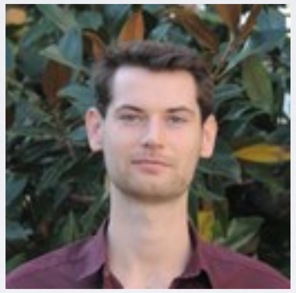
RENORMALIZATION GROUP APPROACH TO COMPETING ORDERS AT CHARGE NEUTRALITY IN TBG

Lucile Savary

Univ. Bremen, from Lyon, Monday, Feb. 8th, 2021

COLLABORATORS

- **Eric Brillaux**



- Andrei Fedorenko

CNRS, ENS de Lyon

- David Carpentier

arXiv:2008.05041

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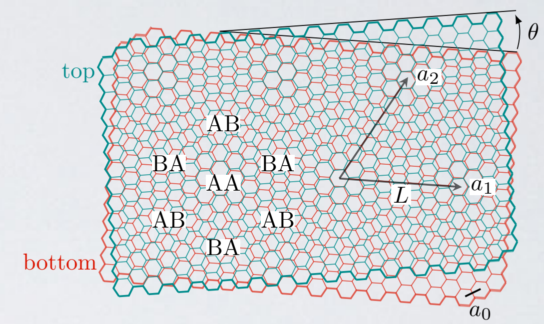
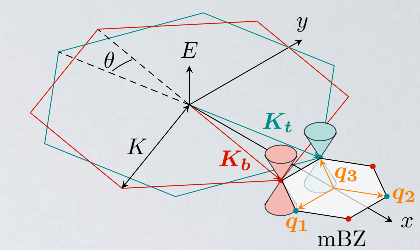
FLAT BAND PREDICTION AT "MAGIC ANGLES"

- prediction that twisted bilayer graphene ought to have flat bands for some specific ("magic") very small twist angles, where v_{Dirac} vanishes

