Strong Correlations, Electronic Ordered States, and Potts-Nematicity in Twisted Bilayer Graphene

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University of Minnesota



In collaboration with:



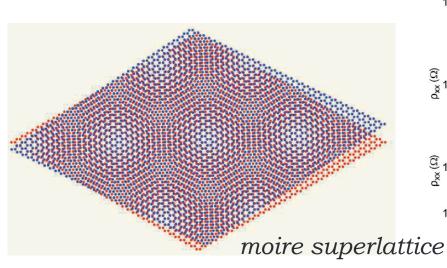
Jörn Venderbos, University of Pennsylvania

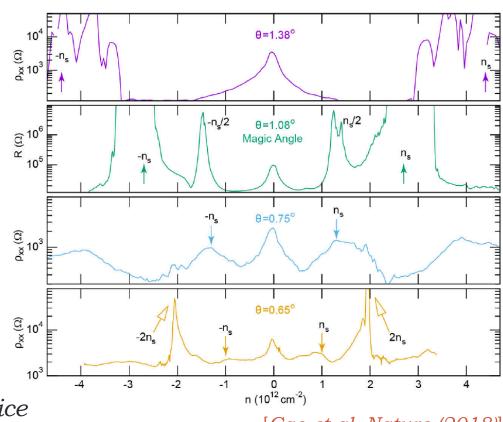
Venderbos and RMF, Phys. Rev. B 98, 245103 (2018)

Acknowledgments:

- O. Vafek and J. Kang (FSU);
- P. Jarillo-Herrero (MIT); L. Fu (MIT)

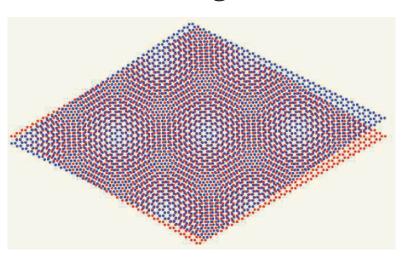
 emergence of correlated insulator at "half filling" for magic twist angle

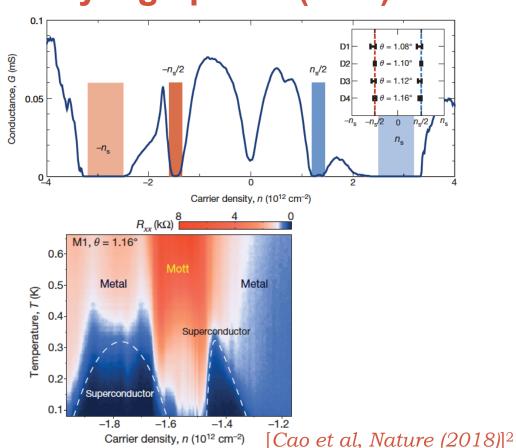




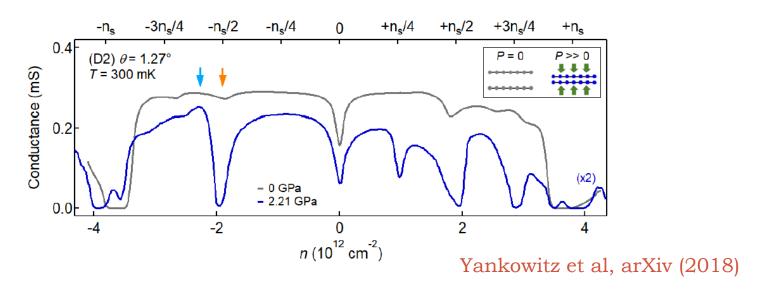
[Cao et al, Nature (2018)]²

- emergence of correlated insulator at "half filling" for magic twist angle
- superconductivity near an insulating state



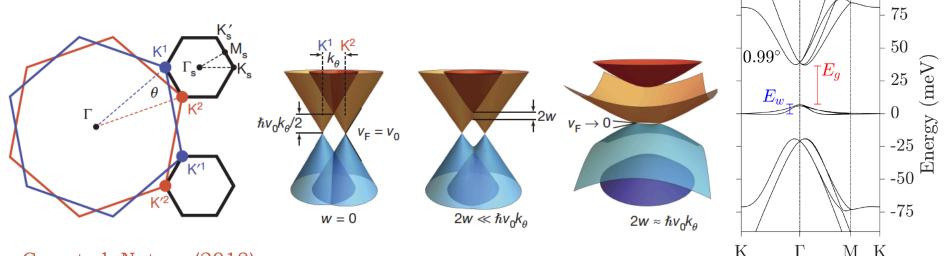


• Electronic states can also be controlled with pressure



• Similar phenomena seen in other twisted systems (TB²G, trilayer graphene, ...) P. Kim group, F. Wang group

- Magic angle: isolated nearly-flat bands in the moiré Brillouin zone. Bistritzer and MacDonald, PNAS (2011)
- Small bandwidth: interactions become important



Cao et al, Nature (2018)

Kaxiras et al, arXiv (2019)

- New platform to understand strong interactions, superconductivity, and their interplay with topology
- Bringing two communities together





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The New York Times

At Rio's Beaches, Kicks Go Over Net

- New platform to understand strong interactions, superconductivity, and their interplay with topology
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Outline

1. Low-energy model and interactions

Strong-coupling phase diagram: spin, orbital, and superconducting degrees of freedom

3. Potts-nematicity and nematic superconductivity

Outline

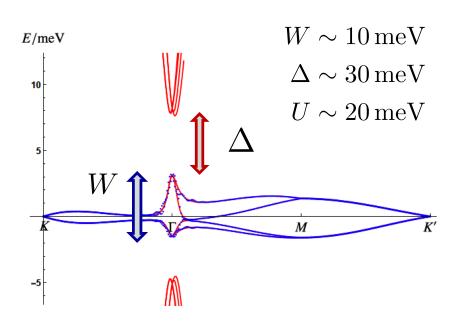
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Low-energy model

