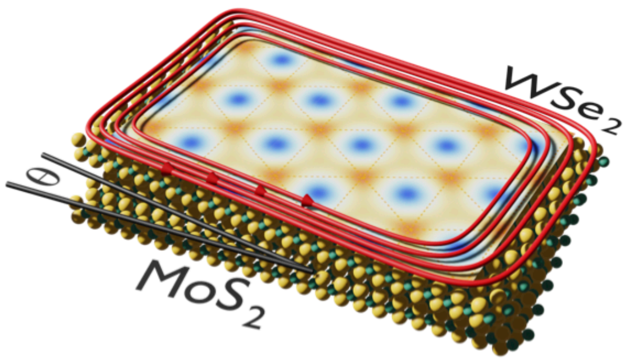
Functional RG for the triangular-lattice extended Hubbard model:

competing instabilities and application to moiré materials



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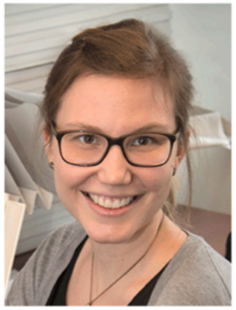
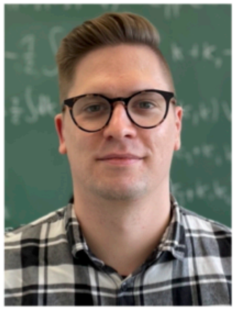
Outline

- Introduction
- **Band structure** of moiré transition metal dichalcogenides
- Effective **frustrated extended superlattice Hubbard model**
- **Functional RG** approach
- Chiral **($g + ig$) superconductivity** and **quantized Hall responses**



Laura Classen
MPI-FKF



Nico Gneist
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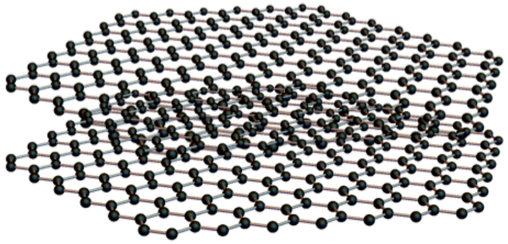
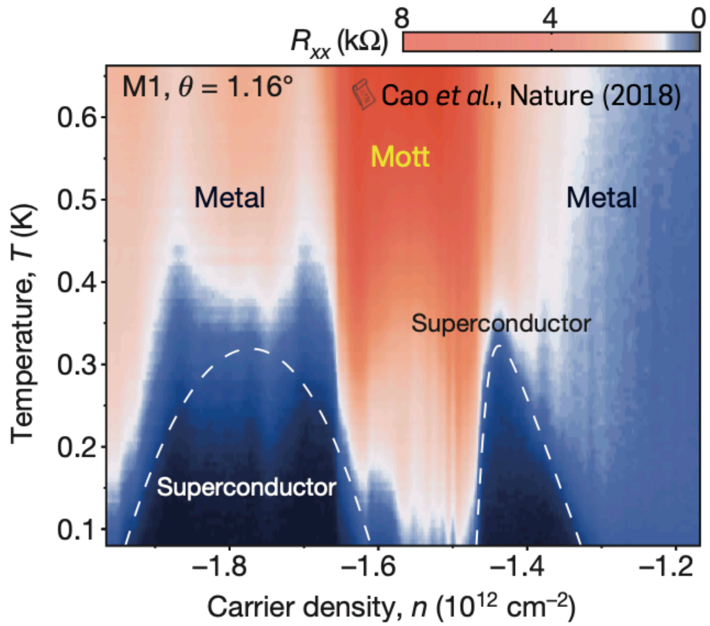
Dante M. Kennes
RWTH Aachen

Introduction



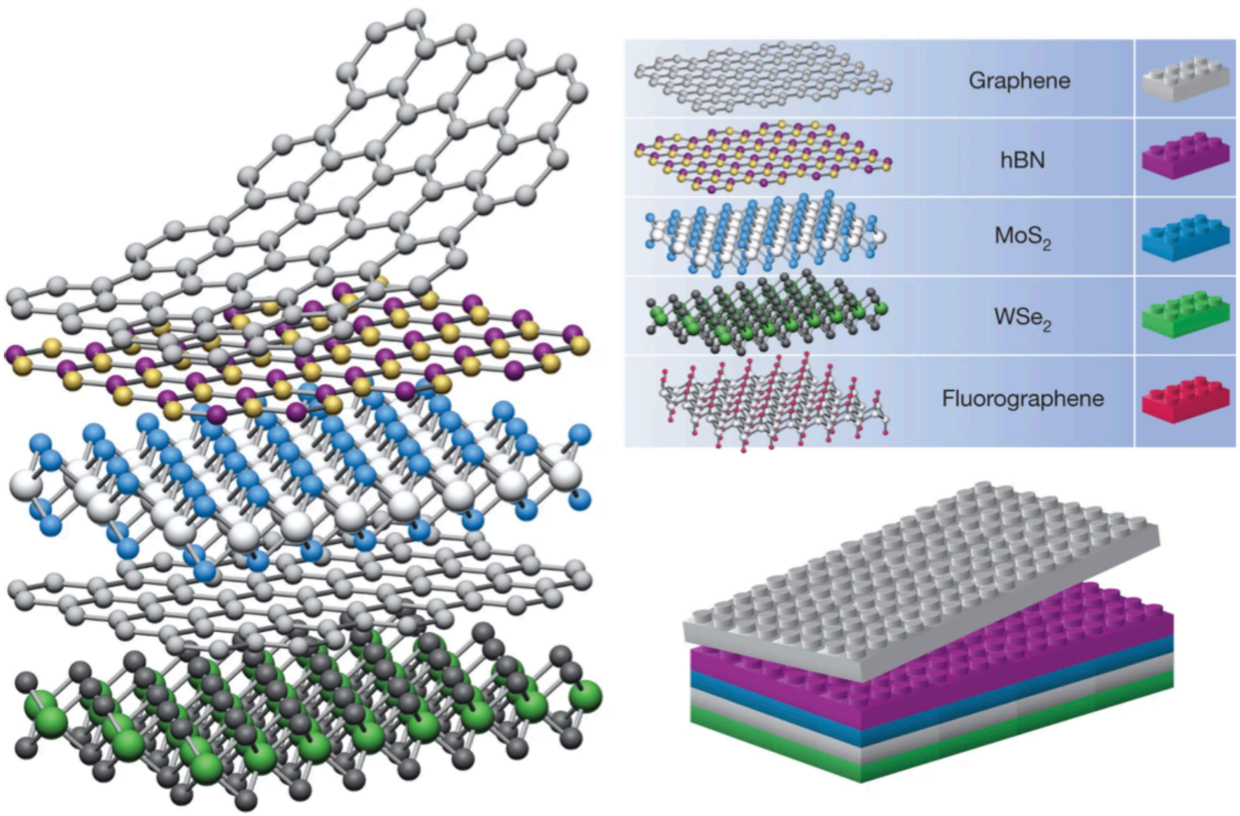
- singlelayer graphene → no strongly-correlated behavior
- bilayer graphene with small twist angle $\theta \sim 1^\circ$ → strongly-correlated behavior!



