Moments and Multiplets in Moiré materials

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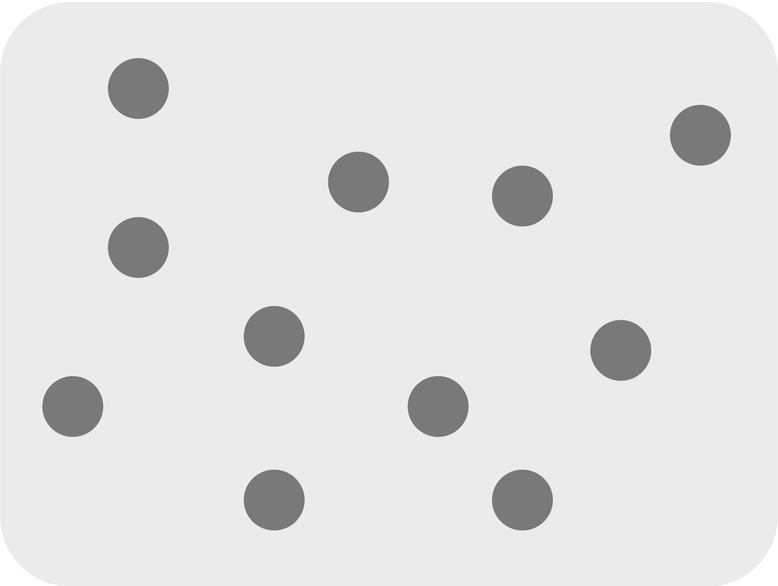
CRC 1238 Control and Dynamics of Quantum Materials

SU(N) physics in condensed matter and cold atoms
virtual, May 2022

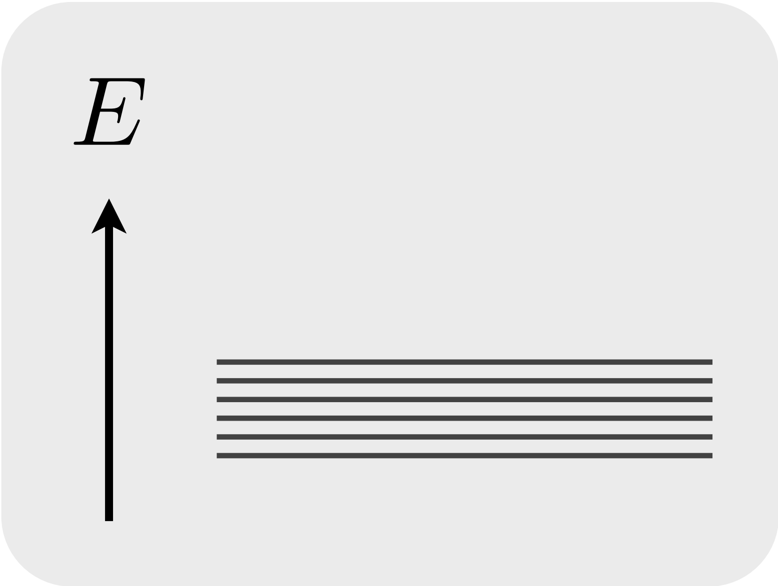
CRC 183 ENTANGLED STATES OF MATTER

When do interesting things happen?

Some of the most intriguing phenomena in condensed matter physics arise from the splitting of **‘accidental’ degeneracies**.



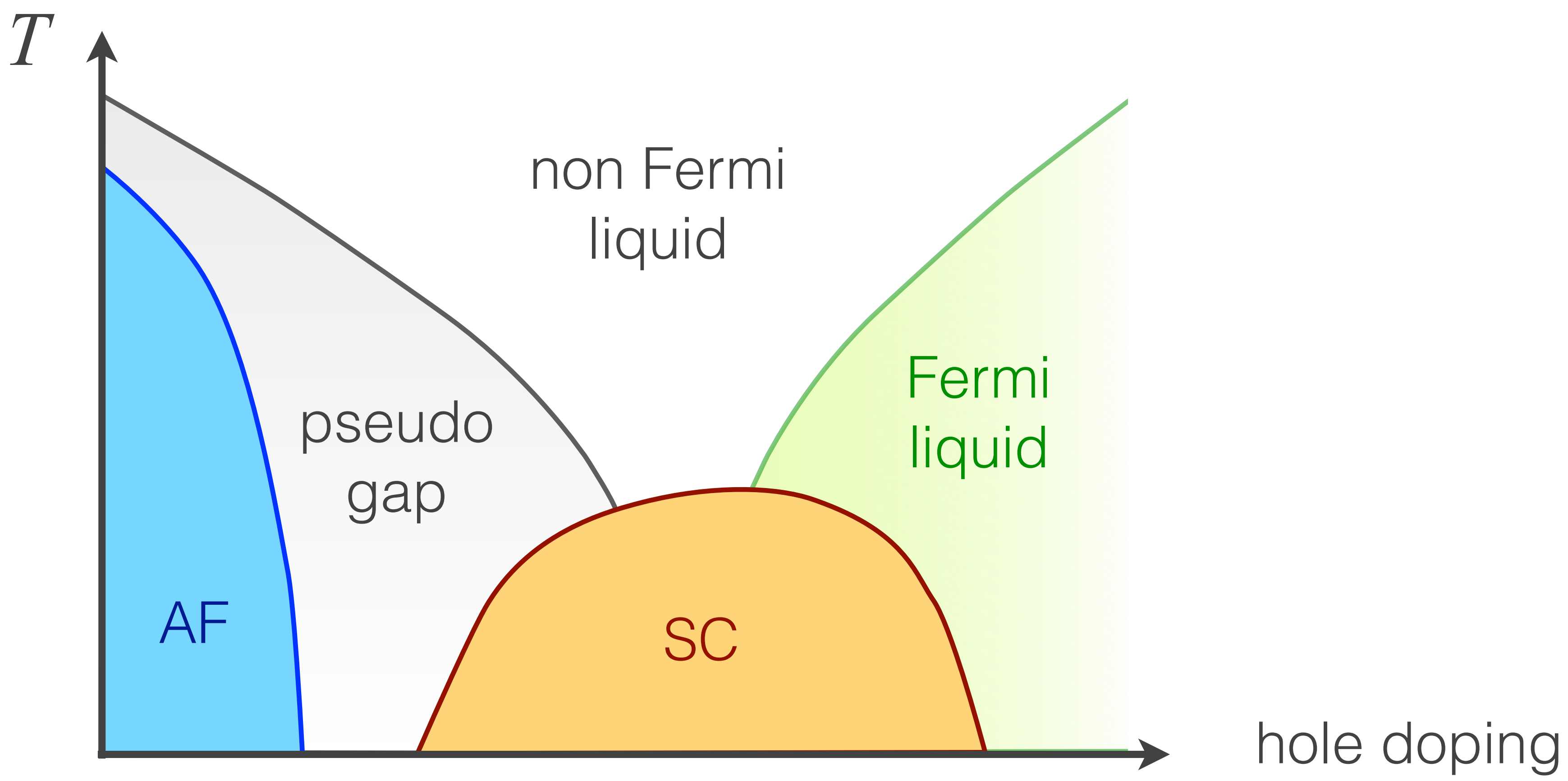
interacting
many-body system



‘accidental’
degeneracy

residual effects
select ground state

phase diagram of
cuprate superconductors



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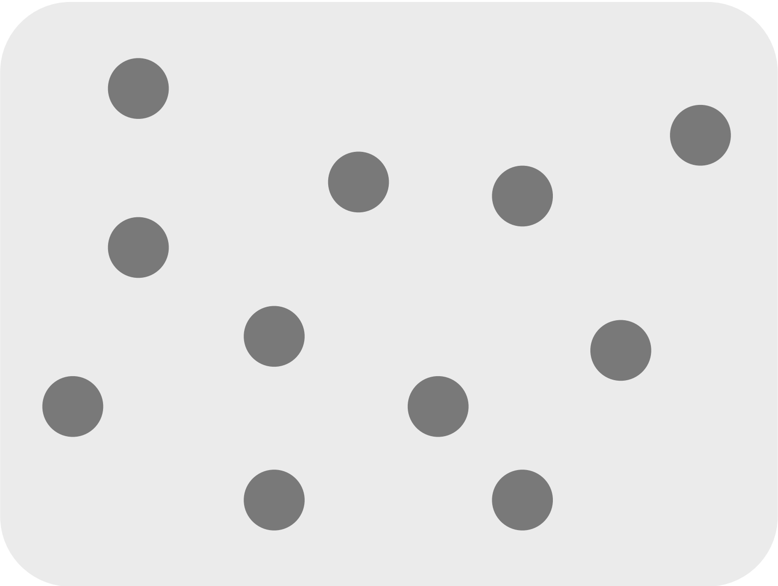

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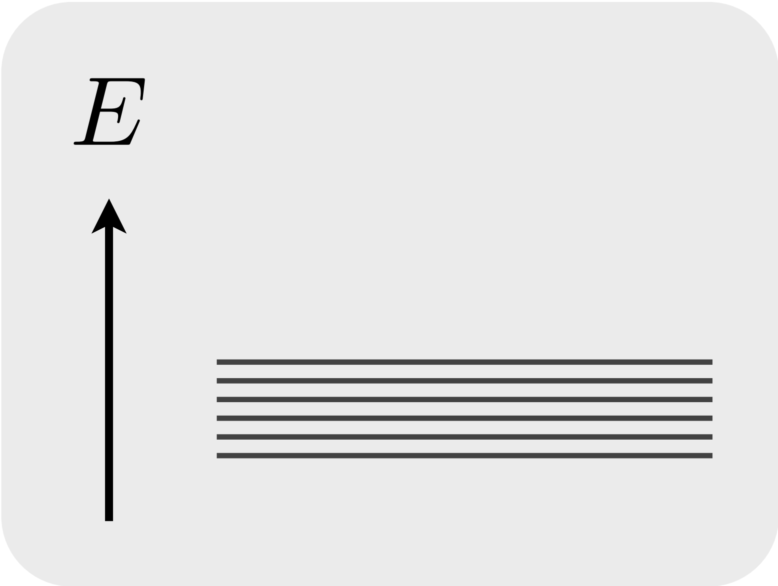

‘accidental’
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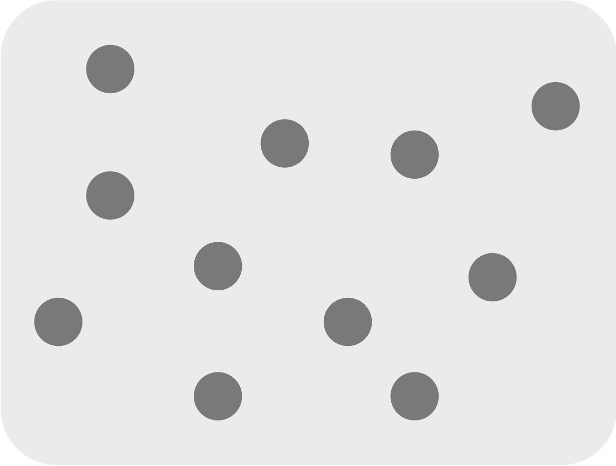
residual effects
select ground state

But they are also **notoriously difficult** to handle, due to

- multiple energy scales
- complex energy landscapes / slow equilibration
- strong coupling
- macroscopic entanglement

Example – frustrated magnetism



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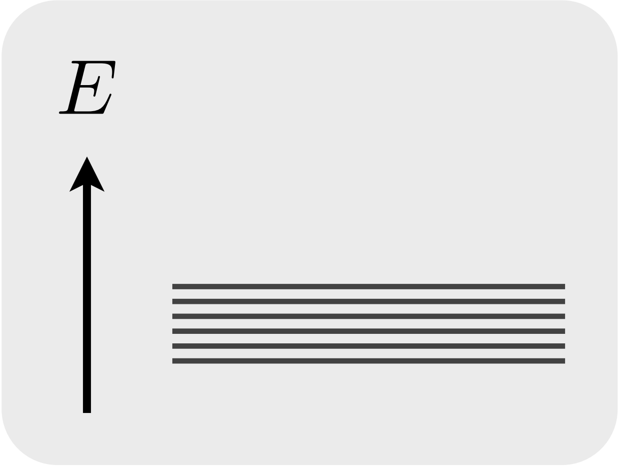

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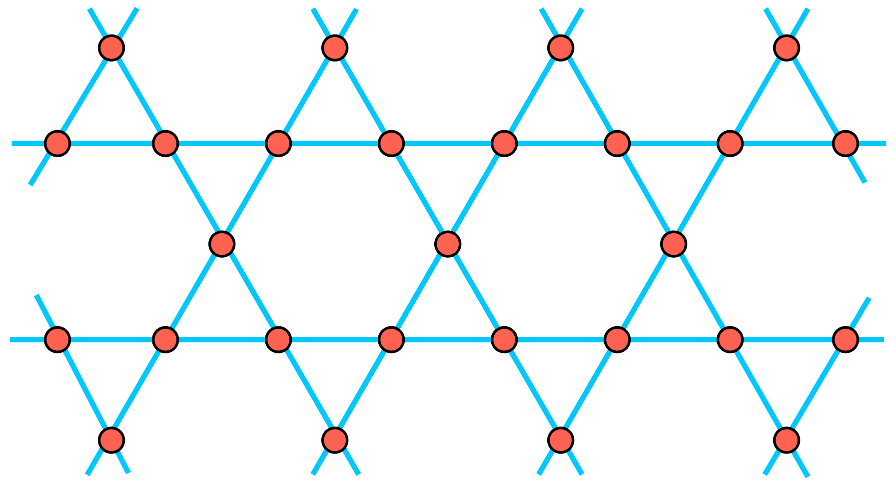
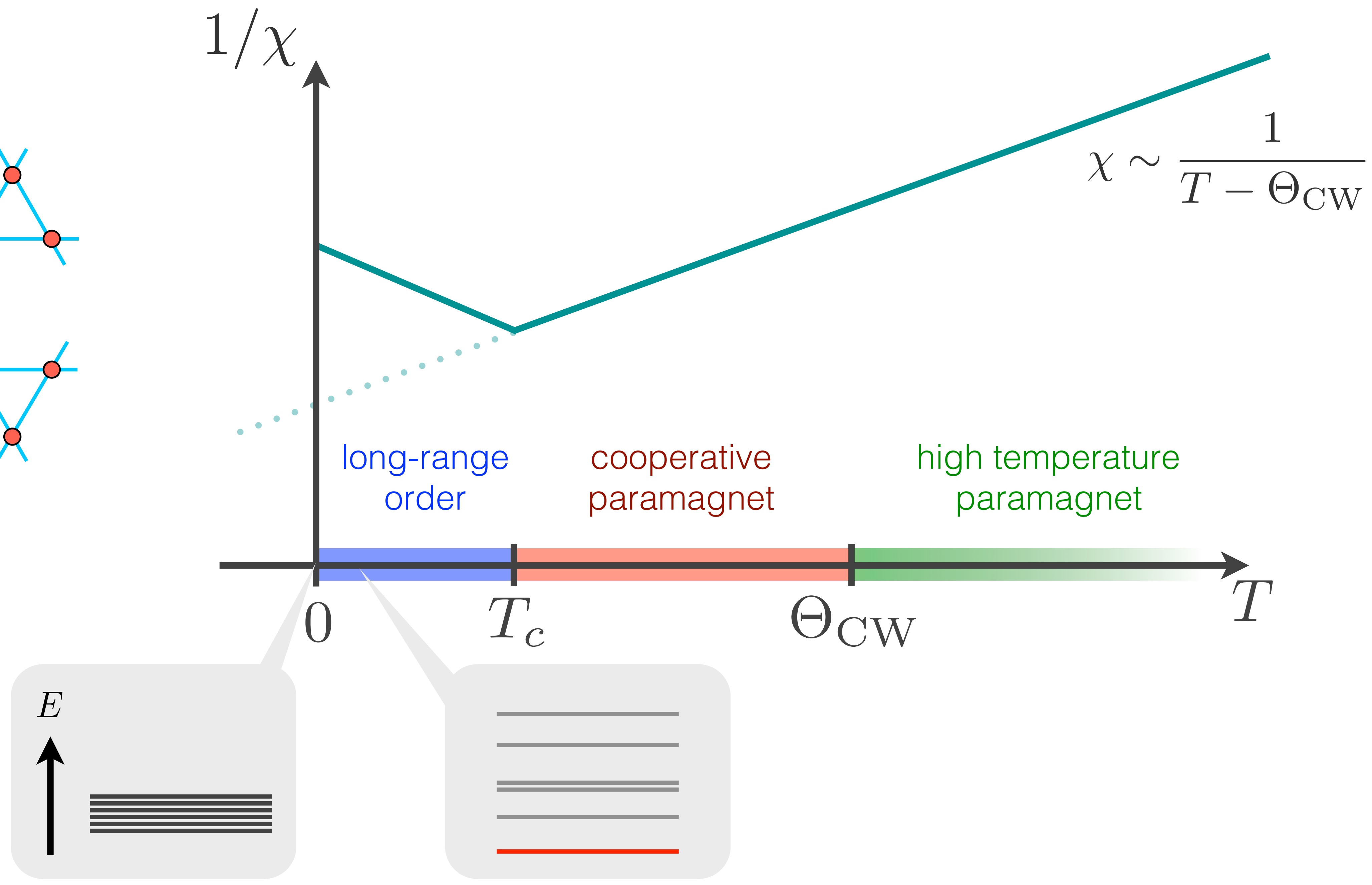
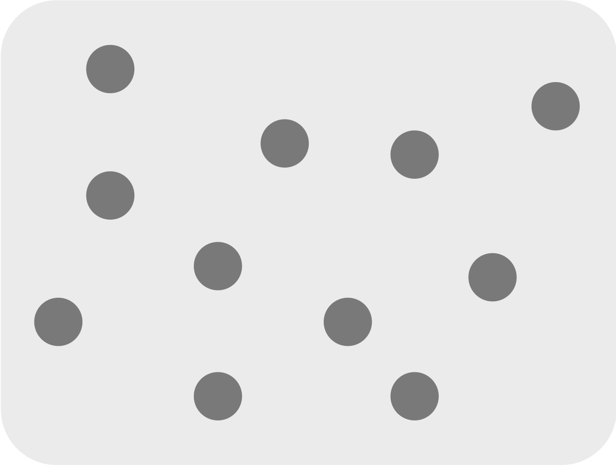