Energy scales (estimates):

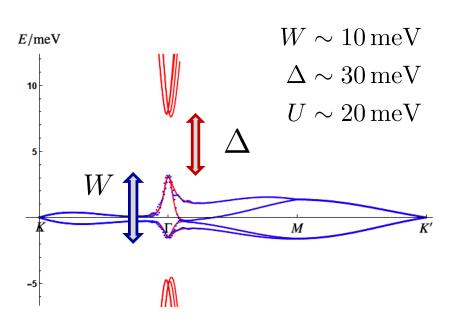


Kang & Vafek, PRX (2018)

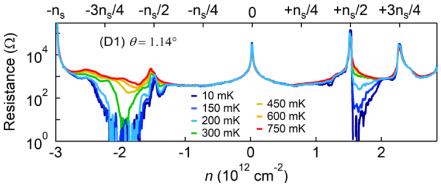
- > focus only on narrow bands as long as $\Delta > U$
- most likely, the narrowband subsystem is in the intermediate coupling regime U ~ W
- starting point: weak-coupling or strong-coupling?

Low-energy model

Energy scales (estimates):



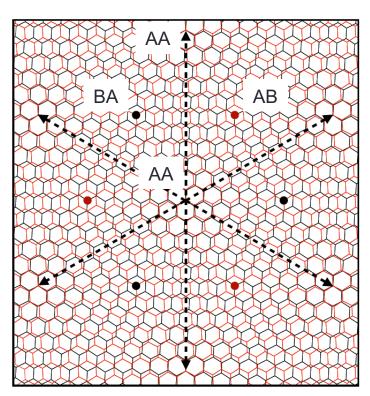
Kang & Vafek, PRX (2018)

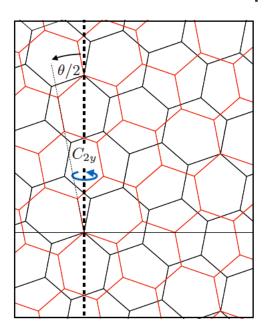


Yankowitz et al, arXiv (2018)

observation of insulating behavior at commensurate filling motivates us to start with a strong-coupling approach

Commensurate twist from AA center: moiré superlattice

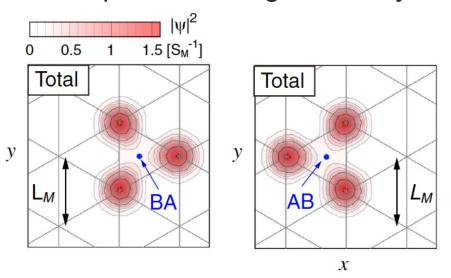


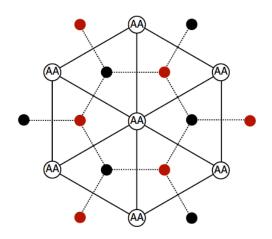


absence of C_{2x} symmetry (D_3 space group) removes any subtleties related to Wannier obstruction

Yuan & Fu, PRB (2018) Kang & Vafek, PRX (2018) Zou, Po, Vishwanath, Senthil, PRB (2018)

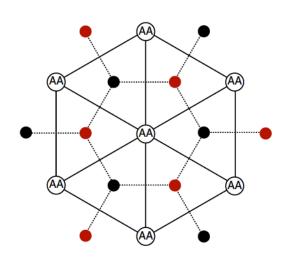
 Wannier states are peaked near AA points, but centered at AB/BA points: emergent honeycomb lattice





Koshino et al, PRX (2018) Kang & Vafek, PRX (2018) 8 states per moiré unite cell: 2 (spin) x 2 (sublattice) x 2 ("orbitals")

Two "p-orbital" honeycomb lattice model:



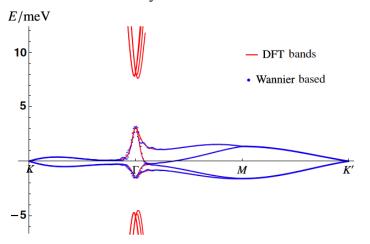
- ➤ the 2 "orbitals" in each honeycomb sublattice site are eigenstates of C_{3z}
- $rackleright > L_z = \pm 1$ angular momentum eigenstates (nearly valley-polarized): equivalent to $p_x \pm i p_y$ "orbitals"
- \blacktriangleright unitary transformation: p_x and p_y "orbitals" on a honeycomb lattice
- hopping amplitudes **not** given by Slater-Koster rules

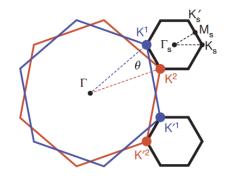
Yuan & Fu, PRB (2018)

Kang & Vafek, PRX (2018)

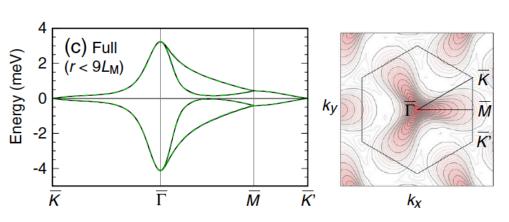
 Two-orbital honeycomb lattice model: tightbinding band dispersions

$$H_K = \sum_{ij} c_i^{\dagger} \hat{T}(\mathbf{r}_{ij}) c_j + \text{H.c.}$$





Brillouin zone is folded due to moiré superlattice



Kang & Vafek, PRX (2018)

Koshino et al, PRX (2018)

Low-energy model: interaction terms

 Extended Hubbard-Kanamori model: density-density and exchange-like interactions

$$H_{I} = \frac{1}{2} \sum_{ij} V_{ij}^{\alpha\beta} n_{i\alpha} n_{j\beta} + \frac{1}{2} \sum_{ij,\alpha\beta} J_{1,ij}^{\alpha\beta} c_{i\alpha\sigma}^{\dagger} c_{j\beta\sigma'}^{\dagger} c_{i\beta\sigma'} c_{j\alpha\sigma}$$

$$+ \frac{1}{2} \sum_{ij,\alpha\neq\beta} J_{2,ij}^{\alpha\beta} c_{i\alpha\sigma}^{\dagger} c_{j\beta\sigma'}^{\dagger} c_{i\alpha\sigma'} c_{j\beta\sigma}$$

$$+ \frac{1}{2} \sum_{ij,\alpha\neq\beta} J_{3,ij}^{\alpha\beta} c_{i\alpha\sigma}^{\dagger} c_{j\alpha\sigma'}^{\dagger} c_{i\beta\sigma'} c_{j\beta\sigma},$$

 Main challenges: determine the most important interaction terms and solve the problem in the intermediate coupling regime.