- **new platform for study of strongly-correlated materials**
- twisted bilayer graphene is not so simple
  - 4 spin-degenerate nearly-flat bands
  - "magic angles"
  - "topological obstruction"

2D materials LEGO® with a twist

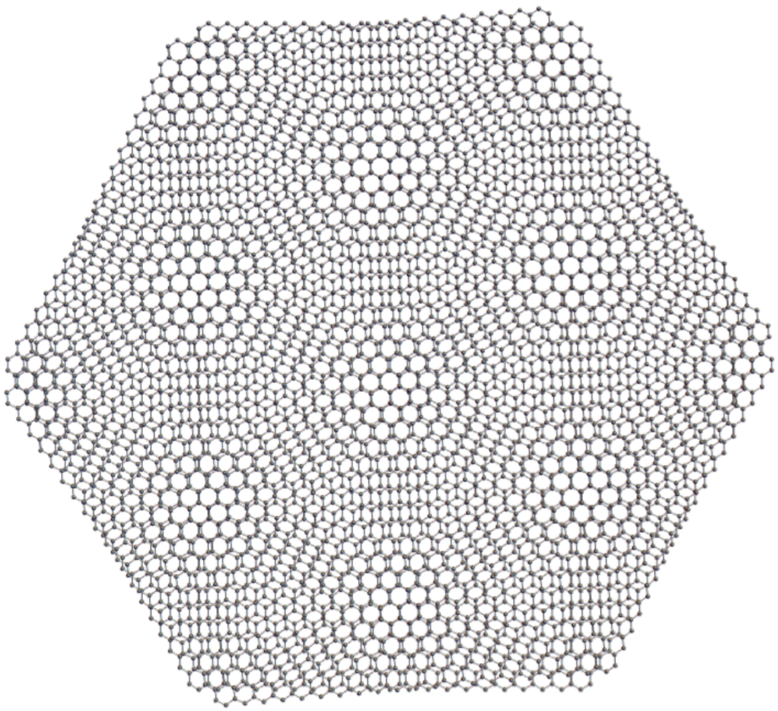
- broader class of 2D materials (semi-conductors, insulators,...)



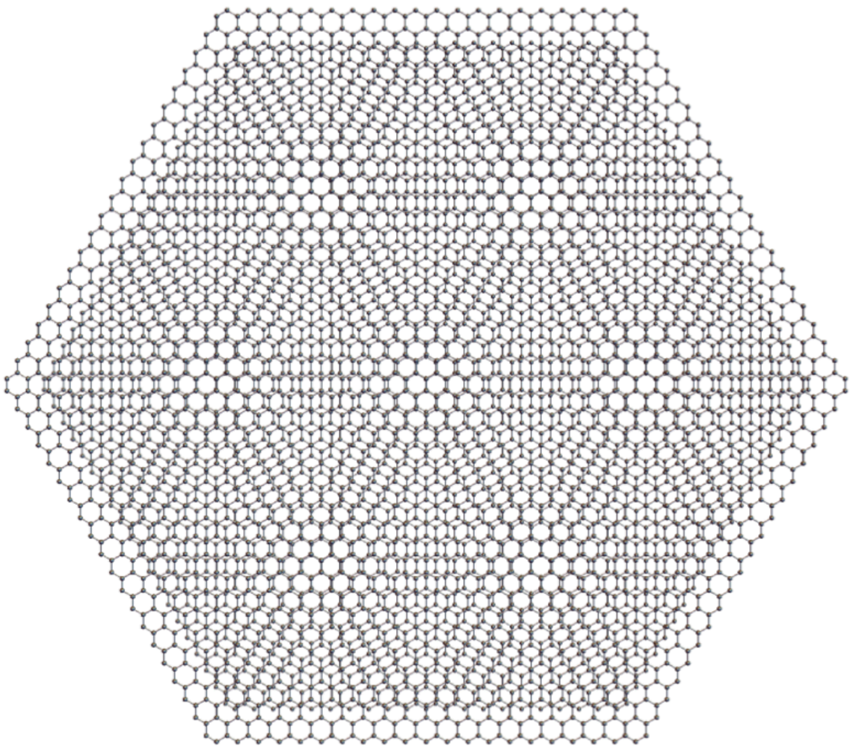
Geim & Grigorieva, Nature (2013)

2D moiré patterns

- overlay of 2 periodic structures with slight mismatch → moiré interference pattern



rotation by $\theta = 5^\circ$

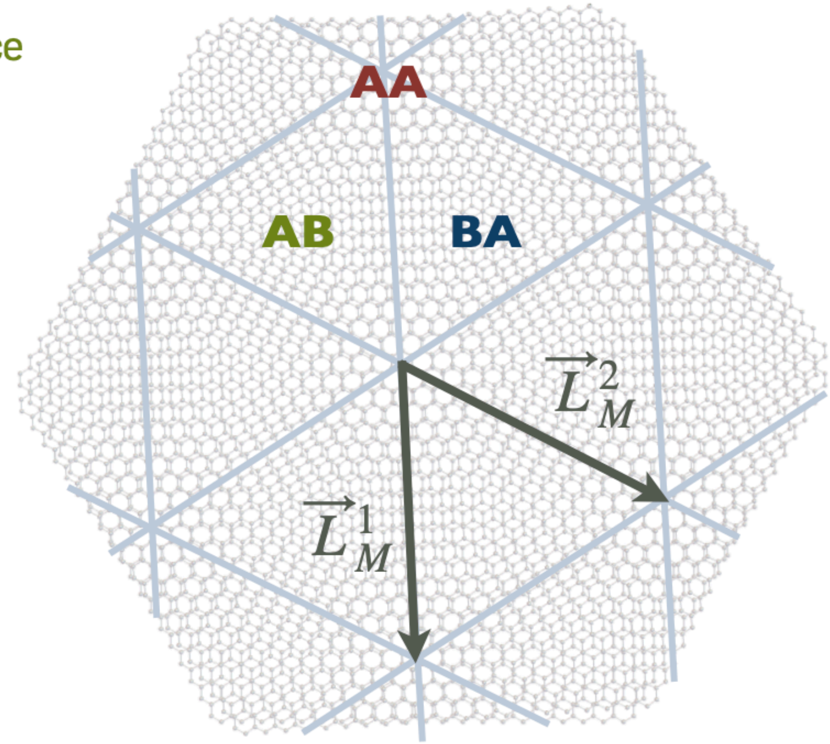


$\theta = 0^\circ$ with different lattice constants

2D moiré patterns

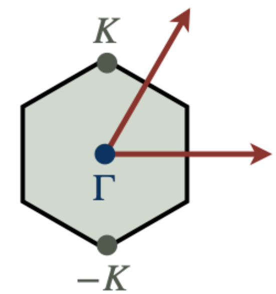
- ions at lattice sites generate crystal potential for electrons
  - superposition of two layers → hexagonal moiré superlattice
- with twist angle θ and lattice-constant mismatch δ
  - **moiré lattice constant** $a_M = |\vec{L}_M^i| \approx \dfrac{a_0}{\sqrt{\theta^2 + \delta^2}}$
  - WSe2: $a_0 \approx 3.32\,\text{Å}$
  - MoS2: $a_0 \approx 3.19\,\text{Å}$

