Contrasting electronic nematicity in rigid lattices and moiré superlattices

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Collaborators

Jörn Venderbos, Draxel University

Venderbos and RMF,
Phys. Rev. B **98**, 245103 (2018)

RMF and Venderbos,
Science Adv. **6**, eaba8834 (2020)

Rhine Samajdar, Harvard

Mathias Scheurer, Harvard

Samajdar, Scheurer, Venderbos, and RMF, *in preparation*

Experimentalists

Pablo Jarillo-Herrero, MIT

Yuan Cao, MIT

Cao, …, RMF, Fu, and Jarillo-Herrero, arxiv:2004.04148

Abhay Pasupathy, Columbia

Carmen Verdú-Rubio, Columbia

Simon Turkel, Columbia

Verdú-Rubio, …, RMF, Rubio, and Pasupathy, arxiv:2009.11645

Outline

1. Brief overview of twisted moiré systems
2. Potts-nematicity in moiré superlattices: static strain
3. Potts-nematicity in moiré superlattices: fluctuating strain
4. Electric control of the nematic director

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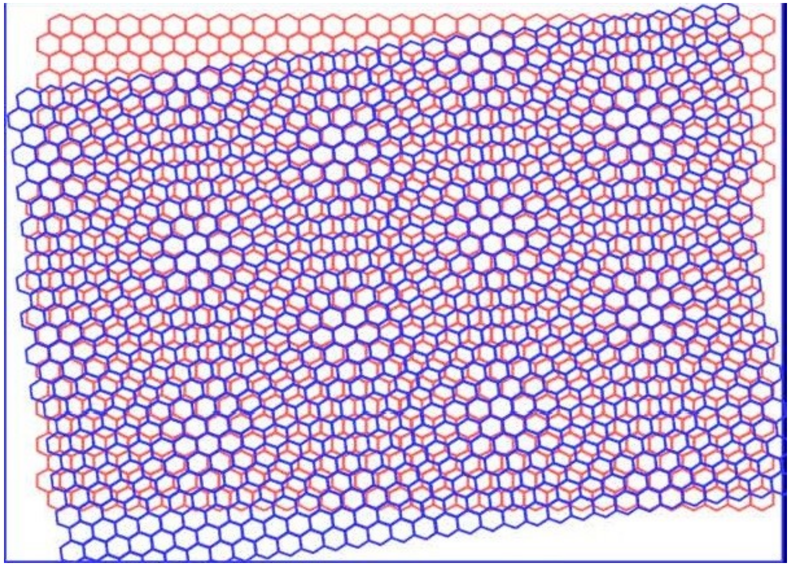
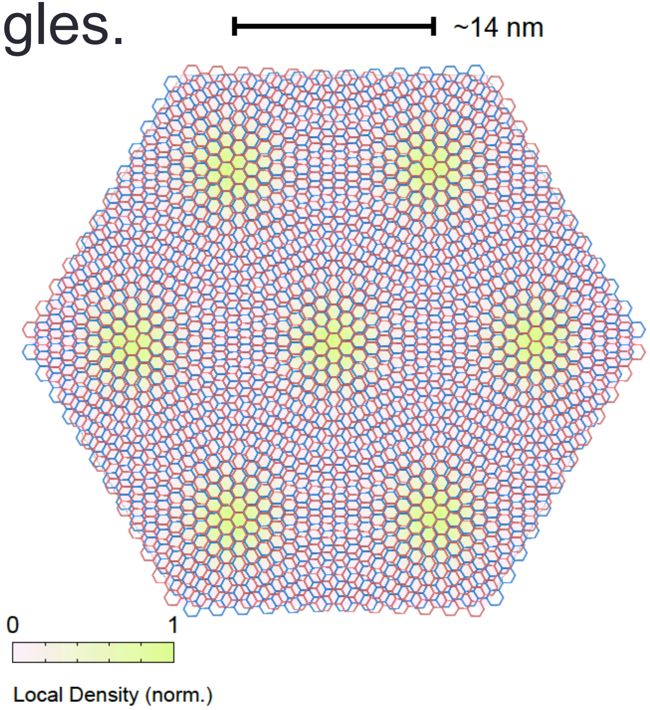
Twisted bilayer graphene (TBG): moiré superlattice

- Two graphene layers twisted by small angles.



Eva Andrei website

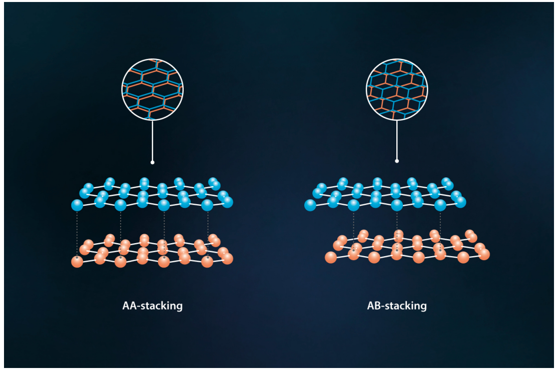


Emergent **moiré lattice**:
huge distance between lattice sites

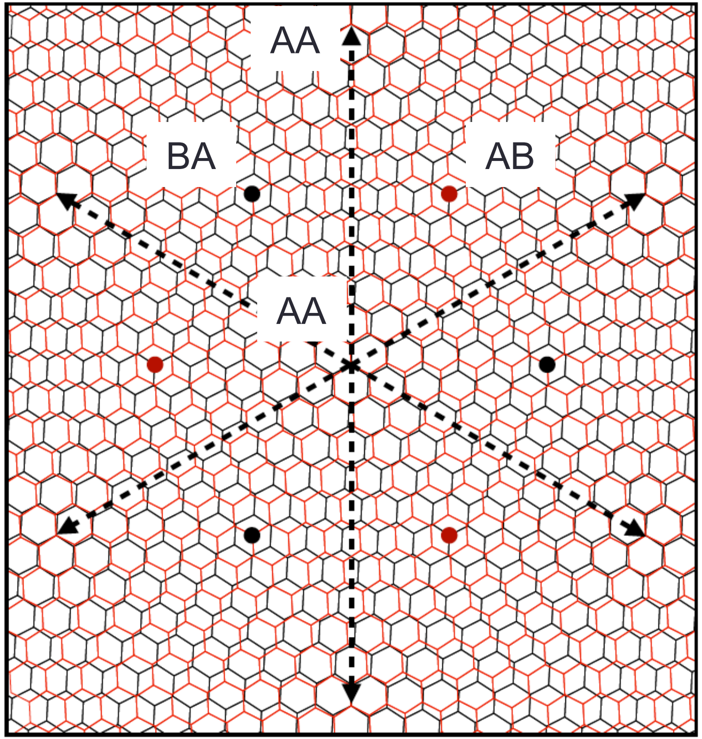
Twisted bilayer graphene (TBG): symmetries

- Emergence of a triangular moiré superlattice

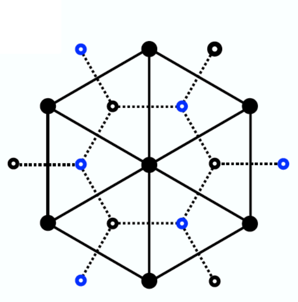
Phys.org

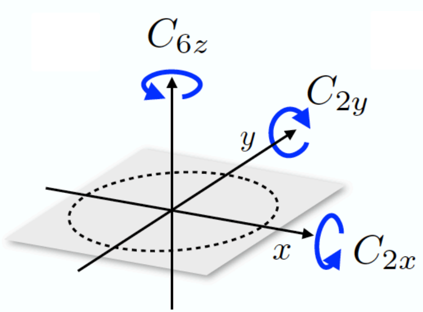


➢ *eight electrons per moiré unit cell*



➢ symmetries: C_{6z}, C_{2x}, C_{2y}





Twisted bilayer graphene (TBG): "flat" bands

- Nearly-flat bands at "magic angle"

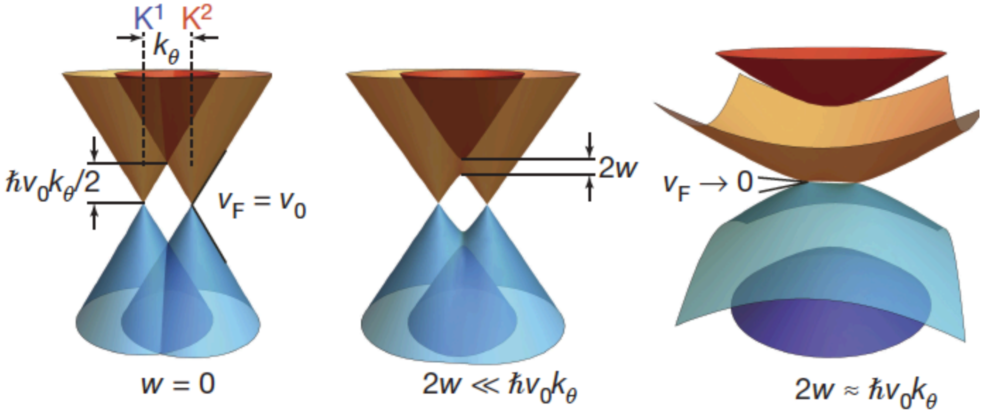
Lopes dos Santos et al, PRL (2007)

Bistritzer and MacDonald, PNAS (2011)

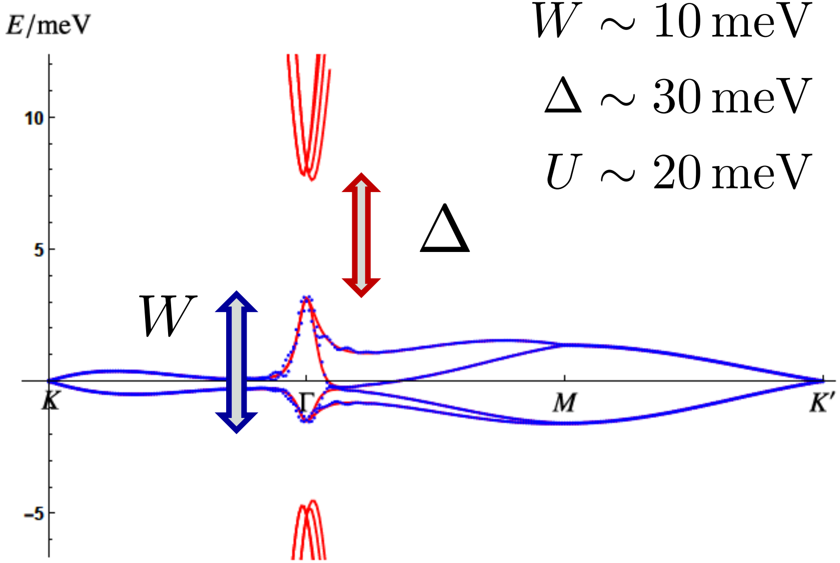
$W \sim 10\,\mathrm{meV}$

$\Delta \sim 30\,\mathrm{meV}$

$U \sim 20\,\mathrm{meV}$



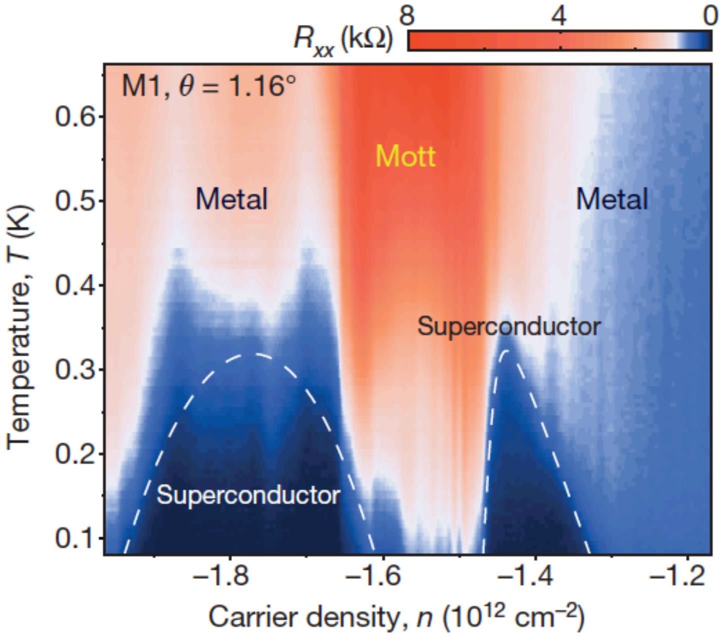
Cao et al, Nature (2018)