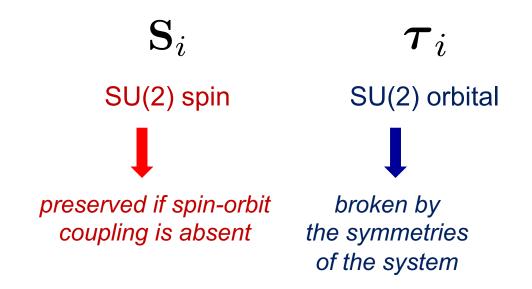
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Strong-coupling phase diagram: spin, orbital, and superconducting degrees of freedom

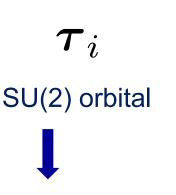
3. Potts-nematicity and nematic superconductivity

• What to expect? In the insulating regime, with one electron per site ("half-filling"), two unquenched degrees of freedom are left.

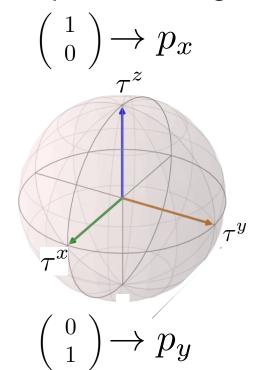


see also: Xu & Balents, PRL (2018); Dodaro et al, PRB (2018)

• What to expect? In the insulating regime, with one electron per site ("half-filling"), two unquenched degrees of freedom are left.



broken by the symmetries of the system



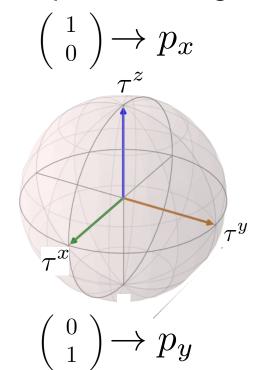
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SU(2) orbital



broken by the symmetries of the system



 au^z : orbital order (C $_{3z}$ symmetry breaking) $n_{p_x}
eq n_{p_y}$

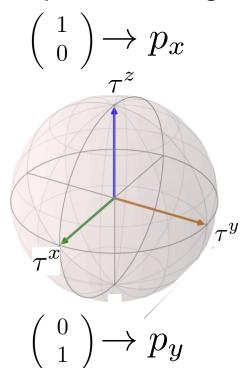
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$$au^z$$
: orbital order (C_{3z} symmetry breaking) $n_{p_x}
eq n_{p_y}$

$$au^x$$
: orbital order (C_{3z} symmetry breaking) $n_{p_x+p_y}
eq n_{p_x-p_y}$

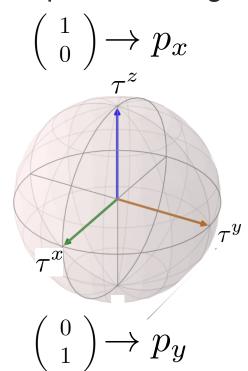
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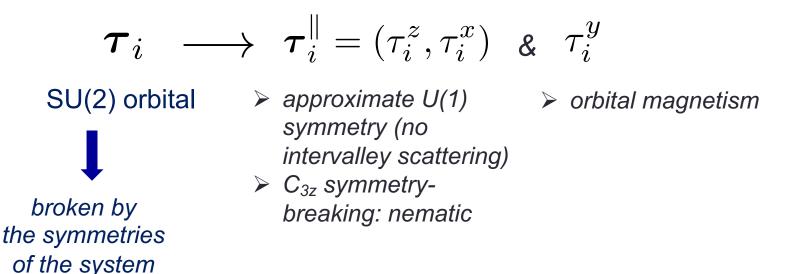


$$au^z$$
: orbital order (C_{3z} symmetry breaking) $n_{p_x}
eq n_{p_y}$

$$au^x$$
: orbital order (C_{3z} symmetry breaking) $n_{p_x+p_y}
eq n_{p_x-p_y}$

$$au^y$$
: orbital magnetism (T symmetry breaking) $n_{p_x+ip_y}
eq n_{p_x-ip_y}$

• What to expect? In the insulating regime, with one electron per site ("half-filling"), two unquenched degrees of freedom are left.