$$a_M \approx \frac{a_0}{\sqrt{0 + \delta^2}} \approx 8.5\,\text{nm}$$

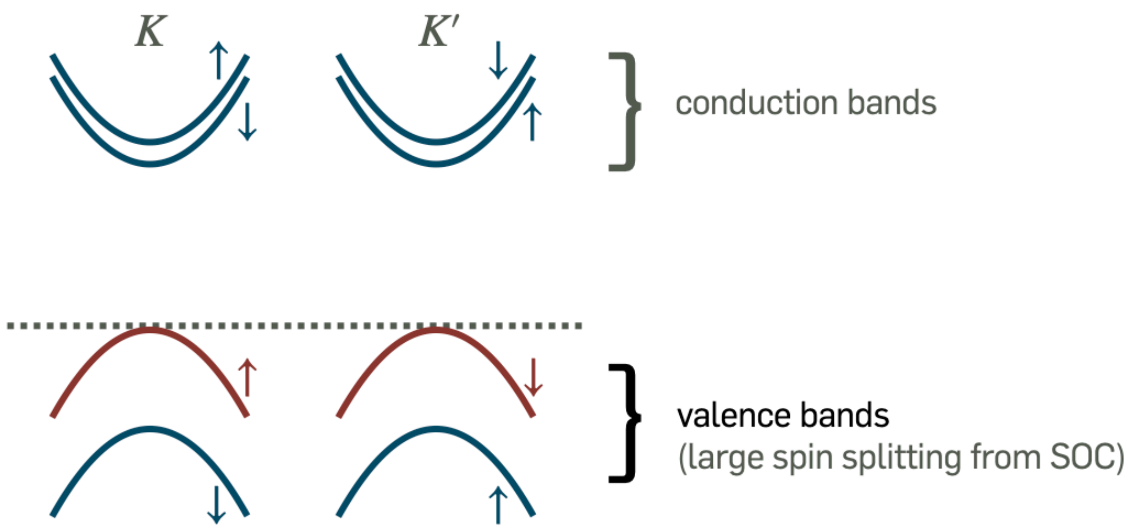


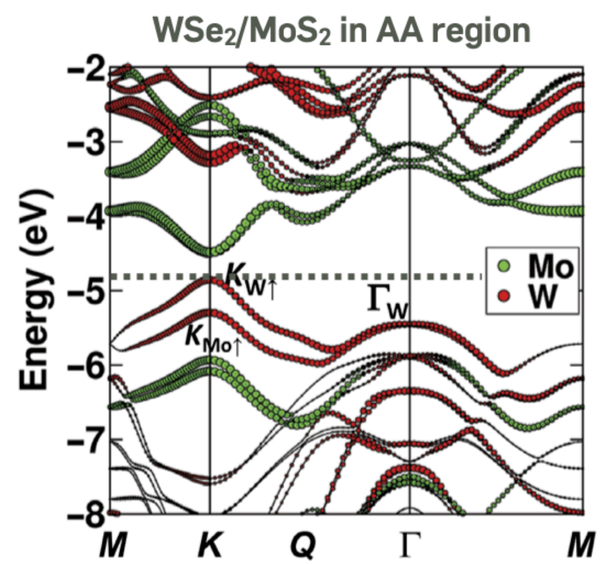
RUB

2D group-VI transition metal dichalcogenides



- schematic band structure of monolayer WSe_2
  - band extrema at BZ corners K and K'



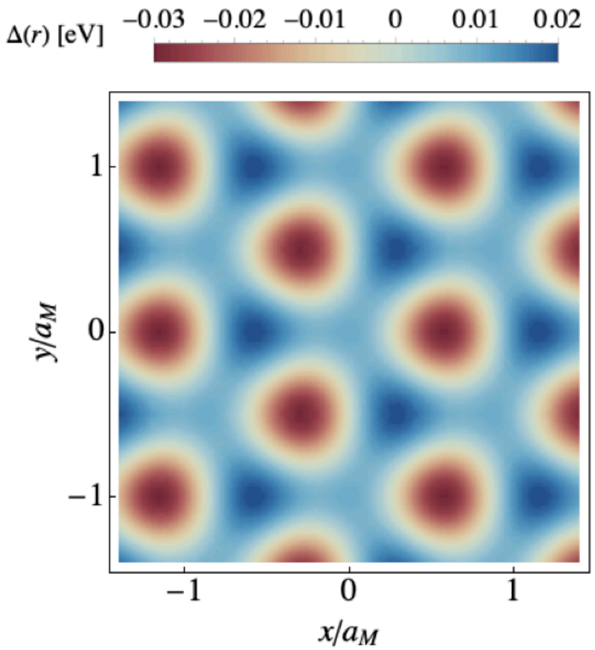


Zhang *et al.*, Sci. Adv. (2017)

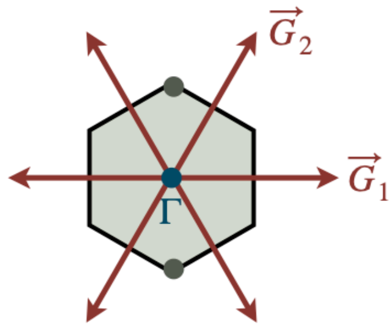
  - focus on states near max of WSe_2 valence bands → lie inside MoS_2 gaps

Moiré potential of WSe_2/MoS_2

- moiré pattern → periodic potential for WSe_2 valence-band states → moiré potential $\Delta(\vec{r})$ w/ period a_M



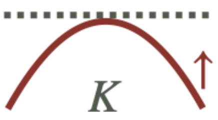
- $\Delta(\vec{r})$ can be approximated by Fourier series $\Delta(\vec{r}) = \sum_{\vec{G}} V(\vec{G})\, e^{i\vec{G}\cdot\vec{r}}$
  - $V(\vec{G})$ fixed by $V(\vec{G}_1) = Ve^{i\psi}$
  - can be measured with STM
  - **parameter fit** $(V, \psi) \approx (5.1\,\text{meV}, -71^\circ)$



Wu, Lovorn, Tutuc, MacDonald, PRL (2018)

Moiré band Hamiltonian of WSe_2/MoS_2

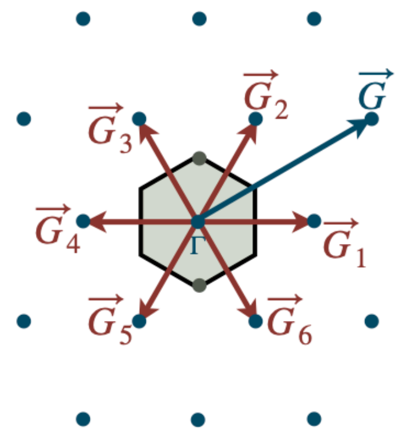
- effective mass approximation for maximum of WSe_2 band



$$\mathscr{H}_{\text{kin}} = -\frac{\hbar^2 \vec{Q}^2}{2m^*} \quad \text{with} \quad m^* \approx 0.35 m_0$$