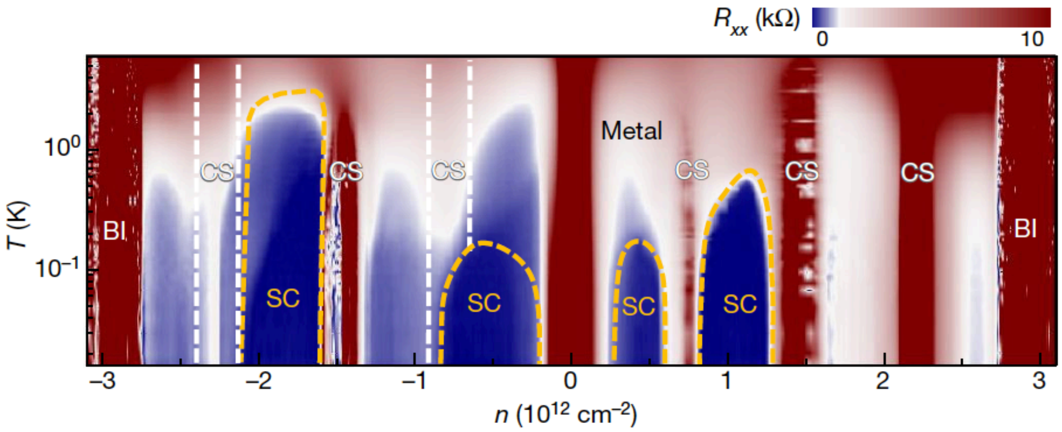


Kang & Vafek, PRX (2018)

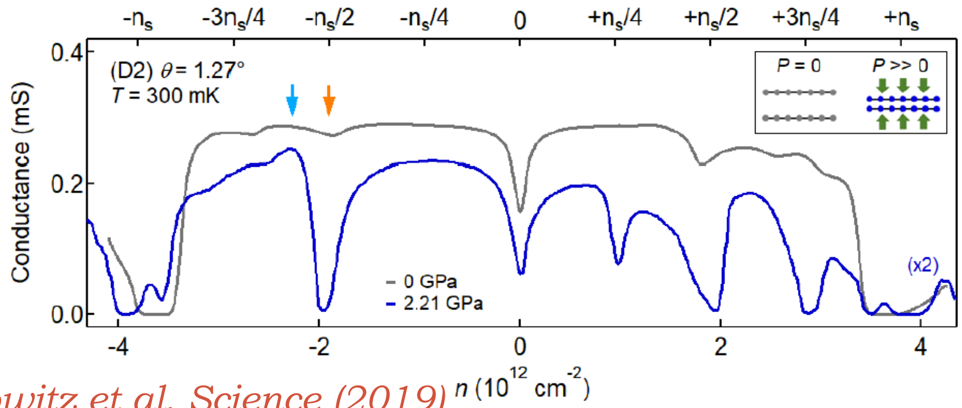
- Interactions give rise to a rich phase diagram and superconductivity.

Cao, ..., Jarillo-Herrero, Nature (2018)





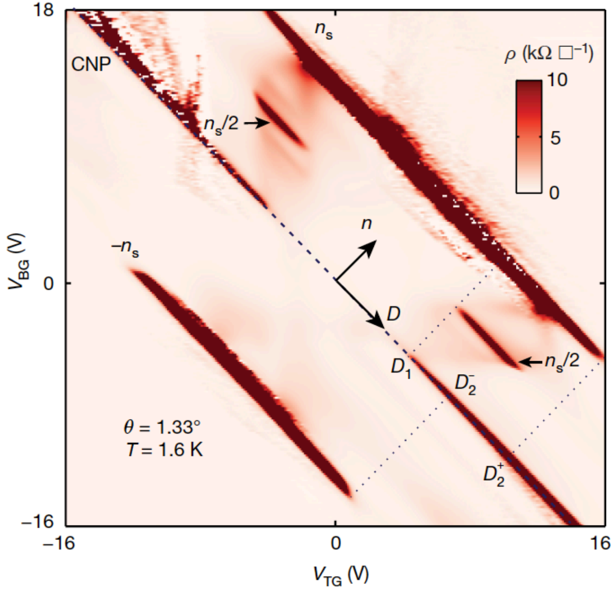
Lu et al, Nature (2019)



Yankowitz et al, Science (2019)

TBG and beyond: twisted moiré systems

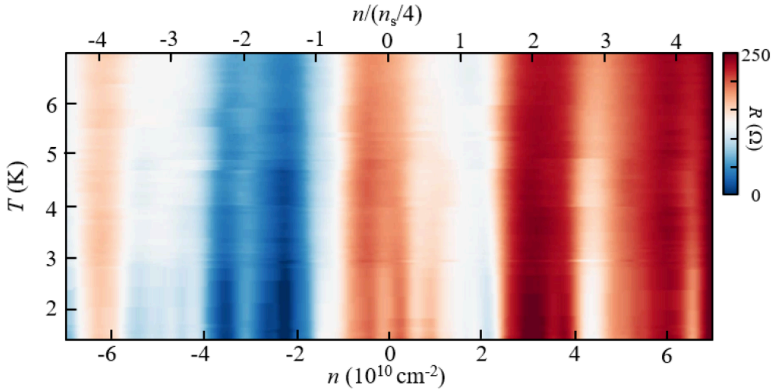
➢ twisted double bilayer graphene (TDBG)



Liu et al, Nature (2020)

Cao et al, Nature (2020)

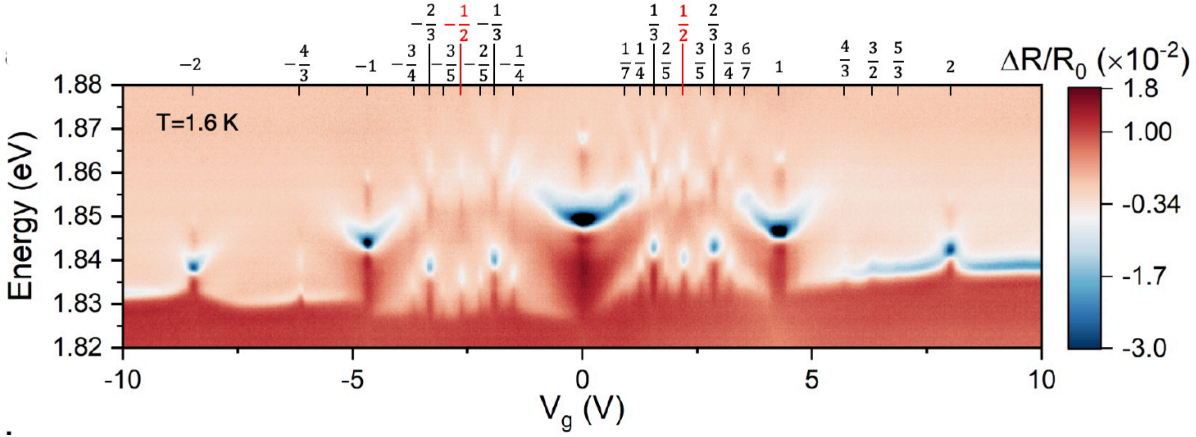
Chen et al, Nature Phys (2020)



➢ twisted trilayer graphene

Tsai et al, arxiv (2020)

➢ dichalcogenide heterobilayers



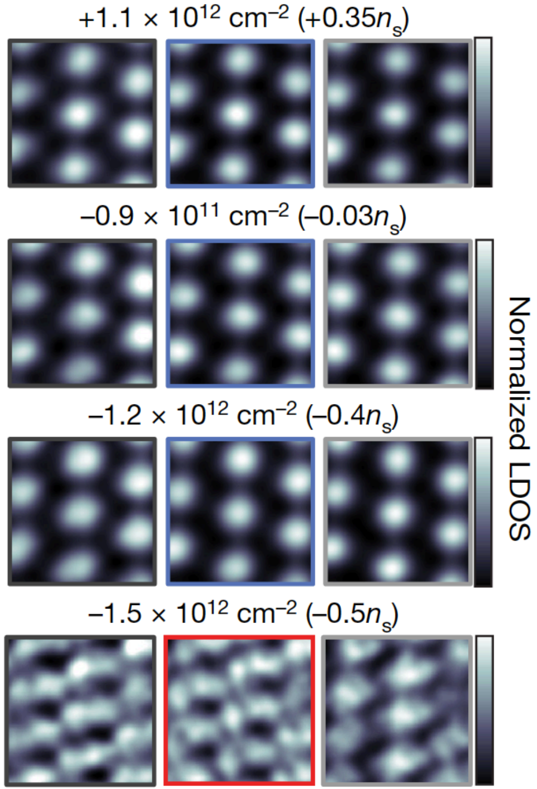
Xu et al, arxiv (2020); Regan et al, Nature Phys (2020)

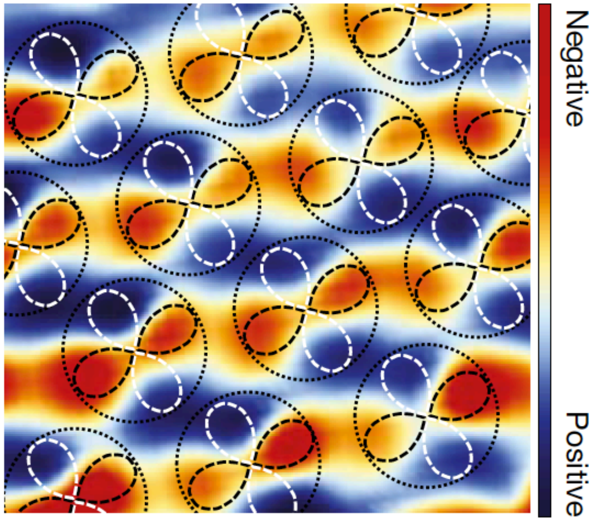
Twisted moiré systems: common properties

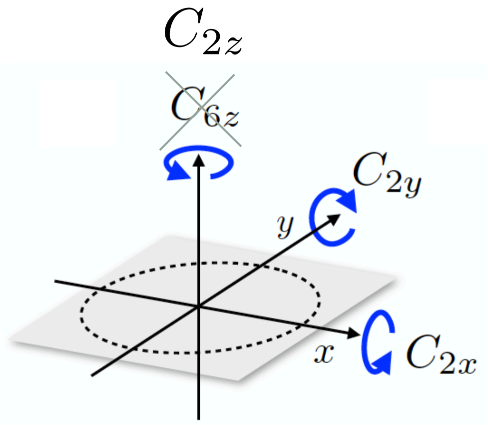
- Are there “universal” features of the phase diagrams?
  - Correlated insulating phases? Yes.
  - Superconductivity? Maybe.
  - Symmetry-breaking phases? Maybe.