- Strong-coupling expansion: Hamiltonian in terms of $\, {f S}_i \,$ and ${m au}_i \,$
 - Kugel-Khomskii Hamiltonian

Crystal structure and magnetic properties of substances with orbital degeneracy

K. I. Kugel' and D. I. Khomskii P. N. Lebedev Physics Institute (Submitted November 13, 1972)

Zh. Eksp. Teor. Fiz. 64, 1429-1439 (April 1973)

• First step: onsite interactions (Hubbard *U* and Hund's *J*) and nearest-neighbor hopping only.

$$H_{I}^{(\text{onsite})} = U \sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + (U - 2J) \sum_{i} n_{ix} n_{iy}$$

$$+ J \sum_{i,\sigma,\sigma'} c_{ix\sigma}^{\dagger} c_{iy\sigma'}^{\dagger} c_{ix\sigma'} c_{iy\sigma}$$

$$+ J \sum_{i,\alpha\neq\beta} c_{i\alpha\uparrow}^{\dagger} c_{i\alpha\downarrow}^{\dagger} c_{i\beta\downarrow} c_{i\beta\uparrow}.$$

$$H_K = \sum_{ij} c_i^{\dagger} \hat{T}(\mathbf{r}_{ij}) c_j$$
 $\hat{T}_1^{(1)} = t_1 + t_1' \tau^z$

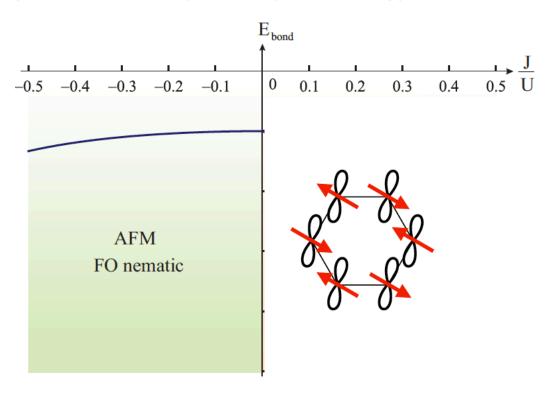
approximately zero
(intervalley scattering)

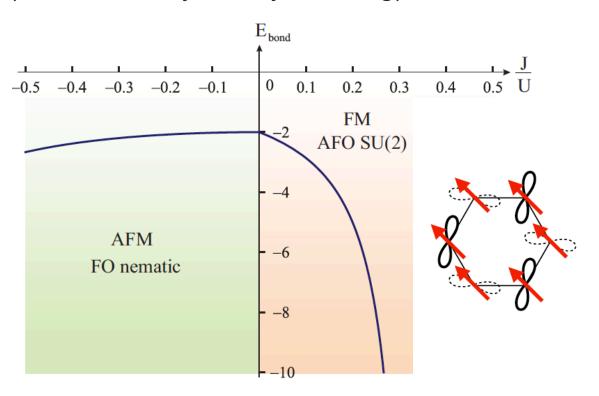
Strong-coupling Hamiltonian

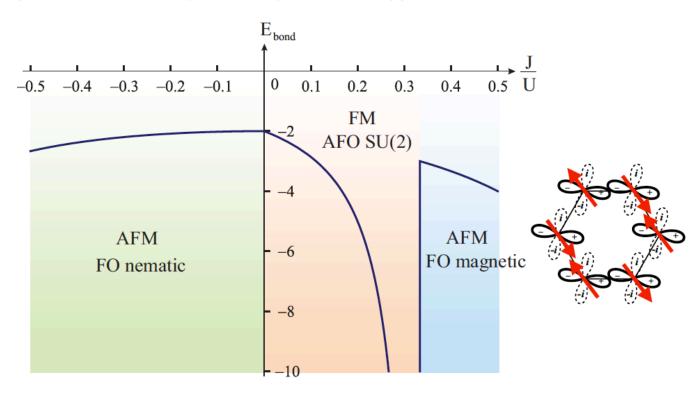
One electron per site ("half-filling", but moiré unit cell is 1/4 filled)

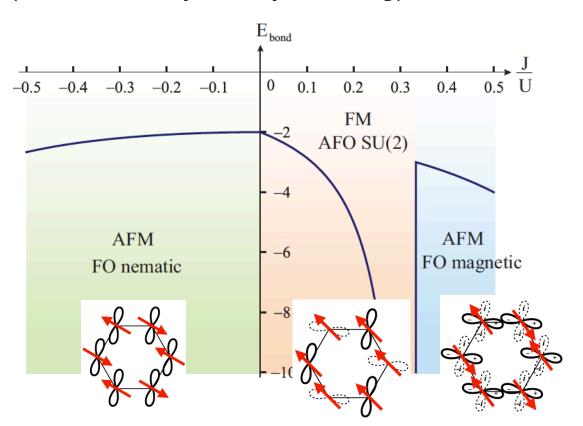
$$\mathcal{H} = \sum_{\langle ij \rangle} \left\{ \frac{t^2}{(U - 3J)} \left(\frac{3}{4} + \mathbf{S}_i \cdot \mathbf{S}_j \right) (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j - 1) - \frac{t^2}{U + J} \left(\frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j \right) (1 + \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j - 2\tau_i^y \tau_j^y) - \frac{2t^2}{U - J} \left(\frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j \right) (\tau_i^y \tau_j^y + 1) \right\}.$$

several approaches to capture the effects of interactions: Balents, Xu, Fu, Vafek, Kang, Isibo, Sachdev, Kivelson, Rademaker, Mellado, Senthil, Vishwanath, Guinea, Bascones, Martin, MacDonald, Lee, Law, Ma, Koshino, Kuroki, Kennes, Thomson, Phillips, Betouras, Nandkishore, Bernevig, Thanos, ...









What about superconductivity?

- Decomposition of the interaction terms in pair operator.
- Three types of **onsite** pairing: $\Delta_{\sigma\sigma'}^{\alpha\alpha'}c_{i,\alpha\sigma}^{\dagger}c_{i,\alpha'\sigma'}^{\dagger}$

$$\Delta = au^0 \otimes (i\sigma^y)$$
s-wave spin-singlet

(A₁ symmetry)

$$\Delta = (au^z, au^x) \otimes (i\sigma^y)$$
 degenerate d-wave

(E symmetry)