T=0 residual entropy

long-range order

Example – quantum Hall liquids



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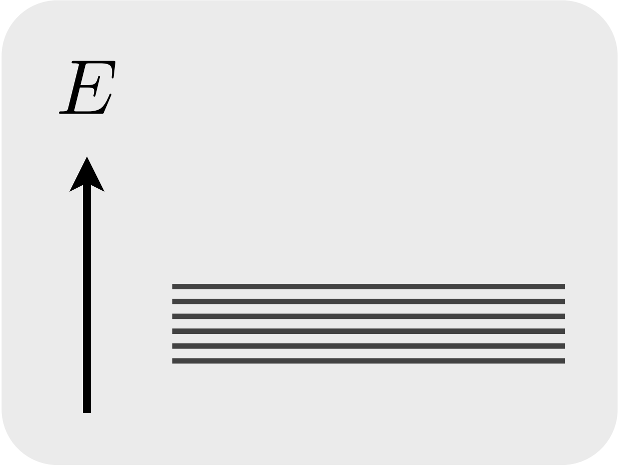
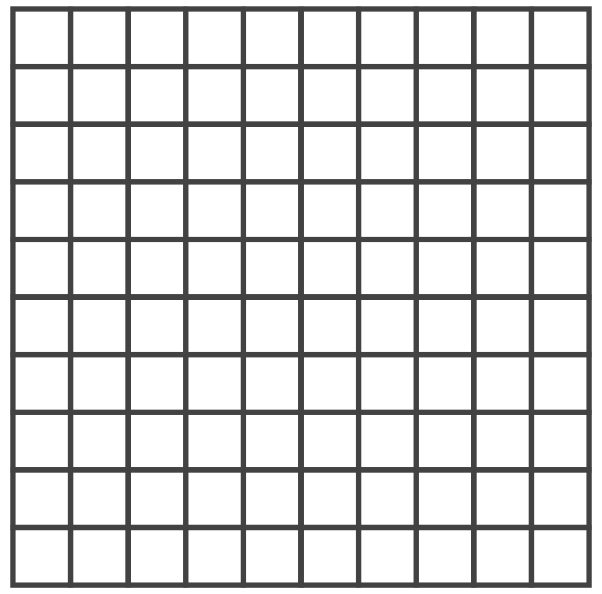


'accidental'
degeneracy

residual effects
select ground state

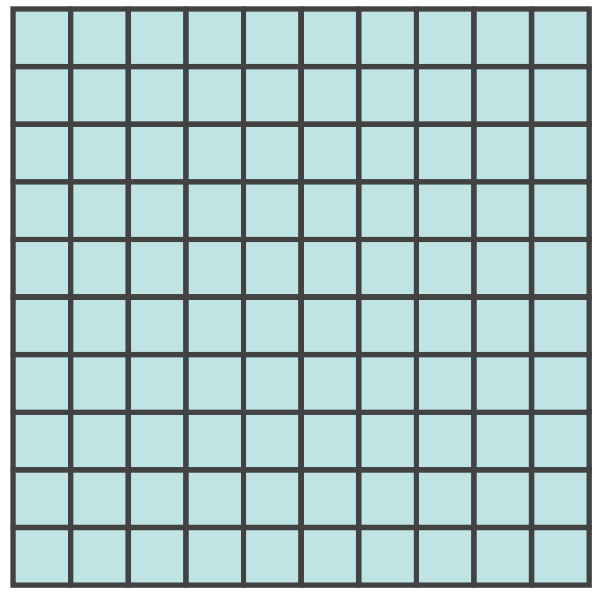
Landau level **degeneracy**



$$2\Phi/\Phi_0$$

orbital states

integer quantum Hall

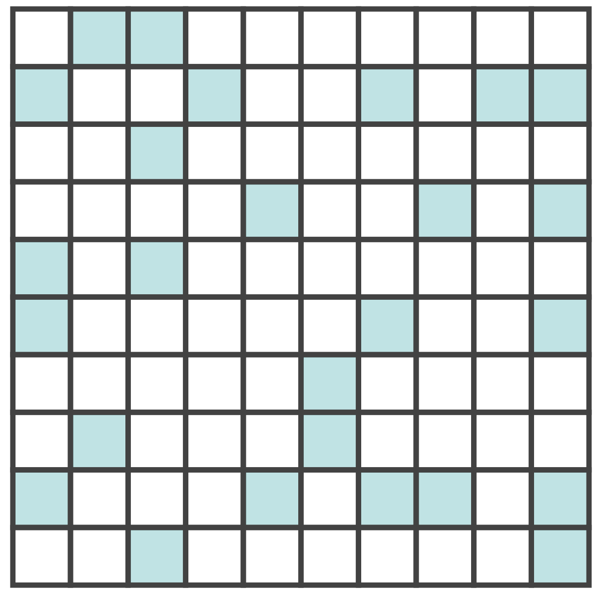


filled level

↓

incompressible liquid

fractional quantum Hall

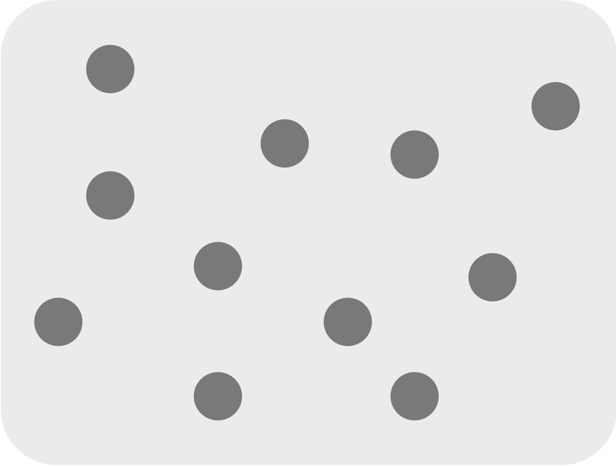


partially filled level

↓ Coulomb repulsion

incompressible liquid

Example – twisted bilayer graphene



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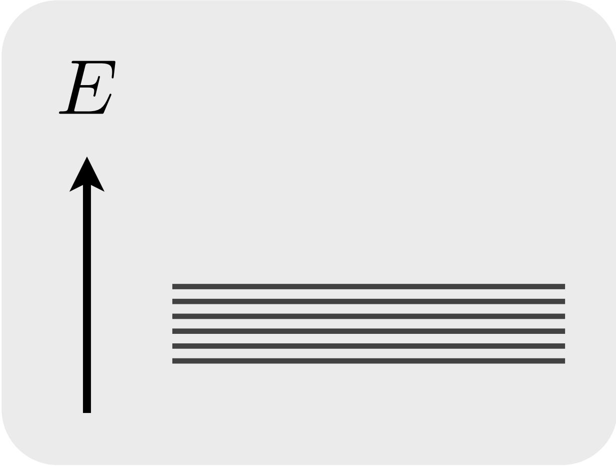

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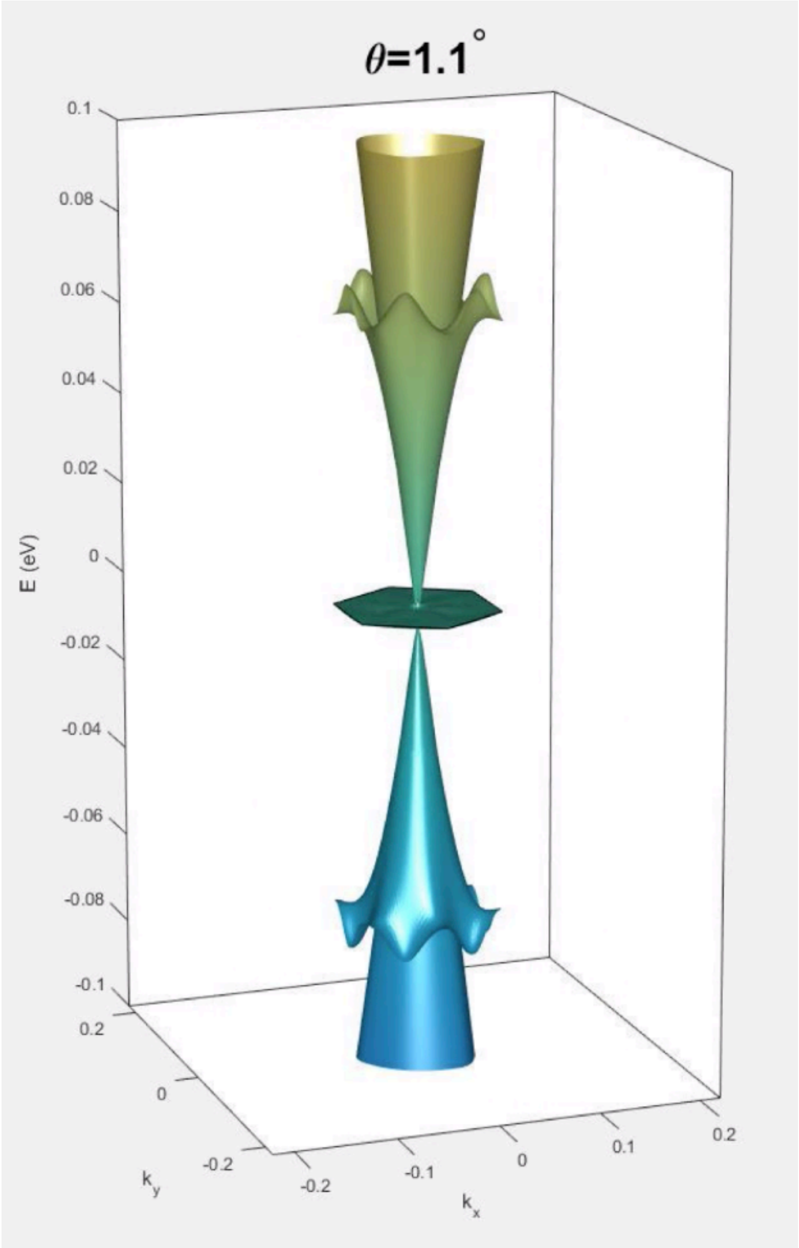
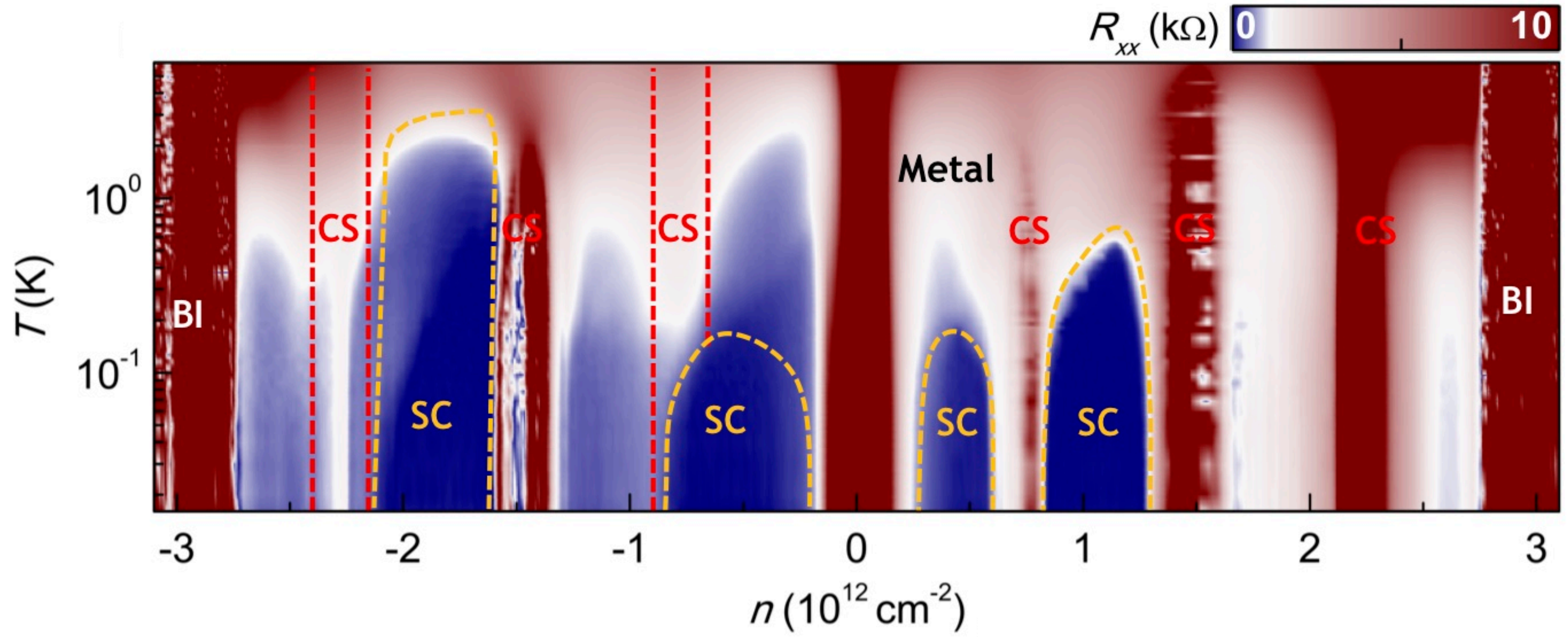


electronic band structure with a **flat band** in twisted bilayer graphene



Efetov group, Nature **574**, 653 (2019)

Jarillo-Herrero group, Nature **556**, 43 (April 2018)