- moiré band Hamiltonian for WSe_2 valence band maximum states

$$\mathscr{H} = \mathscr{H}_{\text{kin}} + \Delta(\vec{r}) \quad \text{with} \quad \Delta(\vec{r}) = \sum_{i=1}^{6} V(\vec{G}_i)\, e^{i\vec{G}_i\cdot\vec{r}}$$



- dispersion from moiré Bloch Hamiltonian in plane wave representation

$$\langle \vec{k} + \vec{G} \,|\, \mathscr{H} \,|\, \vec{k} + \vec{G}' \rangle = -\frac{\hbar^2 |\vec{k} + \vec{G}|^2}{2m^*}\delta_{\vec{G},\vec{G}'} + \sum_{i=1}^{6} V(\vec{G}_i)\delta_{\vec{G}_i,\vec{G}-\vec{G}'}$$

Moiré bands of WSe_2/MoS_2 at $\theta = 0°$

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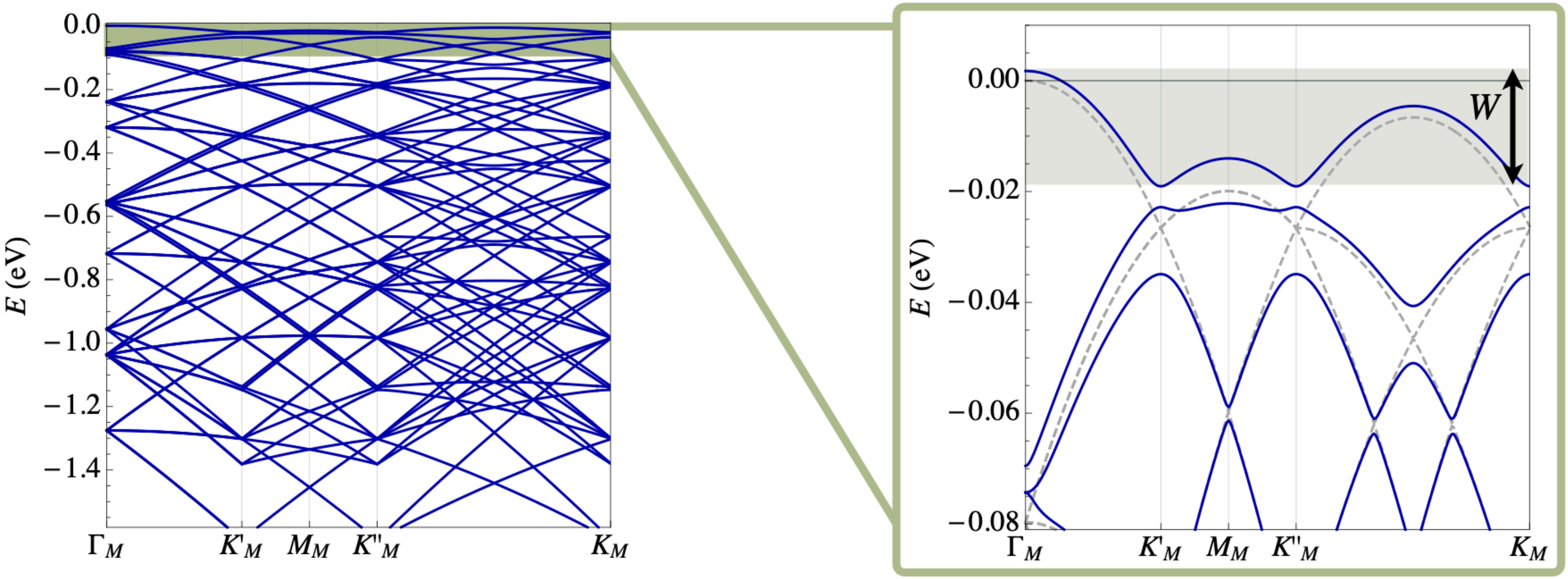
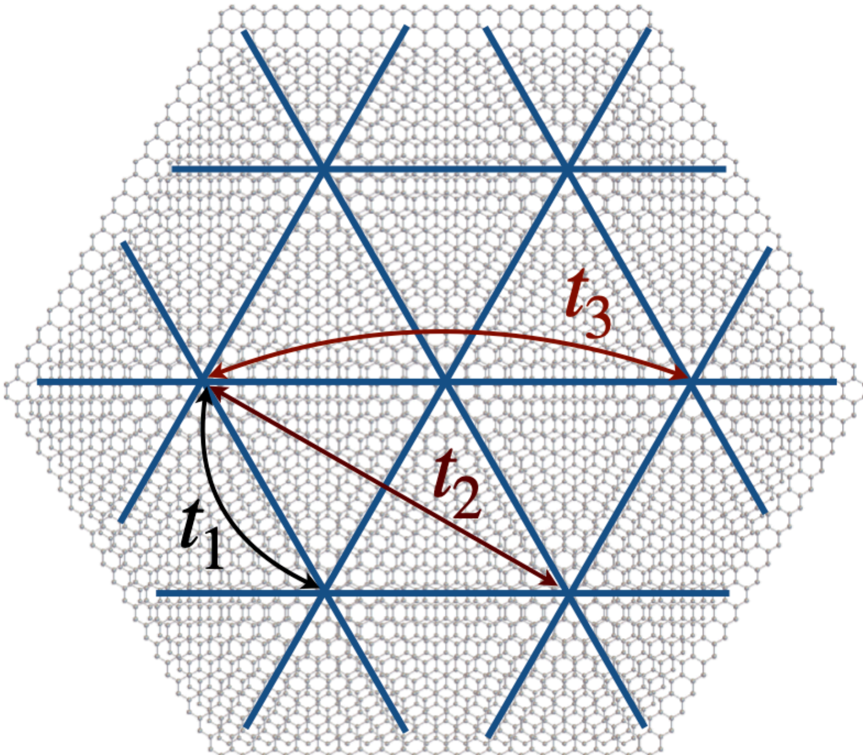
- diagonalization of moiré Bloch Hamiltonian for $\vec{G}, \vec{G}'$ within cutoff circle of radius $4\,|\,\vec{G}_1\,|$



- highest valence moiré band is isolated by band gap and has small bandwidth $W \sim 20\,\mathrm{meV}$

Moiré tight-binding model

- isolated flat band can be described by effective tight-binding model $H_0 = \sum_{\nu=\pm} \sum_{\vec{R},\vec{R}'} t(\vec{R}' - \vec{R}) c^\dagger_{\vec{R},\nu} c_{\vec{R}',\nu}$



