Kekulé spirals in twisted bilayer graphene

arxiv: 2105.05857

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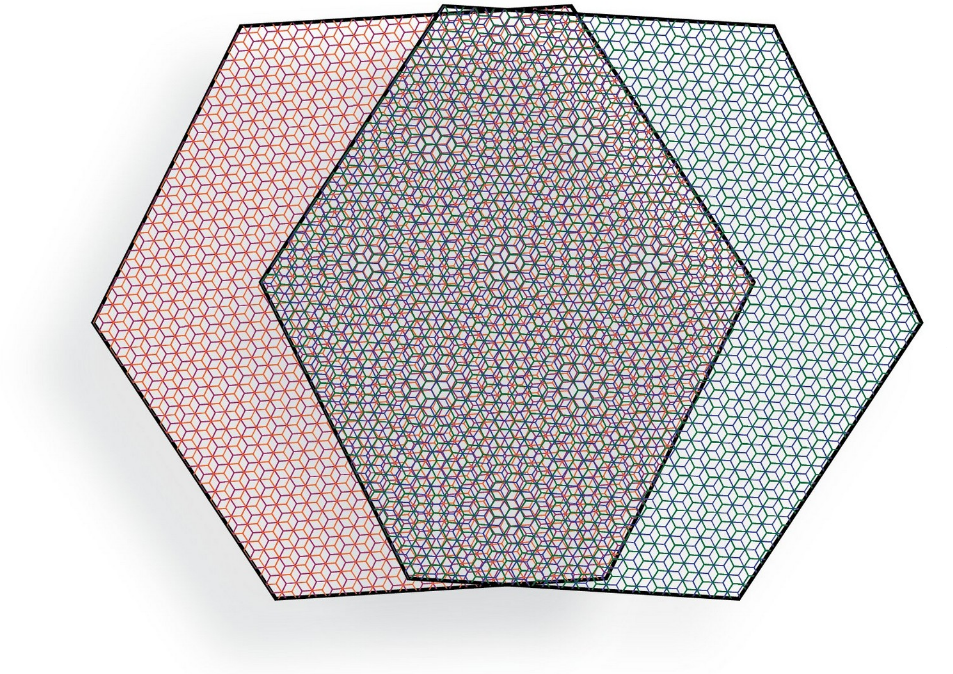
Content

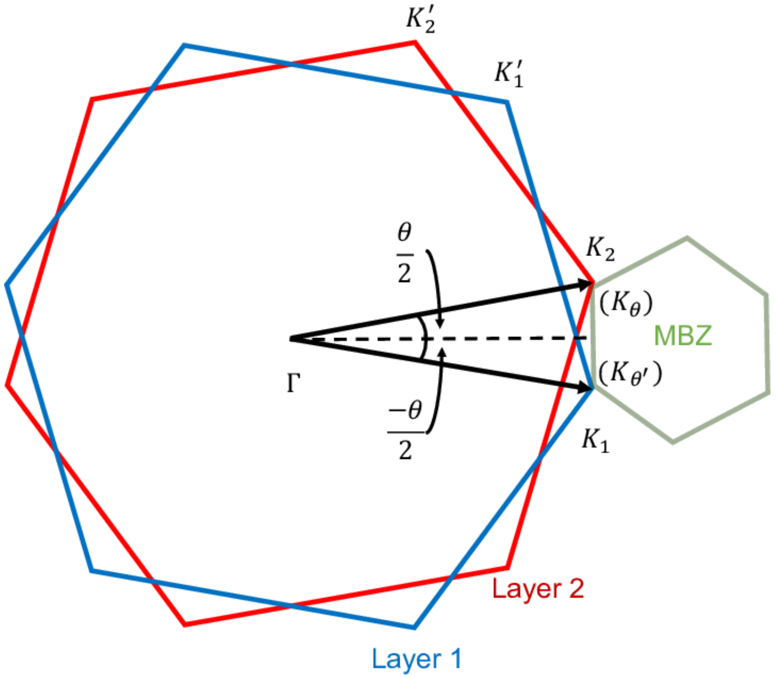
- Continuum model
- Strong coupling phases
- Incommensurate Kekulé spiral
- Experimental features

Continuum model

Moiré pattern



Graphene unit cell expands to moiré unit cell



Graphene BZ shrinks to moiré BZ

Continuum model

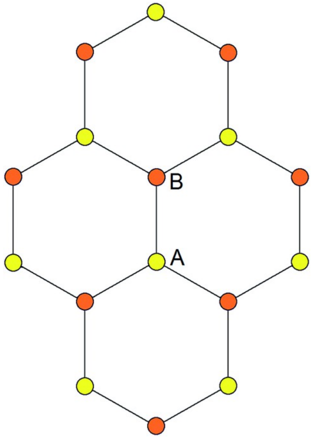
- Rotate Dirac cones

$$\langle \boldsymbol{k}, 1| H |\boldsymbol{k}', 1\rangle = \hbar v_0 \boldsymbol{\sigma}^*_{\theta/2} \cdot (\boldsymbol{k} - \boldsymbol{K}^1)\, \delta_{\boldsymbol{k},\boldsymbol{k}'}$$

$$\langle \boldsymbol{k}, 2| H |\boldsymbol{k}', 2\rangle = \hbar v_0 \boldsymbol{\sigma}^*_{-\theta/2} \cdot (\boldsymbol{k} - \boldsymbol{K}^2)\, \delta_{\boldsymbol{k},\boldsymbol{k}'}$$

- Interlayer tunneling

$$\langle \boldsymbol{k}, 1| H |\boldsymbol{k}', 2\rangle = T_1 \delta_{\boldsymbol{k}-\boldsymbol{k}',\mathbf{0}} + T_2 \delta_{\boldsymbol{k}-\boldsymbol{k}',\mathbf{b}_1^{\mathrm{M}}} + T_3 \delta_{\boldsymbol{k}-\boldsymbol{k}',\mathbf{b}_2^{\mathrm{M}}}$$