meet the team

Lasse Gresista

Dominik Kiese

Ciarán Hickey

Michael Scherer

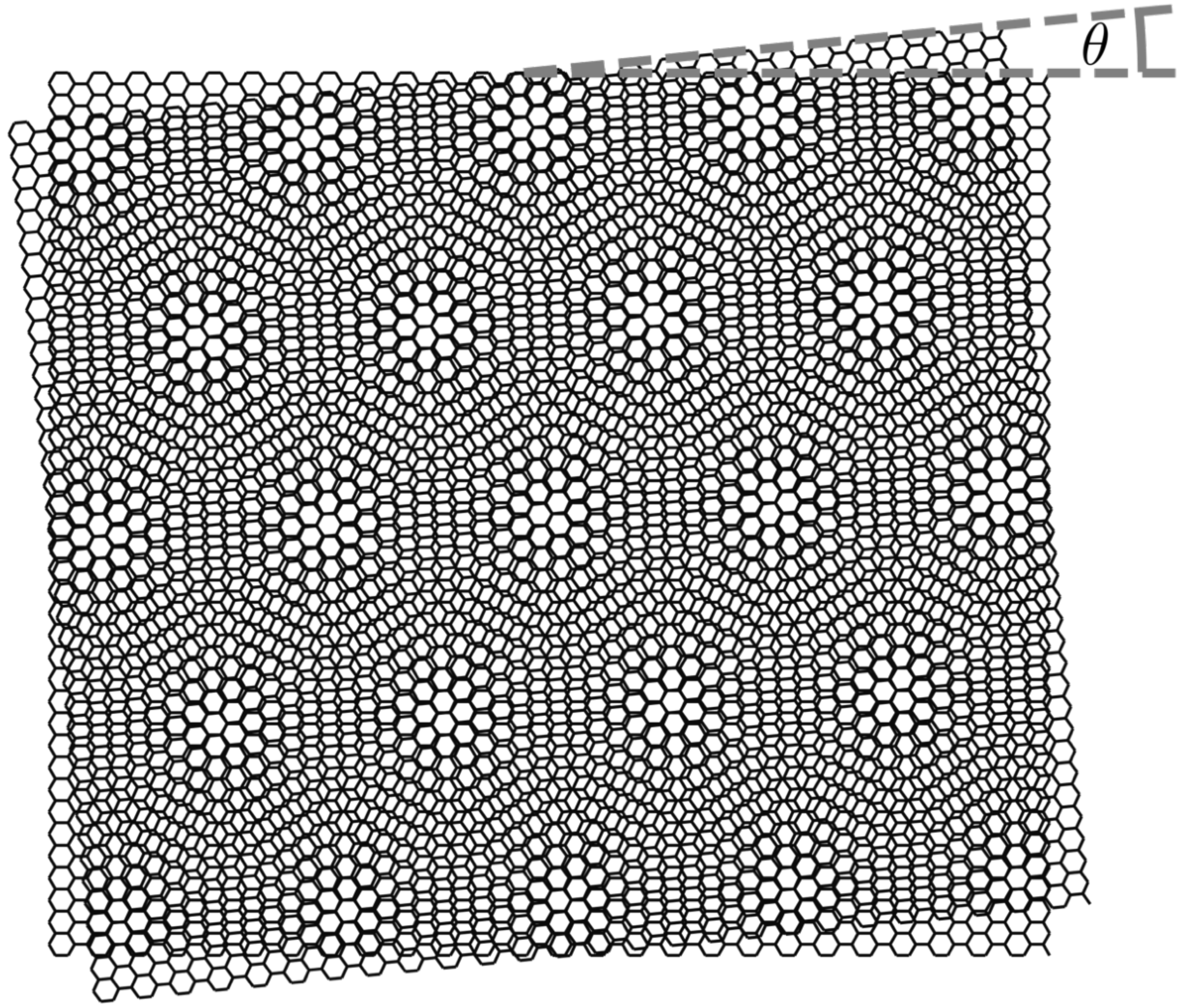
arXiv:2202.05029

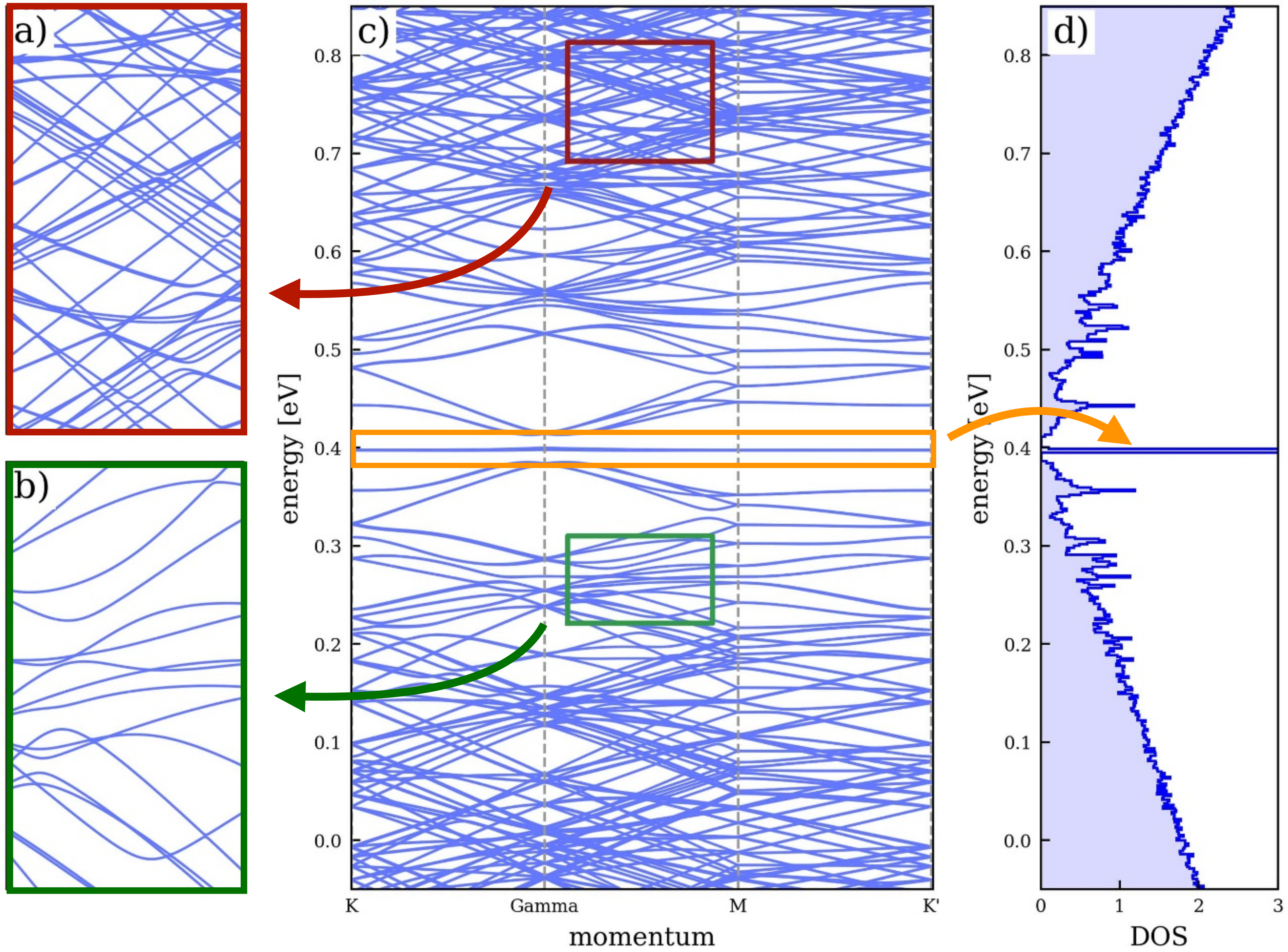
Phys. Rev. Research **2**, 013370 (2020).

moments & multiplets

spin-valley models

hexagonal moiré superlattice



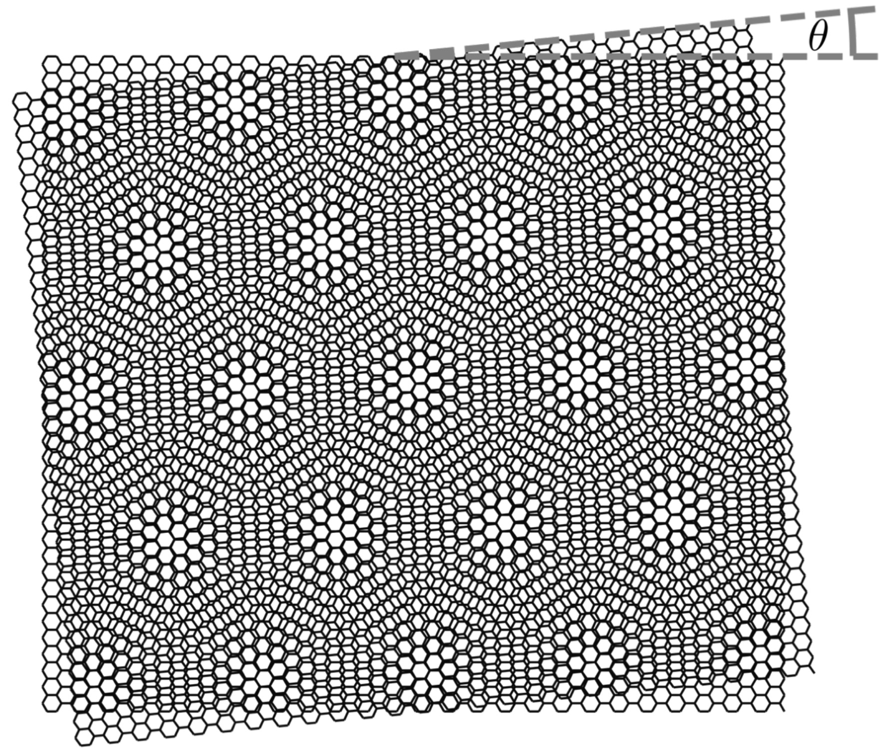


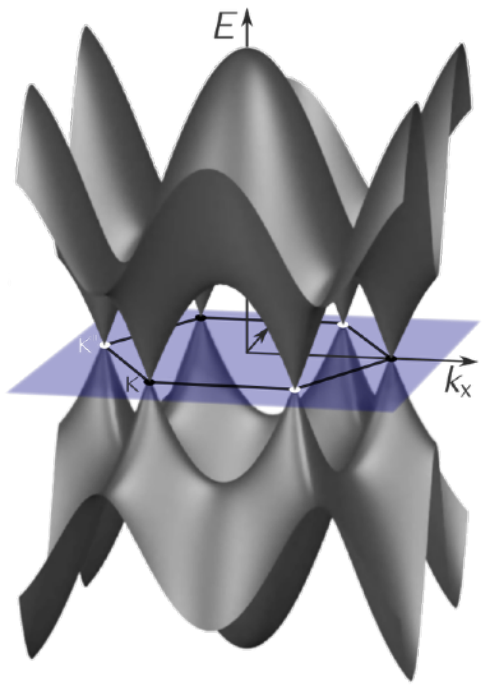
Universal principles of moiré band structures
J. Attig *et al.*, 2D Materials **8**, 044007 (2021)

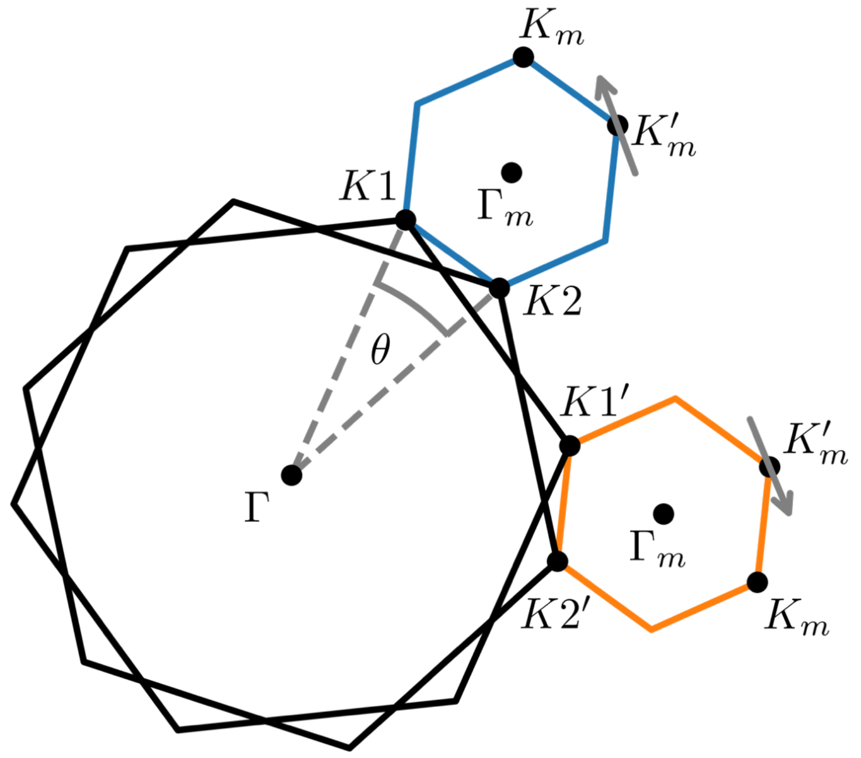
spin-valley models

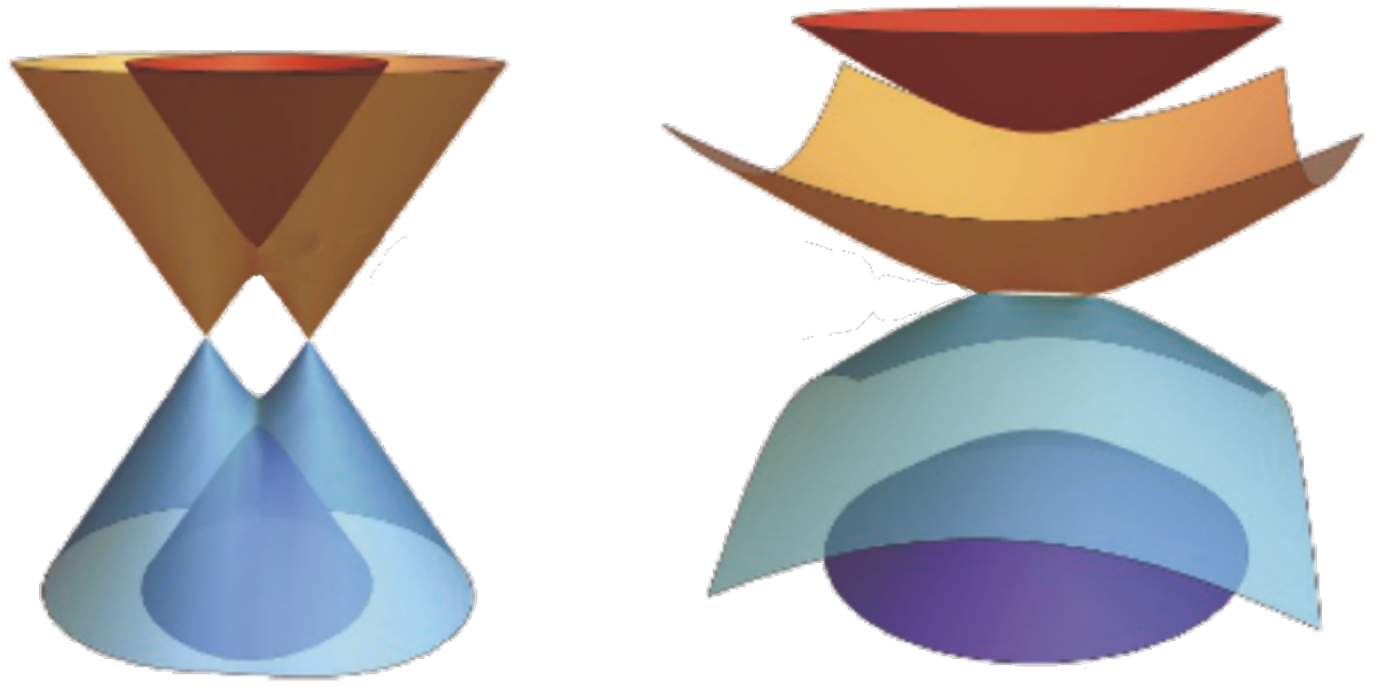
Phys. Rev. Research **2**, 013370 (2020).

hexagonal moiré superlattice | interlayer hybridization at K and K' points (valleys) | electronic correlations









Y. Cao, V. Fatemi, A. Demir et al., Nature **556**, 80 (2018).

$$U, J_\mathrm{H}$$

→ Hubbard model with spin and valley d.o.f. on Moiré super lattice $\xrightarrow{U \gg t}$ spin-valley model

quarter or half filling

$$\sum_{sl} f^\dagger_{isl} f_{isl} = 1,2$$

Example: Trilayer graphene on hexagonal boron nitride (TG/h-BN)

$$H = \frac{J_1}{8}\sum_{\langle ij\rangle}(1+\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)(1+\boldsymbol{\tau}_i\boldsymbol{\tau}_j) + \frac{1}{8}\sum_{\langle ij\rangle} J^1_{p;ij}(1+\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)(\tau^x_i\tau^x_j + \tau^y_i\tau^y_j)$$

$$+\frac{J_2}{8}\sum_{\langle\langle ij\rangle\rangle}(1+\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)(1+\boldsymbol{\tau}_i\boldsymbol{\tau}_j) + \frac{1}{8}\sum_{\langle ij\rangle} J^2_{p;ij}(1+\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)(\tau^x_i\tau^y_j - \tau^y_i\tau^x_j) + O\left(\frac{t^3}{U^2}\right)$$

SU(4) symmetric → (first column of terms)

$\mathrm{SU}(2)_\mathrm{spin} \otimes \mathrm{U}(1)_\mathrm{valley}$ symmetric → (second column of terms)

Y. Zhang and T. Senthil
Phys. Rev. B **99**, 205150 (2019)

spin-valley models

arXiv:2202.05029

SU(2) symmetric Heisenberg model $H = J \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j$ $\mathbf{S} = (S^x, S^y, S^z)$ $[S_i^a, S_j^b] = i\epsilon^{abc} S^c$ $\mathfrak{su}(2)$ Lie algebra

SU(4) symmetric Heisenberg model $H = J \sum_{\langle ij \rangle} \mathbf{T}_i \mathbf{T}_j$ $\mathbf{T} = (T^1, \ldots T^{15})$ $[T_i^a, T_j^b] = i f^{abc} T^c$ $\mathfrak{su}(4)$ Lie algebra

SU(4) spin-valley model

$$H = \frac{J}{8} \sum_{\langle ij \rangle} (1 + \boldsymbol{\sigma}_i \boldsymbol{\sigma}_j)(1 + \boldsymbol{\tau}_i \boldsymbol{\tau}_j)$$

spin $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$

valley $\boldsymbol{\tau} = (\tau^x, \tau^y, \tau^z)$

Represent $\mathfrak{su}(4)$ by "coupled $\mathfrak{su}(2)$ degrees of freedom"