Nematicity in twisted bilayer graphene

- Nematic order = breaking of 3-fold rotational symmetry. STM data:







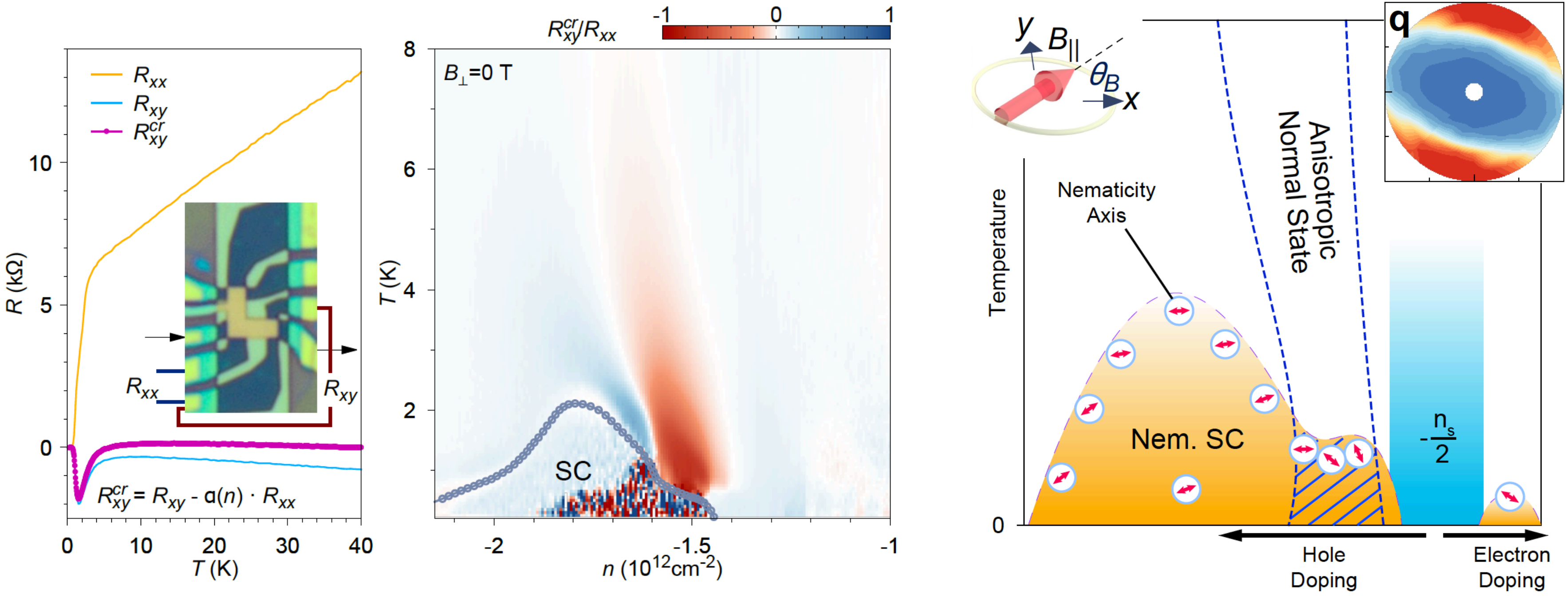
Jian et al, Nature (2019)

Kerelsky et al, Nature (2019)

Choi et al, Nature Phys (2019)

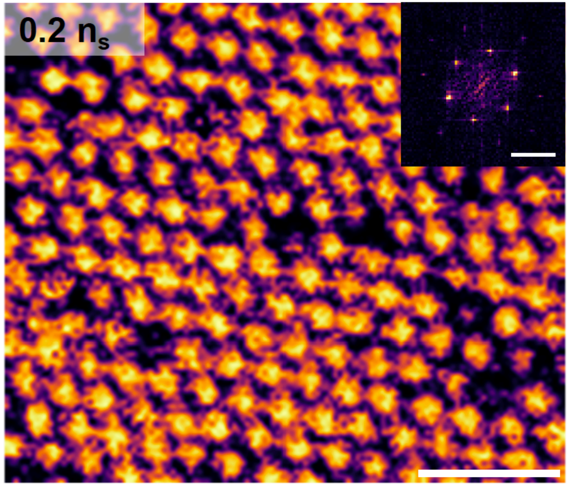
Nematicity in twisted bilayer graphene

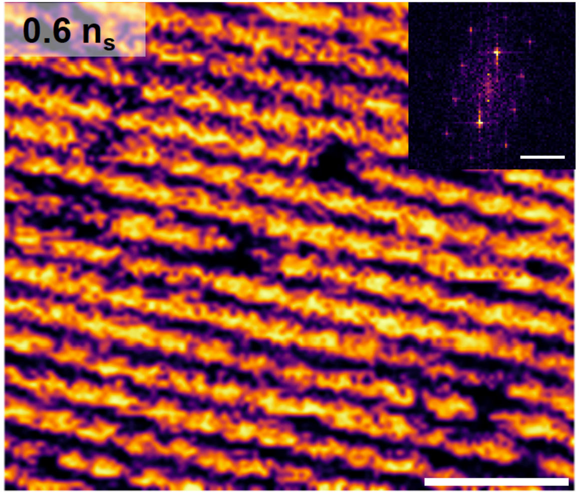
- Nematic order = breaking of 3-fold rotational symmetry. Signatures in transport measurements in the normal and superconducting states.

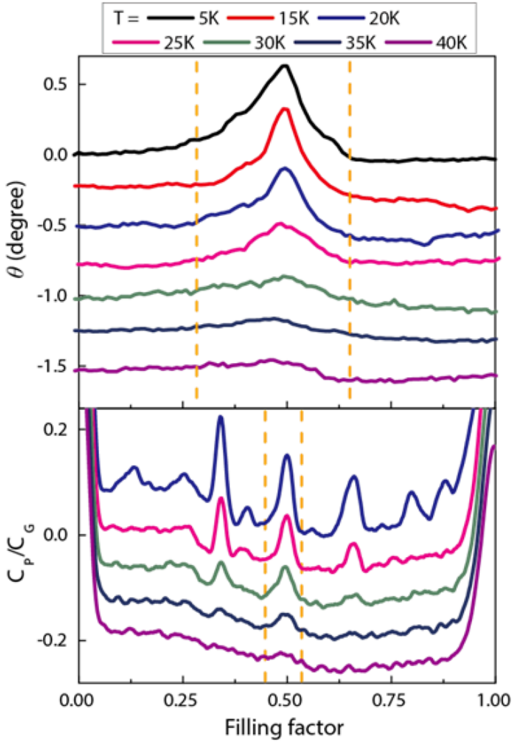


Cao, …, RMF, Fu, and Jarillo-Herrero, arxiv (2020)

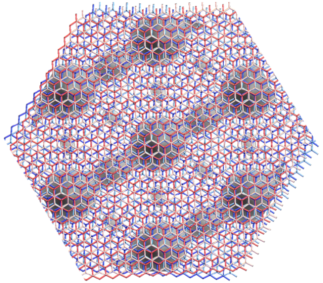
Nematicity in other twisted moiré systems







➢ twisted *double* bilayer graphene



➢ WSe_2/WS_2 heterobilayer

Rubio-Verdú, ..., RMF, Rubio, Pasupathy arxiv (2020)

Jin et al, arxiv (2020)

Nematicity in twisted moiré systems

- General low-energy model to study electronic nematicity in generic moiré superlattices.

- Take-home message: nematicity in moiré superlattices is fundamentally different than in rigid lattices. New effects emerge and unexpected tuning knobs can be used.

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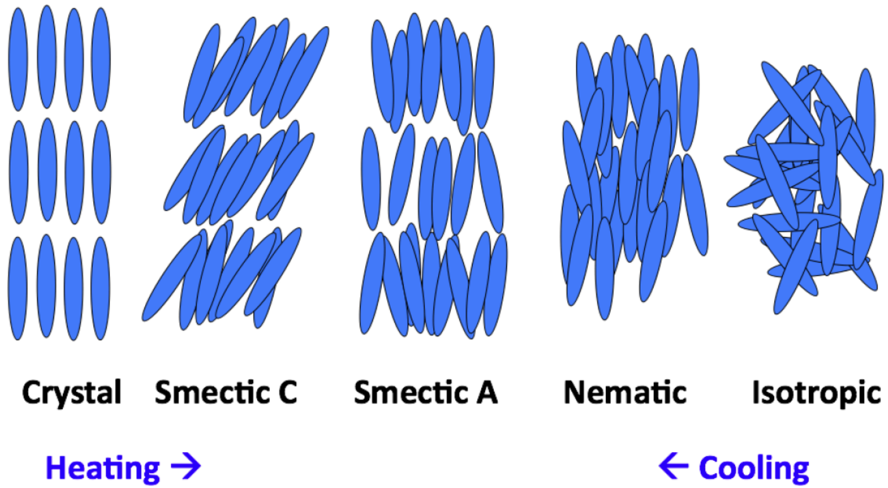
Electronic nematicity: phenomenology

- Nematic order in liquid crystals: orientational order without translational symmetry-breaking.



Mbanga, PhD thesis (2012)

- Order parameter (2D): $Q_{ij} = Q\left(2d_i d_j - \delta_{ij} d^2\right)$

director

Electronic nematicity: phenomenology

- Electronic nematicity: $\hat{Q}_{ij} = \psi^\dagger(\mathbf{r}) \left(2\partial_i\partial_j - \delta_{ij}\nabla^2\right) \psi(\mathbf{r})$

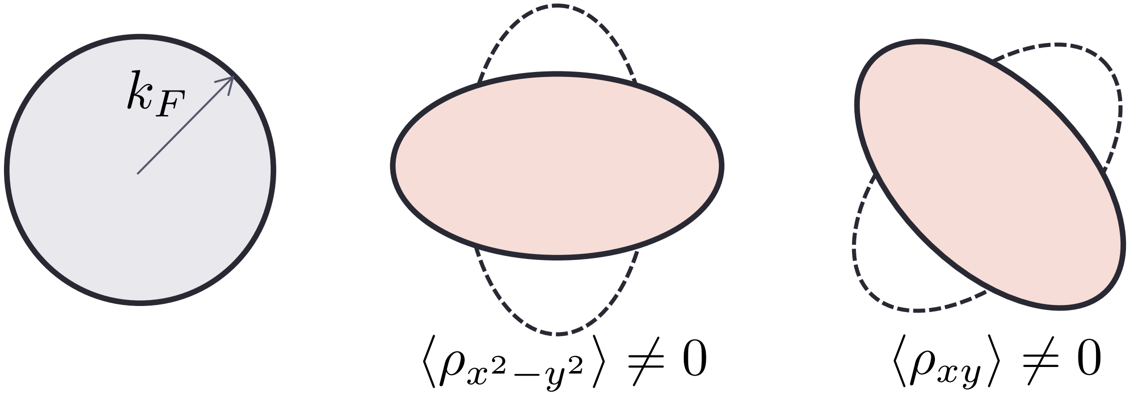
Kivelson, Fradkin, and Emery, Nature (1998)

Electronic nematicity: phenomenology

- Electronic nematicity: $\hat{Q}_{ij} = \psi^\dagger(\mathbf{r})\left(2\partial_i\partial_j - \delta_{ij}\nabla^2\right)\psi(\mathbf{r})$

  - order parameter can be expressed in terms of quadrupolar charge densities:

$$\left\langle \hat{Q} \right\rangle = \begin{pmatrix} \rho_{x^2-y^2} & \rho_{xy} \\ \rho_{xy} & -\rho_{x^2-y^2} \end{pmatrix} \qquad \begin{cases} \rho_{x^2-y^2} \equiv \left\langle (k_x^2 - k_y^2)\hat{\psi}^\dagger(\mathbf{k})\,\hat{\psi}(\mathbf{k})\right\rangle \\ \rho_{xy} \equiv \left\langle (2k_xk_y)\hat{\psi}^\dagger(\mathbf{k})\,\hat{\psi}(\mathbf{k})\right\rangle \end{cases}$$



Electronic nematicity: phenomenology

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  - XY-nematic order parameter $\mathbf{\Phi}$

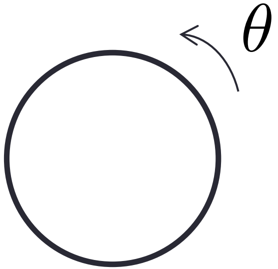
$$\left\langle \hat{Q} \right\rangle = \rho_{x^2-y^2}\sigma^z + \rho_{xy}\sigma^x \qquad \Longrightarrow \qquad \mathbf{\Phi} = \begin{pmatrix} \rho_{x^2-y^2} \\ \rho_{xy} \end{pmatrix}$$

Electronic nematicity: phenomenology

- Electronic nematic free-energy: XY nematics

$$\mathbf{\Phi} = \Phi \begin{pmatrix} \cos 2\theta \\ \sin 2\theta \end{pmatrix}$$

$$\boxed{F_0 = \frac{a}{2}\Phi^2 + \frac{u}{4}\Phi^4}$$



director space

- XY nematics has unique properties: Goldstone mode couples directly (i.e. not via the gradient) to the electronic density, promoting non-Fermi liquid behavior.