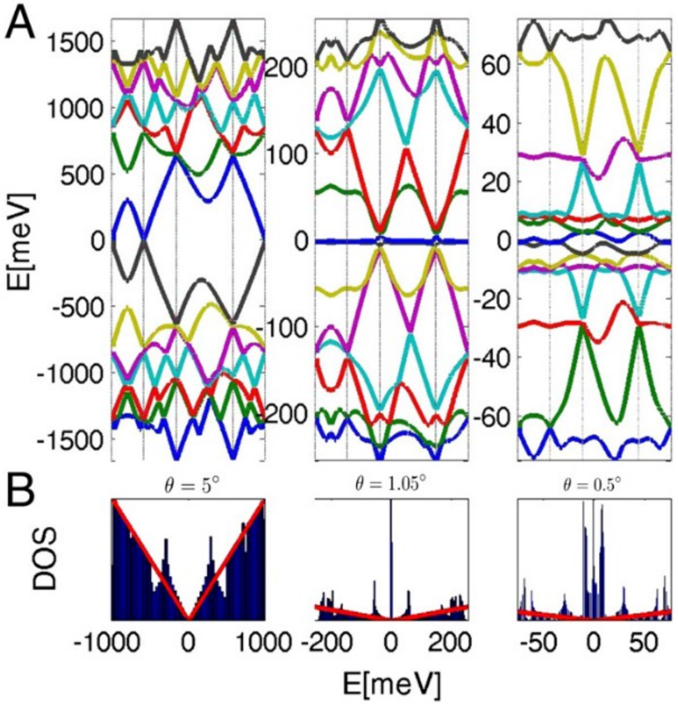


$$T_1 = \begin{pmatrix} w_{AA} & w_{AB} \\ w_{AB} & w_{AA} \end{pmatrix}$$

$w_{AA} = 0$ "chiral limit"

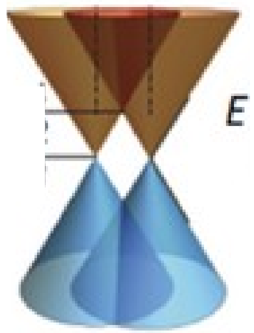
The magic angle

- Flat bands near magic angle of ~1º



$$v_F \frac{\theta}{a} \sim w_{AB}$$

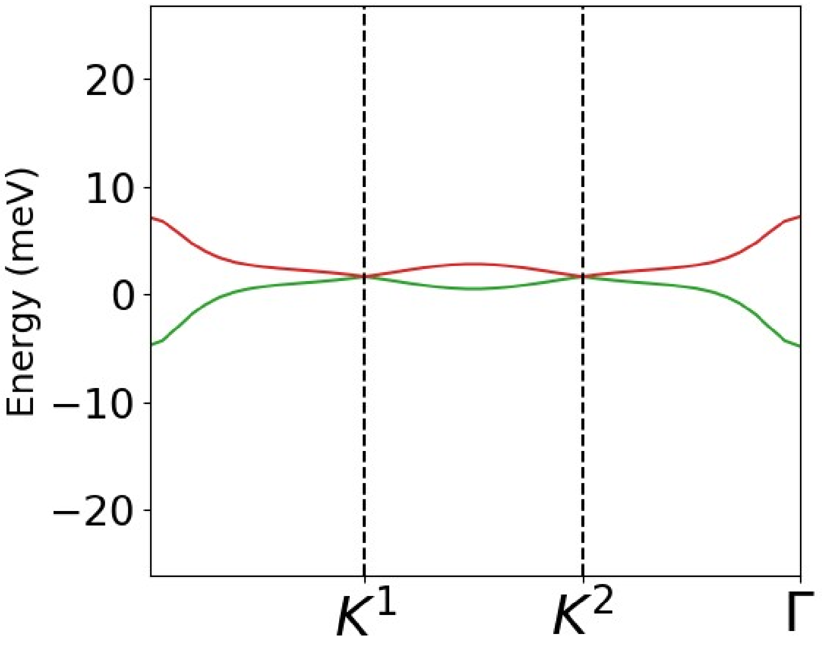
$$\theta \sim \frac{w_{AB}}{v_F/a} \sim 1^\circ$$

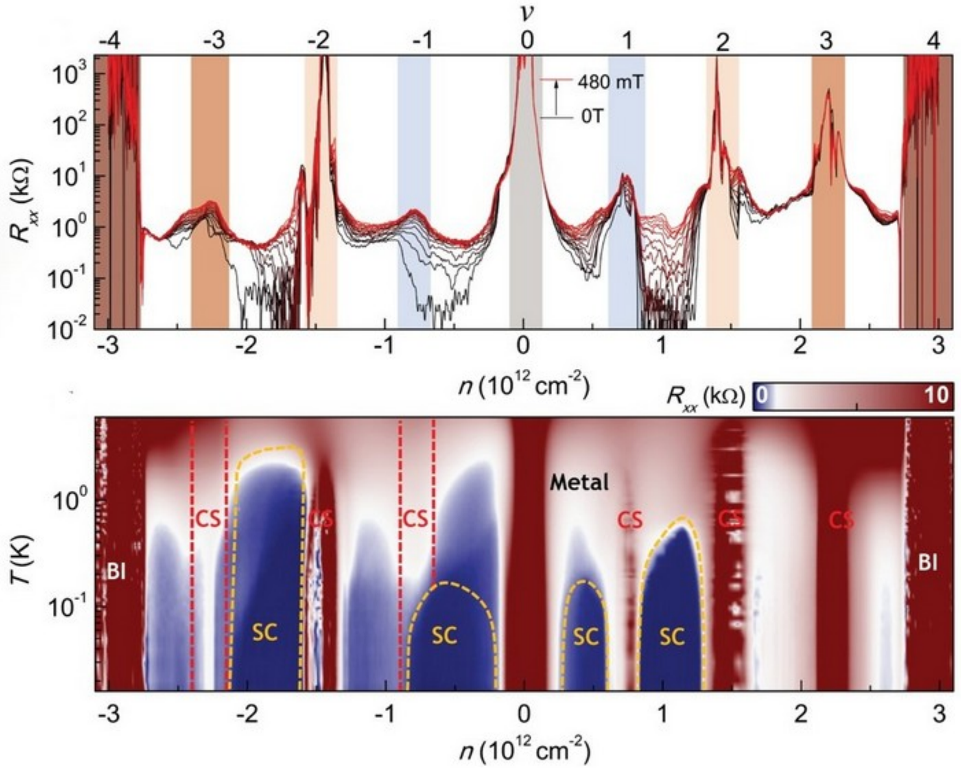


Bistrizer, MacDonald, **PNAS** (2011)

Central bands

$$\nu = \text{electrons/moiré unit cell}$$





Lu, Stepanov,….,Efetov, **Nature** (2019)

Interacting model

$$\mathcal{H}_{\mathrm{eff}} = \sum_{\boldsymbol{k}\in \mathrm{BZ}} c_{\boldsymbol{k}}^{\dagger} h(\boldsymbol{k}) c_{\boldsymbol{k}} + \frac{1}{2A} \sum_{\boldsymbol{q}} V_{\boldsymbol{q}} :\rho_{\boldsymbol{q}} \rho_{-\boldsymbol{q}}:,$$