General **spin-valley Hamiltonian** with symmetry-breaking terms (e.g. Hund's coupling, …)

$$H = \frac{1}{8} \sum_{ij} (\sigma_i^\mu J_{s,ij}^{\mu\nu} \sigma_j^\nu)(\tau_i^\kappa J_{v,ij}^{\kappa\lambda} \tau_j^\lambda) = \frac{1}{8} \sum_{ij} (\sigma_i^\mu \otimes \tau_i^\kappa)\ (J_{s,ij}^{\mu\nu} \otimes J_{v,ij}^{\kappa\lambda})\ (\sigma_j^\nu \otimes \tau_j^\lambda)$$

spin-valley models

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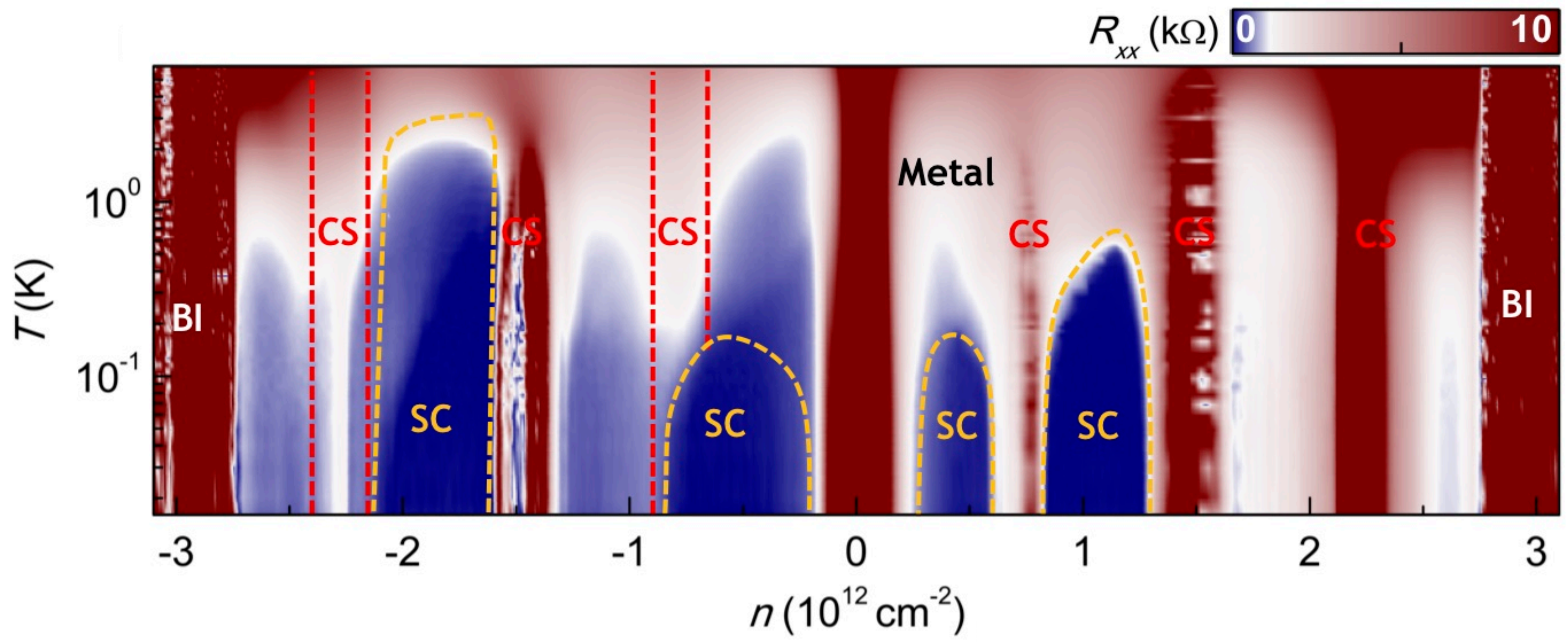
spin-valley operators

$$\sigma_i^\mu \tau_i^\kappa \equiv \sigma_i^\mu \otimes \tau_i^\kappa = f_{isl}^\dagger \theta_{ss'}^\mu \theta_{ll'}^\kappa f_{is'l'}$$

$$\sigma_i^\mu \equiv \sigma_i^\mu \otimes \tau_i^0 = f_{isl}^\dagger \theta_{ss'}^\mu f_{is'l}$$

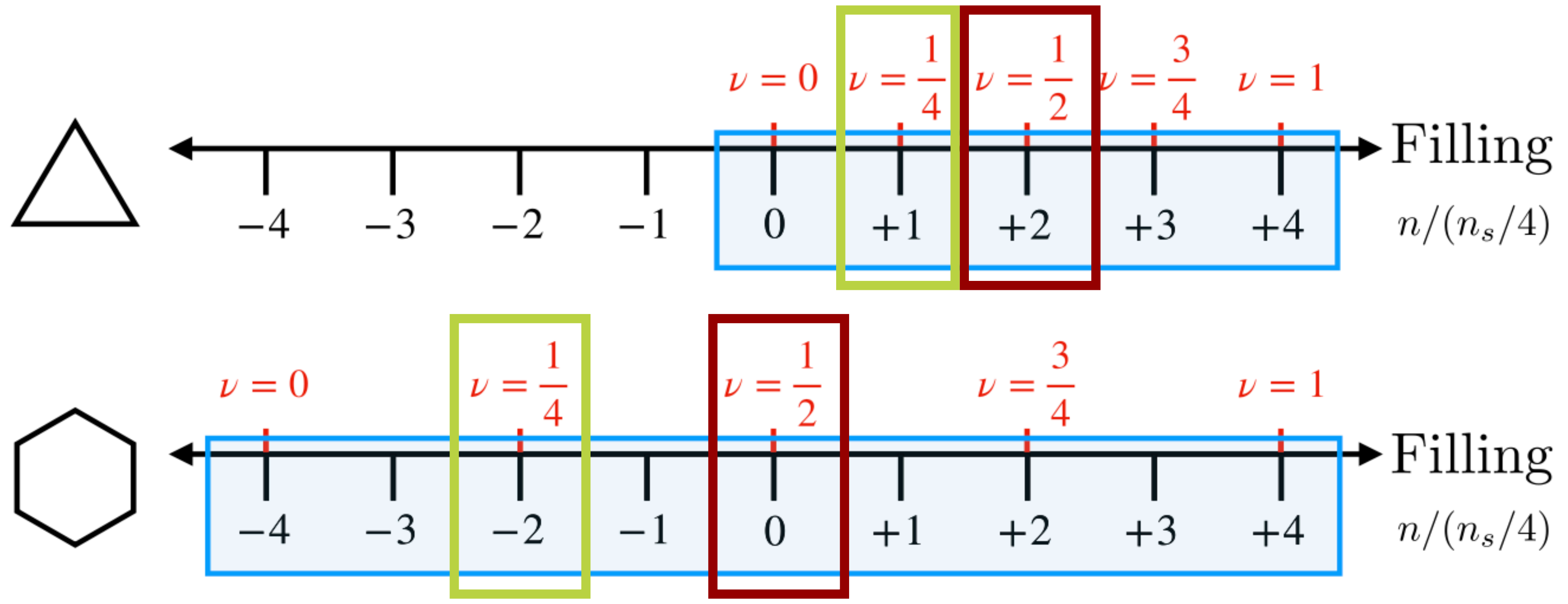
$$\tau_i^\kappa \equiv \sigma_i^0 \otimes \tau_i^\kappa = f_{isl}^\dagger \theta_{ll'}^\kappa f_{isl'}$$



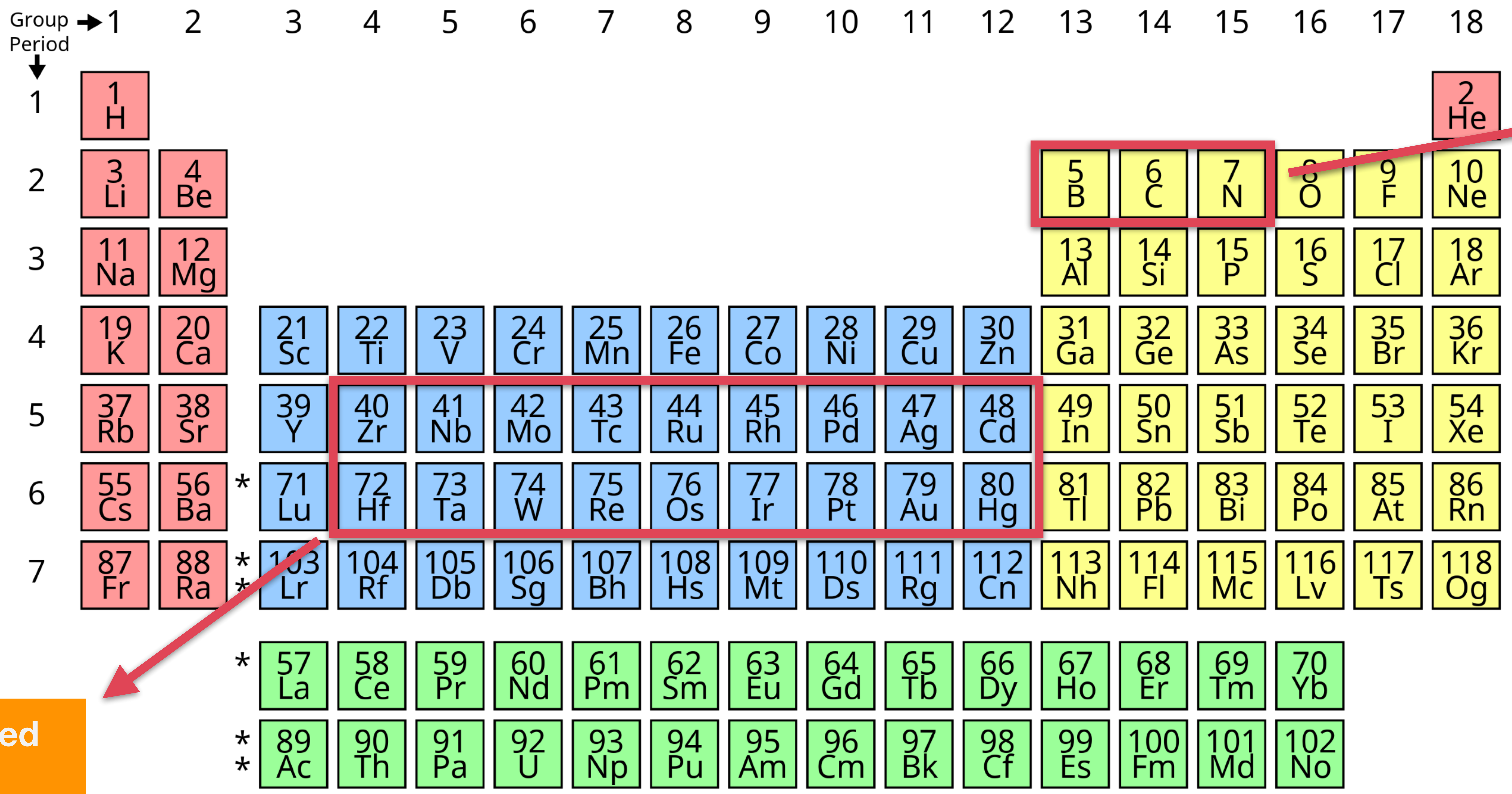
Efetov group, Nature **574**, 653 (2019)

representation fixed by filling

filling	dimensionality	representation
$\sum_{sl} f_{isl}^\dagger f_{isl} = 2$	4 choose 2 = 6	self-conjugate
$\sum_{sl} f_{isl}^\dagger f_{isl} = 1$	4 choose 1= 4	fundamental



spin-valley models



Moiré materials
TBG, TG/h-BN
“spin-valley models”

Spin-orbit entangled Mott insulators
4d and 5d transition metals (Ir, Ru, Zr)
“spin-orbital models”
“Kugel Khomskii model”

spin-valley models

- additional degrees of freedom → **enhanced quantum fluctuations**
- geometric and/or exchange **frustration**

→ suppression of magnetic order → candidates for quantum spin-valley liquid (QSVL) ground states

quantum spin-valley liquids

- no magnetic order even at $T = 0$
- long-range entanglement
- fractional excitations (e.g. Majorana fermions in the Kitaev model)

Goal: Determine ground state spin-valley order (FM/AFM/…) or its absence.

pseudo-fermion FRG

Reuther & Wölfle (2010)

pseudo-fermion FRG

arXiv:2202.05029

general concept

partition function

$$Z = \int \mathcal{D}(\bar{\psi}, \psi) e^{-S}$$

introduce **infrared cutoff Λ**

exact rewriting

infinite hierarchy of differential equations
for one-particle irreducible vertex functions

$$\frac{d}{d\Lambda}\gamma_m^\Lambda = \mathcal{F}^\Lambda(\gamma_1, \gamma_2, \ldots, \gamma_{m+1})$$

flow equations

$\gamma_1(k_{1'}, k_1)$ self-energy

$\gamma_2(k_{1'}, k_{2'}, k_1, k_2)$ two-particle vertex

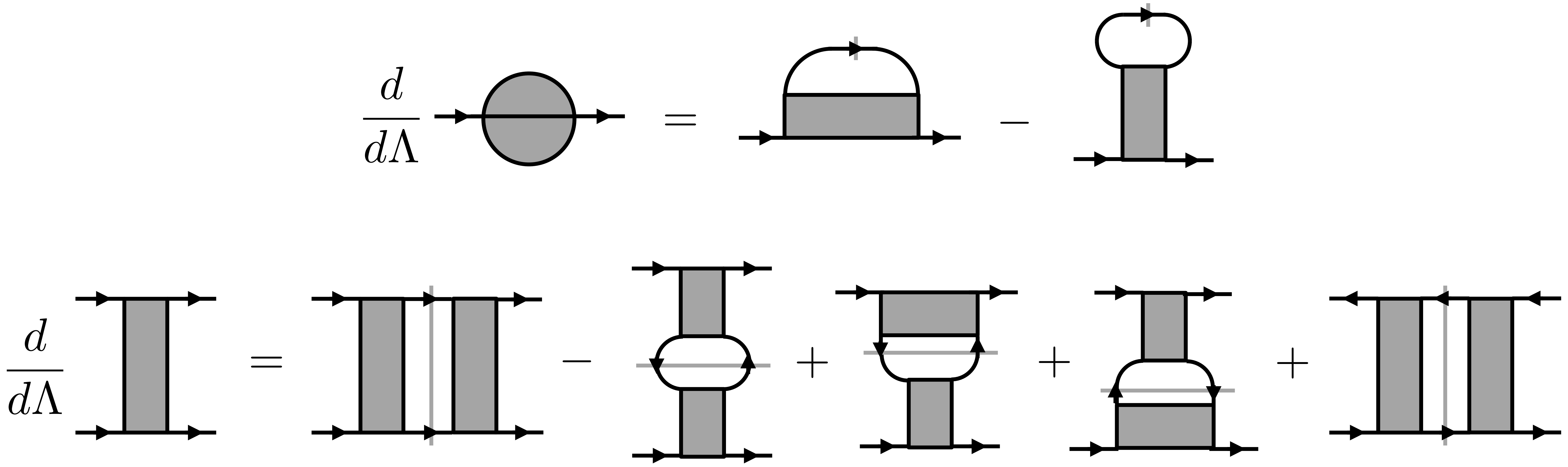
~~3-particle vertex~~

Katanin or multiloop

building blocks of the full correlation functions (tree expansion)

self-energy

two-particle vertex



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$$= \frac{1}{8} \sum_{ij} (\sigma_i^\mu \otimes \tau_i^\kappa) \; (J^{\mu\nu}_{s,ij} \otimes J^{\kappa\lambda}_{v,ij}) \; (\sigma_j^\nu \otimes \tau_j^\lambda)$$

pseudo-fermions

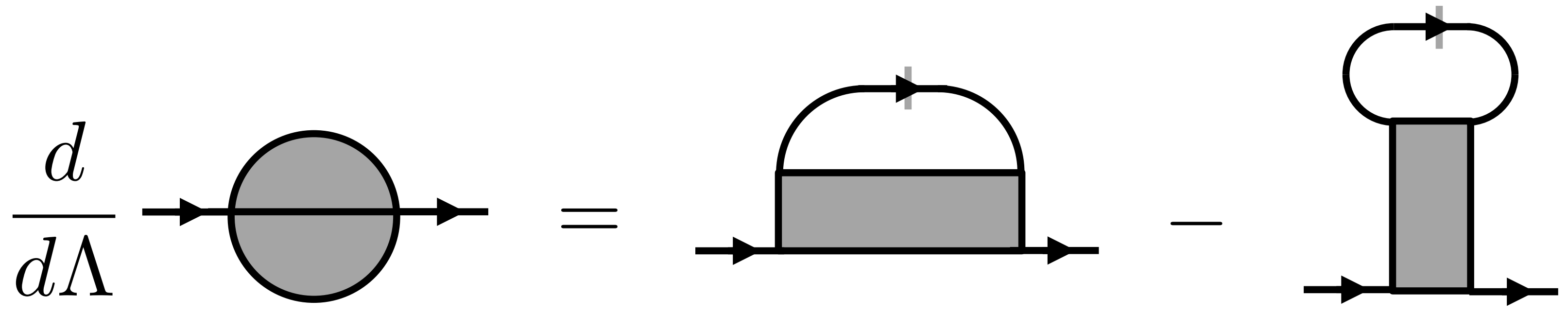
$$\sigma_i^\mu \tau_i^\kappa \equiv \sigma_i^\mu \otimes \tau_i^\kappa = f^\dagger_{isl} \theta^\mu_{ss'} \theta^\kappa_{ll'} f_{is'l'}$$

$$H = \frac{1}{8} \sum_{ij} J^{\mu\nu}_{s,ij} \theta^\mu_{s_1 s_1'} \theta^\nu_{s_2 s_2'} \; J^{\kappa\lambda}_{v,ij} \theta^\kappa_{l_1 l_1'} \theta^\lambda_{l_2 l_2'} \; f^\dagger_{is_1l_1} f^\dagger_{js_2l_2} f_{js_2'l_2'} f_{is_1'l_1'}$$

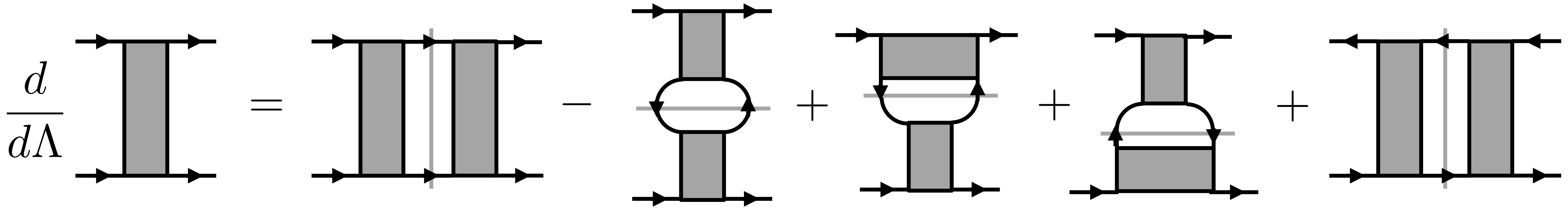
strongly coupled fermions
→ conventional FRG