Oganesyan, Kivelson, and Fradkin, PRB (2001)
Watanabe and Vishwanath, PNAS (2014)

- Underlying crystal: introduces nematic-anisotropy terms.

$$F_{\text{nem}} = F_0 + F_{\text{cr}}$$

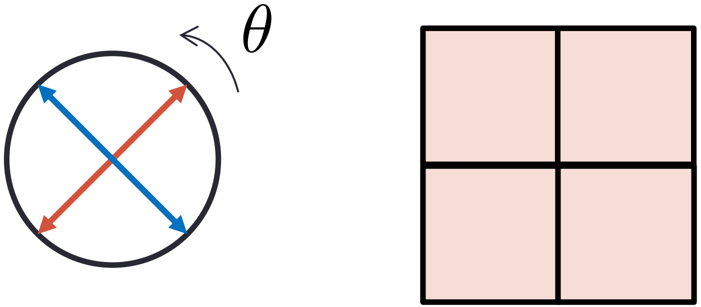
Electronic nematicity: impact of the lattice

- Square lattice: **Ising-nematicity** (cuprates and pnictides)

Fradkin et al, Ann. Rev. Cond. Matter Phys (2010)
RMF, Chubukov, Schmalian, Nature Phys (2014)

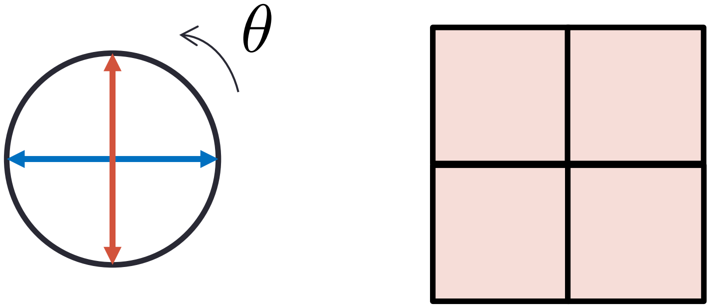
$$F_{\mathrm{cr}} = \gamma\left(\Phi_1^2 - \Phi_2^2\right) = \gamma\Phi^2 \cos 4\theta$$

B_{2g} channel



$\gamma > 0$

B_{1g} channel

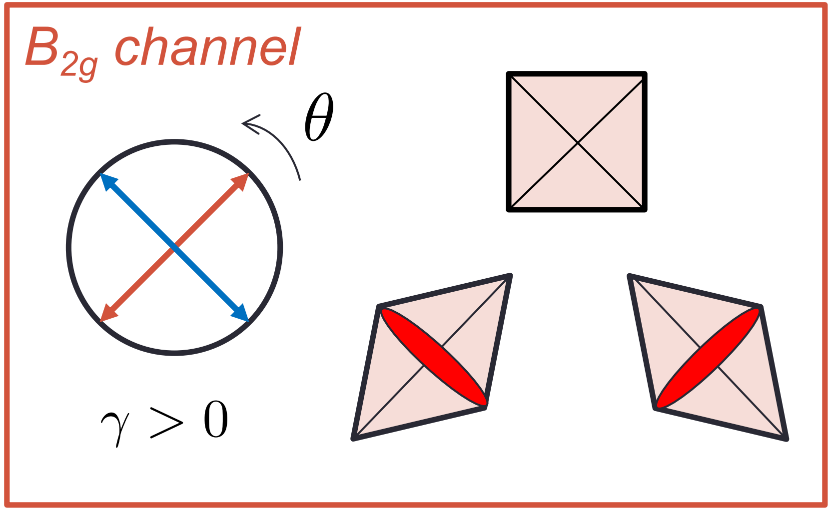


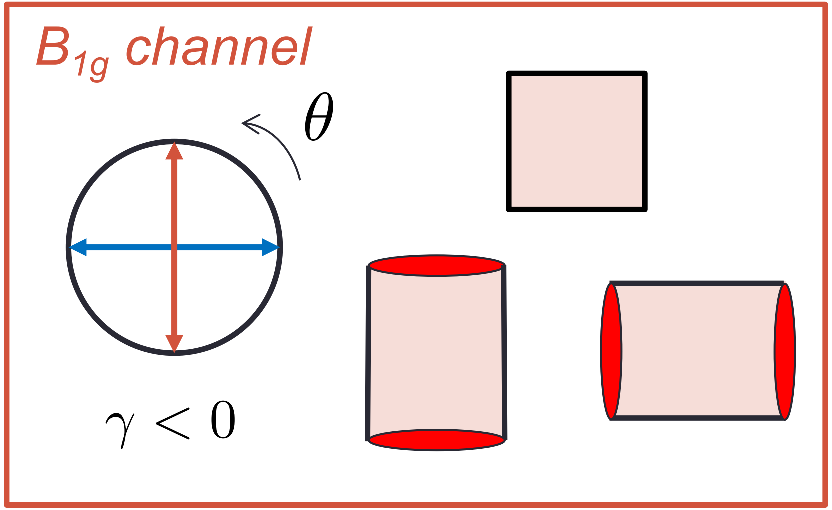
$\gamma < 0$

Electronic nematicity: impact of the lattice

- Square lattice: **Ising-nematicity** (cuprates and pnictides)
- Nematic order *always* triggers a structural distortion.

$$F_{\mathrm{cr}} = \gamma\left(\Phi_1^2 - \Phi_2^2\right) = \gamma\Phi^2\cos 4\theta$$

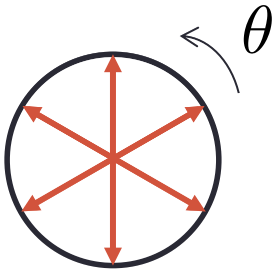


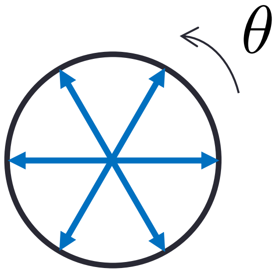


Electronic nematicity: impact of the lattice

- Triangular lattice: the two components of $\mathbf{\Phi}$ transform as the same irreducible representation (E_{2g}). Cubic term is allowed:

$$F_{\rm cr}=\frac{\gamma}{3}\Phi_1\left(\Phi_1^2-3\Phi_2^2\right)=\frac{\gamma}{3}\Phi^3\cos 6\theta$$





Hecker & Schmalian, npj QM (2018)

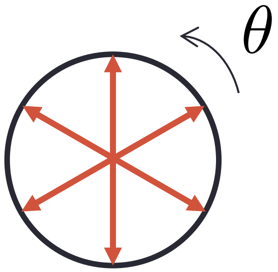
Venderbos & RMF, PRB (2018)

Little et al, Nature Materials (2020)

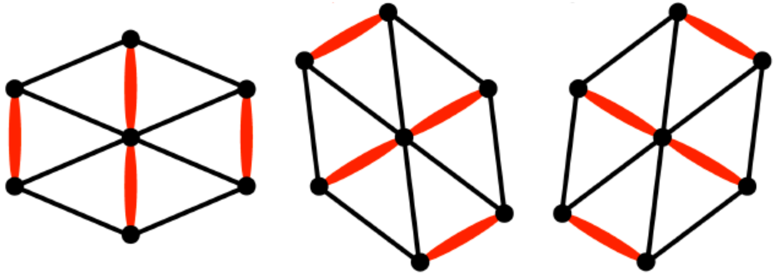
Electronic nematicity: impact of the lattice

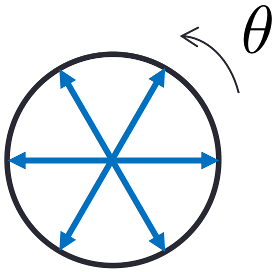
- Triangular lattice: **3-state Potts nematicity** (twisted bilayer graphene, Bi_2Se_3, $Fe_{1/3}NbS_2$)
- Nematic order *always* triggers a structural distortion.

$$F_{\mathrm{cr}} = \frac{\gamma}{3}\Phi_1(\Phi_1^2 - 3\Phi_2^2) = \frac{\gamma}{3}\Phi^3 \cos 6\theta$$



$\gamma > 0$





$\gamma < 0$

Hecker & Schmalian, npj QM (2018)

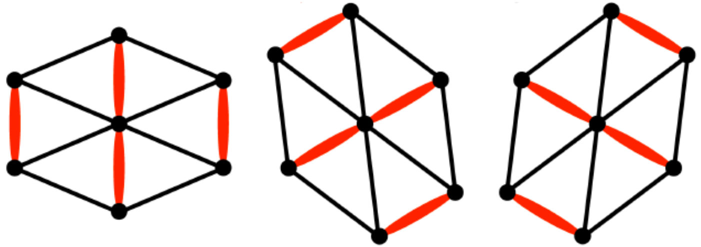
Venderbos & RMF, PRB (2018)

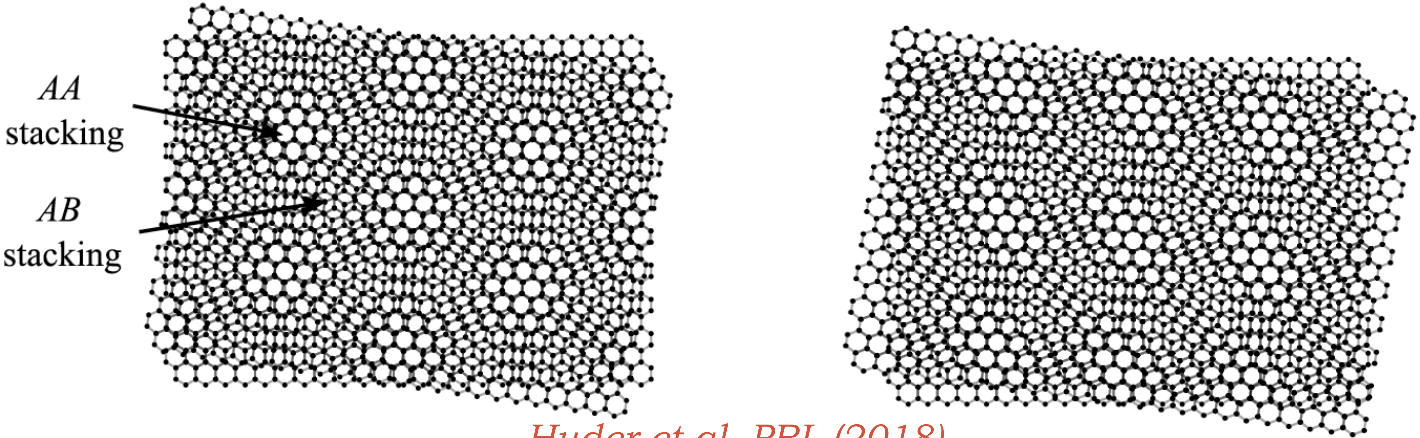
Little et al, Nature Materials (2020)

twofold rotational symmetries are preserved

Nematicity in TBG: static strain

- Build-in strain is unavoidable in TBG. Strain induces structural distortions. How to distinguish effects caused by nematic order from effects caused by strain?



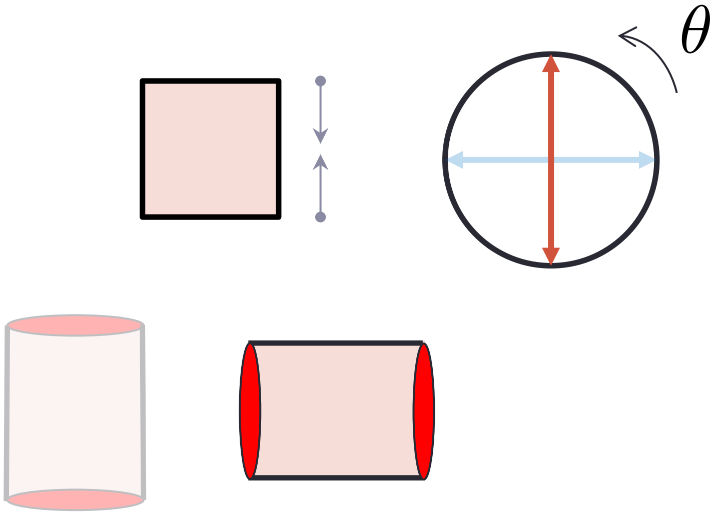


Huder et al, PRL (2018)

Nematicity in TBG: static strain

- Build-in strain is unavoidable in TBG. Can the nematic transition survive?

tetragonal lattice:



