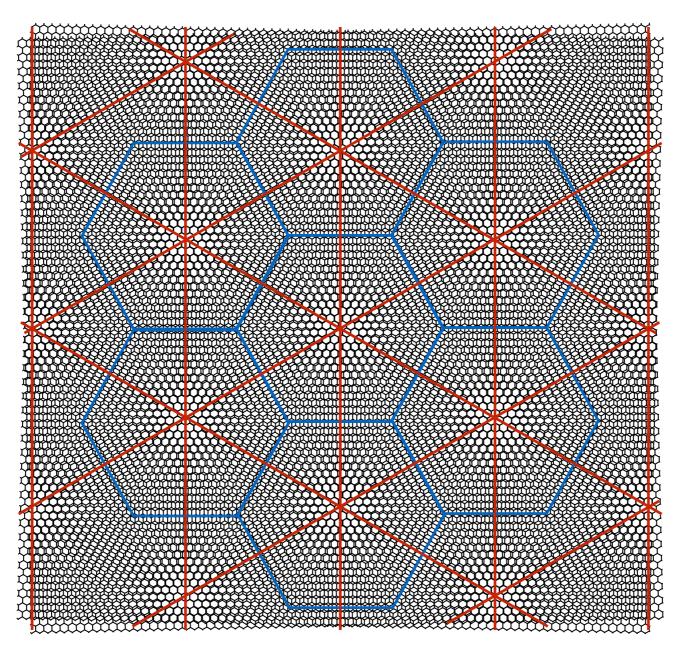
- at magic angles θ_{M} (here: $\theta_{M} = 1.05^{\circ}$)
 - emergence of multiple nearly flat bands
 - well-separated from other bands
 - van Hove singularities in flat bands



Wannier orbitals for flat bands & effective lattice model

• symmetry analysis for tBLG:

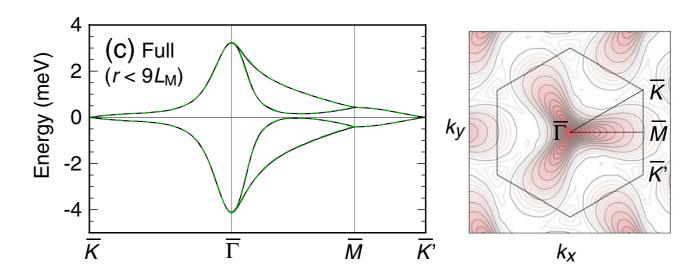
- Wannier orbitals centered at nonequivalent AB and BA spots in moiré pattern
- formation of emergent honeycomb lattice



emergent triangular lattice: ABC trilayer graphene-hBN, twisted double BLG, TMDs

Wannier orbitals for flat bands & effective lattice model

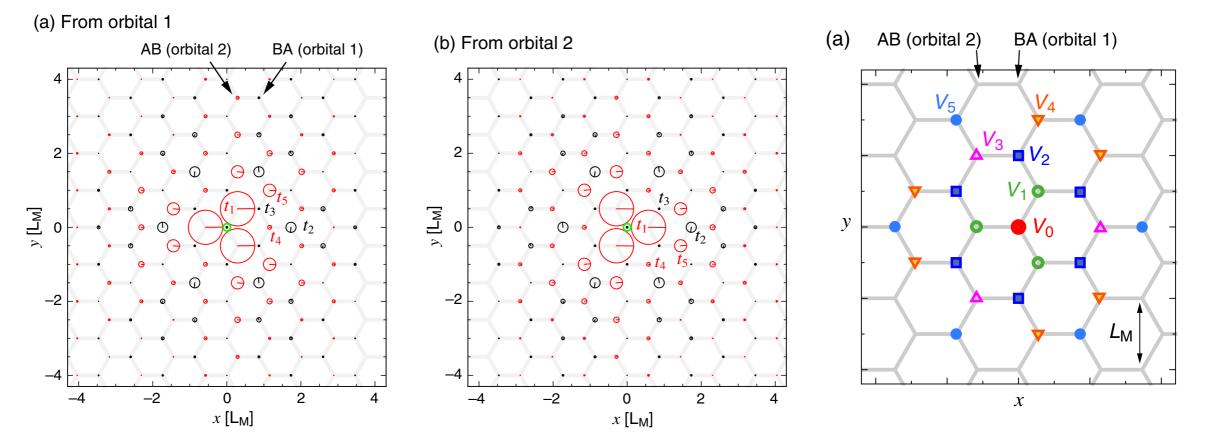
- flat band dispersion from continuum model
 - construct max-localized Wannier orbitals
 - tight-binding + extended Hubbard model