+ half-filling constraint

self-energy



two-particle vertex



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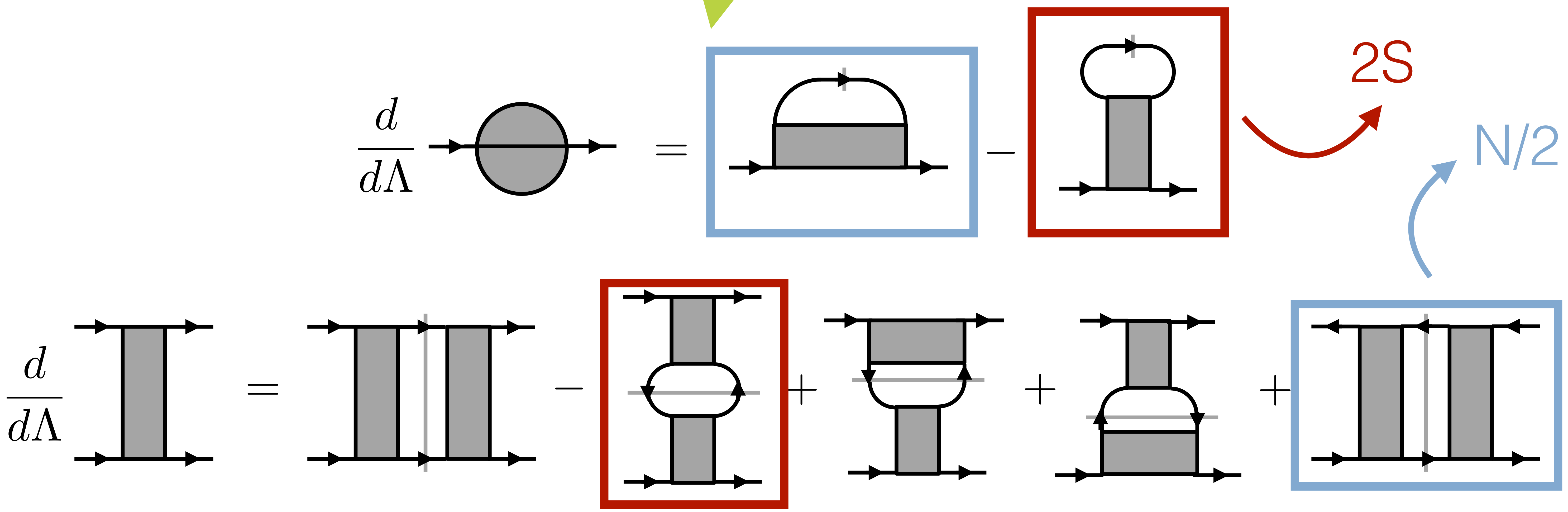
flow equations

$\gamma_1(k_{1'}, k_1)$	$\gamma_2(k_{1'}, k_{2'}, k_1, k_2)$	~~3-particle vertex~~	Katanin or multiloop
self-energy	two-particle vertex		

building blocks of the full correlation functions (tree expansion)

self-energy

two-particle vertex



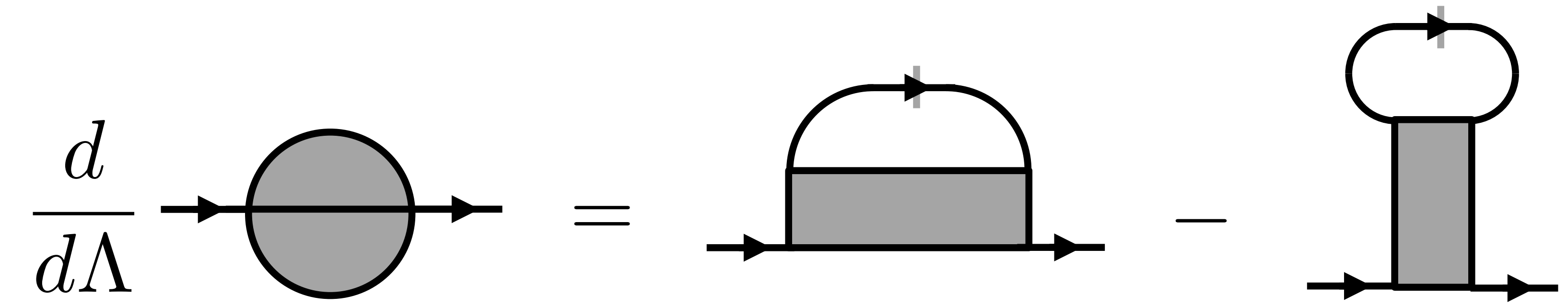
concurrent
1/S and 1/N
expansion

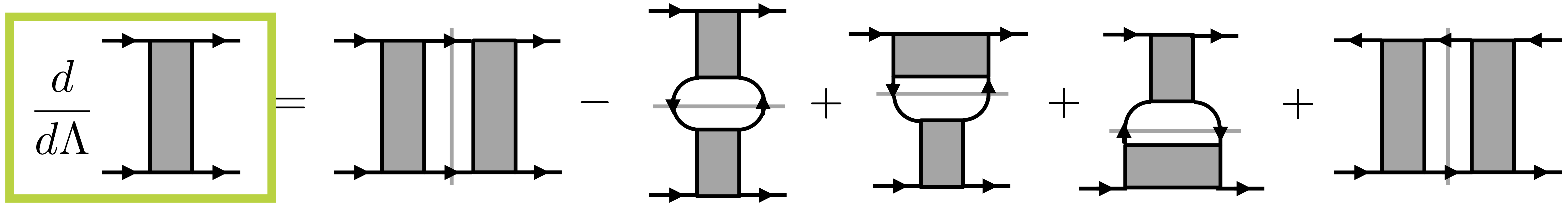
exact in the limits of
$S \to \infty$ and $N \to \infty$

pseudo-fermion FRG

arXiv:2202.05029

numerical solution





$(100 \cdot 4 \cdot 2 \cdot 2)^4 \approx 10^{16}$ vertex components

100 lattice sites, 40 frequencies, 2 spin/valley values

$\sim 10^7$ independent vertex components

using pseudo-fermion Hamiltonian **symmetries**

pf-FRG

PFFRGSolver.jl
official Julia package

Dominik Kiese,
Tobias Müller

arXiv:2011.01269

- adaptive Runge-Kutta algorithm (ODE solver)
- adaptive frequency grids and integration
- multilinear frequency interpolation
- asymptotic frequency parametrization

JUWELS HPC cluster
(Forschungszentrum Jülich)

pseudo-fermion FRG

spin-spin and valley-valley correlations and structure factors

spin-valley spin-valley correlations

$$\chi_{ij}^{\Lambda\mu\nu\kappa\lambda}(i\omega) = \int_0^\infty d\tau e^{i\omega\tau} \left\langle T_\tau \, (\sigma_i^\mu \otimes \tau_i^\kappa)(\tau) \, (\sigma_j^\nu \otimes \tau_j^\lambda)(0) \right\rangle^\Lambda$$

spin-spin correlations

$$\chi_{ij}^{\Lambda s,\mu\nu} \equiv \chi_{ij}^{\Lambda\mu\nu 00} \sim \left\langle \sigma_i^\mu \sigma_j^\nu \right\rangle^\Lambda$$

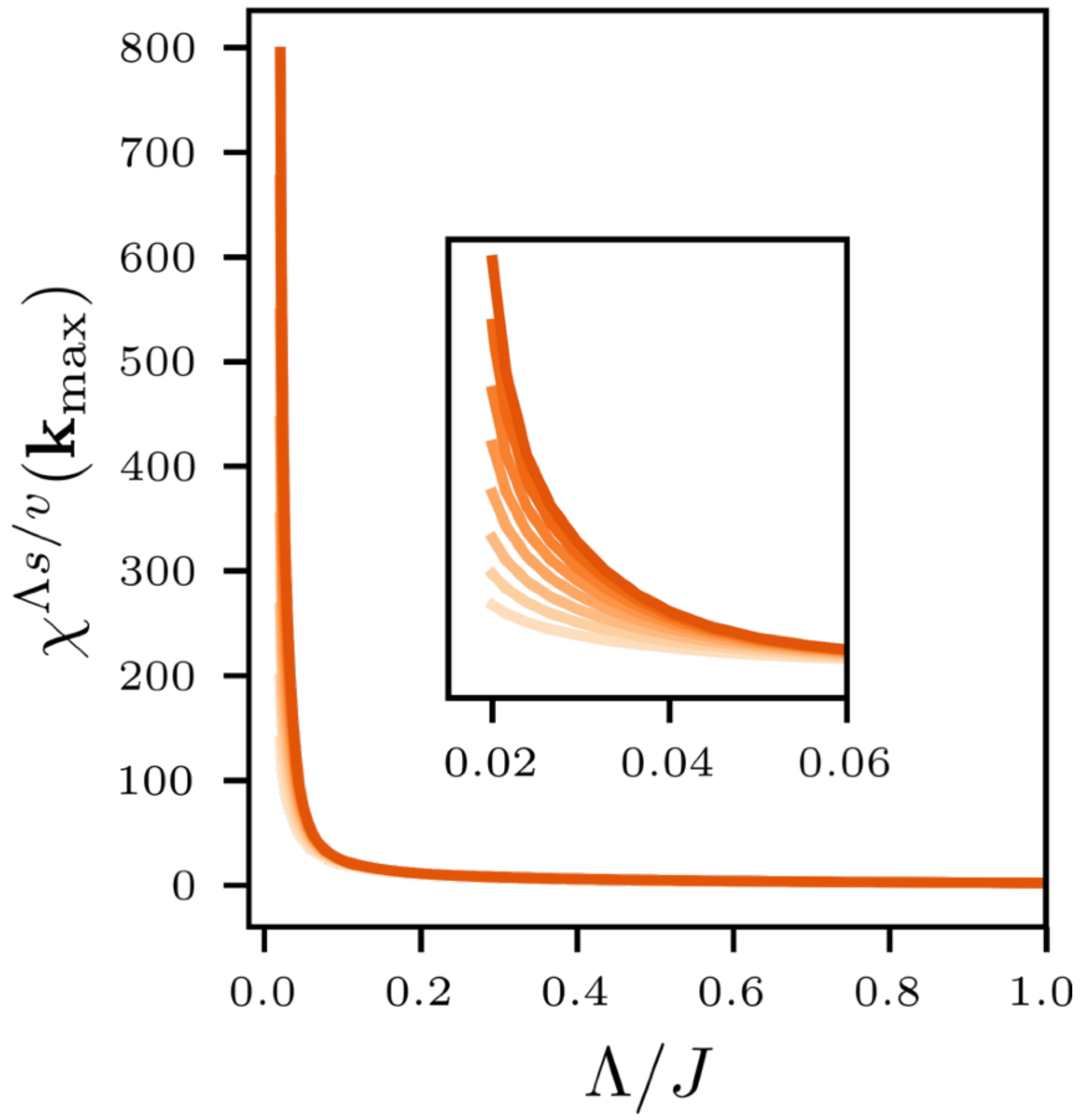
valley-valley correlations

$$\chi_{ij}^{\Lambda v,\kappa\lambda} \equiv \chi_{ij}^{\Lambda 00\kappa\lambda} \sim \left\langle \tau_i^\kappa \tau_j^\lambda \right\rangle^\Lambda$$

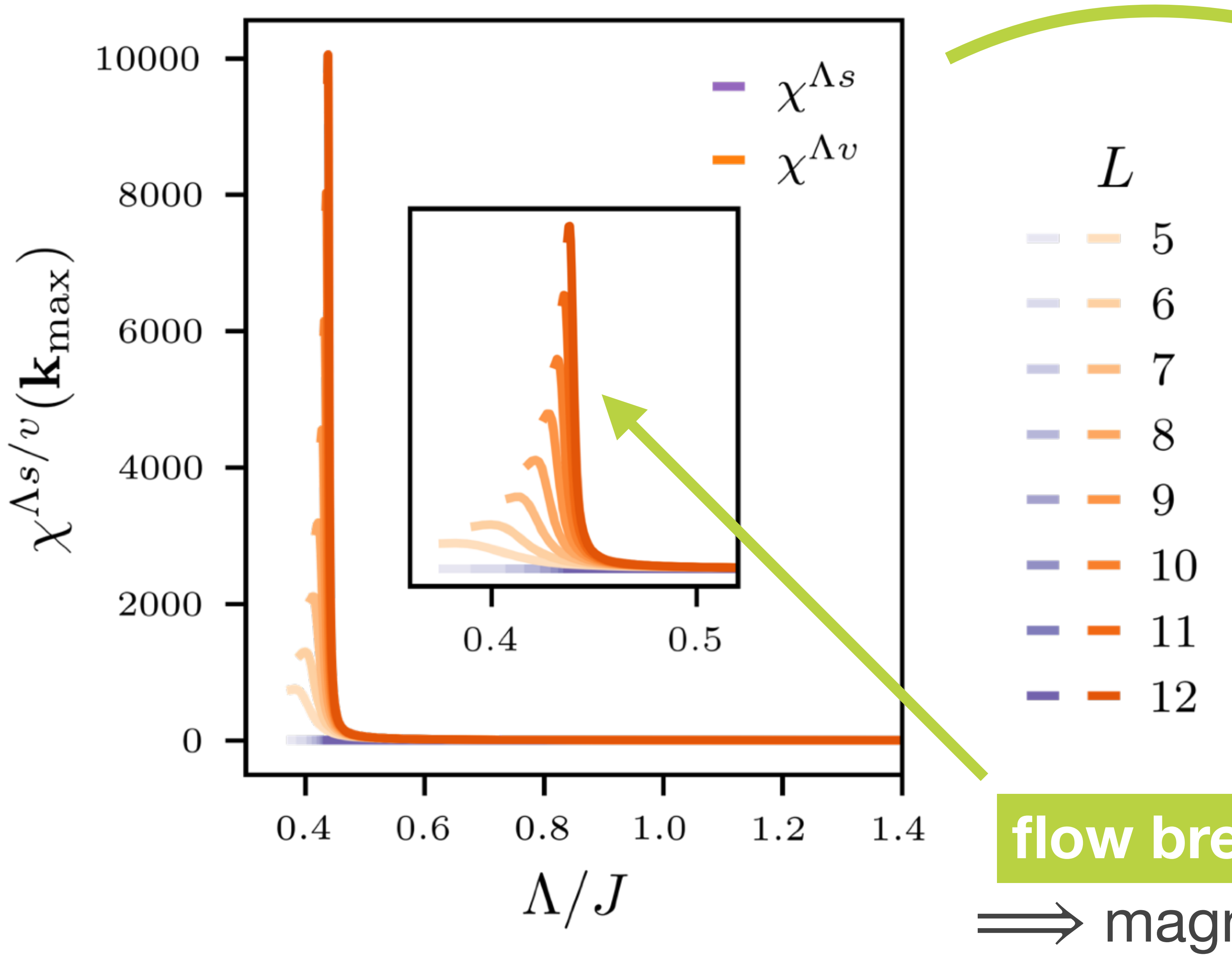
Fourier-transform → **structure factors**

usually consider static contribution ($\omega = 0$)

SU(4) point
(no magnetic order)