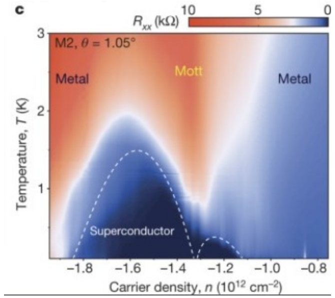
$$\rho_{\boldsymbol{q}} = \sum_{\boldsymbol{k}\in \mathrm{BZ}} c_{\boldsymbol{k}}^{\dagger} \Lambda_{\boldsymbol{q}}(\boldsymbol{k}) c_{\boldsymbol{k}+\boldsymbol{q}}, \qquad [\Lambda_{\boldsymbol{q}}(\boldsymbol{k})]_{\alpha,\beta} = \langle u_{\alpha,\boldsymbol{k}} | u_{\beta,\boldsymbol{k}+\boldsymbol{q}} \rangle,$$

$$V_q = \frac{e^2}{2\epsilon_0 \epsilon_r q} \tanh(qd)$$

Strong coupling phases

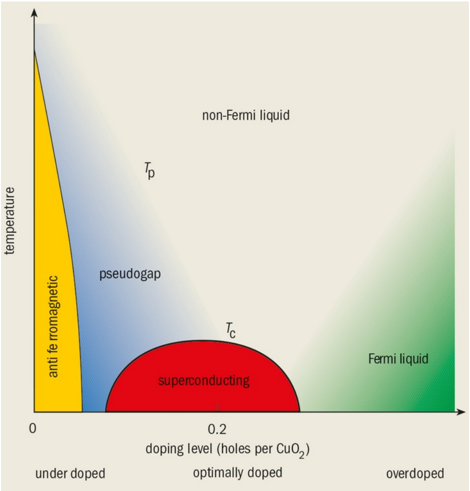
Two paradigms of strong correlations: Hubbard model

Superconducting Domes in TBG

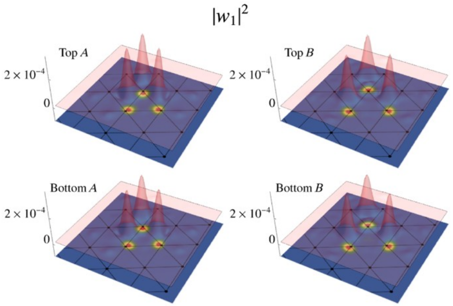


Cao,…, Jarillo-Herrero **Nature** (2018)

cf. cuprates phase diagram



Wannier states



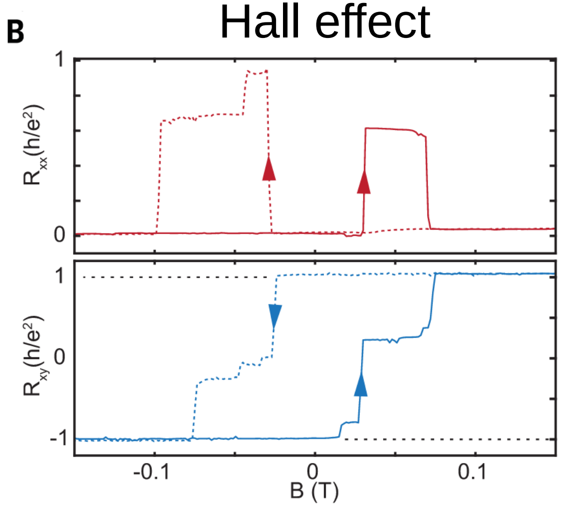
Kang, Vafek, **PRX** (2018)

Doping + further range interactions lead to translational symmetry breaking:

- Charge-density waves
- Spin-density waves
- Pair-density waves

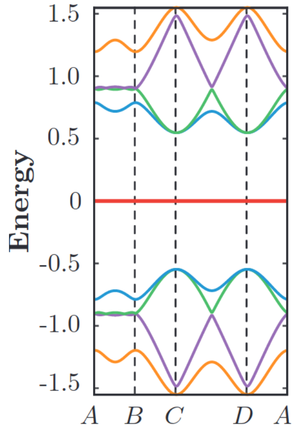
Two paradigms of strong correlations: Quantum Hall effect

Quantized anomalous Hall effect



Serlin, Tschirhart...,Young **Science** (2020)

Flat Chern bands



Tarnopolsky, Kruchkov, Vishwanath, **PRL** (2019)

Hartree potential in high Landau levels leads to translational symmetry breaking:

- Striped phases
- Bubble phases

Quantum Hall systems are in extreme limit of Stoner criterion: Quantum Hall ferromagnetism (QHFM)

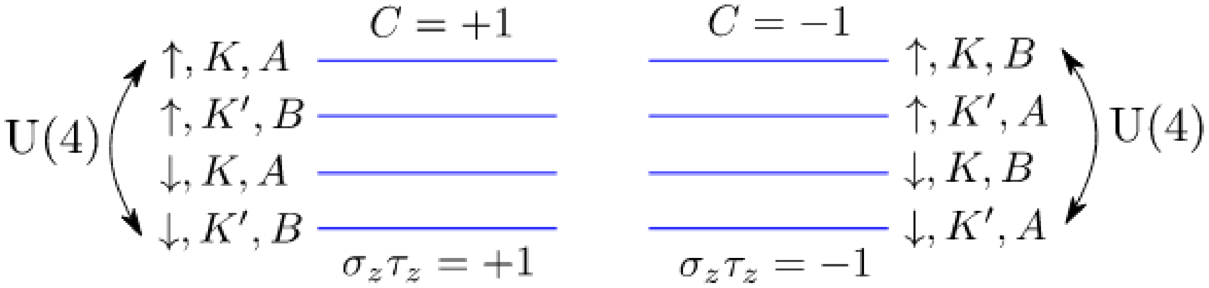
$$|\Psi_{QHFM}\rangle = \prod_k \left(\hat{c}^\dagger_{k\uparrow} + e^{i\varphi}\hat{c}^\dagger_{k\downarrow}\right)|0\rangle$$

Idealized limit

- Full model has
  $$U(2)_K \times U(2)_{K'} \simeq U_C(1) \times U_V(1) \times SU(2)_K \times SU(2)_{K'}$$
- Neglect single-particle dispersion $\rightarrow$ ph symmetry
- Neglect incomplete sublattice polarization $\rightarrow$ chiral symmetry
- Enhanced $U(4) \times U(4)$ symmetry

Bultinck, Khalaf,…,Zalatel, **PRX** (2020)

Idealized limit



$$s_\mu = \text{spin}$$
$$\tau_\mu = \text{valley}$$
$$\sigma_\mu = \text{sublattice}$$

- Two copies of the zeroth Landau level of graphene
- Quantum Hall ferromagnetism