 $H = \sum_{\xi=\pm} \sum_{ij} t(\mathbf{r}_{ij}) e^{i\xi\phi(\mathbf{r}_{ij})} c^{\dagger}_{i\xi} c_{j\xi}$ + **extended Hubbard i.a.**

hopping integrals and electron-electron interaction parameters:

Koshino et al, PRX 8, 031087 (2018)
 Kang & Vafek, PRX 8, 031088 (2018)



Correlated moiré heterostructures - **precis**

Precis

- 2D moiré heterostructures:
 - emergent flat bands, small kinetic energy
 - enhanced interaction effects



- construction of effective models on emergent moiré honeycomb/triangular superlattice
 - universal features:
 - **multi-orbital** structure inherited from two valleys \rightarrow **Hund's couplings**
 - onsite and sizable **further-neighbor interactions**

... starting point for application of **many-body methods...**

what is the nature of the correlated insulating and SC states?

- Kekulé valence bond solid, (anti)ferromagnet, interaction-induced top. states,...?
- featureless Mott insulator?
- gapped quantum spin liquid with neutral spin-1/2 excitations?
- topological/chiral d+id superconductor, f-wave superconductor,...?

Functional renormalization group approach

Effective action

- ▶ system of interacting fermions: $S[\psi, \bar{\psi}] = -(\bar{\psi}, G_0^{-1}\psi) + V[\psi, \bar{\psi}]$ general two-particle i.a.
- bare propagator (translation and spin rotation invariance):

single-particle energy

$$G_0(k_0, \mathbf{k}) = \frac{1}{ik_0 - \xi_\mathbf{k}}, \quad \xi_\mathbf{k} = \epsilon_\mathbf{k} - \mu$$

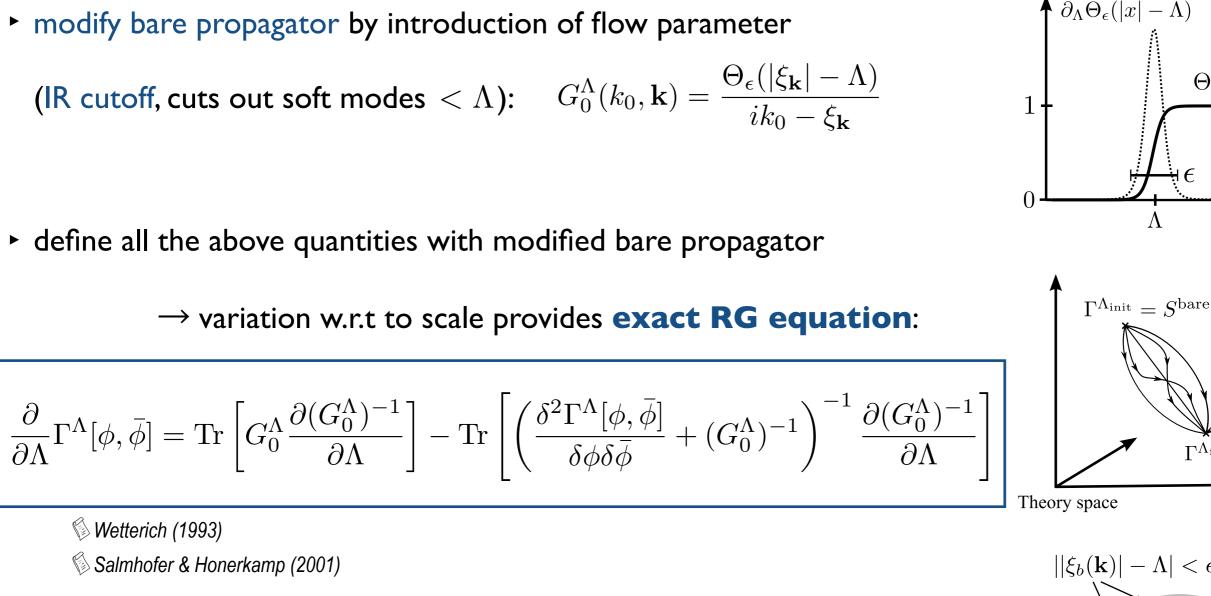
generating functional (for connected Green functions):

$$\mathcal{G}[\eta,\bar{\eta}] = -\ln \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \, e^{\mathcal{S}[\psi,\bar{\psi}]} e^{(\bar{\eta},\psi) + (\bar{\psi},\eta)}$$