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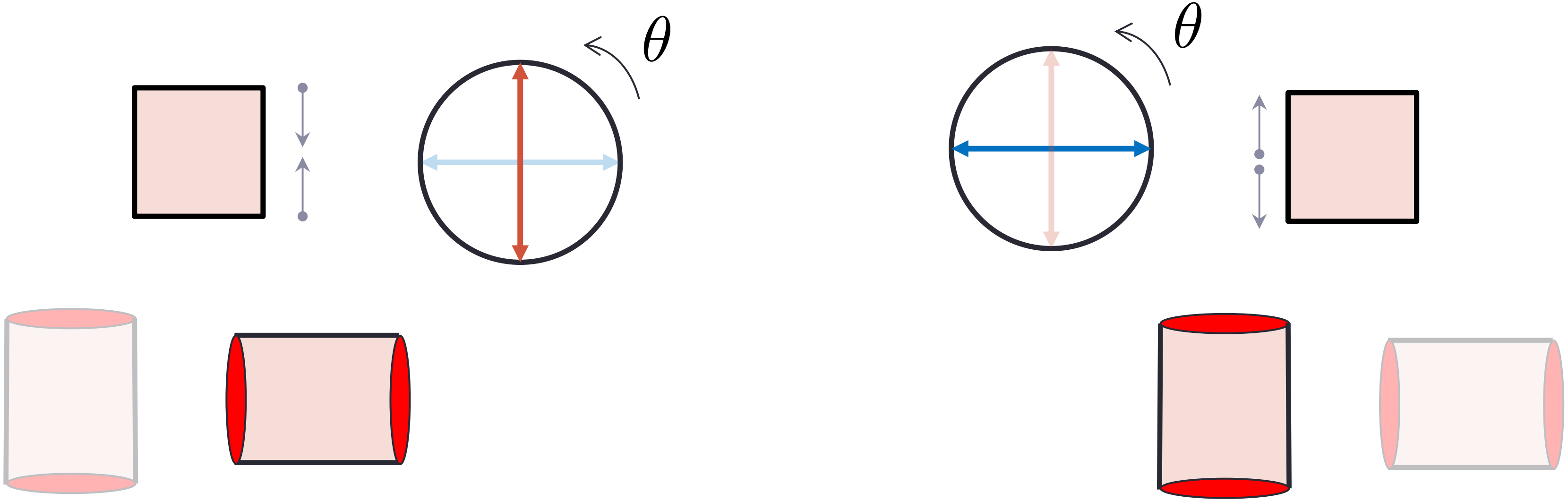
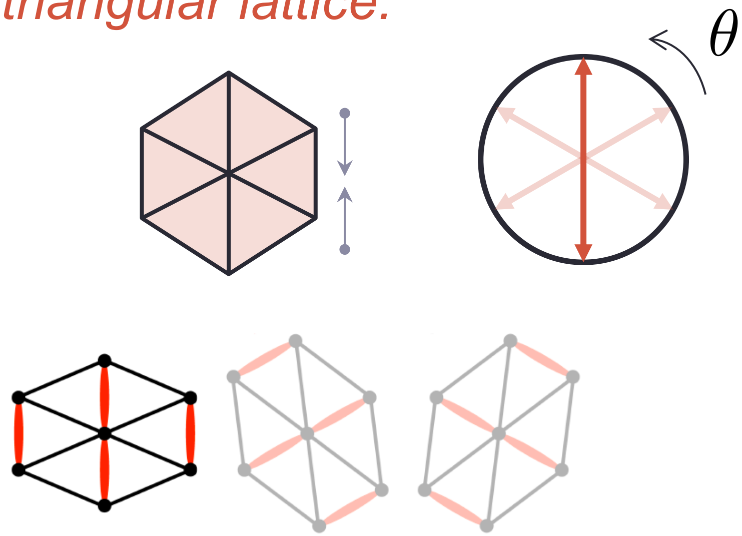


no Ising-nematic transition in the presence of strain

Nematicity in TBG: static strain

- Build-in strain is unavoidable in TBG. Can the nematic transition survive?

triangular lattice:



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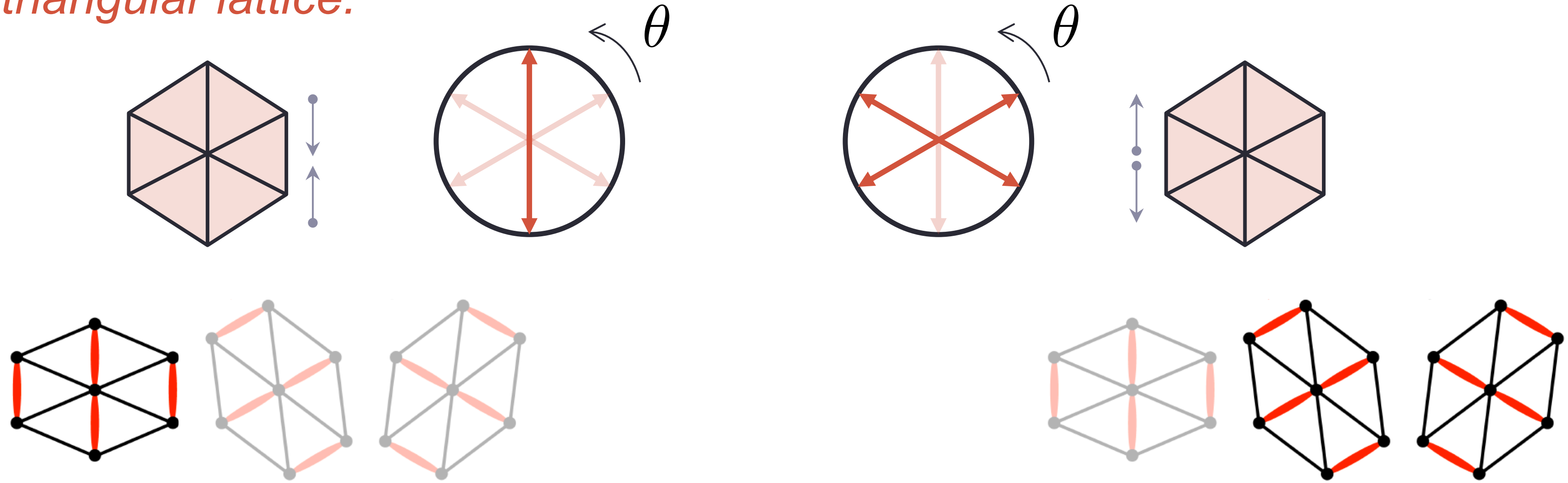


residual Ising symmetry related to in-plane rotations

Nematicity in TBG: static strain

- Nemato-elastic coupling: formalism $\Phi_{\pm} = \Phi_1 \pm i\Phi_2$

$$S_{\text{nem}}\left[\boldsymbol{\Phi}\right] = S_0\left[\Phi\right] + \frac{\gamma}{6}\int_x \left(\Phi_+^3 + \Phi_-^3\right)$$

$$\varepsilon_{ij} = \frac{1}{2}\left(\partial_i u_j + \partial_j u_i\right)$$ *: static strain*

$\mathbf{u}$ *: relative displacement between the two layers*

$$S'\left[\boldsymbol{\Phi}, \hat{\varepsilon}\right] = -\lambda \int_x \left[\left(\varepsilon_{xx} - \varepsilon_{yy}\right)\Phi_1 + 2\varepsilon_{xy}\Phi_2\right]$$

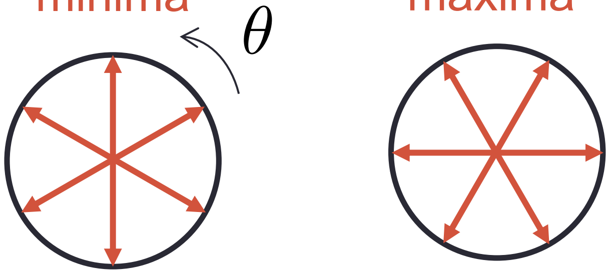
uniaxial strain: frustration of the nematic director

Nematicity in TBG: static strain

- Example: strain along *y* axis with $\lambda<0$ and $\gamma>0$.

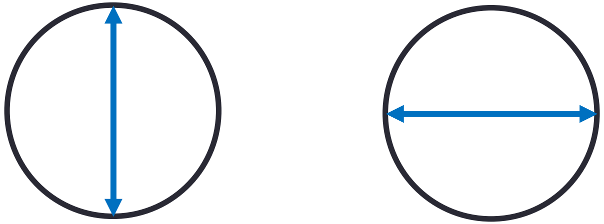
$$S_{\text{nem}}[\mathbf{\Phi}] = S_0[\Phi] + \underbrace{\frac{\gamma}{6}\int_x \left(\Phi_+^3 + \Phi_-^3\right)}_{+\Phi^3 \cos 6\theta}$$

minima maxima



$$S'[\mathbf{\Phi}, \hat{\varepsilon}] = \underbrace{-\lambda \int_x \left[\left(\varepsilon_{xx} - \varepsilon_{yy}\right)\Phi_1 + 2\varepsilon_{xy}\Phi_2\right]}_{-\varepsilon\,\Phi \cos 2\theta}$$

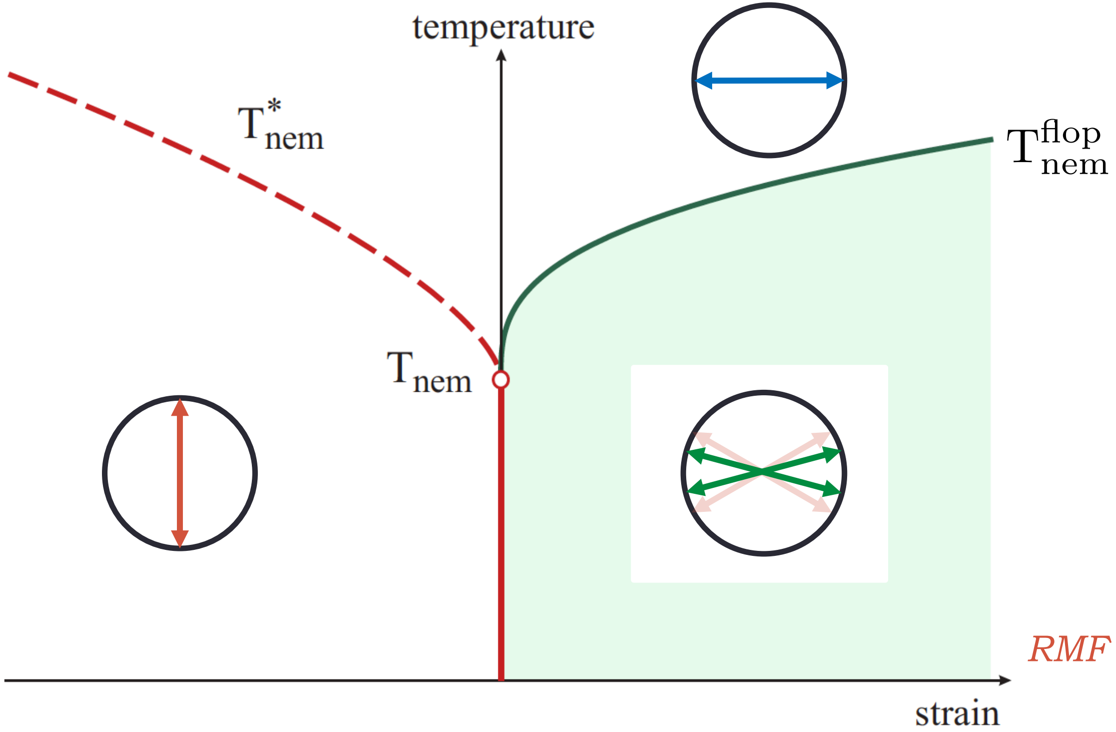
minimum (compressive) minimum (tensile)



maximum (tensile) maximum (compressive)

Nematicity in TBG: static strain

- Ising-like *nematic-flop* transition in the presence of uniaxial strain

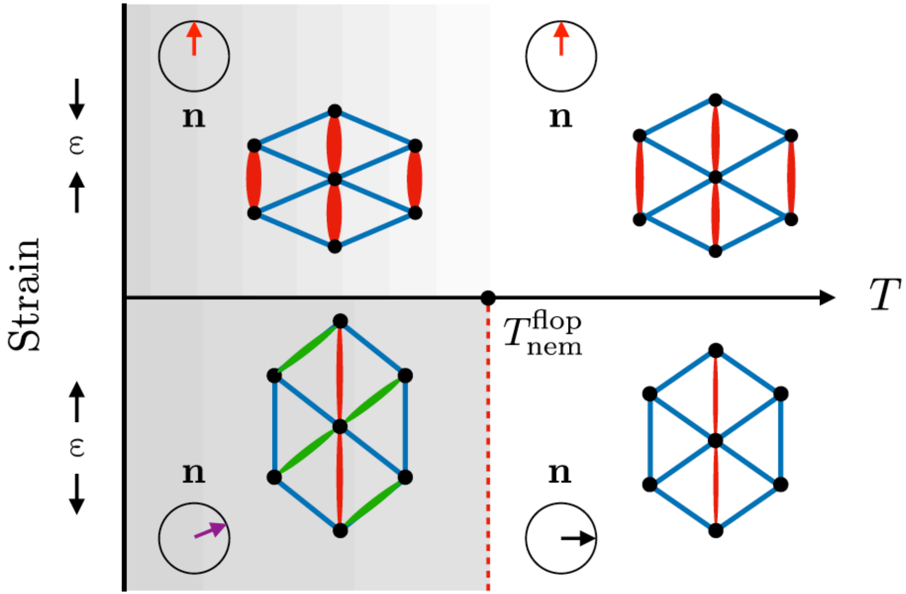


RMF & Venderbos, Sci. Adv. (2020)

can be used to establish long-range nematic order experimentally

Nematicity in TBG: static strain

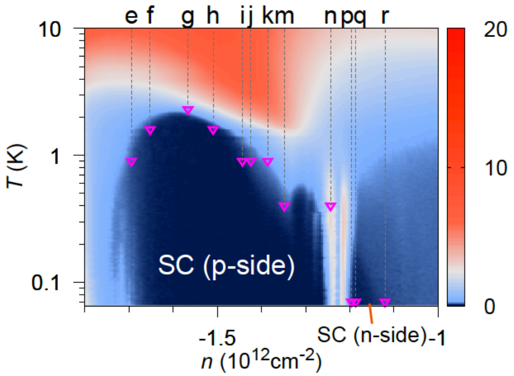
- Ising-like *nematic-flop* transition in the presence of static strain