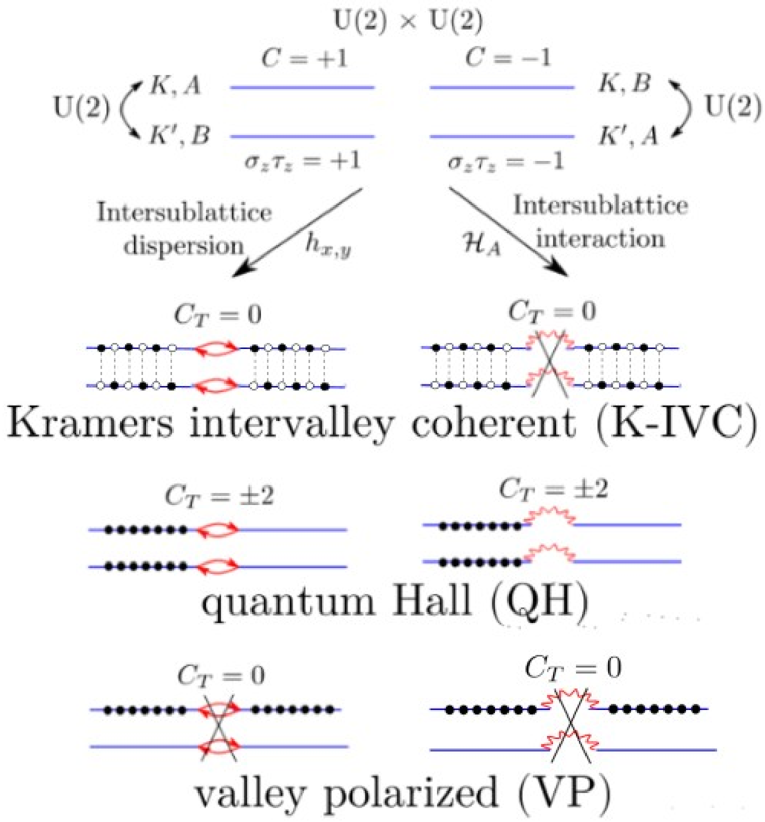
Hierarchy of energy scales

$$\mathcal{H}_{\text{eff}} = \sum_k c_k^\dagger \tilde{h}(\boldsymbol{k}) c_k + \frac{1}{2A} \sum_q V_q \delta\rho_q \delta\rho_{-q}$$

Term	Symmetry	Energy scale
U_S	$\mathrm{U}(4) \times \mathrm{U}(4)$	15-25 meV
t_S	$\mathrm{U}(4)_R$	4-6 meV
U_A	$\mathrm{U}(4)_{\mathcal{PT}}$	4-6 meV
t_A	$\mathrm{U}(2)_K \times \mathrm{U}(2)_{K'}$	0.5-1 meV

Intrasublattice interaction
Intersublattice hopping
Intersublattice interaction
Intrasublattice hopping

Strong coupling orders

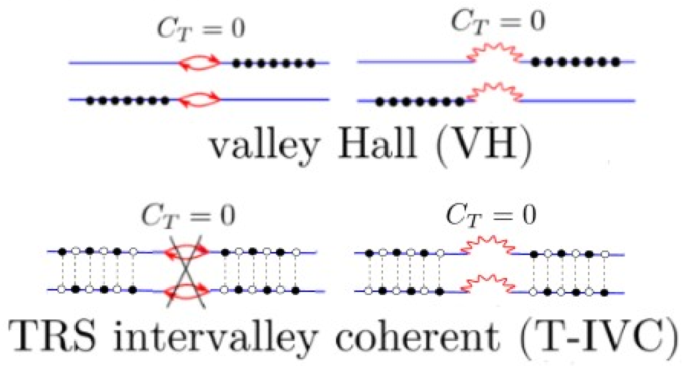


Order	Q	Energy
$\mathcal{T}$-IVC	$\sigma_x\tau_+e^{i\phi} + \text{h.c.}$	λ
QH	$\sigma_z\tau_z$	$\lambda - J$
VH	σ_z	$\lambda - J$
VP	τ_z	0
K-IVC	$\sigma_y\tau_+e^{i\phi} + \text{h.c.}$	$-J$