- $\vec{R}$ on sites of triangular moiré superlattice
- $\nu = \pm$ is valley index from K, K'
- accurate flat-band dispersion at $\theta = 0°$ for

$$t_1 \approx -2.5\,\mathrm{meV}, \quad t_2 \approx 0.5\,\mathrm{meV}, \quad t_3 \approx 0.25\,\mathrm{meV}$$

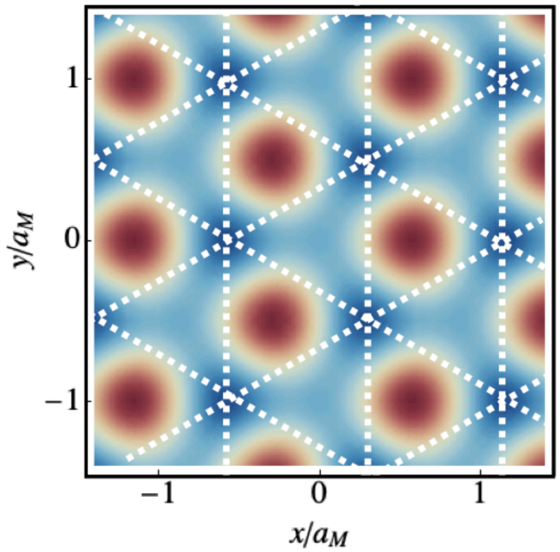
- t_i decrease exponentially with increasing a_M

Wannier wave-functions of isolated band

RUB

- construct localized Wannier functions $w(\vec{r})$ for isolated band centered at moiré potential maxima
- spatial extent a_W of $w(\vec{r})$ increases with a_M as $a_W \propto \sqrt{a_M}$ (harmonic oscillator approximation)

➡ onsite repulsion $U \sim e^2/(\epsilon a_W)$ decreases slowly as a_M increases



➡ ratio of interaction to bandwidth:

$$\frac{U}{W} \text{ increases quickly with } a_M \sim \frac{1}{\theta}$$

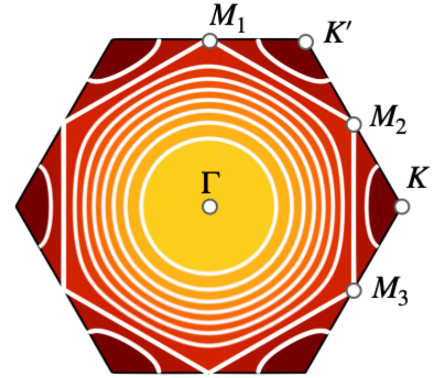
➡ supports formation of strongly correlated states!

Wu, Lovorn, Tutuc, MacDonald, PRL (2018)

Extended Hubbard model on triangular lattice

RUB

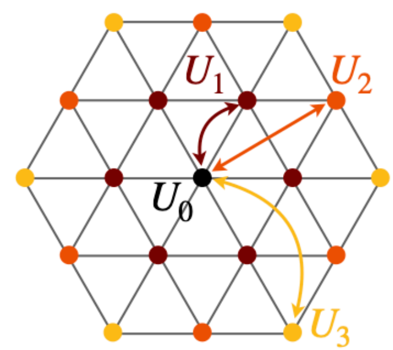
$$H = \sum_{\nu=\pm}\sum_{\vec{R},\vec{R}'} t(\vec{R}'-\vec{R})c^{\dagger}_{\vec{R},\nu}c_{\vec{R}',\nu} + \frac{1}{2}\sum_{\nu,\nu'}\sum_{\vec{R},\vec{R}'} U(\vec{R}'-\vec{R})c^{\dagger}_{\vec{R}\nu}c^{\dagger}_{\vec{R}'\nu'}c_{\vec{R}'\nu'}c_{\vec{R}\nu}$$



- full range of band fillings accessible by electrical gating
- van Hove singularities at 3/4 hole doping
- tunable strength & range of e⁻-e⁻ interactions → sizable non-local terms

➡ complex interplay between electronic interactions and geometric frustration

➡ strongly-correlated phases (MIT, spin liquids, magnetism,… e.g. @ half filling)



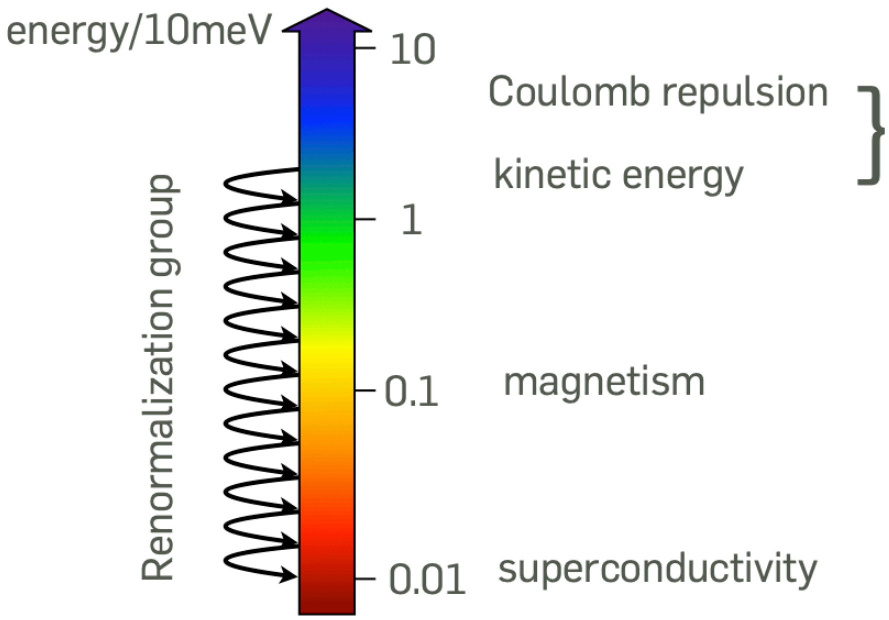
Wietek *et al.*, PRX (2021)
Szasz *et al.*, PRX (2020)
Chen *et al.*, arxiv:2102.05560
Zhu & White, PRB (2015)
Hu, Gong, Zhu, Sheng, PRB (2015)
…

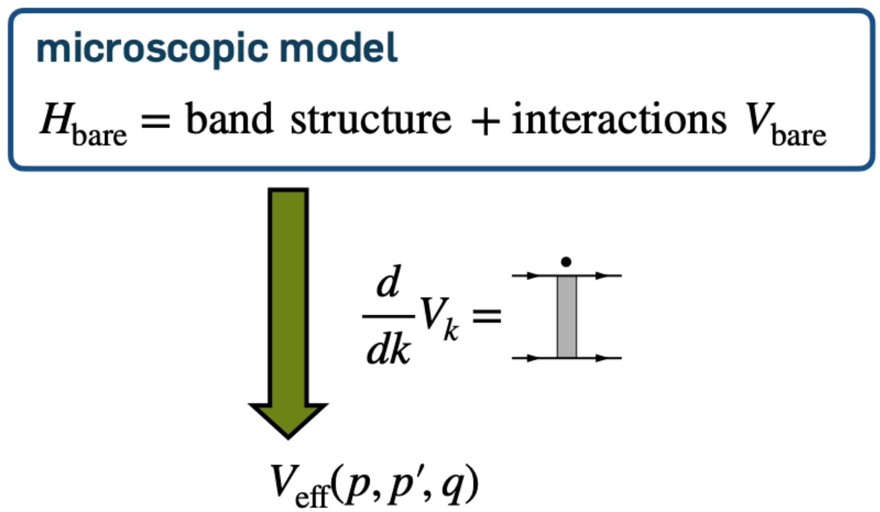
◉ WSe_2/MoS_2 material specific: t_1, t_2, t_3 & sizable non-local interactions V_i

- effect on Van-Hove scenario & superconducting pairing?