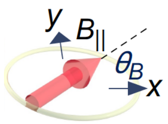


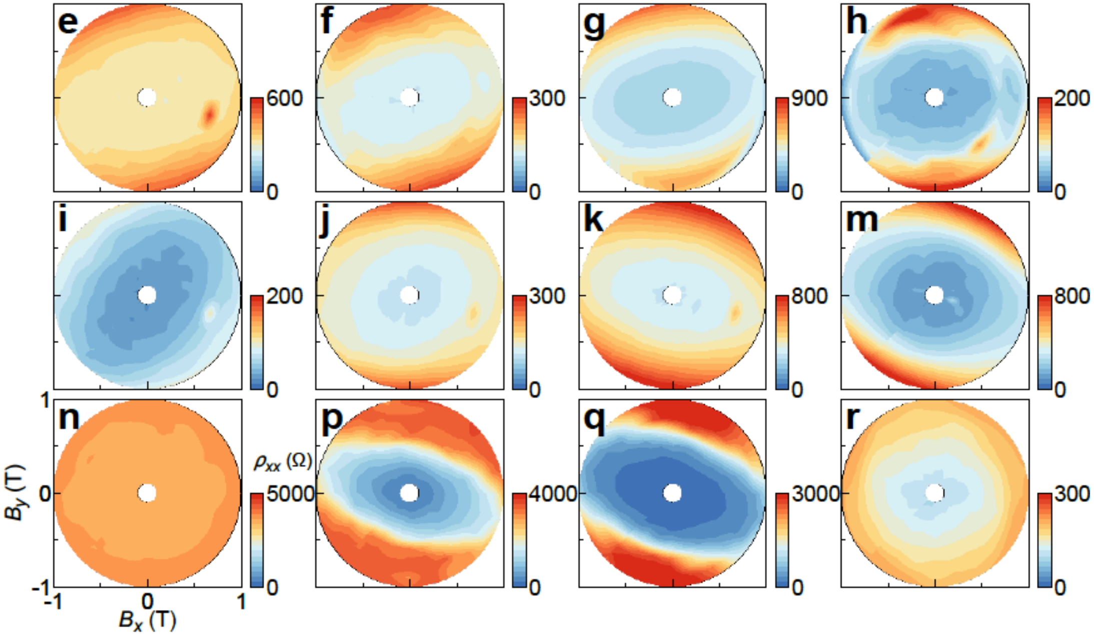
bond-order pattern can establish long-range nematic order experimentally

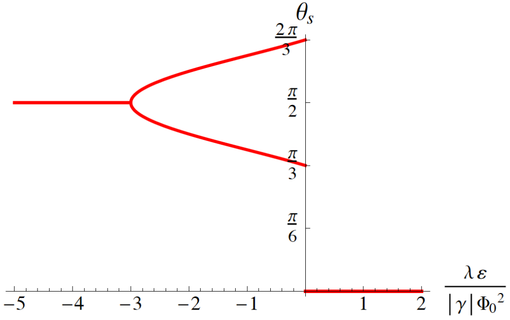
Nematicity in the superconducting state of TBG

- Nematic director rotates as a function of doping inside the superconducting state: evidence for spontaneous nematic order.









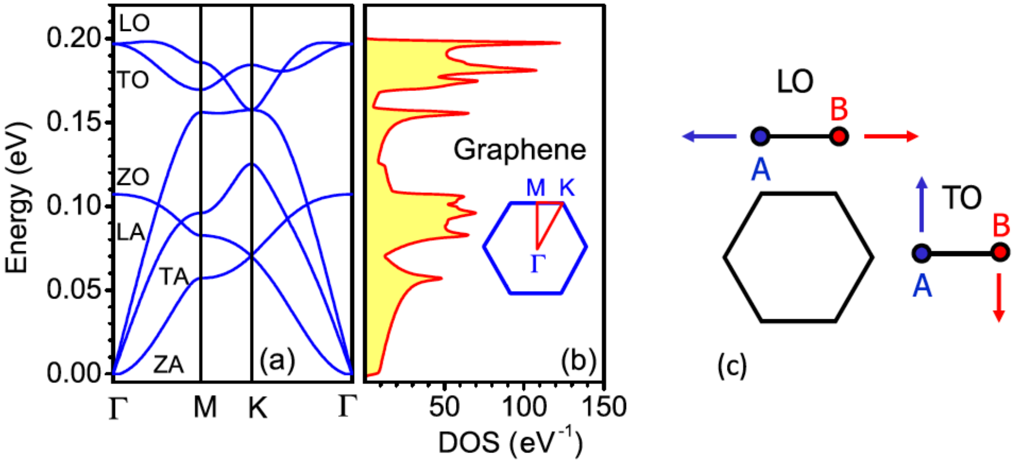
Cao, …, RMF, Fu, and Jarillo-Herrero, arxiv (2020)

Outline

1. Brief overview of twisted moiré systems
2. Potts-nematicity in moiré superlattices: static strain
3. Potts-nematicity in moiré superlattices: fluctuating strain
4. Electric control of the nematic director

Nematicity in TBG: fluctuating strain

- Finite-momentum strain fluctuations: acoustic phonons



$$S_{\mathrm{el}} = \frac{1}{2} \sum_{\mu=L,T} \int_q \tilde{u}_{q,\mu} \left(\omega_n^2 + v_\mu^2 \mathbf{q}^2\right) \tilde{u}_{-q,\mu}$$

$$\hat{\mathbf{e}}_L = (\cos\zeta_{\mathbf{q}}, \, \sin\zeta_{\mathbf{q}})$$

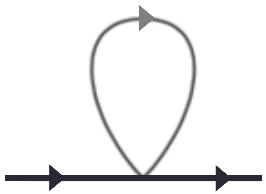
$$\hat{\mathbf{e}}_T = (-\sin\zeta_{\mathbf{q}}, \, \cos\zeta_{\mathbf{q}})$$

Sanders et al, J Phys: Cond Matt (2013)

triangular lattice: purely transversal and purely longitudinal modes

Nematicity in TBG: fluctuating strain

- Acoustic phonons mediate long-range anisotropic nematic interactions



$$\delta S = \int_{\mathbf{r},\mathbf{r}'} \frac{\Phi_i\left(\mathbf{r}\right) A_{ij}\left(\hat{\mathbf{r}}\cdot\hat{\mathbf{r}}'\right)\Phi_j\left(\mathbf{r}'\right)}{\left|\mathbf{r}-\mathbf{r}'\right|^2}$$

Cowley, PRB (1976)

Karahasonovic and Schmalian, PRB (2016)

Paul and Garst, PRL (2017)

Nematicity in TBG: fluctuating strain

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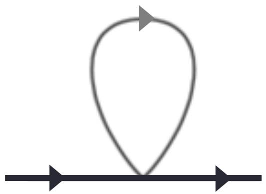


$$\delta S = \int_{\mathbf{r},\mathbf{r}'} \frac{\Phi_i\left(\mathbf{r}\right) A_{ij}\left(\hat{\mathbf{r}}\cdot\hat{\mathbf{r}}'\right)\Phi_j\left(\mathbf{r}'\right)}{\left|\mathbf{r}-\mathbf{r}'\right|^2}$$

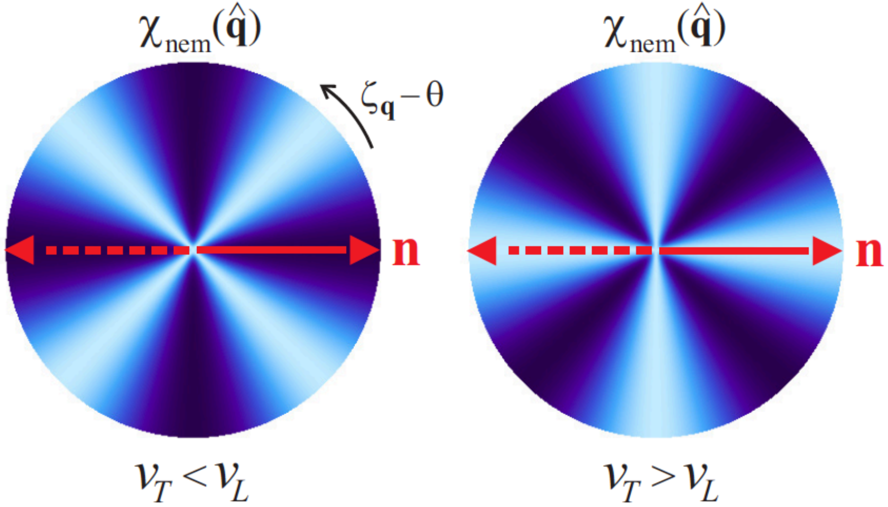
- In momentum-space, this corresponds to a nemato-orbital coupling

$$\delta S = \frac{\lambda^2}{v_T^2}\left(1-\frac{v_T^2}{v_L^2}\right)\int_q \left(\mathbf{\Phi}\cdot\hat{\mathbf{D}}\right)^2 \qquad \hat{\mathbf{D}} = \left(\hat{q}_x^2-\hat{q}_y^2,\, 2\hat{q}_x\hat{q}_y\right)$$

Nematicity in TBG: nemato-orbital coupling

- Nemato-orbital coupling ties the orientation of the nematic director to certain directions in momentum space.

$$\chi_{\mathrm{nem}}^{-1}(q,\zeta_{\mathbf{q}}) = r_0 + q^2 + \left(1 - \frac{v_T^2}{v_L^2}\right)\cos^2\left(2\theta - 2\zeta_{\mathbf{q}}\right)$$

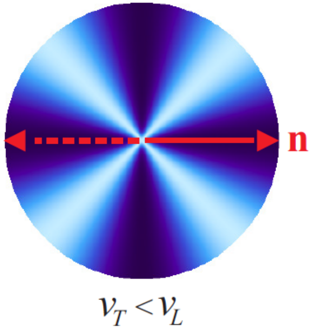


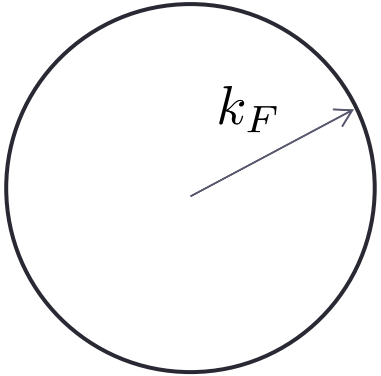
restriction of phase space is expected to render the transition mean-field and first-order (d_c=3)

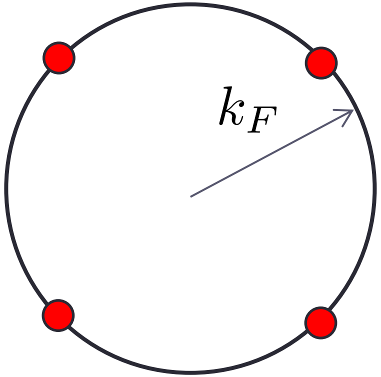
RMF & Venderbos, Sci. Adv. (2020)