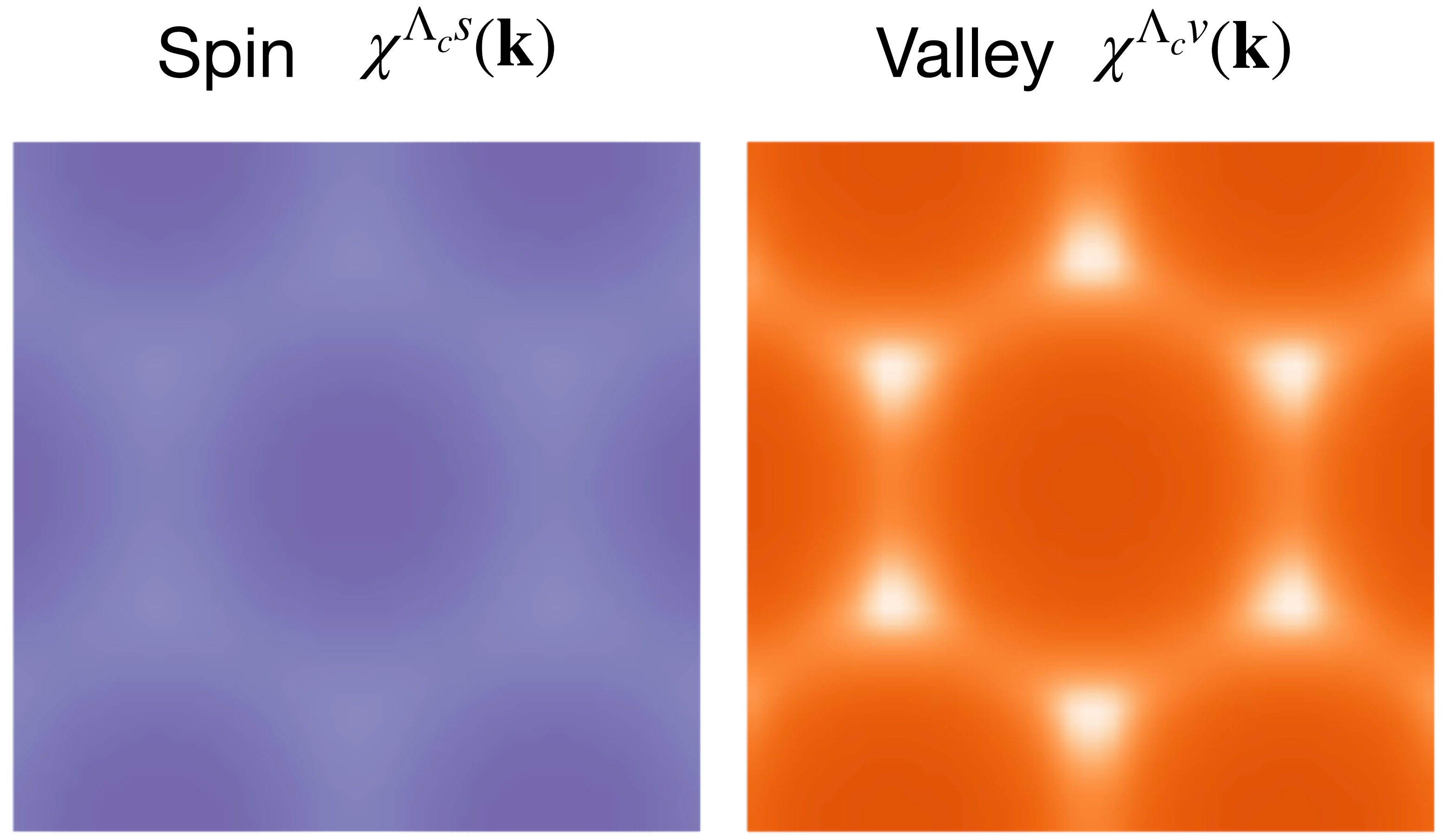


phase with dominant
valley order



flow breakdown

⟹ magnetic order



dominant 120° valley order

spin-valley quantum liquids

$\mathrm{SU}(2)_{\mathrm{spin}} \otimes \mathrm{SU}(2)_{\mathrm{valley}}$

spin-valley model

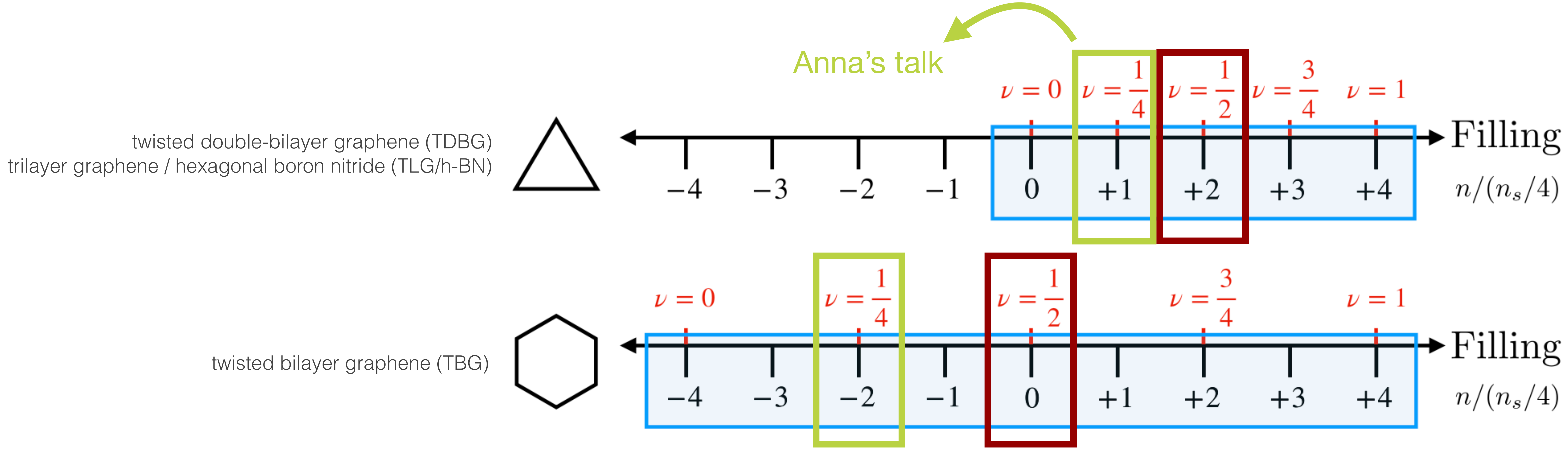
Phys. Rev. Research **2**, 013370 (2020).

spin-valley coupling in presence of **Hund's coupling** gives $\mathrm{SU}(2)_{\mathrm{spin}} \otimes \mathrm{SU}(2)_{\mathrm{valley}}$ model

Heisenberg coupling — Hund's coupling

$$\mathcal{H} = \sum_{\langle ij \rangle} J(\hat{\sigma}_i^a \otimes \hat{\tau}_i^b)(\hat{\sigma}_j^a \otimes \hat{\tau}_j^b) + J_s \hat{\sigma}_i^a \hat{\sigma}_j^a + J_v \hat{\tau}_i^b \hat{\tau}_j^b$$

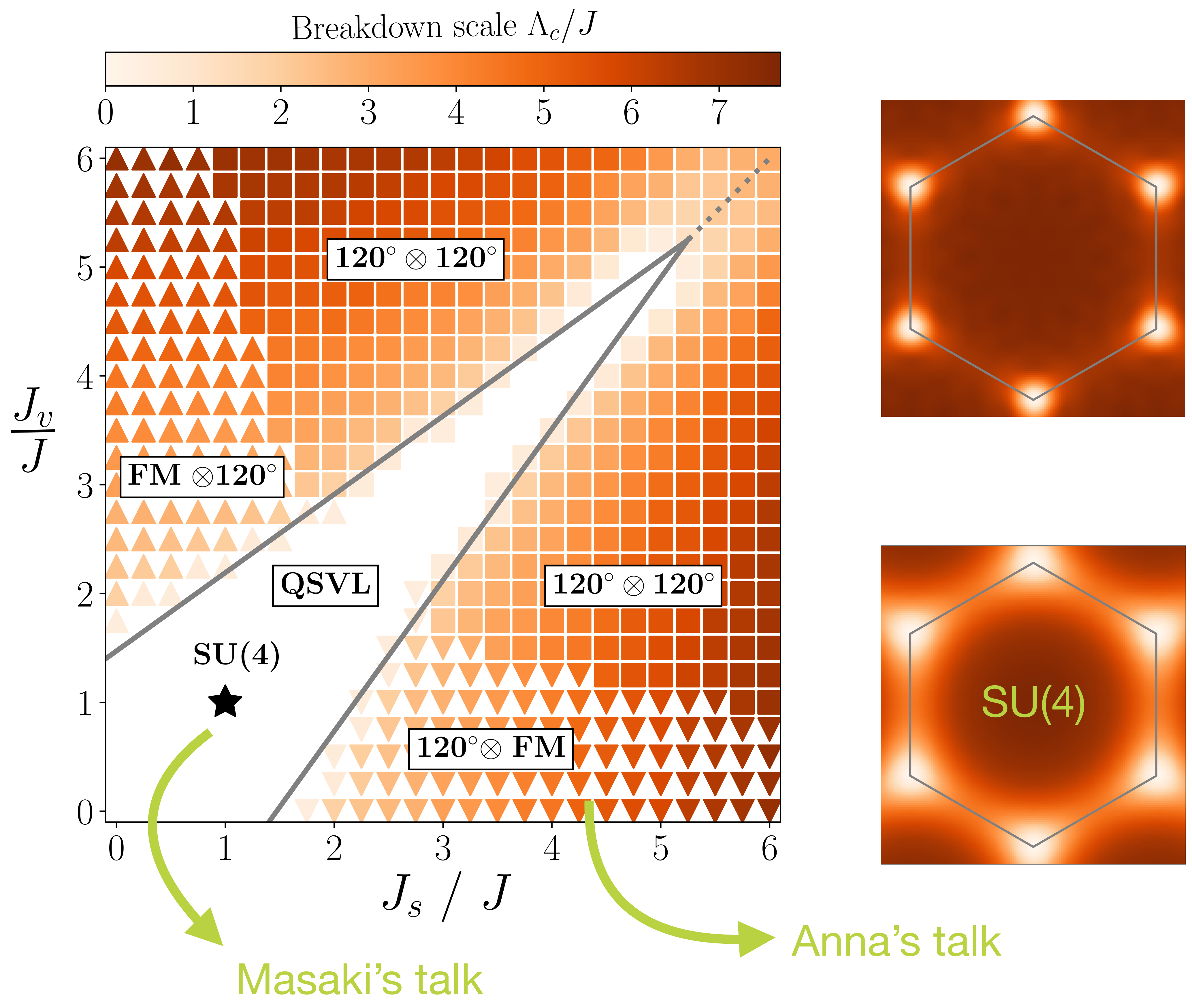
SU(4) symmetric — $\mathrm{SU}(2)_{\mathrm{spin}} \otimes \mathrm{SU}(2)_{\mathrm{valley}}$ symmetric



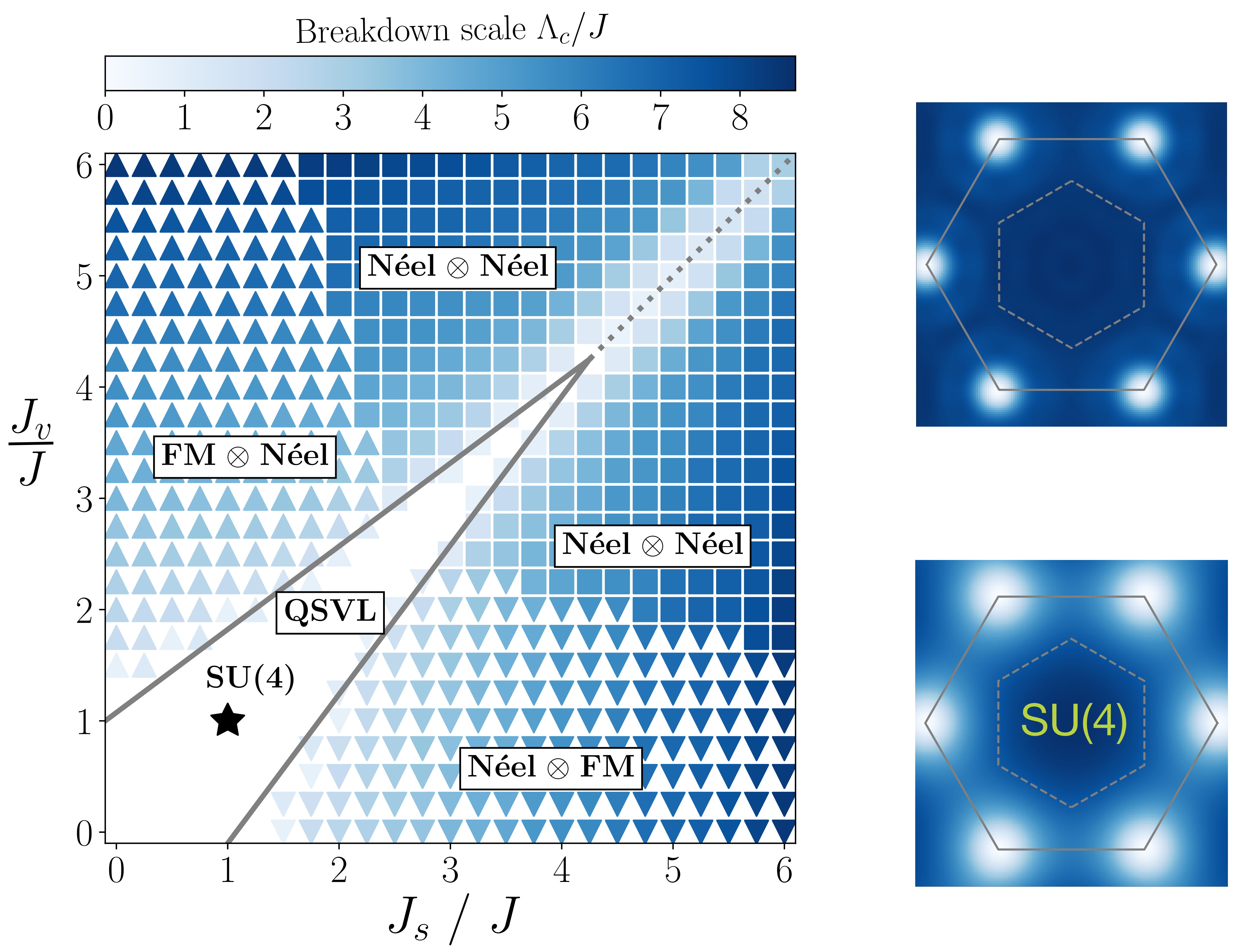
spin-valley model / Hund’s coupling

Phys. Rev. Research **2**, 013370 (2020).

triangular lattice



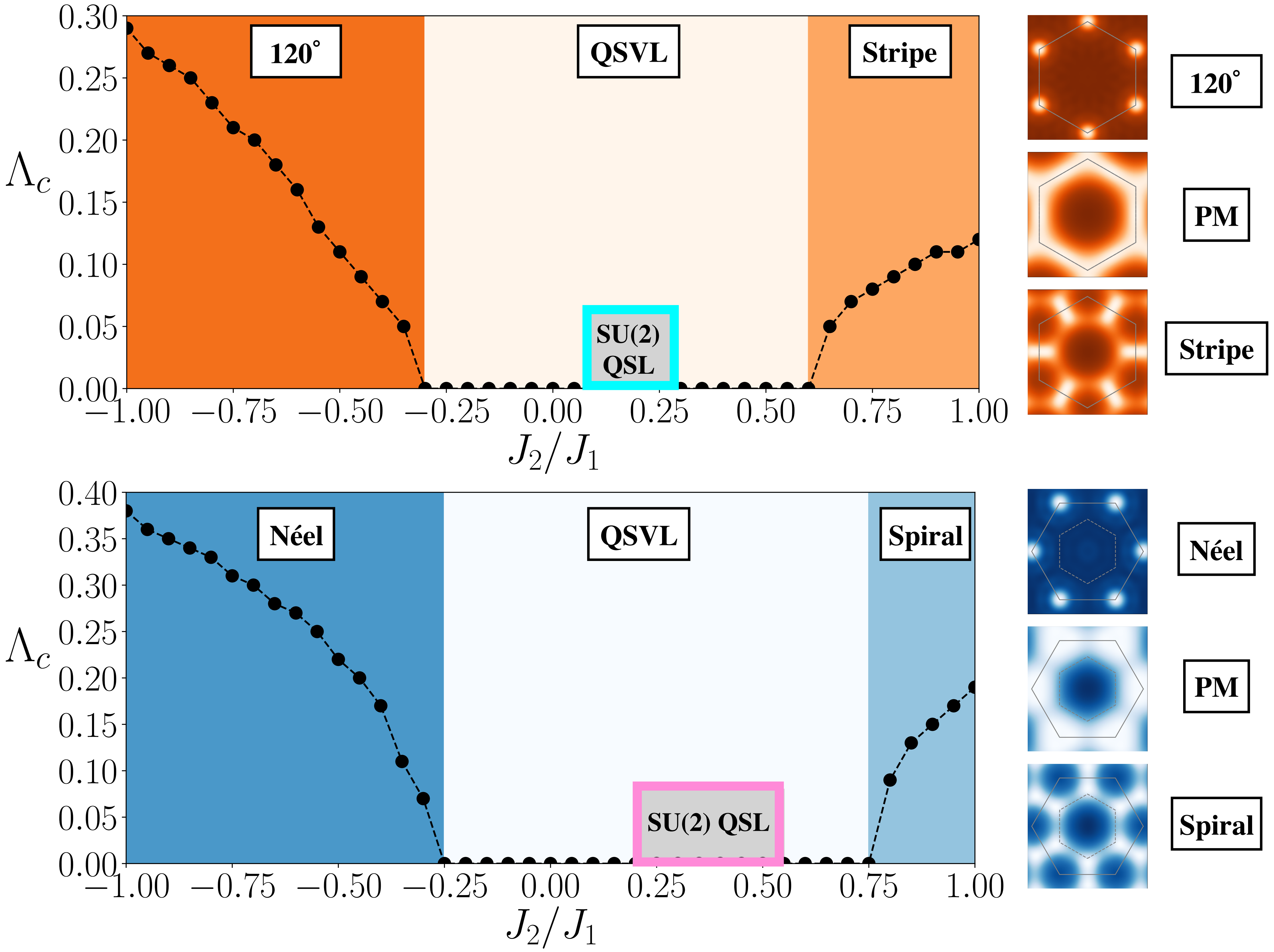
honeycomb lattice



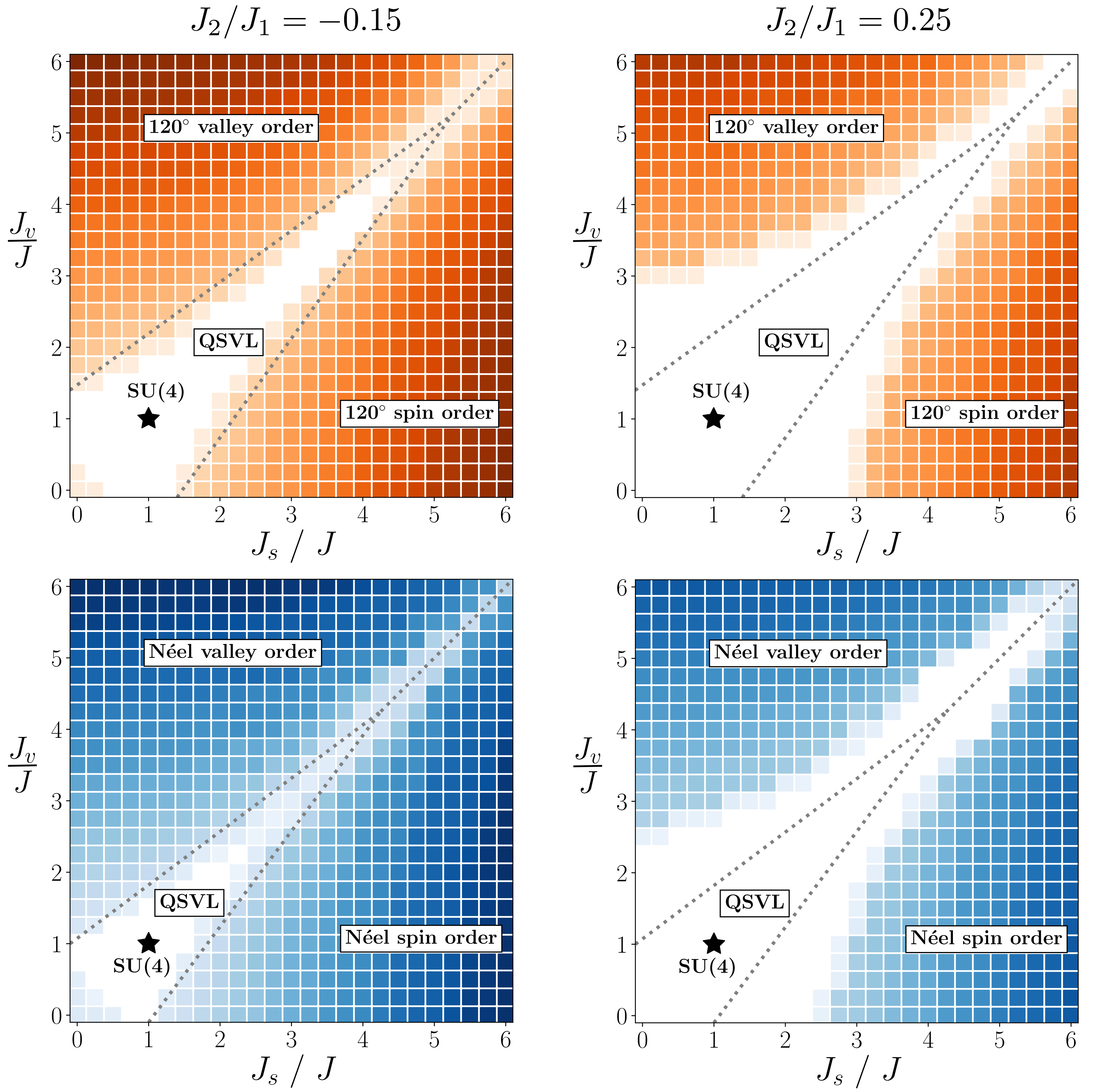
spin-valley model / longer-range couplings

Phys. Rev. Research **2**, 013370 (2020).