Electron functional renormalization group — schematics

- discovery tool for ordering tendencies





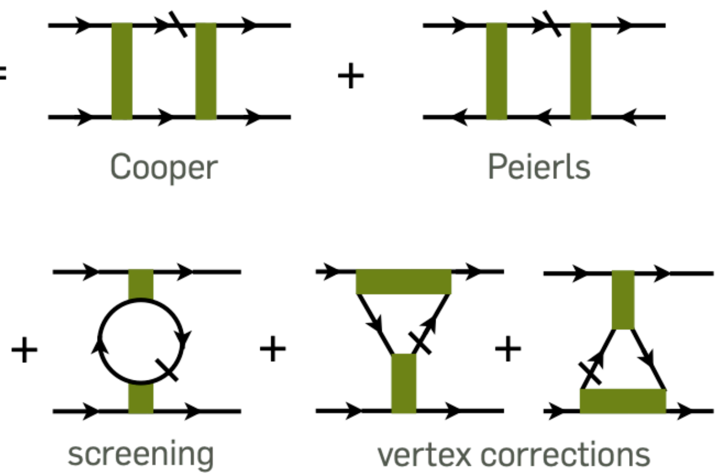
- can simultaneously deal w/ full band structure, non-local interactions, and competing interactions

Electron functional renormalization group — basic truncation

RUB

- consider RG flow of 2-particle interaction vertex $V^{\Lambda}(k_1, k_2, k_3, k_4)$

$$\frac{d}{d\Lambda} V^{\Lambda}(k_1, k_2, k_3, k_4) =$$

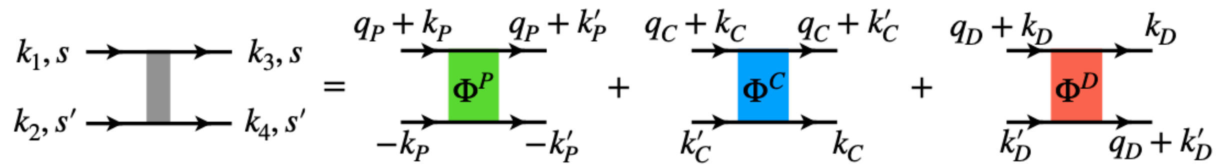


- neglect 6-point vertex and higher
- neglect self-energy feedback
- neglect frequency dependence

  - treats all fermionic fluctuation channels on equal footing
  - infinite-order resummation of all fermionic 1-loop diagrams

Electron functional renormalization group — implementation

- channel decomposition $V^{\Lambda} =$

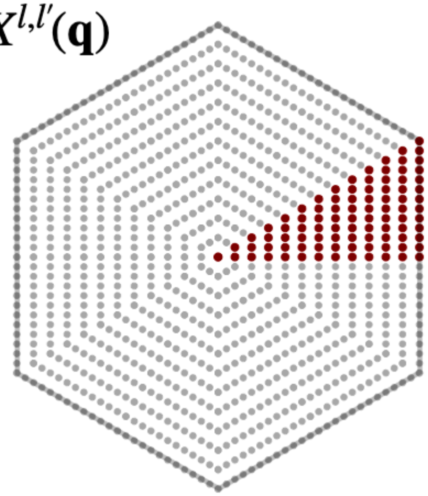


  - transfer momentum & form-factor expansion

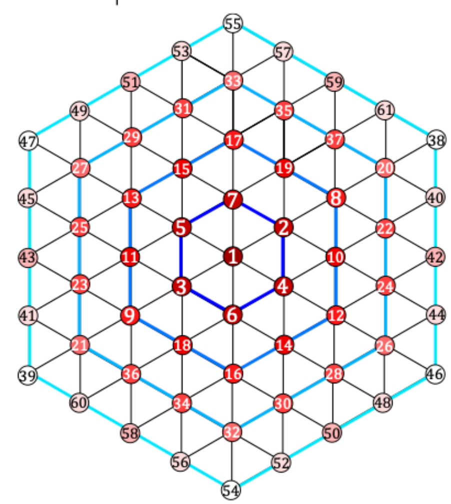
$$\Phi^X(\boldsymbol{q}, \boldsymbol{k}, \boldsymbol{k}') = \sum_{l,l'} X^{l,l'}(\boldsymbol{q}) f_l(\boldsymbol{k}) f^*_{l'}(\boldsymbol{k}')$$

Channel X	P	C	D
Interaction type	Pairing	Magnetic	Density
Transfer momentum q_X	$\boldsymbol{k}_1 + \boldsymbol{k}_2$	$\boldsymbol{k}_1 - \boldsymbol{k}_4$	$\boldsymbol{k}_1 - \boldsymbol{k}_3$
Momentum k_X	$-\boldsymbol{k}_2$	$\boldsymbol{k}_4$	$\boldsymbol{k}_3$
Momentum k'_X	$-\boldsymbol{k}_4$	$\boldsymbol{k}_2$	$\boldsymbol{k}_2$

  - obtain flow equations for $X^{l,l'}(\mathbf{q})$
  - choose momentum mesh



and form-factors $f_l(\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{R}_l}$