Nematicity in TBG: coupling to electrons

- **Hot spots:** electrons efficiently exchange soft nematic fluctuations







Nematicity in TBG: coupling to electrons

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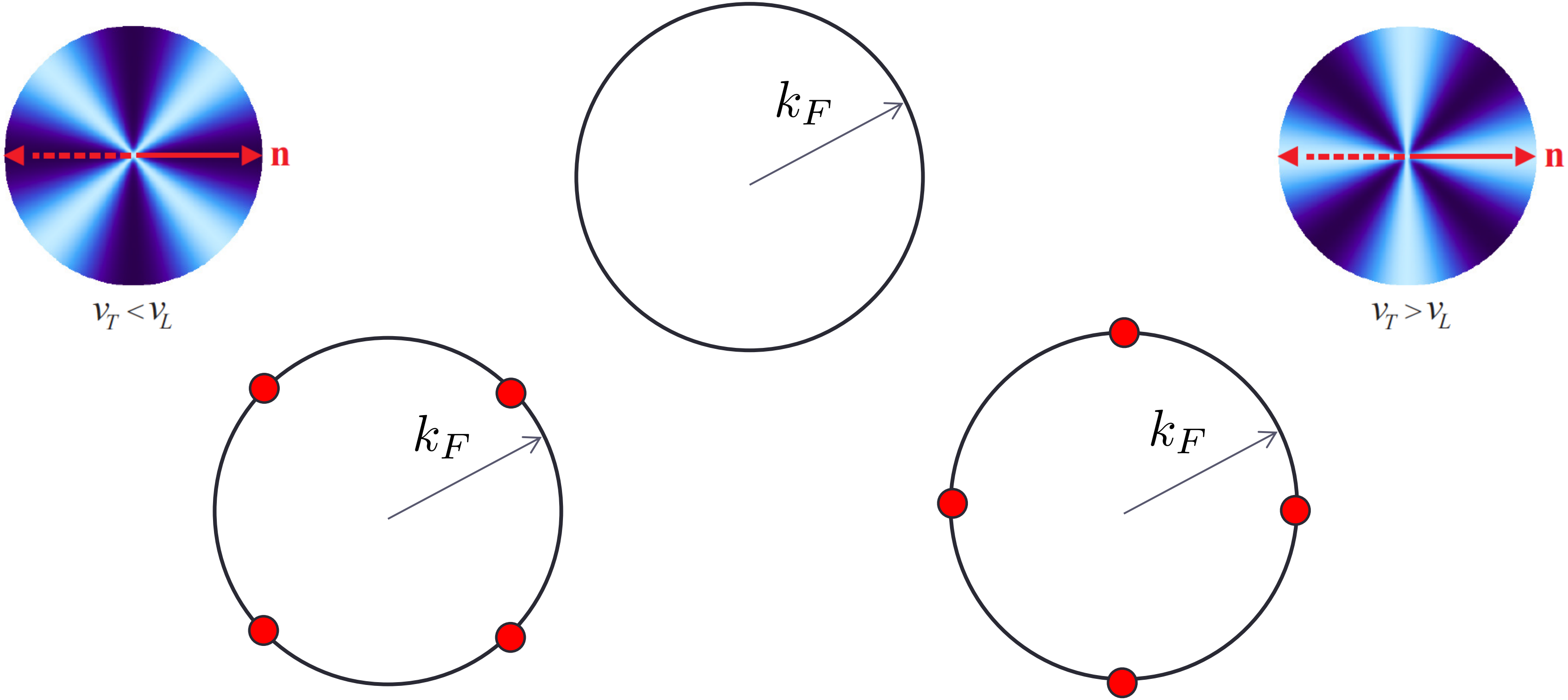
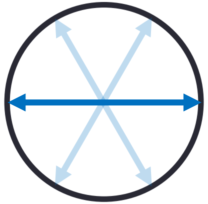
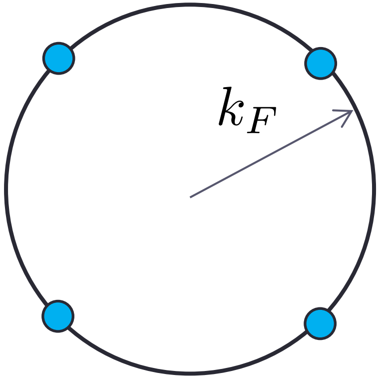


Nematicity in TBG: coupling to electrons

- **Cold spots:** vanishing of the nematic form factor.



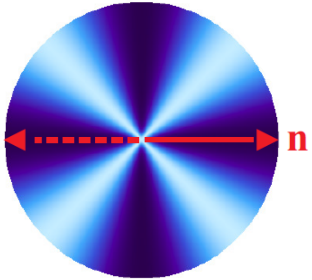
$$H = \sum_{\mathbf{k},\mathbf{q}} \cos\left(2\theta - 2\theta_{\mathbf{k}}\right) \Phi_{\mathbf{q}}\, \hat{\psi}^{\dagger}_{\mathbf{k}-\mathbf{q}/2} \hat{\psi}_{\mathbf{k}-\mathbf{q}/2}$$



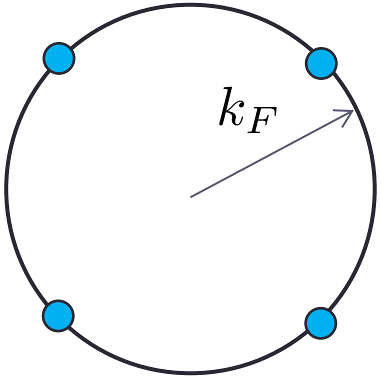
Nematicity in TBG: coupling to electrons

- When the transverse sound velocity is *smaller* than the longitudinal one, hot spots overlap with cold spots: **decoupling between low-energy nematic fluctuations and the electrons**.

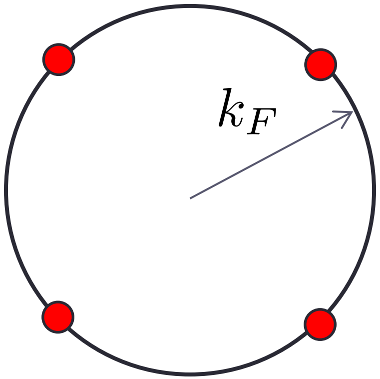
similar to Ising-nematic case:
Paul & Garst, PRL (2017)



$v_T < v_L$



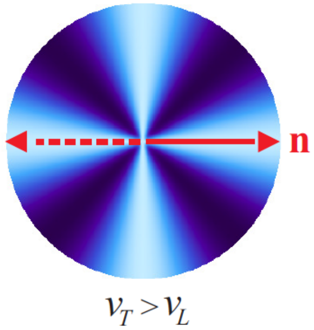
cold spots
vanishing of nematic form factor

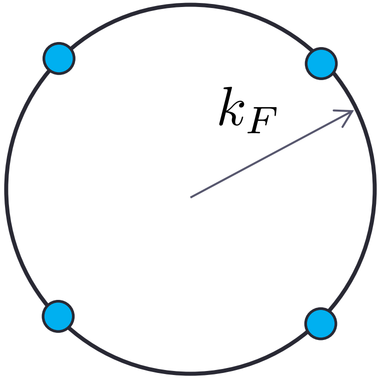


hot spots
exchange of nematic fluctuations

Nematicity in TBG: coupling to electrons

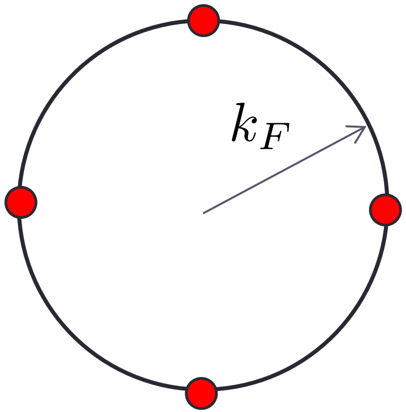
- When the transverse sound velocity is *larger* than the longitudinal one, hot spots do not overlap with cold spots: **maximum coupling between low-energy nematic fluctuations and the electrons**.





cold spots

vanishing of nematic form factor



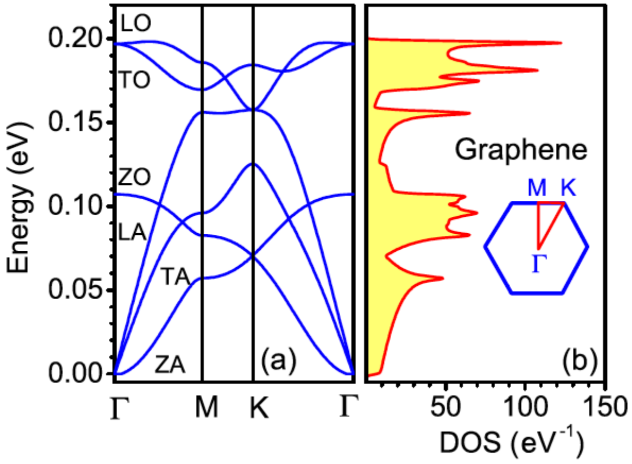
hot spots

exchange of nematic fluctuations

Nematicity in TBG: coupling to electrons

- Rigid lattice: lattice stability requires $v_T < v_L$

$$F_s(\mathbf{u}) = \frac{C_{11}}{2}\left(\varepsilon_{xx}^2 + \varepsilon_{yy}^2\right) + C_{12}\varepsilon_{xx}\varepsilon_{yy} + (C_{11} - C_{12})\,\varepsilon_{xy}^2$$



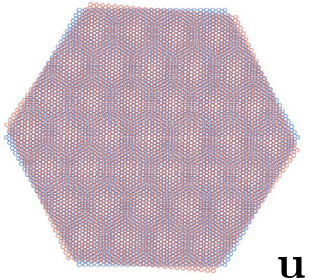
$$\begin{cases} v_L = \sqrt{\dfrac{C_{11}}{\rho}} \\ v_T = \sqrt{\dfrac{C_{11} - C_{12}}{2\rho}} \end{cases}$$

$$|C_{12}| < C_{11}$$

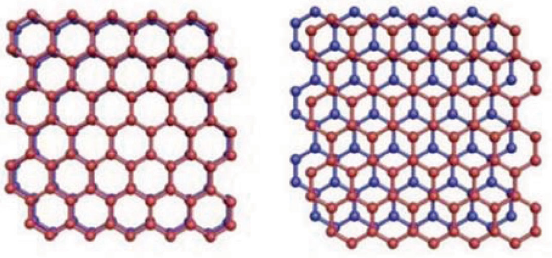
➢ *in the rigid lattice, electrons are nearly decoupled from low-energy nematic fluctuations*

Nematicity in TBG: coupling to electrons

- Rigid lattice: lattice stability requires $v_T < v_L$
- But the moiré superlattice is not a rigid lattice.
  - ➢ adhesion potential favors AB stacking



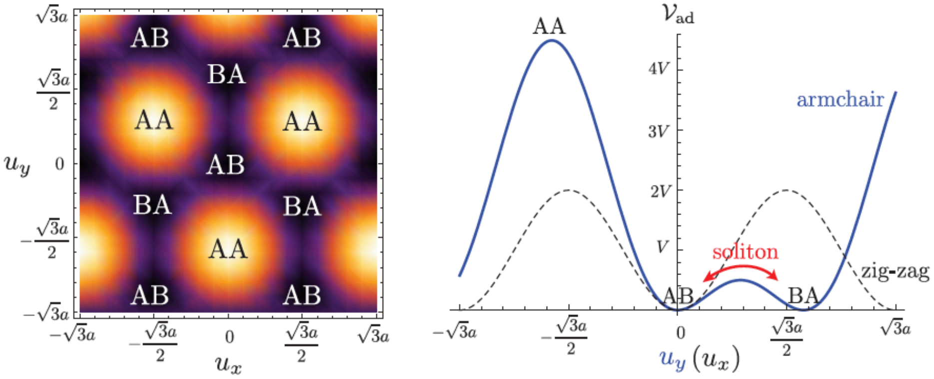
$$\mathbf{u} = \mathbf{u}_{\text{top}} - \mathbf{u}_{\text{bot}}$$



AA-stacked bilayer-graphene

AB-stacked bilayer-graphene

Huang et al, Current Graphene Science (2018)