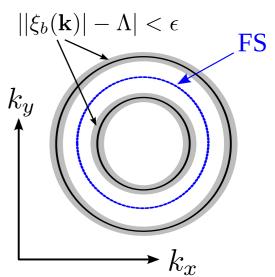
► effective action:
$$\Gamma[\phi, \bar{\phi}] = (\bar{\eta}, \phi) + (\bar{\phi}, \eta) + \mathcal{G}[\eta, \bar{\eta}], \quad \phi = -\frac{\partial \mathcal{G}}{\partial \bar{\eta}}, \quad \bar{\phi} = \frac{\partial \mathcal{G}}{\partial \eta}$$

(generates one-particle irreducible vertex functions)

Functional flow equations



- exact RG equation has one-loop structure
- removing cutoff ($\Lambda \to 0$) yields the full effective action
- Iowering cutoff corresponds to momentum-shell integration



 $\Theta_{\epsilon}(|x| - \Lambda)$

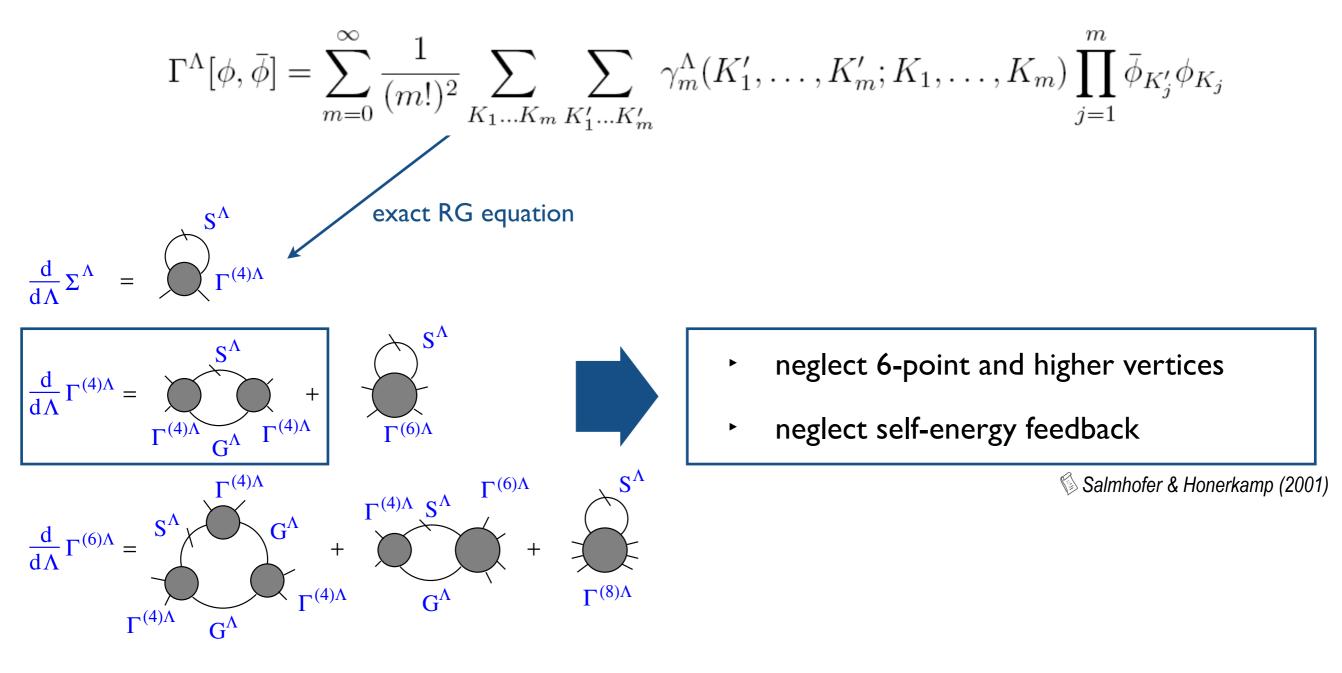
 $\Gamma^{\Lambda_{\text{final}}} = \Gamma$