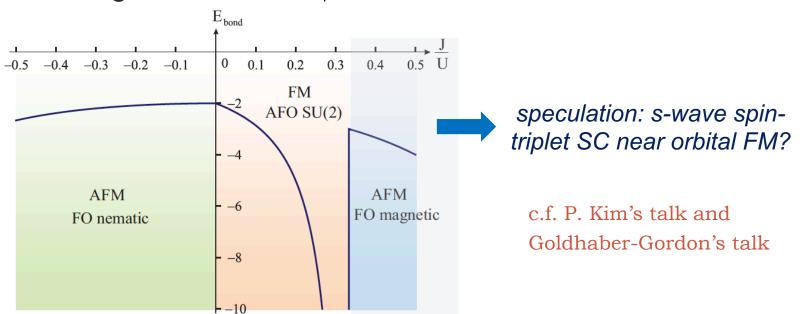
$$\Delta = (i au^y)\otimes (\mathbf{d}\cdotoldsymbol{\sigma}\,i\sigma^y)$$
s-wave spin-triplet

(A₂ symmetry)

superconductivity proposals: Balents, Xu, Fu, Kivelson, Rademaker, Mellado, Guinea, Scalletar, Martin, MacDonald, Lee, Ma, Kennes, Nandkishore, Bernevig, ...

What about superconductivity?

• s-wave spin-triplet channel is attractive already in the bare level in the regime of the phase diagram dominated by orbital ferromagnetism. J>U/3



Our onsite approximation neglects the impact of extended interactions,
 which are expected due to the extended nature of the Wannier functions.

Koshino et al, PRX (2018)

• Kang and Vafek: assisted-hopping interaction favors "ferro" alignment of both \mathbf{S}_i and $\boldsymbol{\tau}_i$ already in the atomic limit. Kang & Vafek, PRX (2018) see also Senthil's talk

$$U \approx \frac{V_0}{2} \sum_{\mathbf{R}} \left(\sum_{j=\pm 1} \sum_{\sigma=\uparrow,\downarrow} O_{j,\sigma}(\mathbf{R}) \right)^2 \qquad O_{j,\sigma}(\mathbf{R}) = \frac{1}{3} Q_{j,\sigma}(\mathbf{R}) + \alpha_1 T_{j,\sigma}(\mathbf{R})$$

 Hopping beyond nearest neighbors are fundamental to correctly describe the narrow bands dispersions. Can they introduce frustration?

Outline

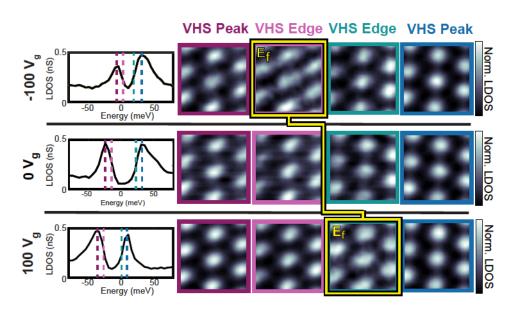
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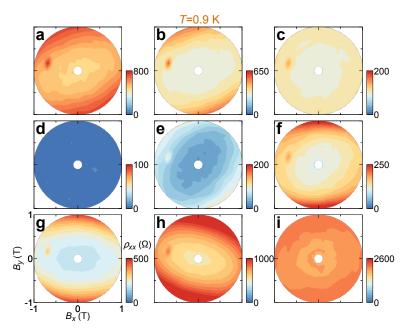
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Electronic nematicity in TBG: experimental hints

> STM: spatial map of the local density of states is not three-fold symmetric



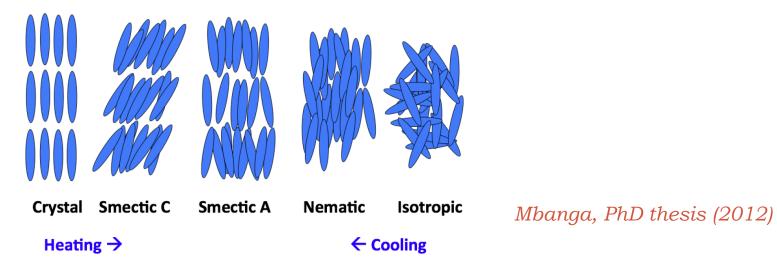
superconducting upper critical field is two-fold symmetric



Kerelsky et al, arXiv (2018)

Jarillo-Herrero's talk

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



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

• 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, Emery Nature (1998)

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Kivelson, Fradkin, Emery Nature (1998)

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

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

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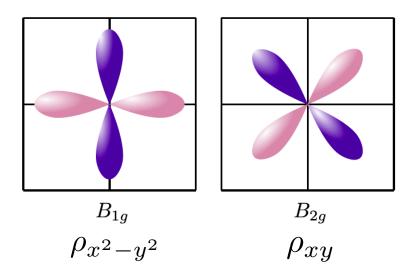
> XY-nematic order parameter Φ

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

Lattice generally breaks the continuous symmetry of the nematic OP:

> square lattice: the two components of Φ transform as two different irreducible representations

$$oldsymbol{\Phi} = \left(egin{array}{c}
ho_{x^2-y^2} \
ho_{xy} \end{array}
ight)$$

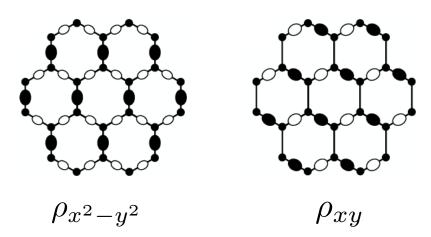


Ising-nematicity: cuprates, pnictides, ruthenates, heavy fermions, ...