J1 - J2 scans



modified phase diagrams

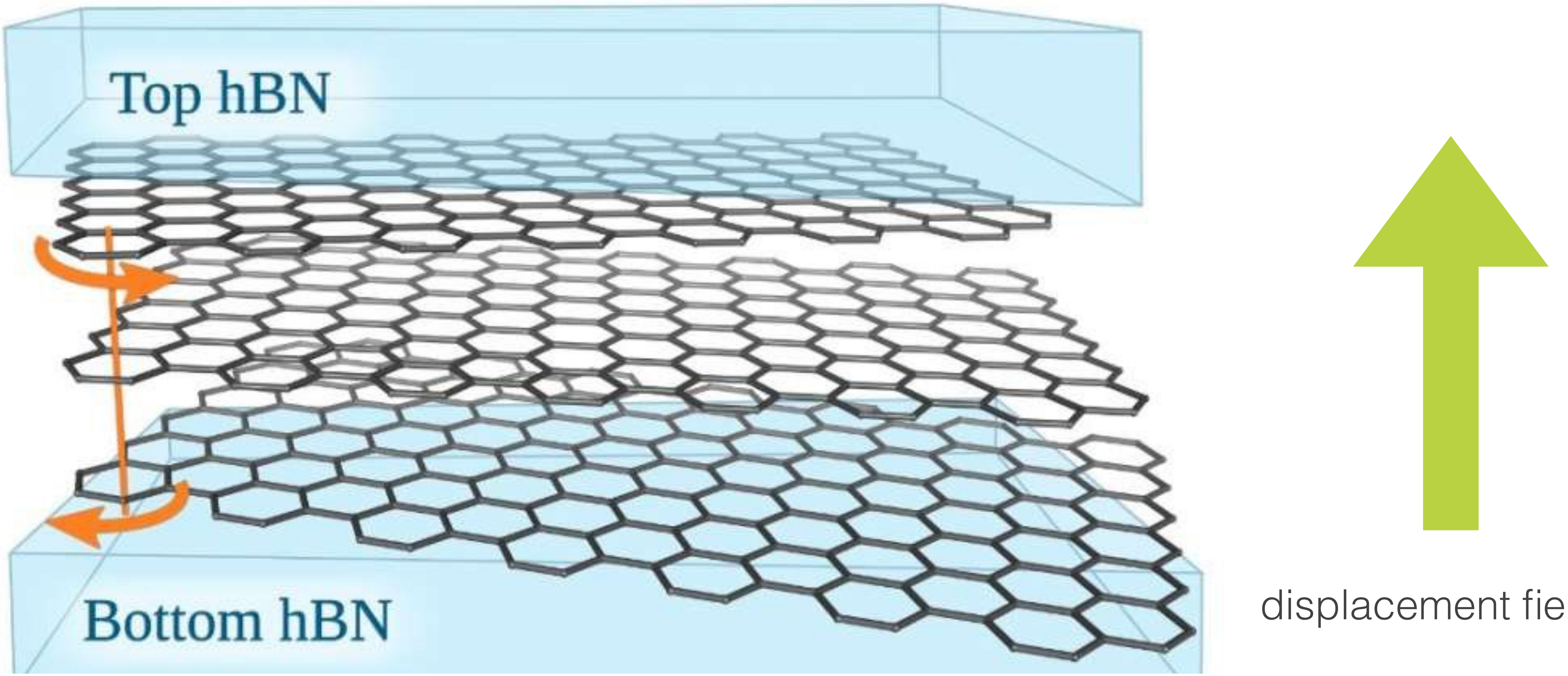


trilayer graphene / h-BN

$SU(2)_{spin} \otimes U(1)_{valley}$

spin-valley model for TLG/h-BN

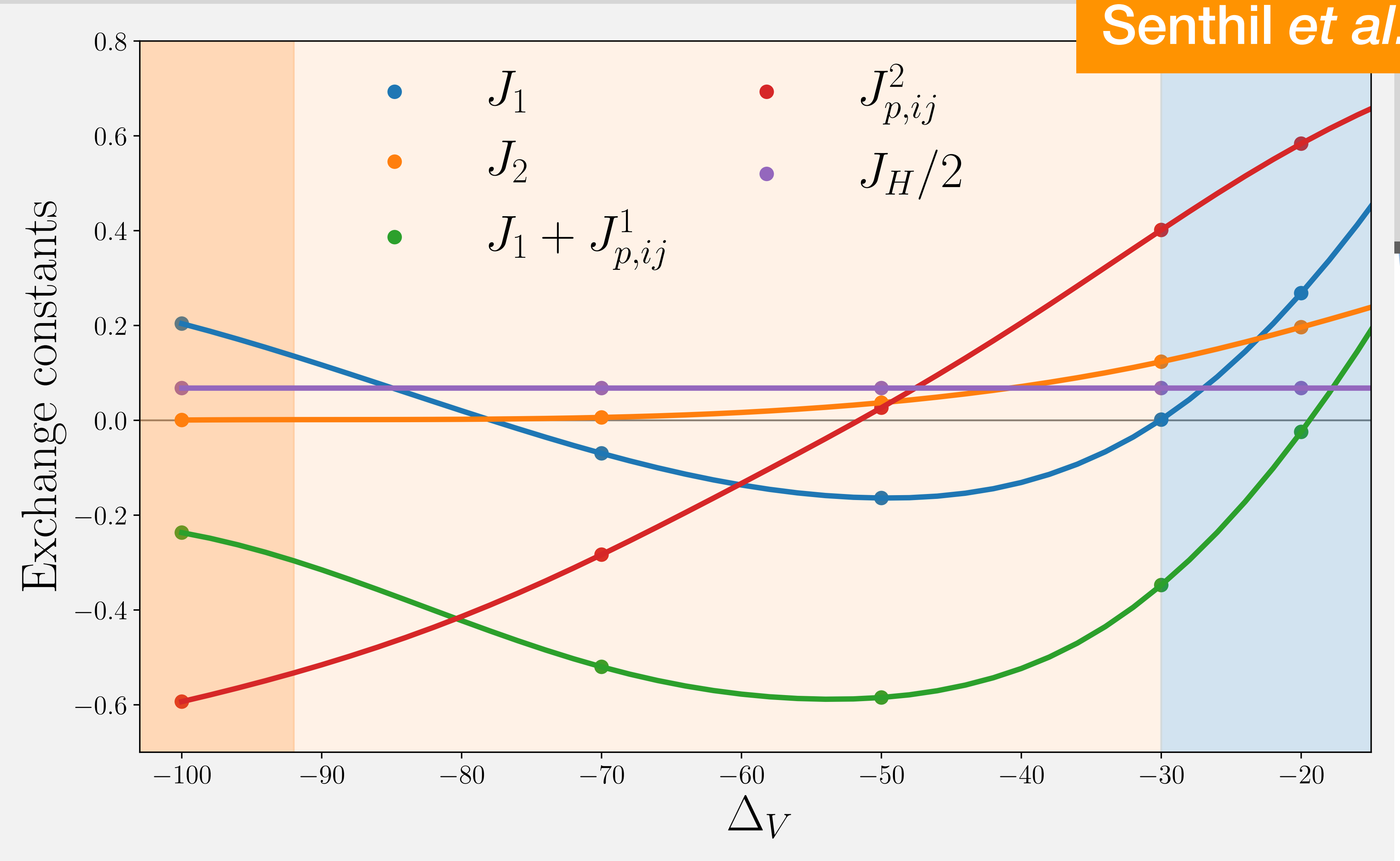
X. Zhang *et al.*, PRL **127**, 166802 (2021)



displacement field *D*

spin-valley model for

Senthil *et al.*



$\mathrm{SU(2)_{spin}} \otimes \mathrm{U(1)_{valley}}$ spin-valley model

SU(4) symmetric

$$H = \frac{J_1}{8}\sum_{\langle ij\rangle}(1+\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)(1+\boldsymbol{\tau}_i\boldsymbol{\tau}_j) + \frac{J_2}{8}\sum_{\langle\langle ij\rangle\rangle}(1+\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)(1+\boldsymbol{\tau}_i\boldsymbol{\tau}_j)$$

$$+\frac{1}{8}\sum_{\langle ij\rangle} J^1_{p;ij}(1+\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)(\tau^x_i\tau^x_j+\tau^y_i\tau^y_j) + \frac{1}{8}\sum_{\langle ij\rangle} J^2_{p;ij}(1+\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)(\tau^x_i\tau^y_j-\tau^y_i\tau^x_j) + \frac{J_H}{4}\sum_i (n_{+i}n_{-i}+\boldsymbol{\sigma}_{+i}\boldsymbol{\sigma}_{-i}) + O\left(\frac{t^3}{U^2}\right)$$

$\mathrm{SU(2)_{spin}} \otimes \mathrm{U(1)_{valley}}$ symmetric

Half-filling

$$\sum_{sl} f^\dagger_{isl} f_{isl} = 2$$

parameters **tunable** by displacement **field** D → potential difference Δ_V

Translated into **matrix form**

$$H = \frac{1}{8}\sum_i \sigma^\mu_i\sigma^\mu_i\ \tau^\kappa_i \begin{pmatrix} -J_H/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \\ 0 & 0 & 0 & J_H/2 \end{pmatrix}^{\kappa\lambda} \tau^\lambda_i + \frac{1}{8}\sum_{\langle ij\rangle}\sigma^\mu_i\sigma^\mu_j\ \tau^\kappa_i \begin{pmatrix} J_1 & 0 & 0 & 0 \\ 0 & J_1+J^1_{p;ij} & J^2_{p;ij} & 0 \\ 0 & -J^2_{p;ij} & J_1+J^1_{p;ij} & 0 \\ 0 & 0 & 0 & J_1 \end{pmatrix}^{\kappa\lambda} \tau^\lambda_j + \frac{1}{8}\sum_{\langle\langle ij\rangle\rangle} J_2\sigma^\mu_i\sigma^\mu_j\tau^\kappa_i\tau^\kappa_j$$

spin valley model for TG/h-BN

spin-spin correlations

SU(2) symmetric

$$\chi_{ij}^{\Lambda s} \equiv \chi_{ij}^{\Lambda s,xx} = \left\langle \sigma_i^x \sigma_j^x \right\rangle = \left\langle \sigma_i^y \sigma_j^y \right\rangle = \left\langle \sigma_i^z \sigma_j^z \right\rangle$$