 \mathcal{X}

[§] from Platt, Hanke, Thomale (2013)

Truncation and approximations

- exact RG equation cannot be solved exactly!
- starting point for systematic approximations (vertex expansion)

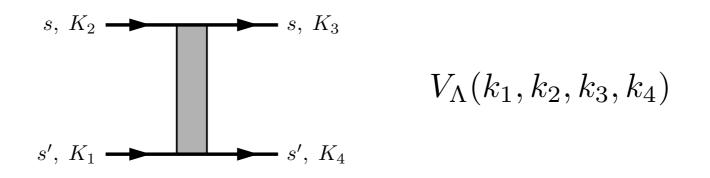


... infinite hierarchy of flow equations!

Symmetries and approximations

- system with spin-rotational invariance:
 - RG flow of general 4-point function $\Gamma^{(4)\Lambda}$: $\Gamma^{(4)\Lambda}_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} = V^{\Lambda}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} V^{\Lambda}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}$

interaction vertex V^A:



- momentum arguments include frequency, wavevector and orbital indices
- round-state properties: neglect frequency dependence, set external frequencies to zero

Symmetries and approximations

- system with spin-rotational invariance:
 - RG flow of general 4-point function $\Gamma^{(4)\Lambda}$: $\Gamma^{(4)\Lambda}_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} = V^{\Lambda}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} V^{\Lambda}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}$

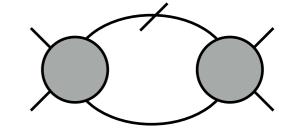
flow of spin-independent interaction vertex V^A:

$$\frac{d}{d\Lambda}V^{\Lambda}(K_{1}, K_{2}; K_{3}, K_{4}) = \int dK V^{\Lambda}(K_{1}, K_{2}, K) L^{\Lambda}(K, -K + K_{1} + K_{2}) V^{\Lambda}(K, -K + K_{1} + K_{2}, K_{3}),$$

$$+ \int dK \left[-2V^{\Lambda}(K_{1}, K, K_{3}) L^{\Lambda}(K, K + K_{1} - K_{3}) V^{\Lambda}(K + K_{1} - K_{3}, K_{2}, K) + V^{\Lambda}(K_{1}, K, K + K_{1} - K_{3}) L^{\Lambda}(K, K + K_{1} - K_{3}) V^{\Lambda}(K + K_{1} - K_{3}, K_{2}, K) + V^{\Lambda}(K_{1}, K, K_{3}) L^{\Lambda}(K, K + K_{1} - K_{3}) V^{\Lambda}(K_{2}, K + K_{1} - K_{3}, K) \right],$$

$$+ \int dK V^{\Lambda}(K_{1}, K + K_{2} - K_{3}, K) L^{\Lambda}(K, K + K_{2} - K_{3}) V^{\Lambda}(K, K_{2}, K_{3}).$$

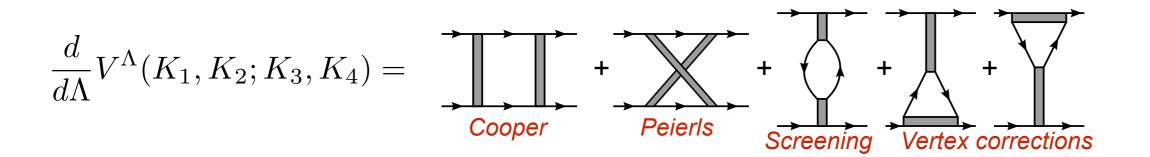
- where
$$L^{\Lambda}(K,K') = \frac{d}{d\Lambda}[G_0^{\Lambda}(K)G_0^{\Lambda}(K')]$$



Symmetries and approximations

- system with spin-rotational invariance:
 - RG flow of general 4-point function $\Gamma^{(4)\Lambda}$: $\Gamma^{(4)\Lambda}_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} = V^{\Lambda}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} V^{\Lambda}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}$

flow of spin-independent interaction vertex V^A:



- corresponds to infinite order summation of one-loop pp and ph terms
- unbiased investigation of competition between various correlations
- flow to strong coupling indicates ordering transition: analyze components of V^{Λ}