Lattice generally breaks the continuous symmetry of the nematic OP:

honeycomb lattice: the two components of Φ transform as the same two-dimensional irrep E

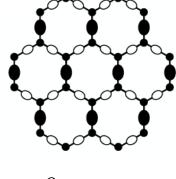
$$oldsymbol{\Phi} = \left(egin{array}{c}
ho_{x^2-y^2} \
ho_{xy} \end{array}
ight)$$



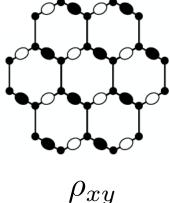
Lattice generally breaks the continuous symmetry of the nematic OP:

honeycomb lattice: the two components of Φ transform as the same two-dimensional irrep *E*

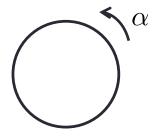
$$\mathbf{\Phi} = \begin{pmatrix} \rho_{x^2 - y^2} \\ \rho_{xy} \end{pmatrix} \equiv \Phi_0 \begin{pmatrix} \cos 2\alpha \\ \sin 2\alpha \end{pmatrix}$$







XY-nematicity?

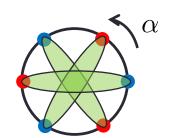


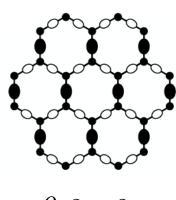
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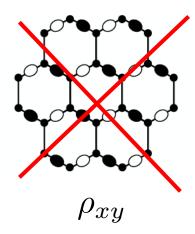
$$f = \frac{a}{2}\Phi_0^2 + \frac{\lambda}{3}\Phi_0^3\cos(6\alpha) + \frac{u}{4}\Phi_0^4$$

3-state Potts nematicity!





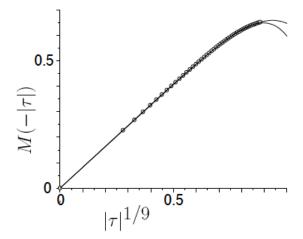
$$\rho_{x^2-y^2}$$



see also:

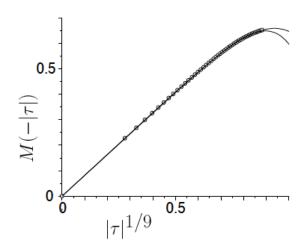
Hecker & Schmalian, npj Quant Mat (2017) Fu et al, PRB (2016)

- General properties of the two-dimensional 3-state Potts model:
- despite the cubic invariant, transition is second order



Shchur et al, PRB (2008)

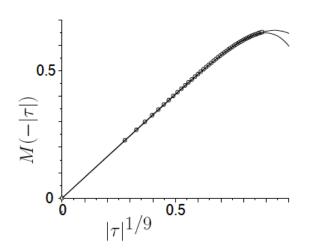
- General properties of the two-dimensional 3-state Potts model:
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- \blacktriangleright Harris inequality is violated: $d\nu = \frac{5}{3} < 2$



importance of disorder, which is ubiquitous in TBG

Shchur et al, PRB (2008)

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importance of disorder, which is ubiquitous in TBG

may explain the financial market \$\$\$

Simulations of financial markets in a Potts-like model

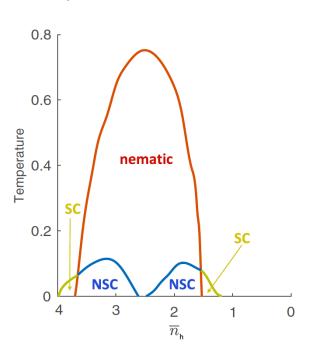
Tetsuya Takaishi

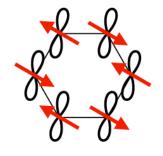
CERN, Physics Department, TH Unit, CH-1211 Genève 23, Switzerland Hiroshima University of Economics, Hiroshima 731-0124, Japan

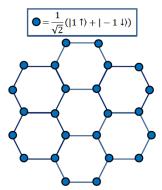
June 29, 2018

Shchur et al, PRB (2008)

- Possible microscopic origins:
 - > spontaneous order of the emergent "orbital" degrees of freedom.

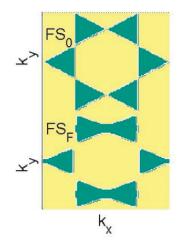


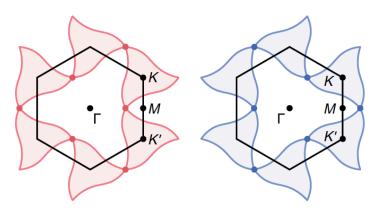




Dodaro et al, PRB (2018) Venderbos & RMF, PRB (2018) Kang & Vafek, arxiv (2018)

- Possible microscopic origins:
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in the context of graphene doped to the vHS: Valenzuela & Vozmediano, NJP (2008)

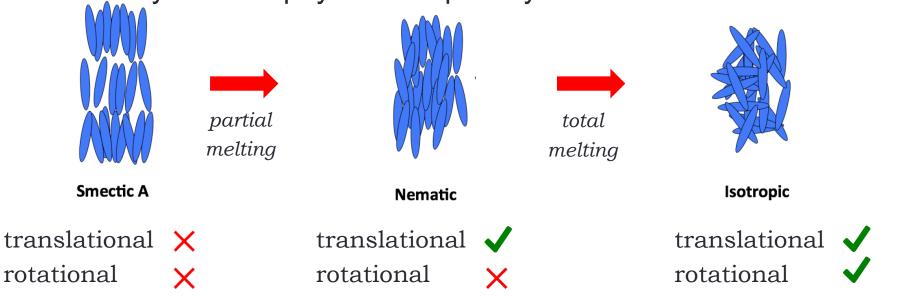
Isobe et al, PRX (2018)

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Venderbos & RMF, PRB (2018)

Vestigial order: partial melting of an ordered state

Similarity with the physics of liquid crystals



• In quantum matter: composite order $\langle \eta_{\alpha} \rangle = 0 \ \mathrm{but} \ \langle \eta_{\alpha} \eta_{\beta} \rangle \neq 0$

RMF, Orth, Schmalian, Ann. Rev. Cond. Matt. Phys, in press

One of the candidates for the superconducting state:

Balents, Xu, Fu, Rademaker, Mellado, Ma, Yang, Lin, Kennes, Nandkishore, ...