hopping parameter w and twist angle θ in single parameter $\alpha \sim 1/\theta$

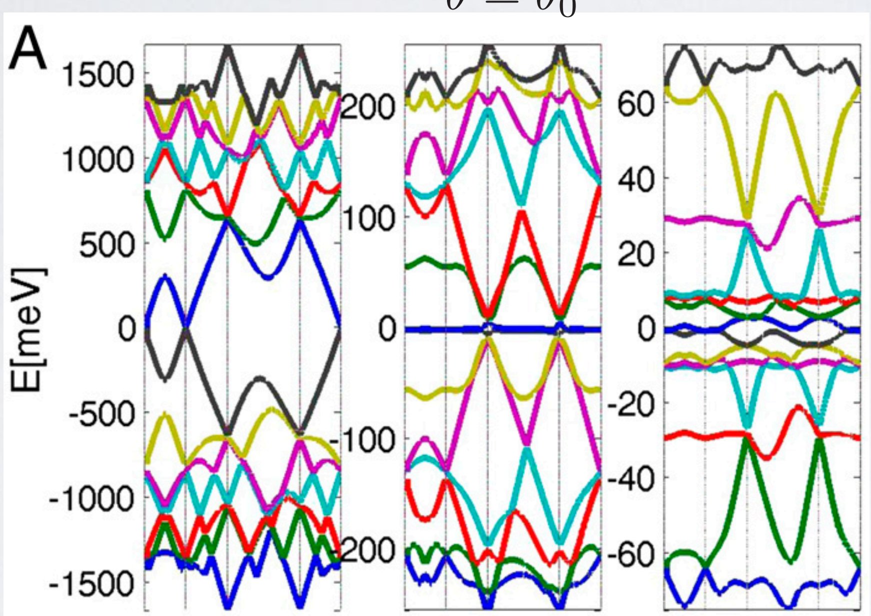




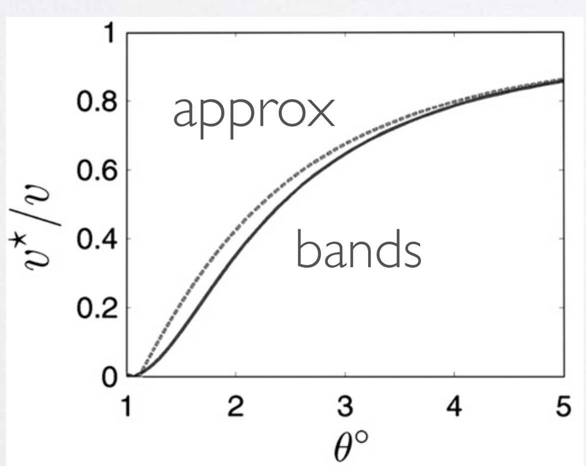
$\theta = \theta_0$

entirely numerical

100-1000 plane wave states



$$\frac{v^\star}{v} = \frac{1 - 3\alpha^2}{1 + 6\alpha^2}$$

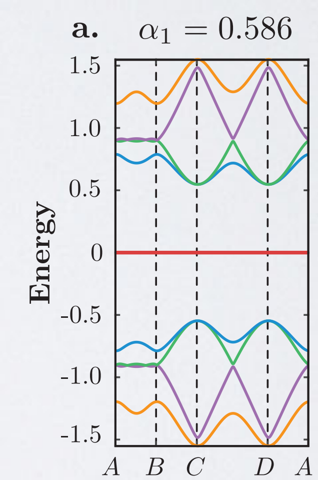


very accurate!

simple

Bistritzer and MacDonald

important note for later: Tarnopolsky et al find a simple limit where bands *exactly* flat

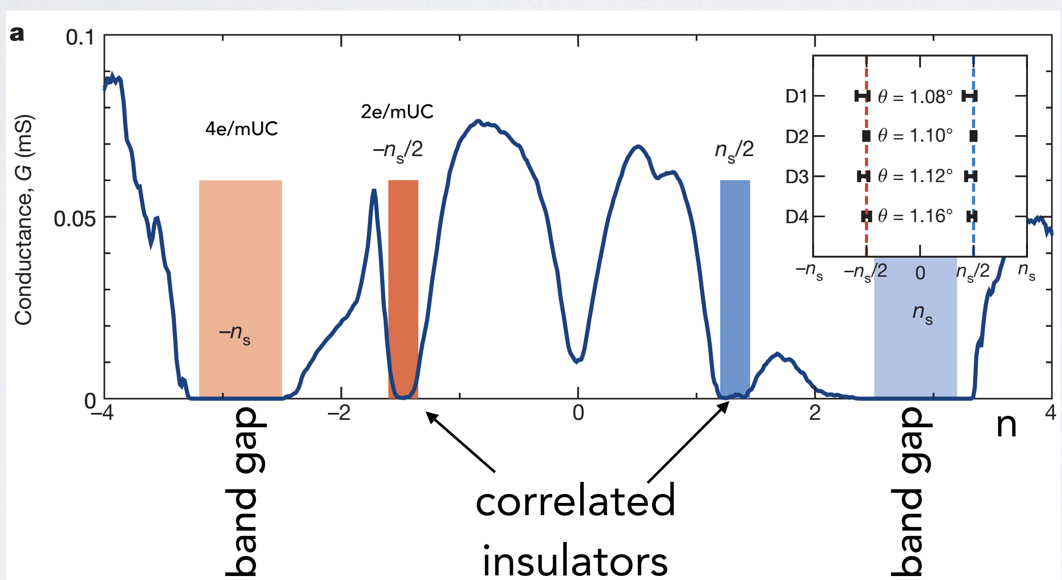


Tarnopolsky et al

2018-NOW: EXPERIMENTAL CONFIRMATION

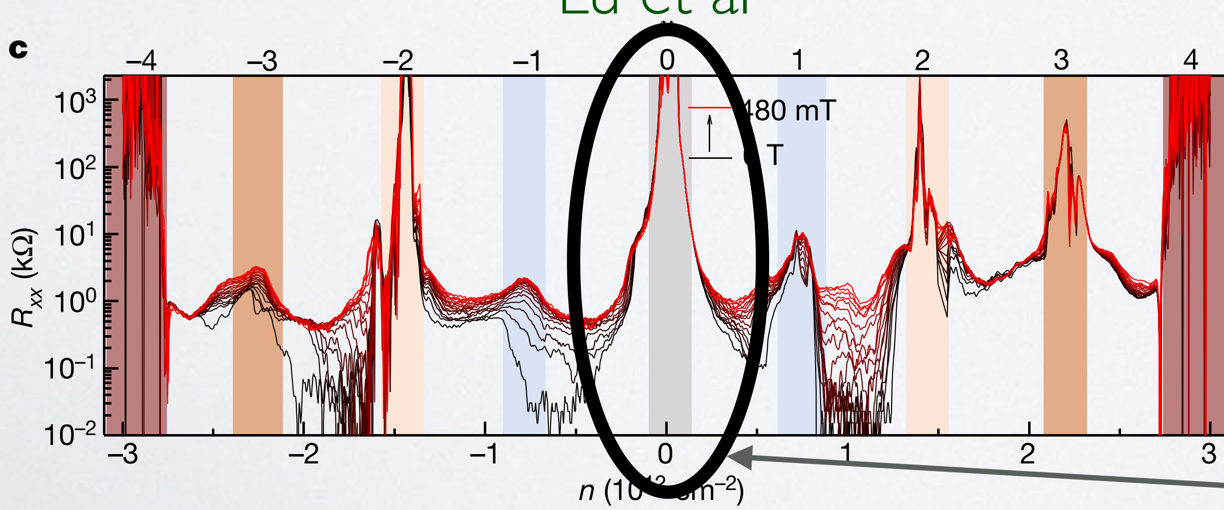
- appearance of insulating and superconducting behaviors at different fillings