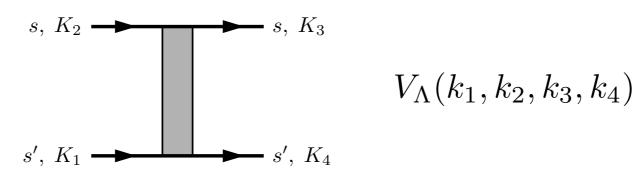
Multi-orbital models

- orbital degrees of freedom:
 - valley d.o.f. in tBLG, *d*-orbitals of iron pnictides and transition-metal oxides
 - sublattice index of bipartite/multi-layer lattice (e.g., graphene's honeycomb lattice)
 - general non-interacting part of multi-orbital model: $H_0 = \sum_{\vec{k},s} \sum_{o,o'} c^{\dagger}_{o,s,\vec{k}} K_{o,o'}(\vec{k}) c_{o',s,\vec{k}}$ - unitary transformation to **energy band representation**:

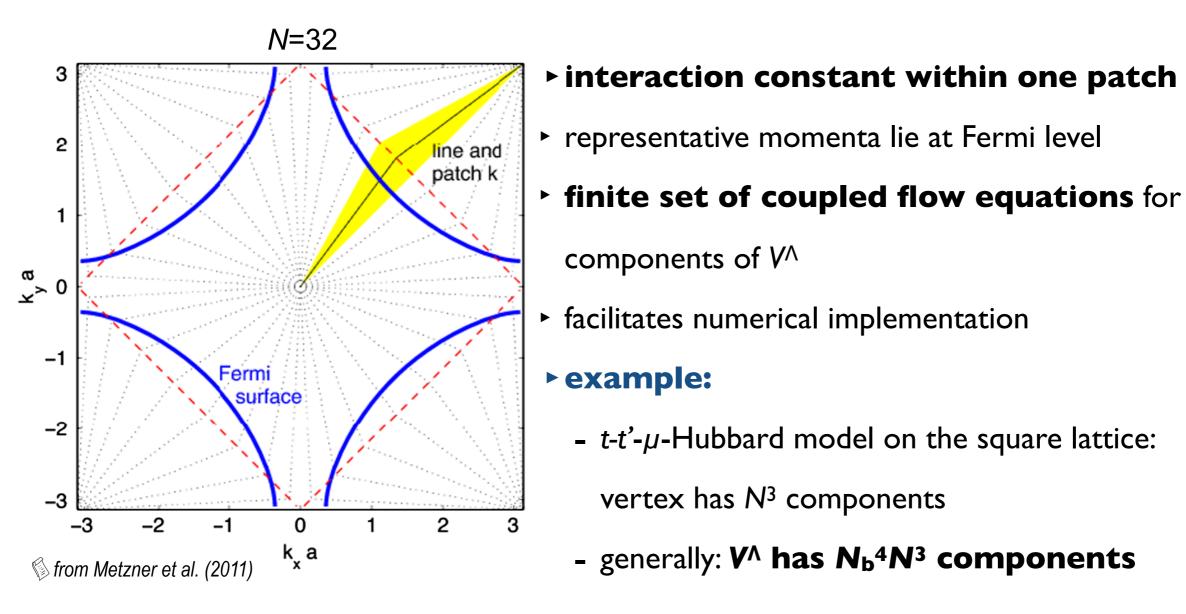
- interaction part of Hamiltonian has to be transformed accordingly