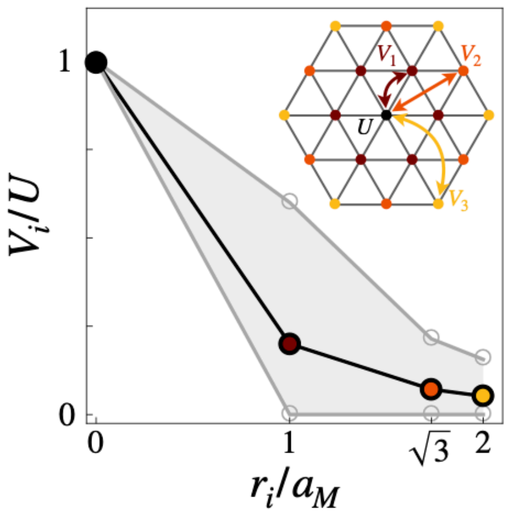


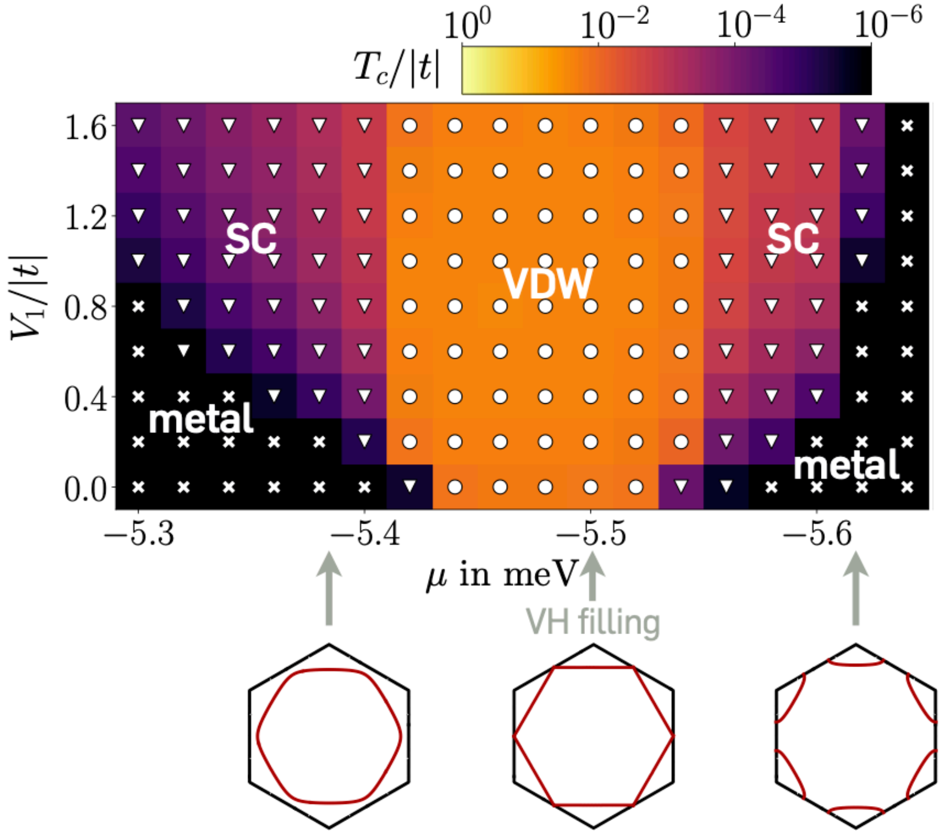
Gneist, Classen, MS (2022)

Electron FRG phase diagram for moiré TMD model

RUB

$t_1 \approx -2.5\,\mathrm{meV}, \quad t_2 \approx 0.5\,\mathrm{meV}, \quad t_3 \approx 0.25\,\mathrm{meV}, \quad U/|t_1| = 4, \quad V_2/V_1 \approx 0.36, \quad V_3/V_1 \approx 0.26$ Zhou, Sheng, Kim, PRL (2022)

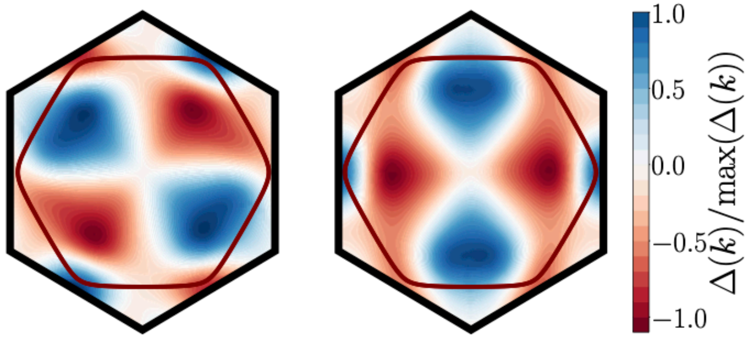


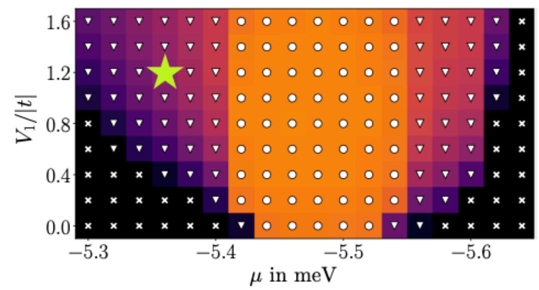


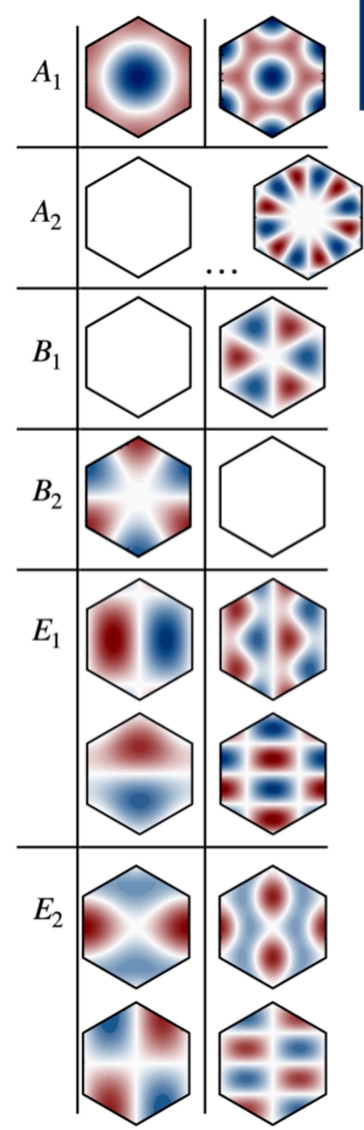
Gneist, Classen, MS (2022)

Pairing instability and symmetry

- SC gap $\Delta(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} \Phi^P(\boldsymbol{k},\boldsymbol{k}') \frac{\Delta(\boldsymbol{k}')}{2\xi_{\boldsymbol{k}'}} \tanh\left(\frac{\xi_{\boldsymbol{k}'}}{2T_c}\right)$







  - fitted well by 2nd-nn lattice harmonics $g_1(\mathbf{k}), g_2(\mathbf{k})$ of 2D irrep E_2
  - same symmetry properties under C_{6v} as 1st-nn E_2
  - can we distinguish d_1, d_2 vs. g_1, g_2 if symmetries are the same? ...