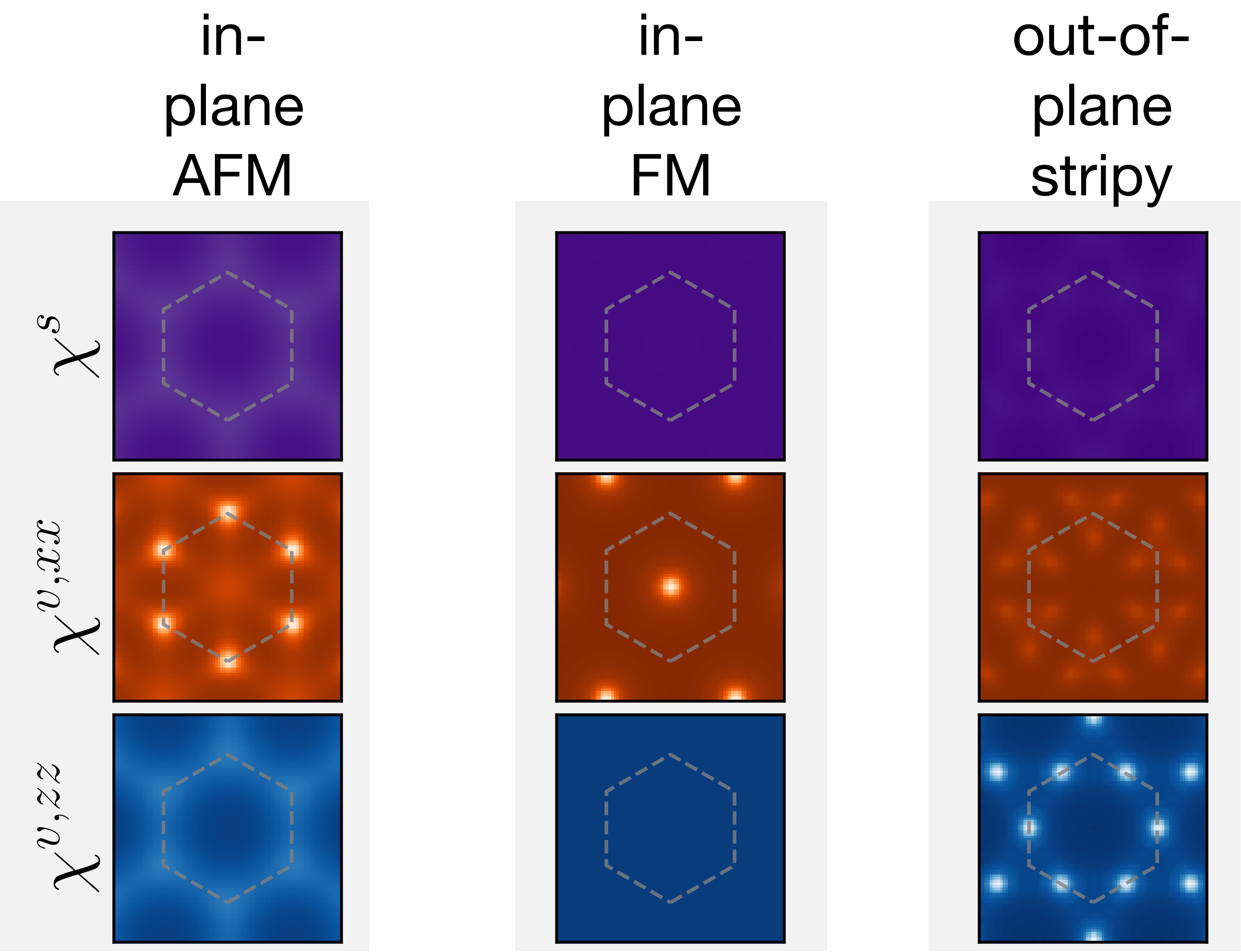
valley-valley correlations

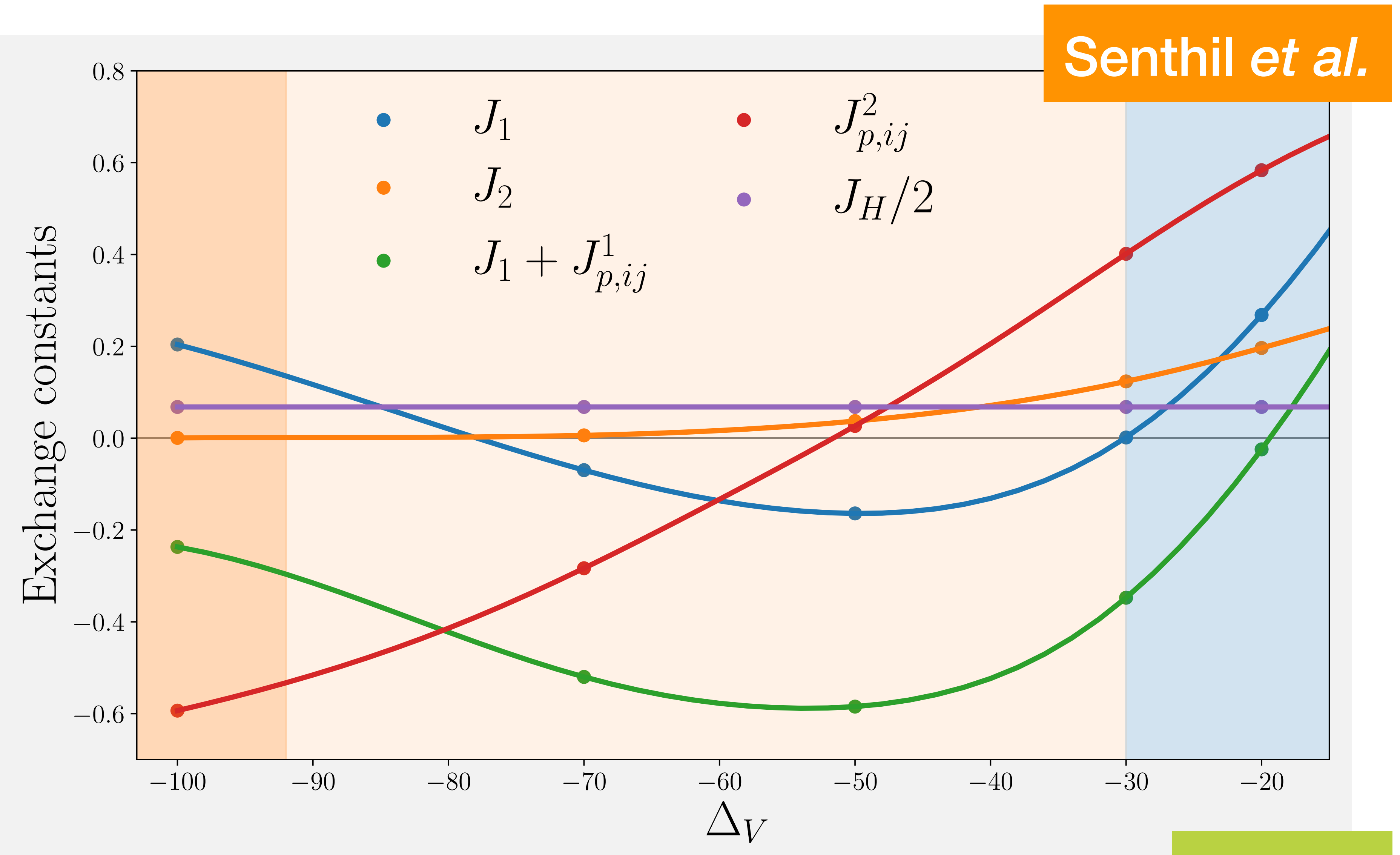
in-plane

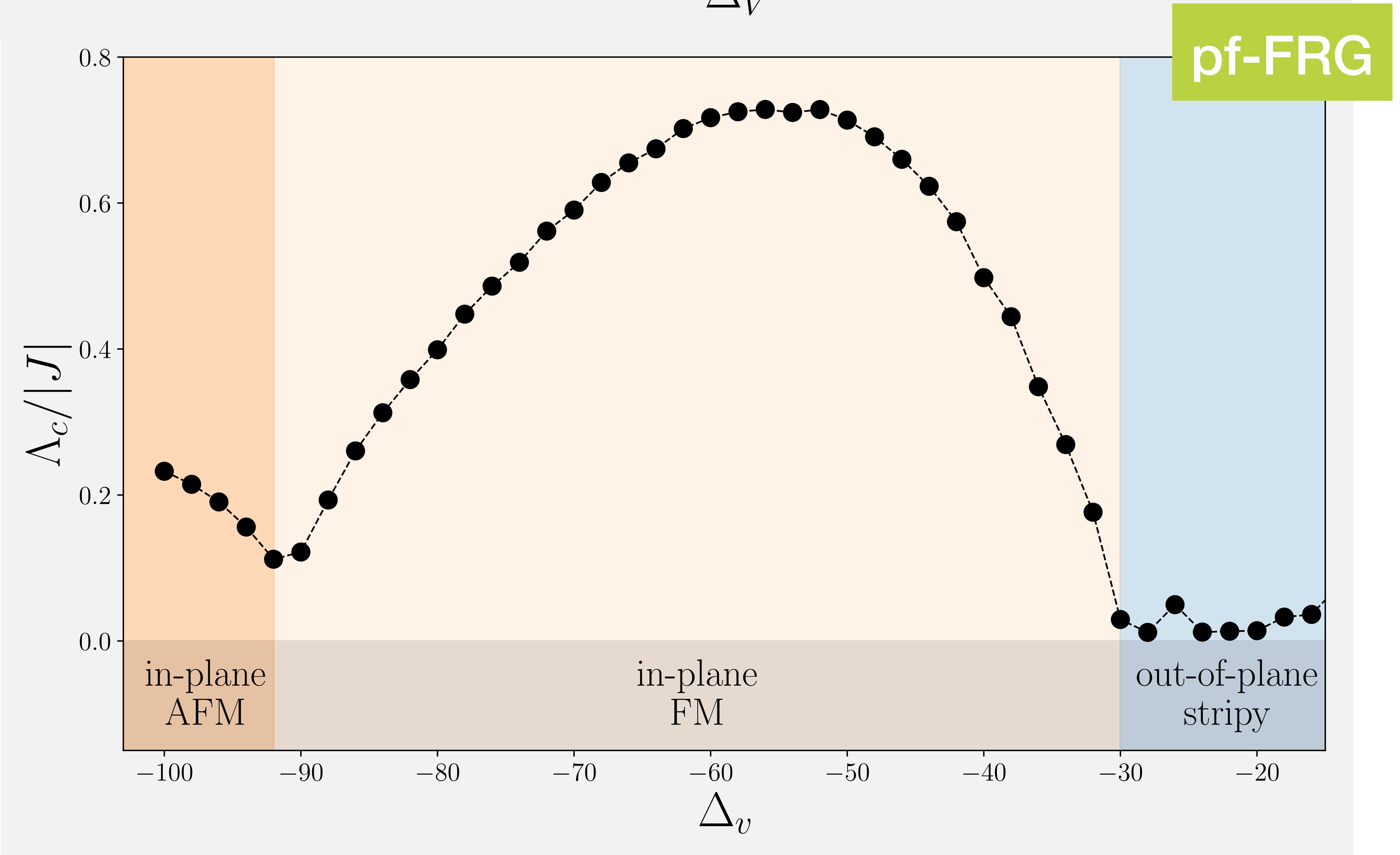
$$\chi_{ij}^{\Lambda v,x} \equiv \chi_{ij}^{\Lambda v,xx} = \left\langle \tau_i^x \tau_j^x \right\rangle = \left\langle \tau_i^y \tau_j^y \right\rangle$$

out-of-plane

$$\chi_{ij}^{\Lambda v,z} \equiv \chi_{ij}^{\Lambda v,zz} = \left\langle \tau_i^z \tau_j^z \right\rangle$$

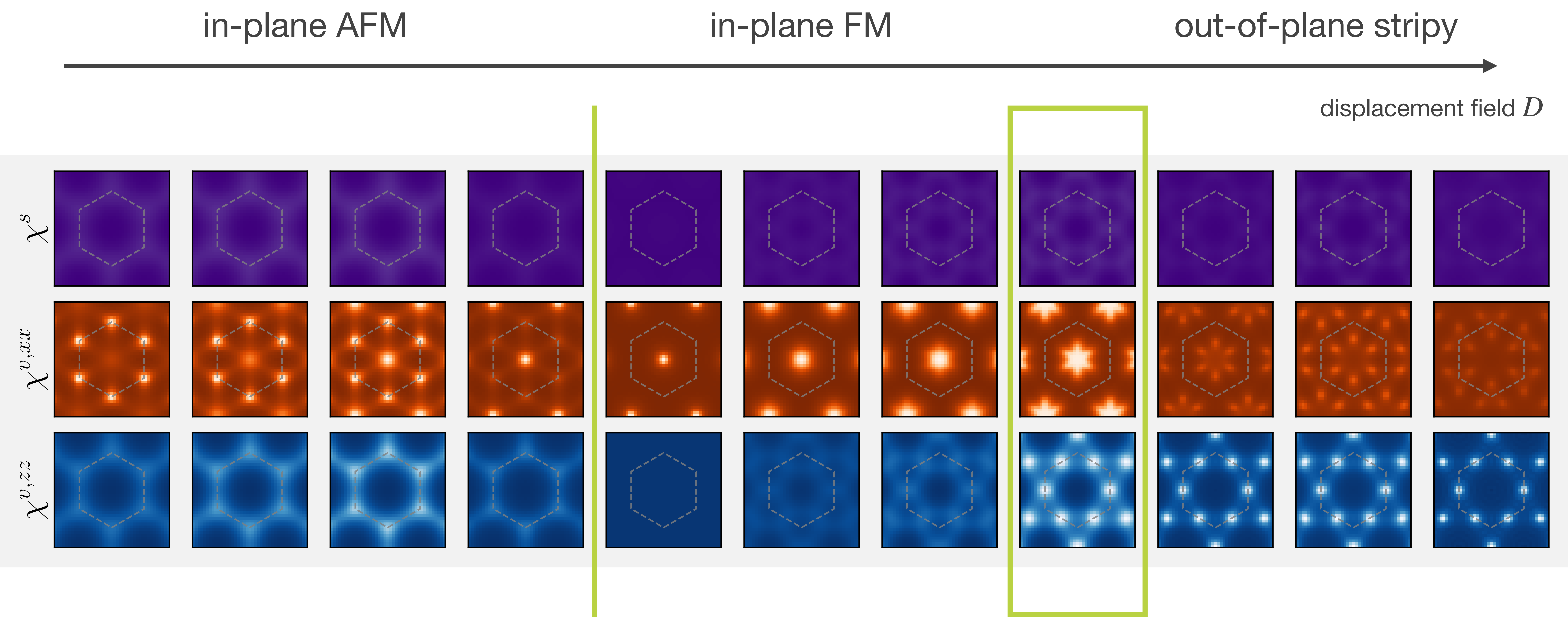






spin valley models for TG/h-BN

L. Gresista *et al.*, in preparation



Where to go from here?

summary

arXiv:2202.05029

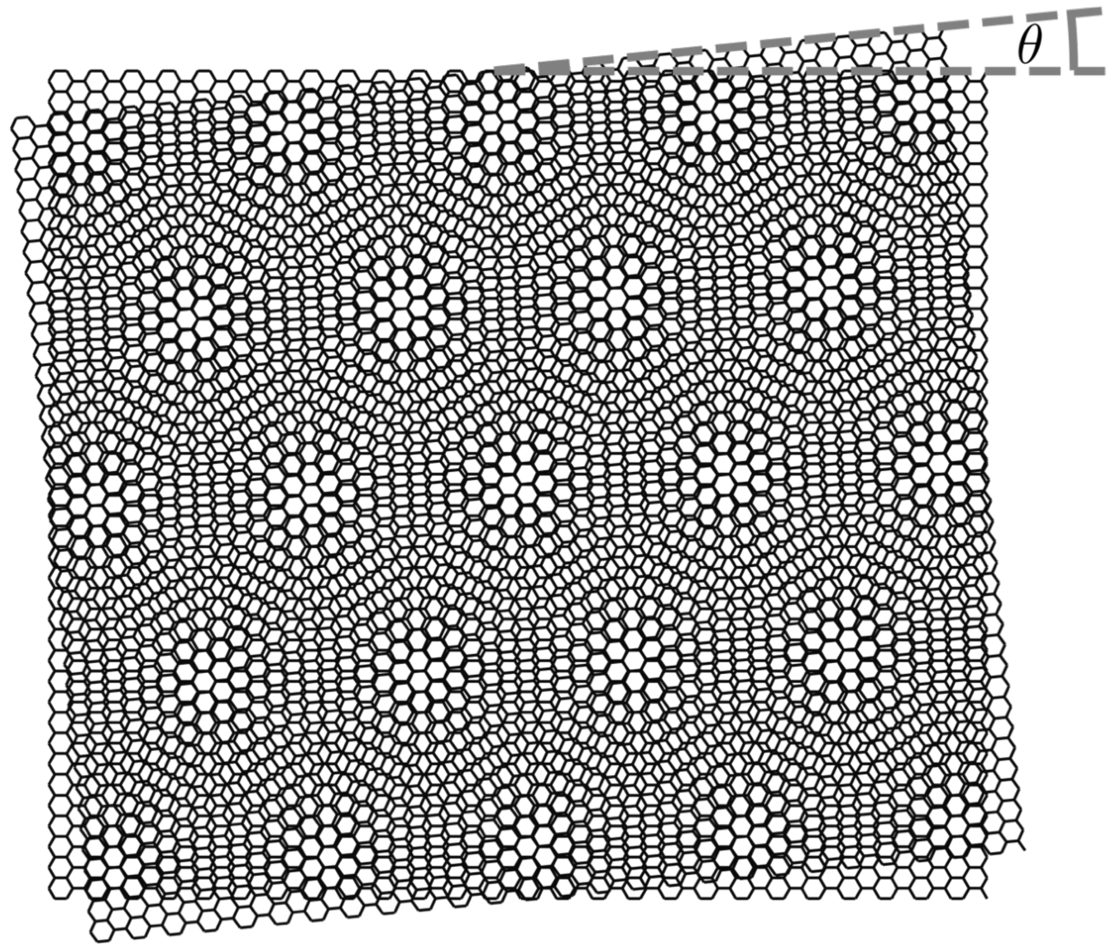
Phys. Rev. Research **2**, 013370 (2020).

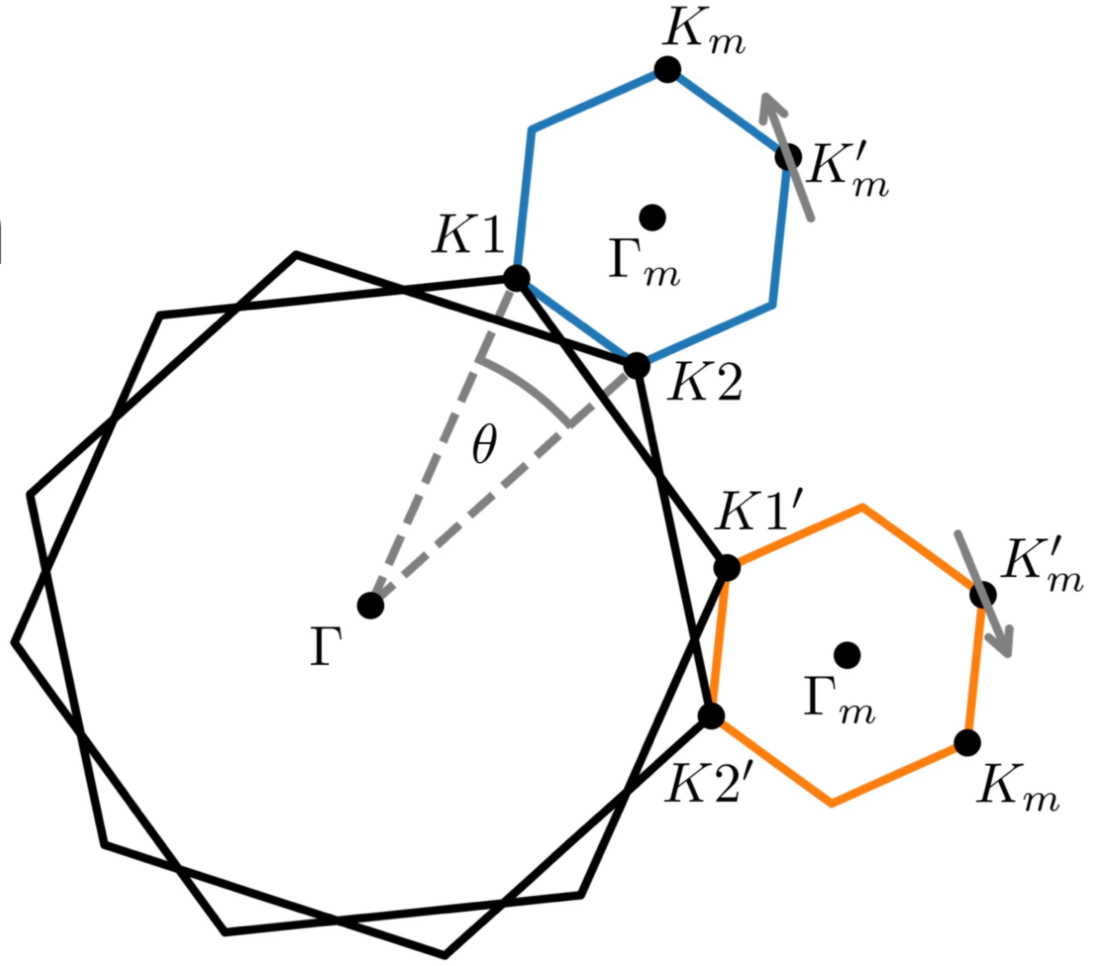
Take-away messages

- Moiré materials are a **new platform** for SU(N) physics

- Interplay of spin and valley degrees of freedom gives rise to **rich phase diagrams**

- In proximity of SU(4) symmetry we find **spin-valley quantum spin liquid** states





Outlook

- Like for their SU(2) counterparts the **intermediate coupling regime** between weakly coupled **Hubbard** physics and strongly coupled **spin-valley SU(4) models** might be most interesting.