adds momentum dependence to interaction vertex at bare level - orbital makeup

Fermi-surface patching scheme

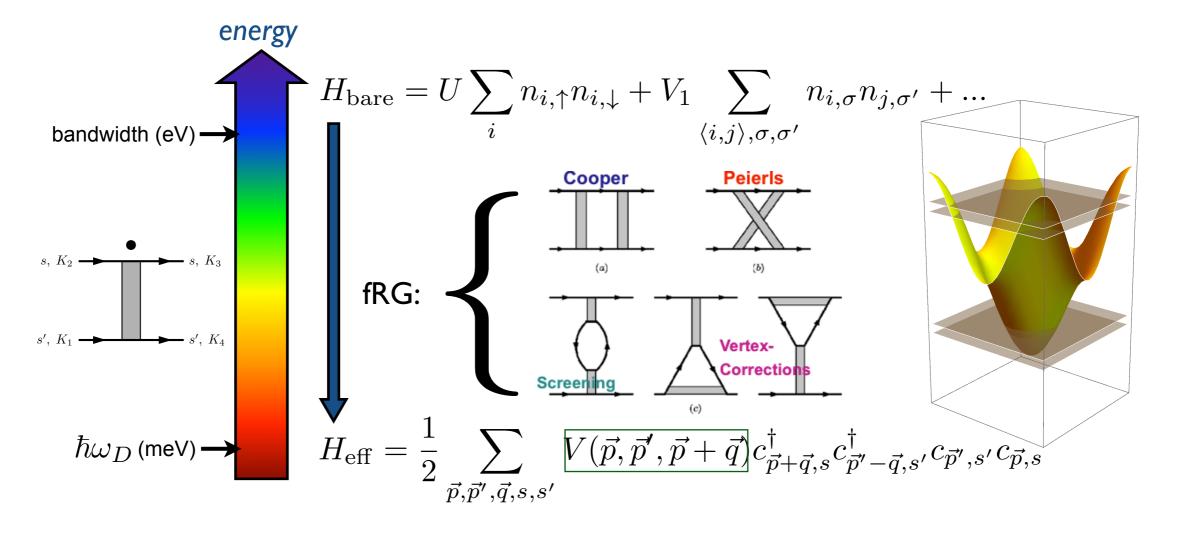


• wavevector dependence of Fermi surface from discretization in N patches:



fRG: from **bare** to **effective interaction**

• excitations at intermediate scales generate momentum structure in low-energy interaction



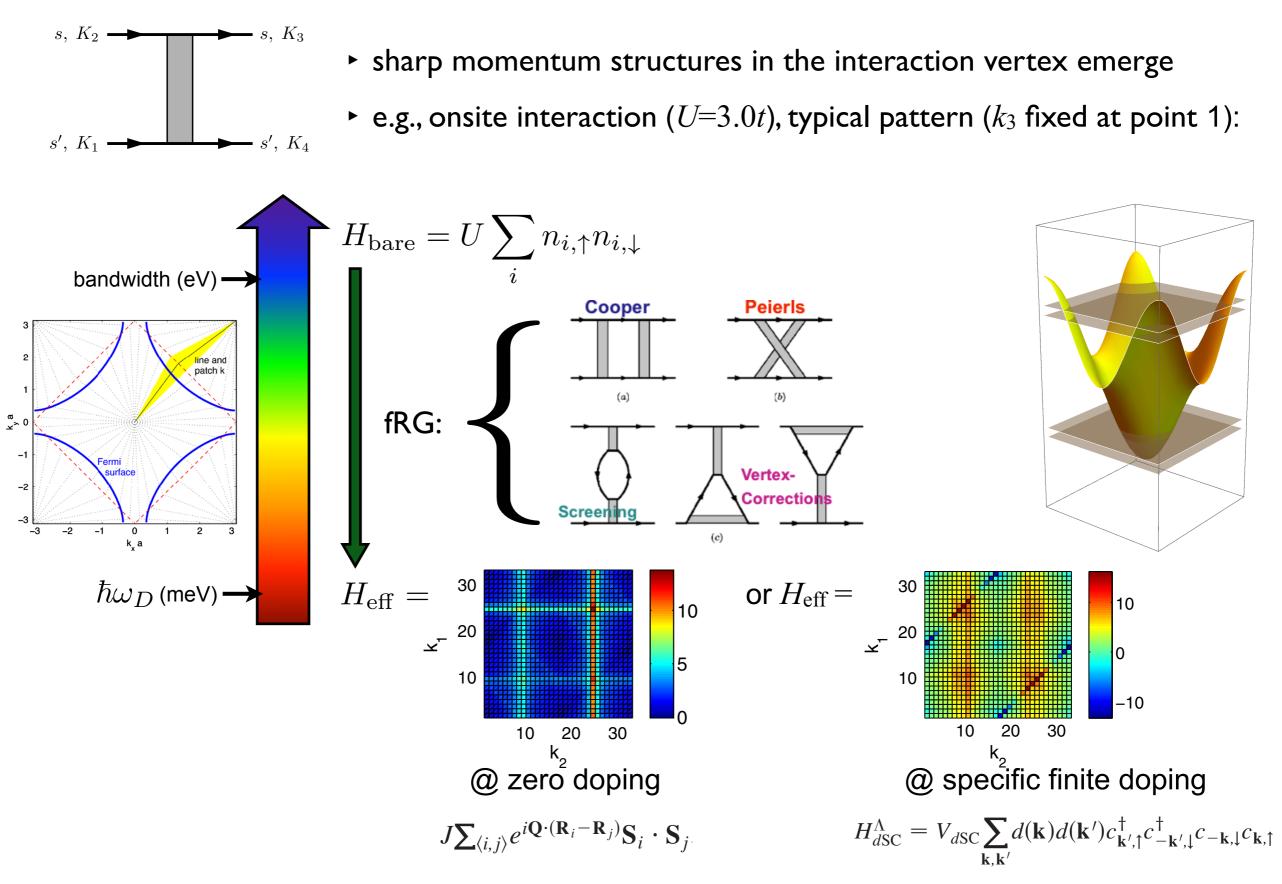
Iow-energy effective action & momentum structure