Gneist, Classen, MS (2022)

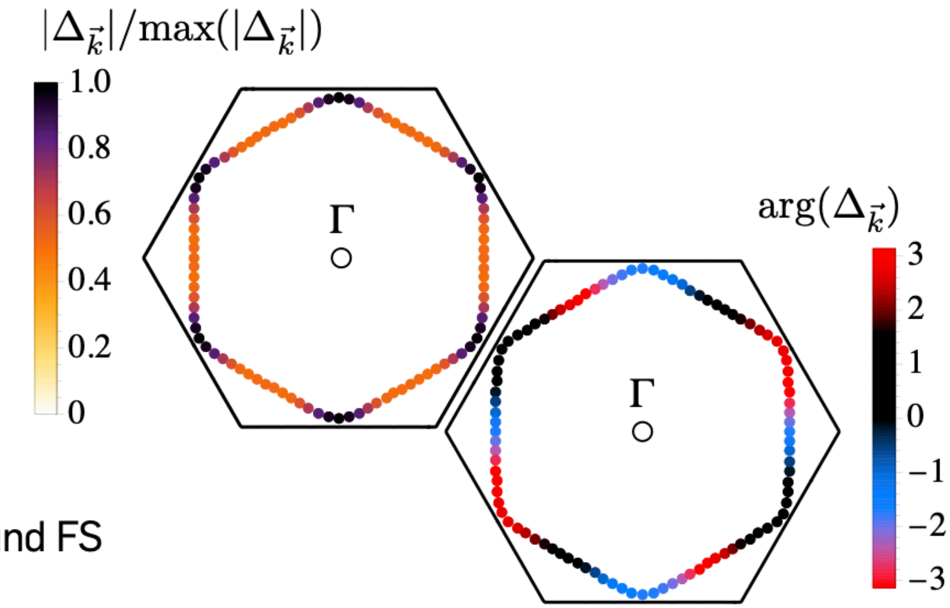
Properties of SC phase

- 2 degenerate pairing solutions $\rightarrow$ $\Delta(\vec{k}) = \Delta_1 \, g_1(\vec{k}) + \Delta_2 \, g_2(\vec{k})$
  - ground state is generally a linear combination
  - minimize Landau functional $\mathscr{L} = \alpha(|\Delta_1|^2 + |\Delta_2|^2) + \beta(|\Delta_1|^2 + |\Delta_2|^2)^2 + \gamma|\Delta_1^2 + \Delta_2^2|^2$
  - get α, β, γ by integrating out fermions with FRG data

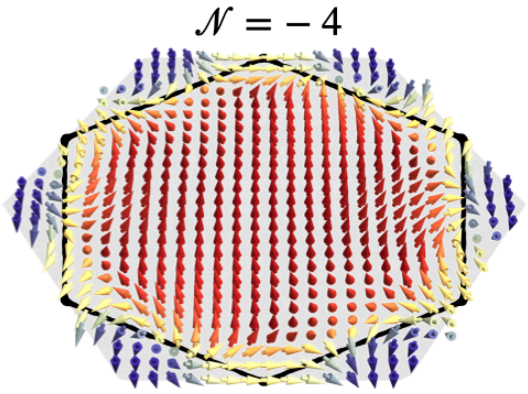
    $\Rightarrow \gamma > 0$

    $\Rightarrow$ $\Delta_2 = \pm i\Delta_1$ **minimizes $\mathscr{L}$**

    $\Rightarrow \Delta(\vec{k}) = \hat{\Delta}\,[g_1(\vec{k}) \pm i g_2(\vec{k})]$
  - $|\Delta(\vec{k})|$ has no nodes & arg $\Delta(\vec{k})$ winds 4 times around FS



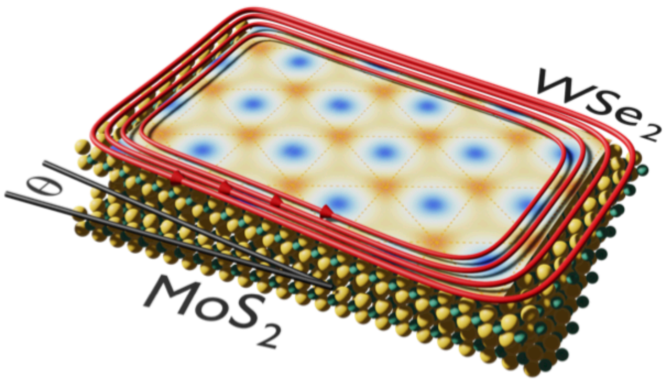
Properties of SC phase



- spont. breaking of TRS: $g_1 + ig_2$ vs. $g_1 - ig_2$
  - define "pseudo-spin" $\vec{m} = \frac{1}{\sqrt{(\epsilon_{\vec{k}} - \mu)^2 + \Delta_{\vec{k}}^2}} \begin{pmatrix} \mathrm{Re}\Delta_{\vec{k}} \\ \mathrm{Im}\Delta_{\vec{k}} \\ \epsilon_{\vec{k}} - \mu \end{pmatrix}$
  - topological invariant → winding number $\mathcal{N} = \frac{1}{4\pi} \int_{\mathrm{BZ}} d^2k\, \vec{m} \cdot \left(\frac{\partial \vec{m}}{\partial k_x} \times \frac{\partial \vec{m}}{\partial k_y} \right)$
  - *g+ig*: $\mathcal{N} = \pm 4$
  - *d+id*: $\mathcal{N} = \pm 2$

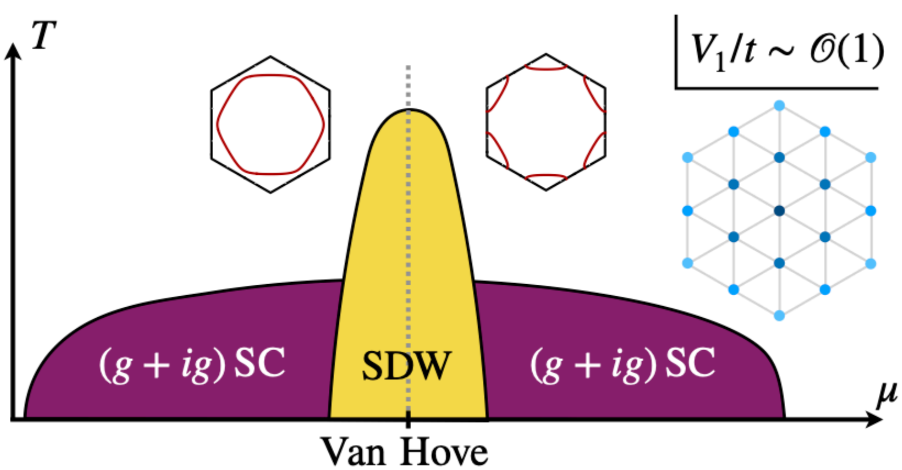
  } same symmetries under C_{6v} but different topological states!

- $\mathcal{N}$ chiral edge modes → **enhanced quantized Hall responses**
  - spin Hall conductance $\sigma_{xy}^s = \mathcal{N}\hbar/(8\pi)$
  - thermal Hall conductance $\kappa = \mathcal{N}\pi k_B^2/(6\hbar)$



Summary

- simulate **extended Hubbard model on triangular lattice** w/ moiré TMDs
- non-local Coulomb interactions are relevant
- Van-Hove filling accessible (and all other fillings)
- resolve competing orders with electron FRG
  - **chiral (g+ig)-wave superconductivity in extended parameter region**
    - breaks time-reversal
    - topological with Chern number $|\mathcal{N}| = 4$
    - enhanced quantized Hall responses



MS, Kennes, Classen, *accepted in* npj Quantum Materials, arxiv:2108.11406

Gneist, Classen, MS, *accepted in* PRB, arxiv:2203.01226