$$J \sim \frac{t_S^2}{U_S}, \ \lambda \sim \frac{U_A^2}{U_S}$$

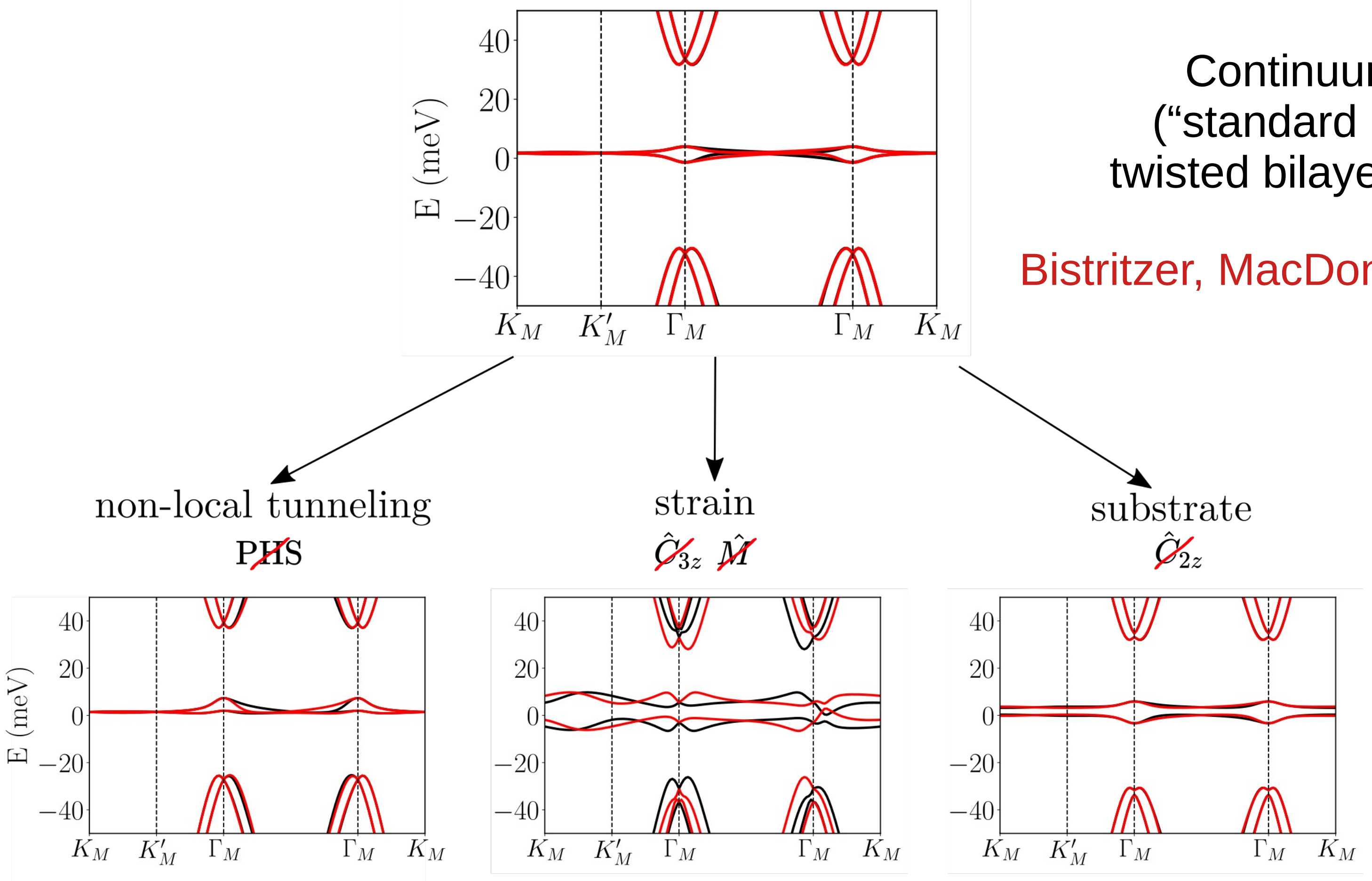
$$\mathcal{T} = \tau_x\mathcal{K}$$

$$\mathcal{T}' = \tau_y\mathcal{K}$$



Incommensurate Kekulé spiral

Realistic perturbations



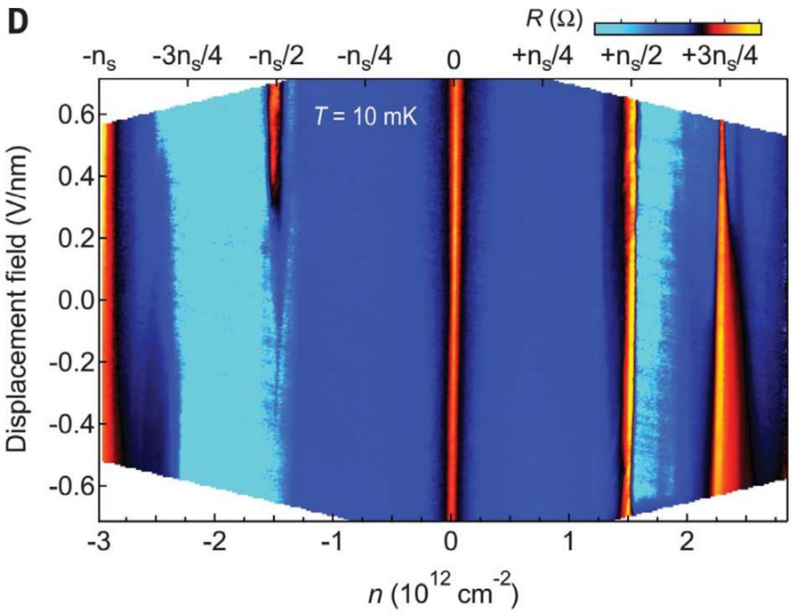
Continuum model
(“standard model” of
twisted bilayer graphene)

Bistritzer, MacDonald, **PNAS** (2011)

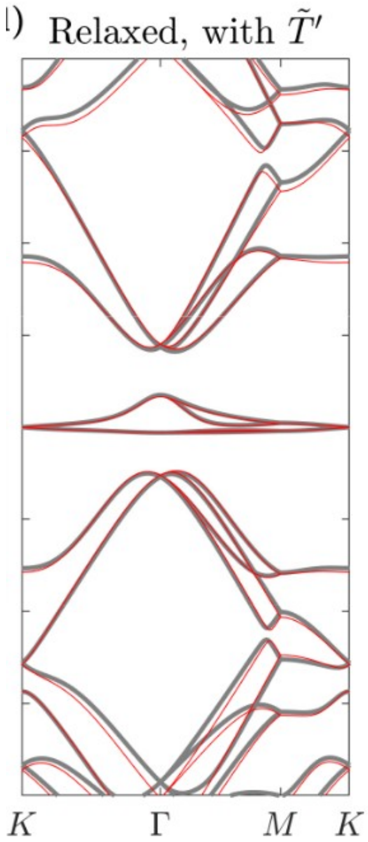
+Coulomb
(Hartree-Fock)

Importance of ph breaking

- BM model almost ph symmetric
- ph broken by non-local tunneling



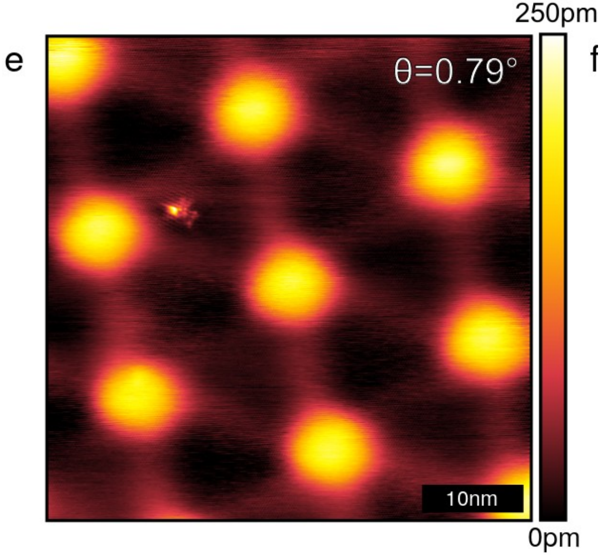
Yankowitz, …, Dean, **Science** (2019)



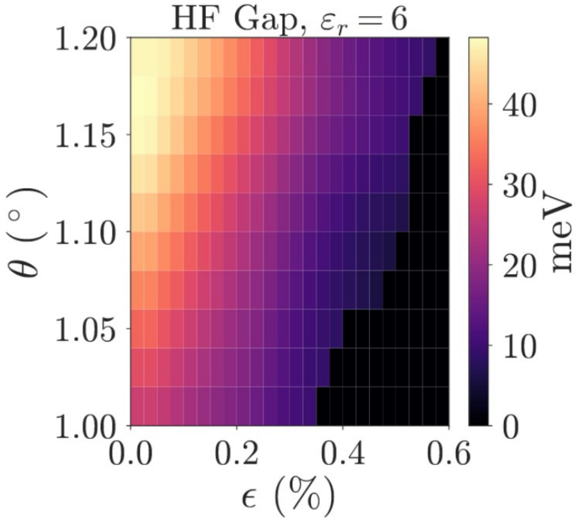
Fang, …,Kaxiras, **arxiv** (2019)

Importance of strain

- STM observes strain in many samples, 0.1-0.7%
- Strain explains presence of semimetal at $\nu = 0$