two-particle interaction vertex $V(\vec{p}, \vec{p}', \vec{p} + \vec{q})$

```
> flow to strong coupling: singularity for \Lambda \to \Lambda^*
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read off dominant interactions and e.g. extract form factors of order parameters

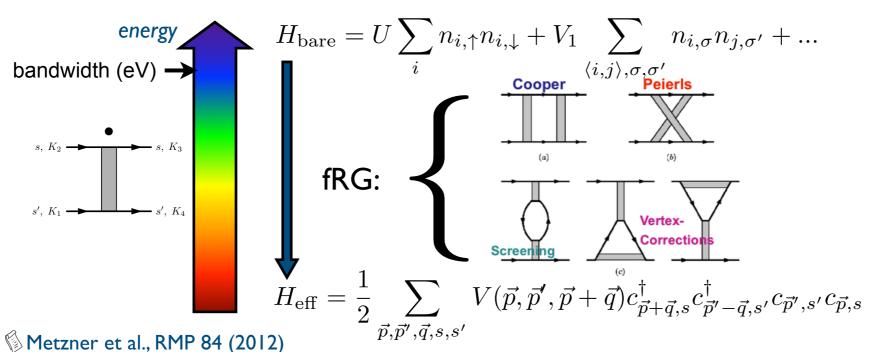
fRG: from bare to effective interaction

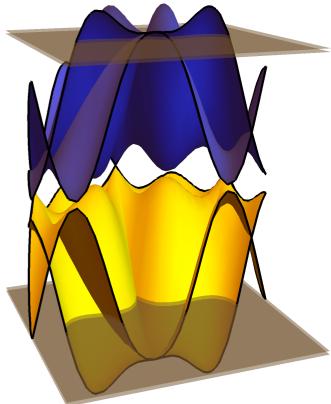


▶ mean-field decoupling \rightarrow antiferromagnetic SDW (**AF-SDW**) or **d-wave SC**

fermion fRG approach — Precis

• *fermion fRG*: discovery tool for leading many-body instabilities





- treats all fermionic fluctuation channels on equal footing
- infinite-order resummation of all fermionic I-loop diagrams
- can deal with multi-orbital band structures, non-local i.a. & competing correlations
- due to truncations/approximations: qualitative (not quantitative) tool
- prediction of different types of magnetism / superconductivity / bond order states / ...

Minimal phenomenological model for tDBLG

- I. *triangular* lattice near van-Hove filling (twisted **double** bilayer graphene)
- 2. weak tunnelling between nearest-neighbor unit supercells dominates kinetic energy
- 3. each cell hosts two degenerate orbitals from original valleys +/-
- 4. no mixing of orbitals due to large momentum space separation
- 5. spin-independent hopping of electrons Balents & Xu, PRL 121, 087001 (2018)

two-orbital tight-binding model $H_{kin} = -t \sum_{\langle ij \rangle} \sum_{\sigma=\uparrow,\downarrow} \sum_{o=\pm} \left(c^{\dagger}_{i\sigma o} c_{j\sigma o} + h.c. \right)$

- 4 flavours: α ∈ {(↑,+), (↓,+), (↑,-), (↓,-)} → effective SU(4) symmetry
- add SU(4) symmetric Hubbard interaction as minimal interaction

$$H_{\rm int} = U \sum_{i} \left(\sum_{\alpha=1}^{4} n_{i\alpha} \right)^2$$

dominant interaction depends only on total charge of site