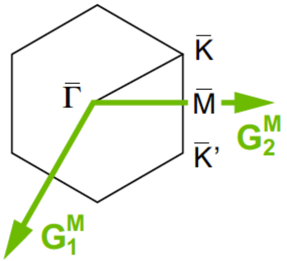


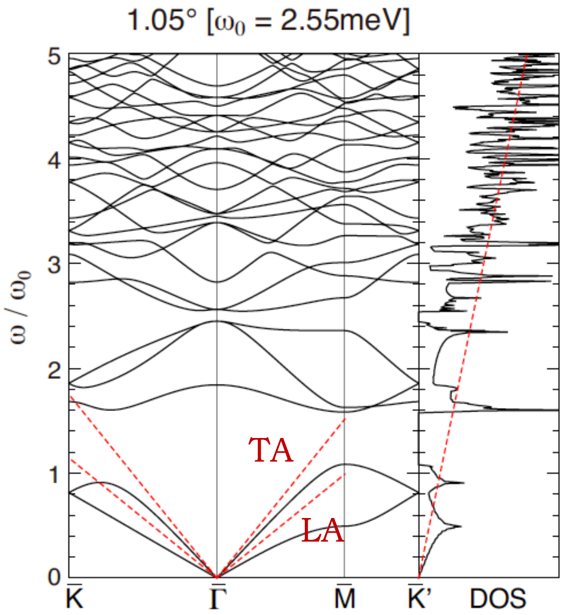
Ochoa, PRB (2019)

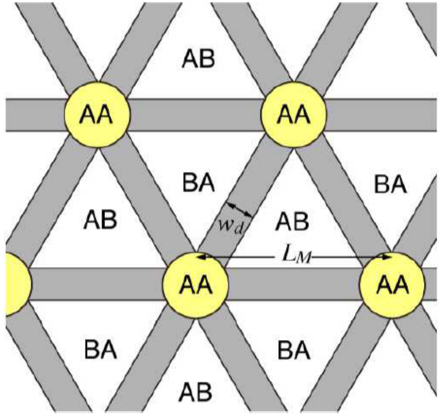
Nematicity in TBG: coupling to electrons

- Rigid lattice: lattice stability requires $v_T < v_L$

- But the moiré superlattice is not a rigid lattice: $v_T > v_L$







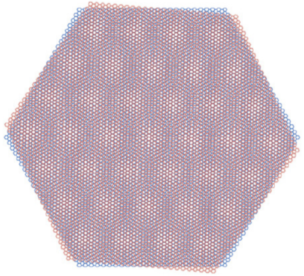
Koshino, PRB (2019)
Ochoa, PRB (2019)

➢ *in the moiré superlattice, electrons are maximally coupled to low-energy nematic fluctuations*

Nematicity in TBG: elastic degrees of freedom

- Adhesion potential favors sharp domain walls between AB/BA stacking regions.
- In contrast to a rigid crystal, rotations of the moiré superlattice cost energy.

$$F_s(\mathbf{u}) = \frac{C_{11}}{2}\left(\varepsilon_{xx}^2 + \varepsilon_{yy}^2\right) + C_{12}\varepsilon_{xx}\varepsilon_{yy} + \left(C_{11} - C_{12}\right)\varepsilon_{xy}^2 + \frac{K}{2}\omega_{xy}^2$$



$$\mathbf{u} = \mathbf{u}_{\text{top}} - \mathbf{u}_{\text{bot}}$$

$$\begin{cases} \varepsilon_{ij} = \frac{1}{2}\left(\partial_i u_j + \partial_j u_i\right) \\ \omega_{ij} = \frac{1}{2}\left(\partial_i u_j - \partial_j u_i\right) \end{cases}$$

Ochoa, PRB (2019)

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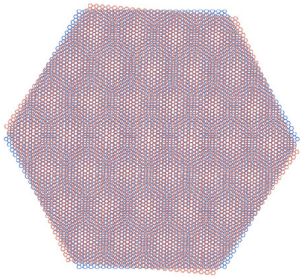

$$\mathbf{u} = \mathbf{u}_{\mathrm{top}} - \mathbf{u}_{\mathrm{bot}}$$

$$\begin{cases} v_L = \sqrt{\dfrac{C_{11}}{\rho}} \\ v_T = \sqrt{\dfrac{C_{11} - C_{12} + \frac{K}{2}}{2\rho}} \end{cases}$$

$$\hat{\mathbf{e}}_L = \left(\cos\zeta_{\mathbf{q}}, \sin\zeta_{\mathbf{q}}\right)$$

$$\hat{\mathbf{e}}_T = \left(-\sin\zeta_{\mathbf{q}}, \cos\zeta_{\mathbf{q}}\right)$$

➢ *rotation term contributes only to the transverse phonon velocity*

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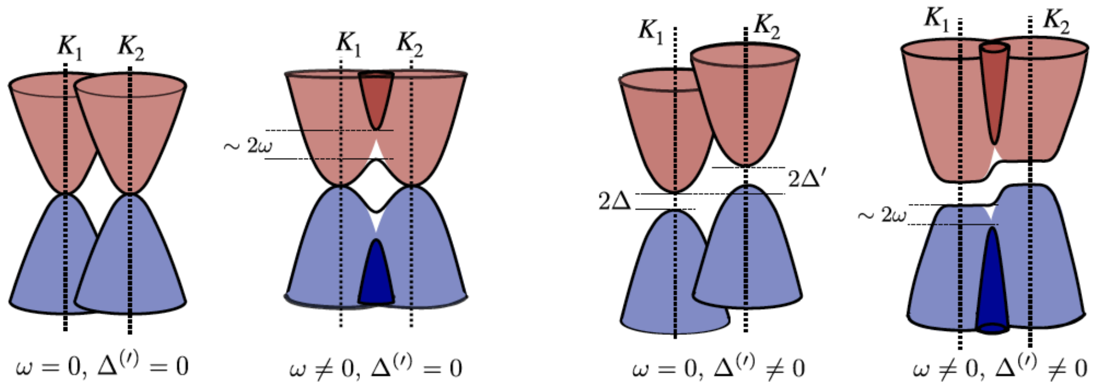
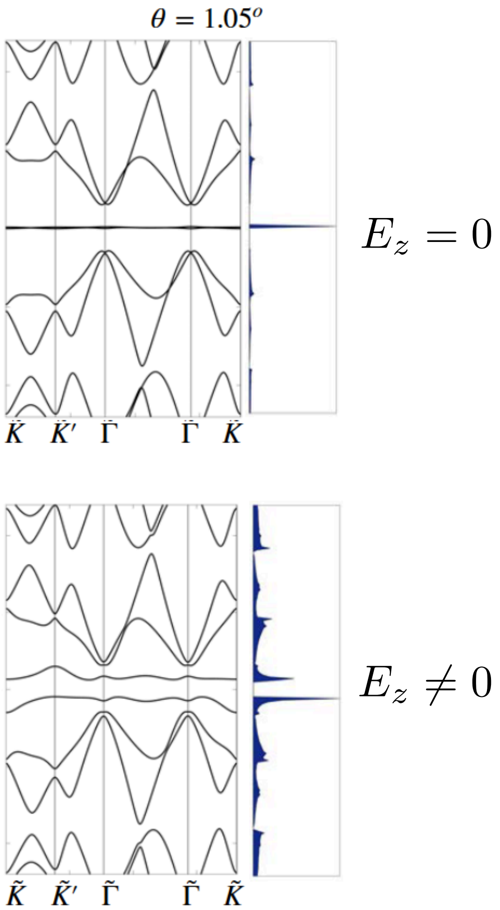
Nematicity in TDBG: electric field control

- Band structure of twisted double-bilayer graphene can be efficiently tuned by a perpendicular electric field.



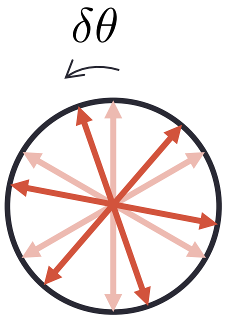


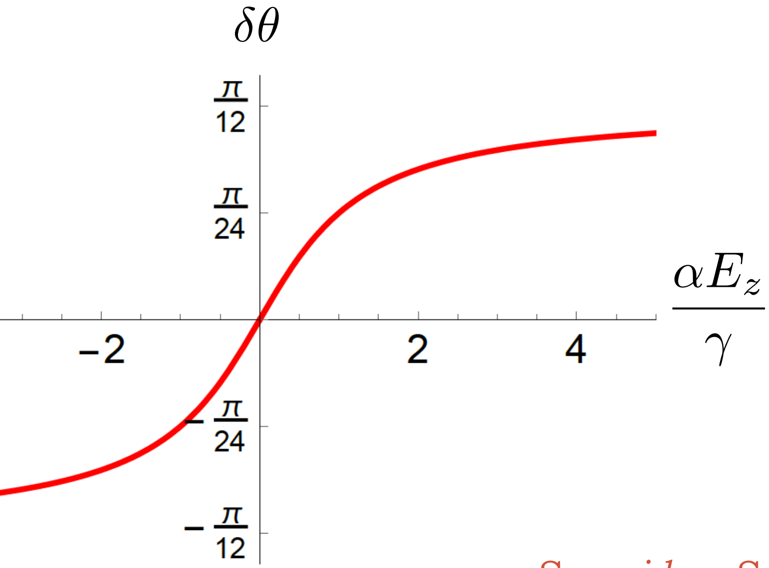
Chebrolu et al, PRB (2019)

Nematicity in TDBG: electric field control

- Perpendicular electric field lowers the symmetry from D_3 to C_3.

$$S_{\text{nem}}[\boldsymbol{\Phi}] = S_0[\Phi] + \frac{\gamma}{6}\int_x \left(\Phi_+^3 + \Phi_-^3\right) + \frac{\alpha E_z}{6i}\int_x \left(\Phi_+^3 - \Phi_-^3\right)$$

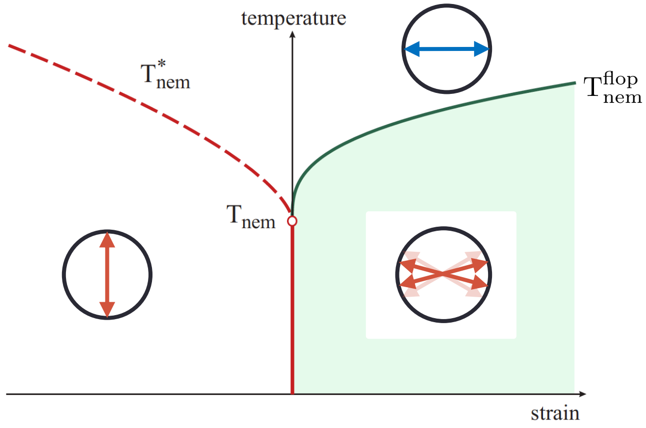


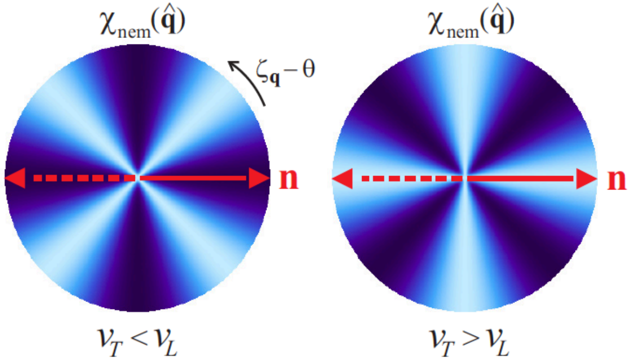


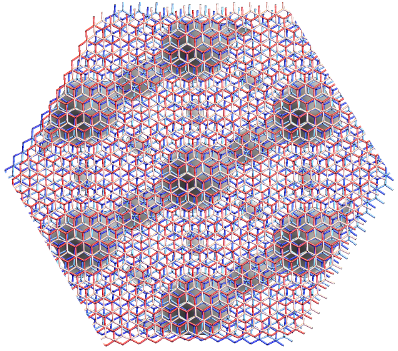
- ➢ *nematic director is no longer pinned to high-symmetry directions*
- ➢ *nematic director (and related thermodynamic quantities) can be rotated by the electric field*

Samajdar, Scheurer, Venderbos, and RMF, in preparation

Conclusions







- Nematic order in twisted moiré systems belongs to the 3-state Potts-model universality class.
- Nematic transition can survive in the presence of static strain, becoming an Ising-like nematic-flop transition.
- Impact of the nematic-acoustic phonon coupling on the electronic properties is fundamentally different in moiré superlattices as compared to rigid lattices.
- Electric control of the nematic director may be possible in twisted double-bilayer graphene