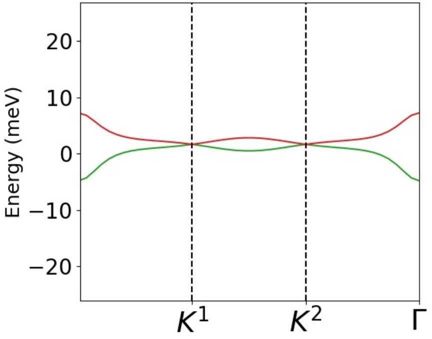
Kerelsky,…, Pasupathy, **Nature** (2019)

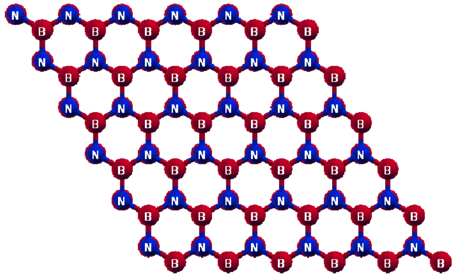


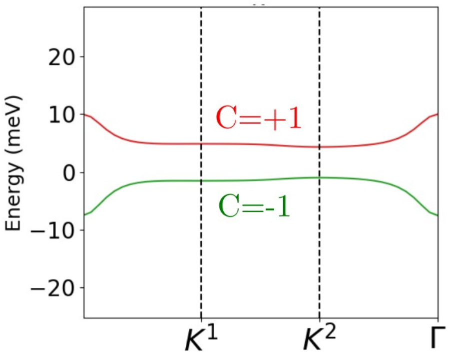
Parker,…, Bultinck, **PRL** (2021)

Importance of substrate

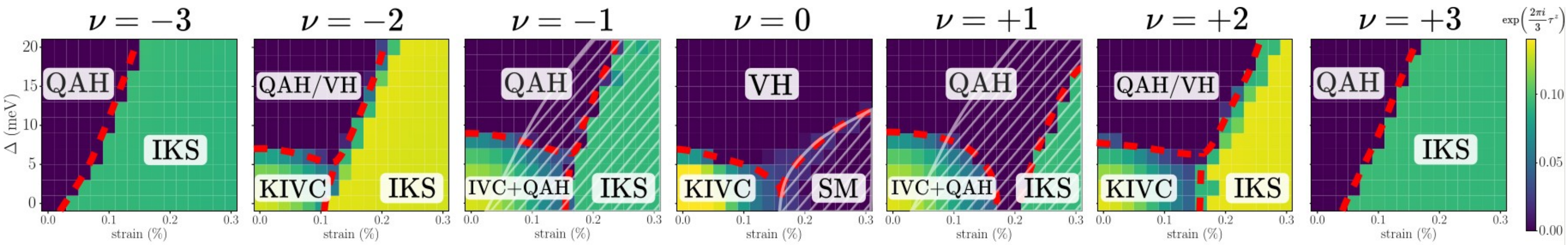
- hBN substrate acts as a sublattice potential
- Breaks C_2 and gaps out Dirac points
- Experiments see QAH at $\nu = +3$ in cases where hBN is aligned with graphene







Phase diagram

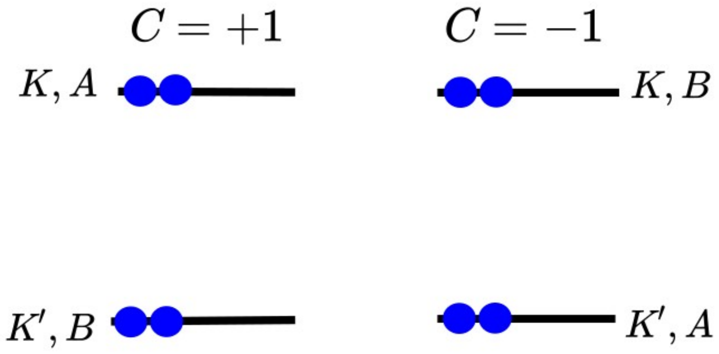


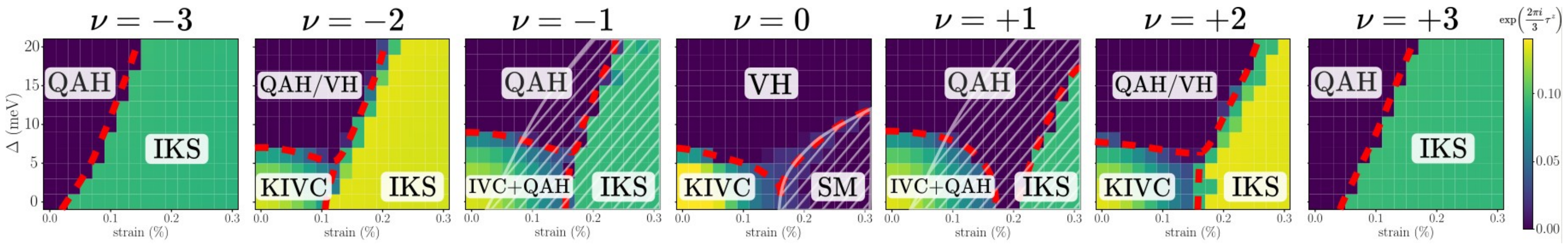
IKS: incommensurate Kekulé spiral
QAH: quantized anomalous Hall state
KIVC: Kramers intervalley coherent state
VH: valley Hall state
IVC: intervalley coherence
SM: semi-metal

- Self-consistent HF with Coulomb interactions
- Allowing for completely general translational symmetry breaking

SM (semi-metal)