Next-to-minimal model

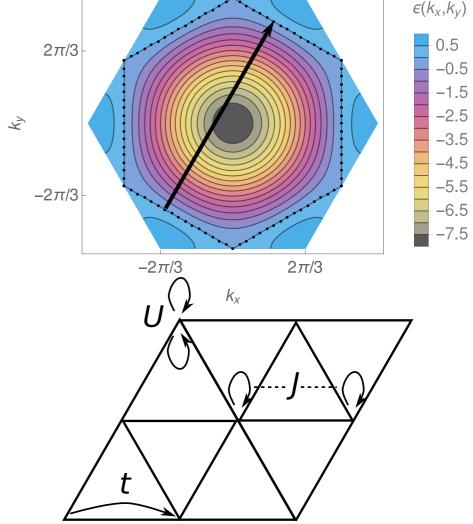
- Include Hund's couplings: $H_h = -V_h \sum_{i} \vec{S}_i \cdot \vec{S}_i$
 - with $\vec{S}_i = rac{1}{2} c^{\dagger}_{i\sigma o} \vec{\sigma}_{\sigma\sigma'} c_{i\sigma'o}$
 - breaks SU(4)
 - alternatively "orbital" Hund's coupling (anti-Hund):

$$H_K = -K \sum_i \vec{L}_i \cdot \vec{L}_i \quad \text{with} \quad \vec{L}_i = \frac{1}{2} c^{\dagger}_{i\sigma o} \vec{\tau}_{oo'} c_{i\sigma o'}$$

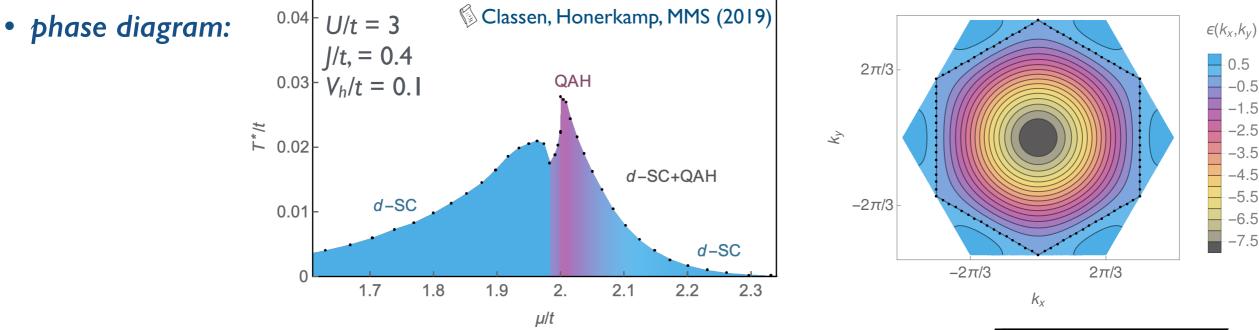
- also add SU(4) exchange coupling J
- hierarchy of model parameters:
 - strong onsite interaction U > J, V_h ,
 - approximate $SU(4): U > V_h, K$
 - tune filling by chemical potential μ

fRG phase diagram...

Xu & Balents
Dodaro, Kivelson, Schattner, Sun, Wang
Yuan & Fu
Po, Zou, Vishwanath, Senthil



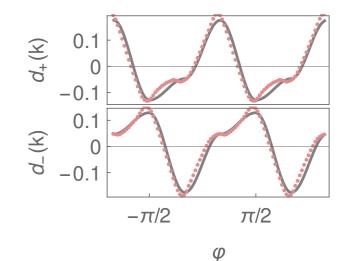
Next-to-minimal models — functional RG approach



• interaction-induced quantum anomalous Hall state:

- robust near van-Hove filling, fully gapped spectrum
- breaks time-reversal symmetry
- Chern insulator: Haldane-like loop current $V(\varphi, \varphi', \varphi_0)$
- d±id superconductivity:
 - SC form factor superposition of $d_{xy}(k)$ and $d_{x^2}^{\pi/2}$.
 - expect lowest energy for full gap $\rightarrow d_{xy} \pm i d_{x^2}$
 - for $V_h > K$: (spin-singlet) x (orbital-triblet) pairing function $\pi/2$

-20 0 20 40



...next: implementation of realistic lattice models...

Conclusions & Outlook

Conclusions and **Outlook**

- Superlattice modulation of moiré heterostructures
 - flat bands, strongly-correlated physics, "high-T_c" phase diagrams, highly tunable

Open questions

- appropriate models and characterization of correlated states
- weak-coupling vs. strong coupling perspective
- Competing orders/instabilities → fermion fRG (for tdBLG)