$$\Delta = au^0 \otimes (i\sigma^y)$$
s-wave spin-singlet

s-wave spin-singlet (A₁ symmetry)

$$\Delta = (au^z, au^x) \otimes (i\sigma^y)$$
 degenerate d-wave

degenerate d-wave (E symmetry)

$$\Delta = \eta_1 \tau^z \left(i \sigma^y \right) + \eta_2 \tau^x \left(i \sigma^y \right)$$

$$\downarrow$$

$$d_{x^2 - y^2} \text{-wave} \qquad d_{xy} \text{-wave}$$

$$\Delta = (i\tau^y) \otimes (\mathbf{d} \cdot \boldsymbol{\sigma} \, i\sigma^y)$$

s-wave spin-triplet $(A_2 \text{ symmetry})$

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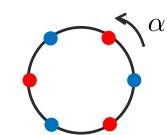
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$$\Delta = (i\tau^y) \otimes (\mathbf{d} \cdot \boldsymbol{\sigma} \, i\sigma^y)$$

s-wave spin-triplet (A₂ symmetry)

$$\Delta = \eta_1 \tau^z \left(i\sigma^y \right) + \eta_2 \tau^x \left(i\sigma^y \right)$$

- > d+id chiral superconductivity $oldsymbol{\eta} = \left(egin{array}{c} 1 \ \pm i \end{array}
 ight)$
- > d+d nematic superconductivity $\eta = \begin{pmatrix} \cos \alpha \\ \sin \alpha \end{pmatrix}$



Vestigial nematic order in TBG $\,$ • What are the possible composite operators? $\,\eta=\left(\begin{array}{c}\eta_1\\\eta_2\end{array}\right)$

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A₂ chiral order, breaks time-reversal symmetry

$$m{\Phi} = \left(egin{array}{c} |\eta_1|^2 - |\eta_2|^2 \ \eta_1^* \eta_2 + \eta_1 \eta_2^* \end{array}
ight)$$

E nematic order, breaks three-fold rotational symmetry

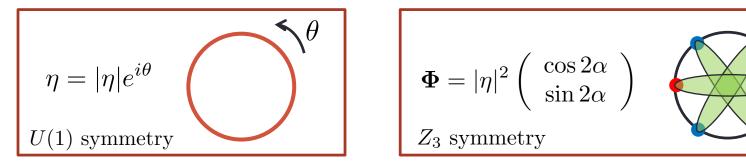
none of them break U(1) symmetry

- Can the composite nematic order parameter condense even in the absence of long-range superconductivity?
- Two phase variables: global phase and relative angle.

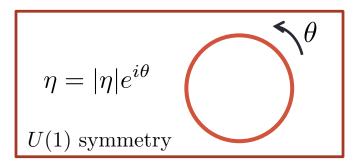
$$\eta = |\eta|e^{i\theta} \begin{pmatrix} \cos \alpha \\ \sin \alpha \end{pmatrix}$$

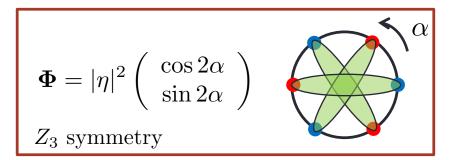
$$\eta = |\eta| e^{i\theta} \begin{pmatrix} \cos \alpha \\ \sin \alpha \end{pmatrix}$$

$$\Phi = \begin{pmatrix} |\eta_1|^2 - |\eta_2|^2 \\ \eta_1^* \eta_2 + \eta_1 \eta_2^* \end{pmatrix} \equiv |\eta|^2 \begin{pmatrix} \cos 2\alpha \\ \sin 2\alpha \end{pmatrix}$$

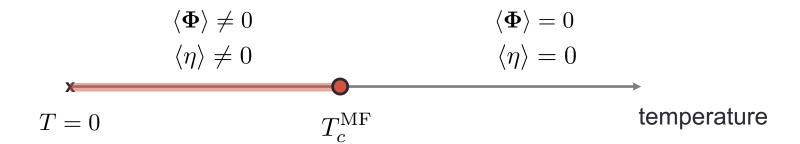


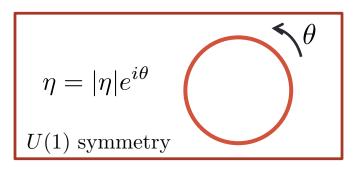
$$\Phi = |\eta|^2 \begin{pmatrix} \cos 2\alpha \\ \sin 2\alpha \end{pmatrix}$$
 Z_3 symmetry

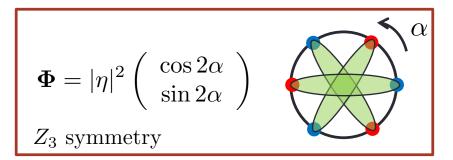




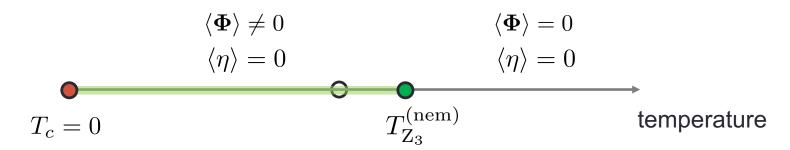
Mean-field: both order parameters condense simultaneously

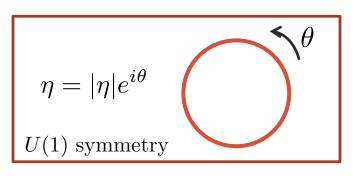


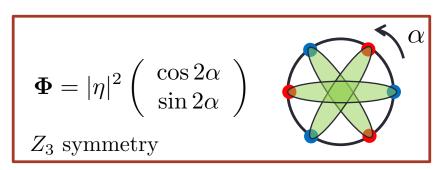




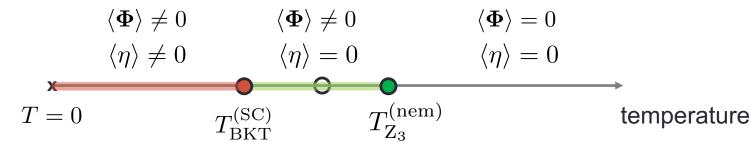
• Fluctuations kill superconductivity in 2D (Mermin-Wagner), but enhance the Potts transition. $\chi_{\rm nem}^{-1} \propto C - \xi_{\rm SC}^{-2}$