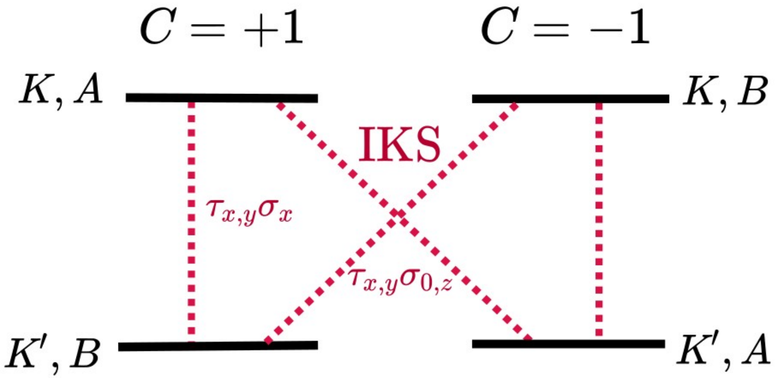
- No spontaneous symmetry breaking

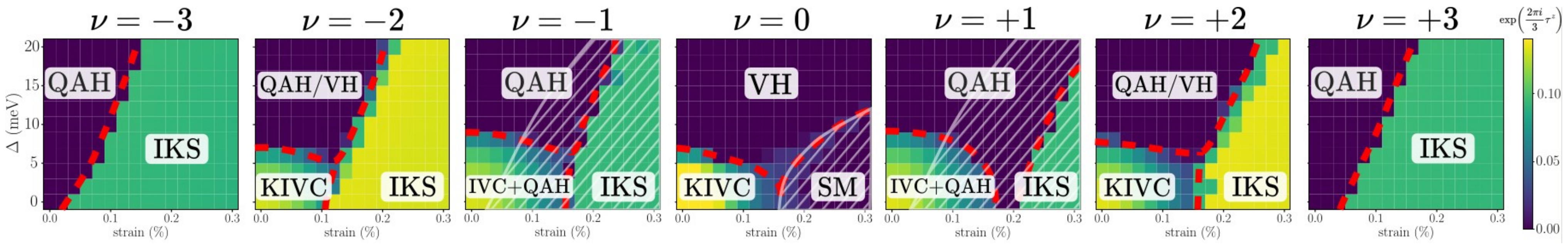




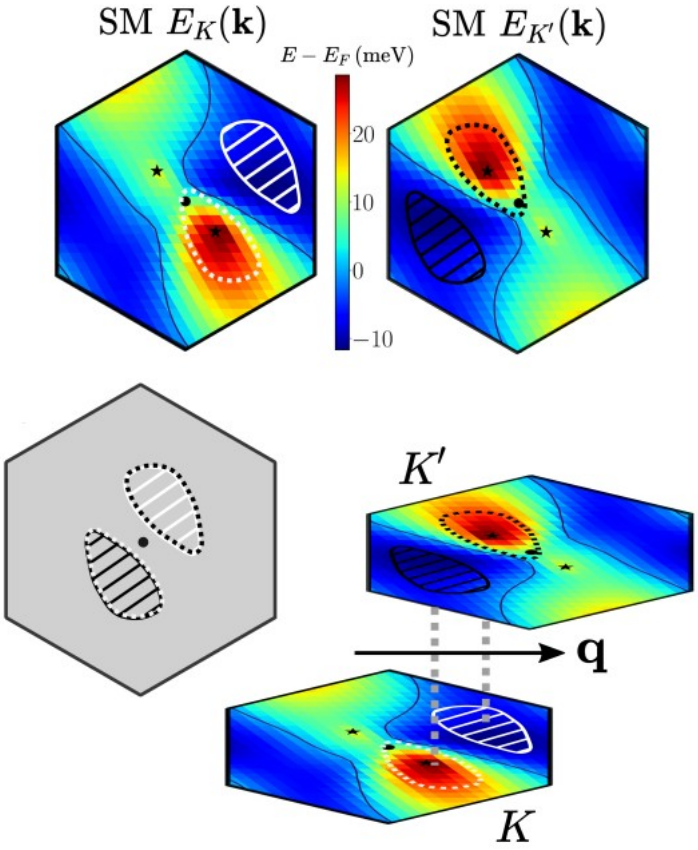
IKS (incommensurate Kekulé spiral)

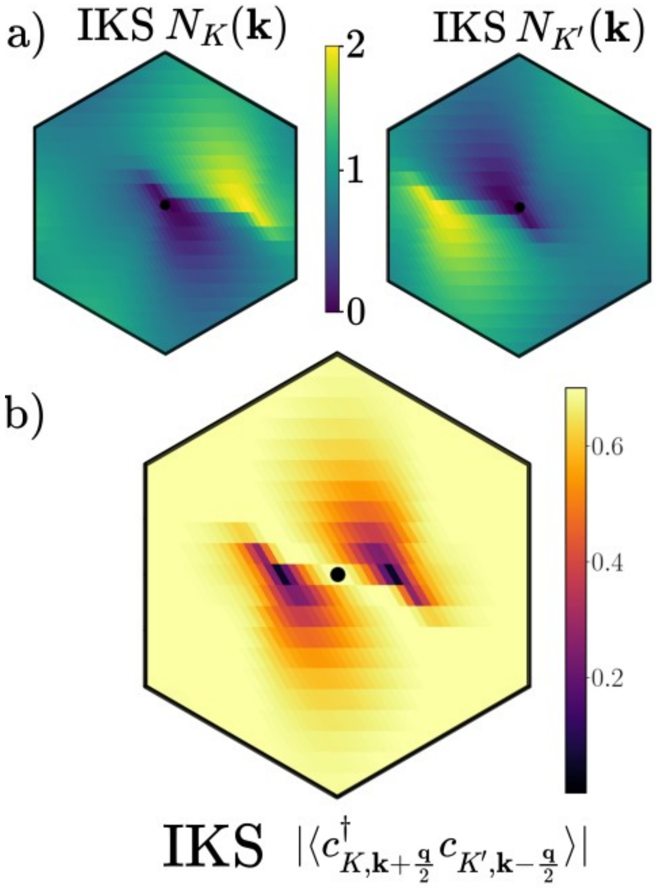
- Intervalley coherence at a finite wavevector





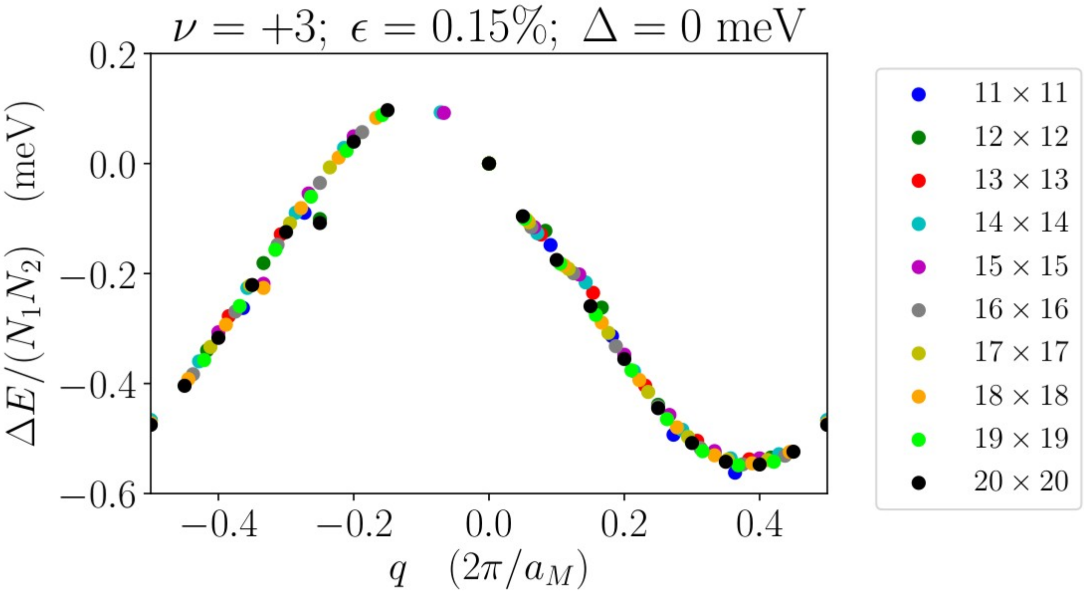
Physical mechanism





IKS order parameter

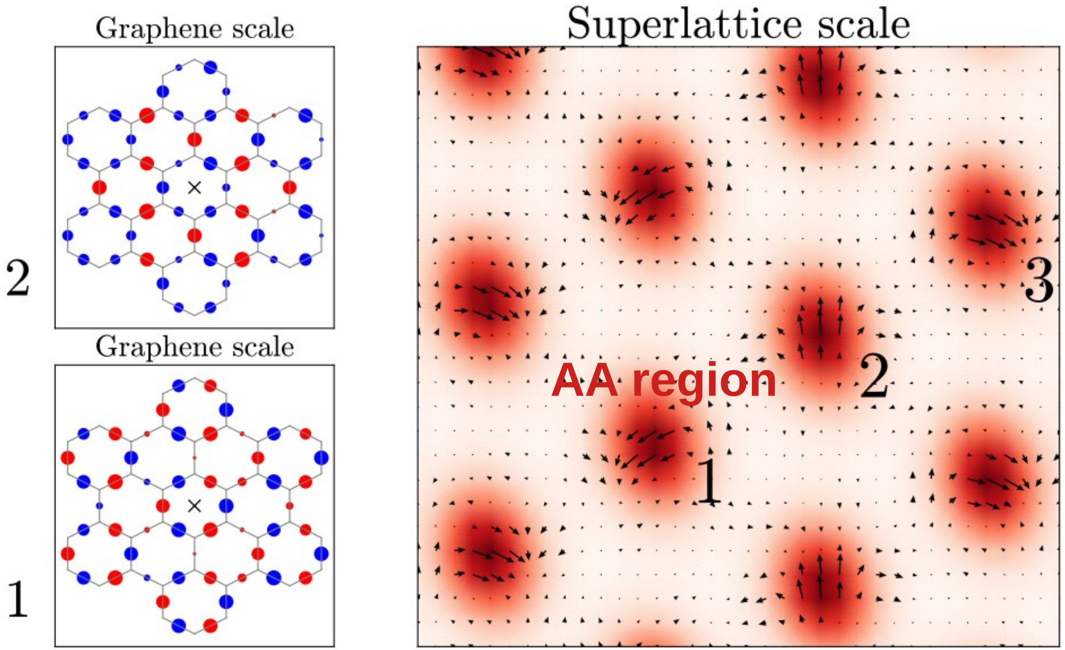
Dispersion relation



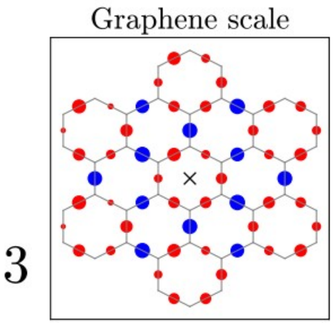
$T_{\mathrm{BKT}} \sim 7\mathrm{K}$

Incommensurate!

Real space picture



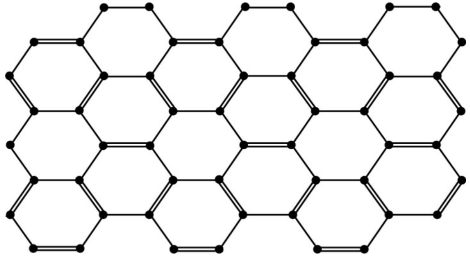
$$\langle c_A^\dagger c_B + c_B^\dagger c_A \rangle > 0$$



$$\langle c_A^\dagger c_B + c_B^\dagger c_A \rangle < 0$$

KIVC=Kekulé distortion (tripling of graphene unit cell)

IKS=spatially modulating Kekulé distortion



Kekulé pattern!

Properties

- Satisfies generalized translation symmetry

$$\hat{T}'_{\mathbf{a}_i} \equiv \hat{T}_{\mathbf{a}_i} e^{i\mathbf{a}_i \cdot \mathbf{q}\, \tau_z/2}$$

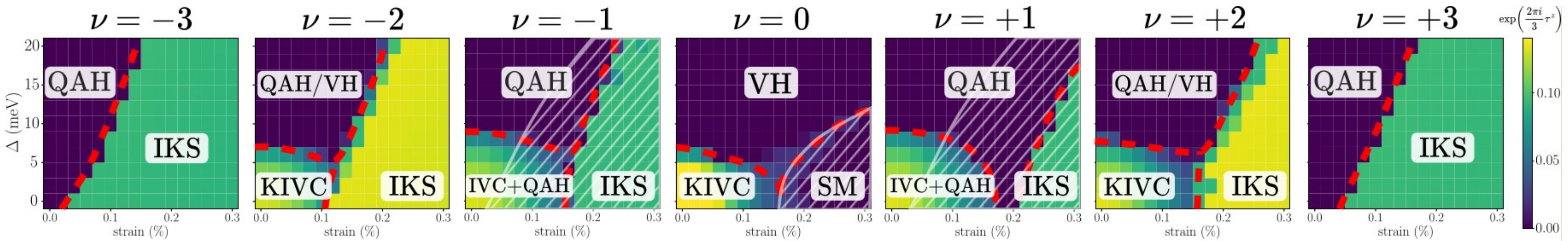
- Generalized Bloch theorem $\psi_{\tilde{\mathbf{k}}}(\mathbf{r}) = e^{i\mathbf{r}\cdot(\tilde{\mathbf{k}} - \tau_z \mathbf{q}/2)} u_{\tilde{\mathbf{k}}}(\mathbf{r})$
- Generalized LSM theorem:

IKS state only gapped at integer ν unless there is additional topological or symmetry breaking order

Experimental features

Experiments

- Semimetal at $\nu = 0$
- Metallic at $\nu = \pm 1$
- Spin-unpolarized insulators at $\nu = \pm 2$
- C=0 insulators at $\nu = +3$
- Nematic superconductivity between $\nu = -3, -2$



Direct Experimental observations?

- First-order strain induced transition from KIVC to IKS at $\nu = \pm 2$ visible in spin moment
- Detect Kekulé pattern using STM
- Interplay between IKS eccentricity and charge order

Summary: Incommensurate Kekulé spiral

- Candidate for insulators seen in TBG
- Stabilized by strain
- Pseudospin spiral at incommensurate wavevector
- Real space: Kekulé distortion