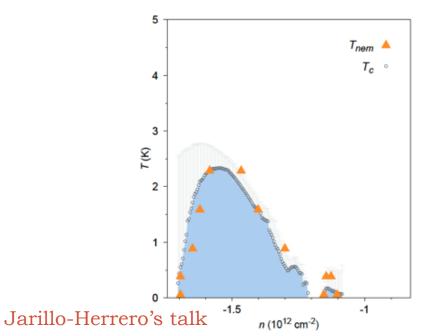


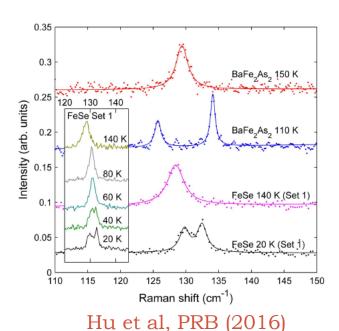


• Kosterlitz-Thouless transition: quasi-long-range SC order (microscopic similar results for Cu_xBi₂Se₃, but in 3D Hecker and Schmalian, npj Quant. Mat. (2018)



- Experiments indicate that the entire superconducting dome is nematic.
- Possible nematicity in the normal state could be probed, for instance, by the Raman splitting of the E_g phonon mode (like in pnictides).

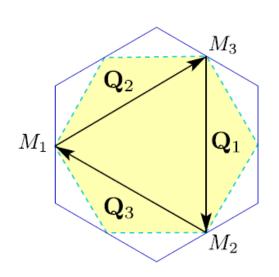




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 - vestigial phase of a spin-density wave (SDW).

Vestigial nematic order in TBG: SDW case

 Similarly to monolayer graphene doped to the van Hove singularity, TBG may be unstable towards a SDW.



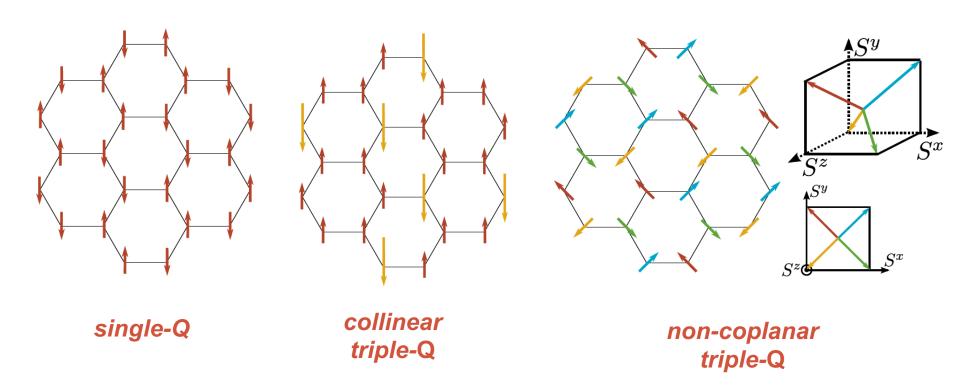
Nandkishore et al, Nat Phys (2013) Platt et al, Adv Phys (2013) Wang et al, PRB (2012) Chern et al, PRB (2011)

$$\mathbf{S}\left(\mathbf{r}\right) = \sum_{a=1,2,3} \mathbf{m}_a \cos\left(\mathbf{Q}_a \cdot \mathbf{r}\right)$$

three-fold degenerate SDWs

Vestigial nematic order in TBG: SDW case

Three possible magnetic ground states

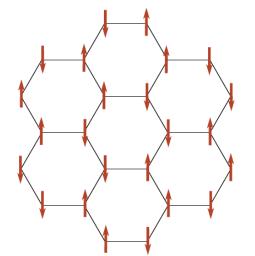


Vestigial nematic order in TBG: SDW case

- Composite 3-state Potts (Z₃) nematic order parameter can condense already in the paramagnetic phase.
 - ➤ long-range SDW not allowed in 2D

$$\phi_{(1,0)}^{\nu} = \left\{ m_1^2 - m_2^2, \, \frac{1}{\sqrt{3}} \left(m_1^2 + m_2^2 - 2m_3^2 \right) \right\}$$

bond order

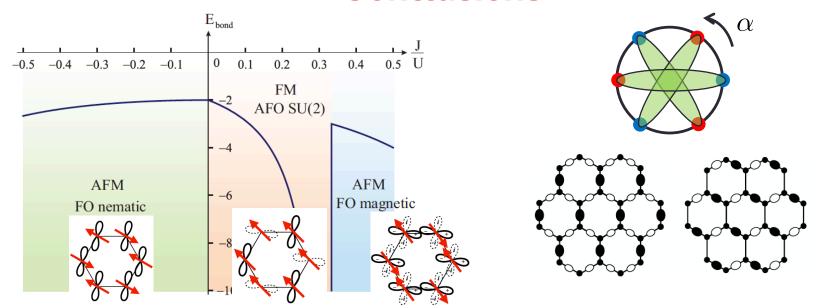


single-Q

RMF, Orth, Schmalian,

Ann. Rev. Cond. Matt. Phys, *in pres*s

Conclusions



- Rich interplay between spin and emergent orbital degrees of freedom in the strong-coupling insulating state of TBG.
- Potts-nematicity offers a new window to explore electronic nematic order.
- Nematic order expected to survive in the normal state as a vestigial order.

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