Cao et al



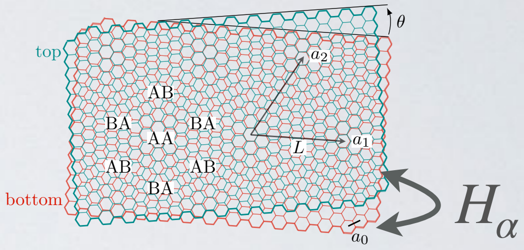
MIT, UCSB, Columbia, Harvard, ICFO, Rutgers, Stanford, Berkeley, Princeton ……

Lu et al



charge neutrality

OUR APPROACH AND RESULTS



- two decoupled twisted sheets of graphene — H_0
- coupled in perturbation theory — $H_0' = H_0 + H_\alpha$
  - obtain velocity as a function of parameters — $v_0 \to v(\alpha, \beta)$
- classify contact interactions (find 12)
- weak-coupling RG approach

$$-\frac{\partial \log g_i}{\partial \log \mu} = -\epsilon + v^{-1} \sum_{l=1}^{12} f_{il}(\alpha, \beta) g_l$$

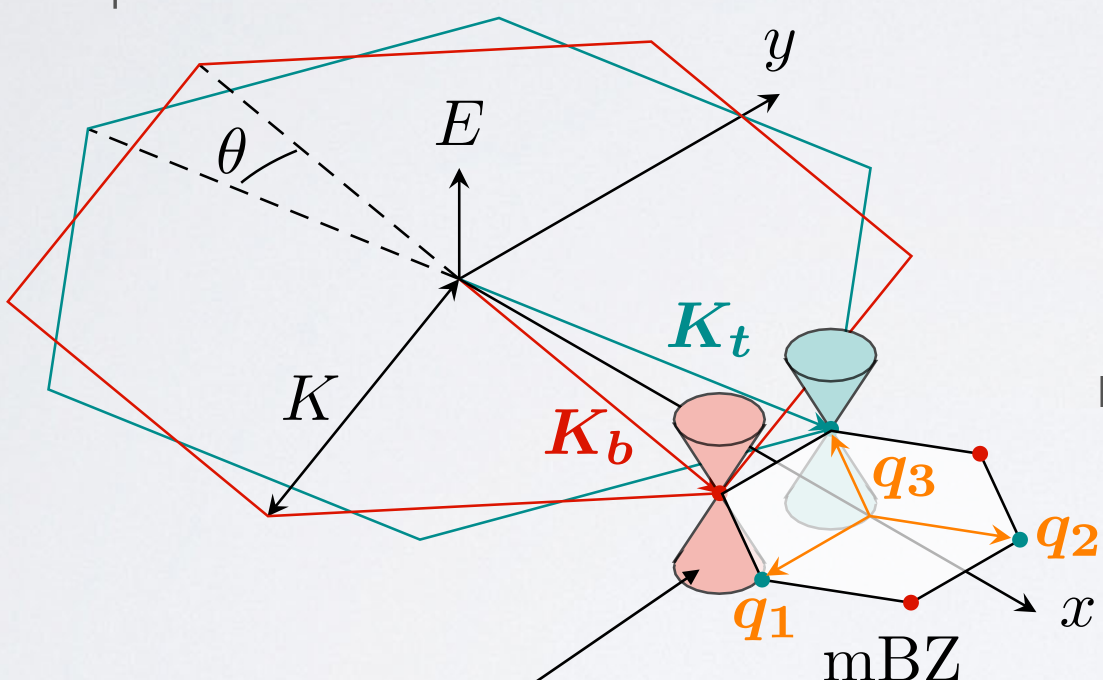
  - define how flow works — collapse of fixed points towards origin
  - obtain flows — nematic phase appears

one other RG paper from 09/20 Kang-Vafek which uses Coulomb

DECOUPLED TWISTED LAYERS

two noninteracting sheets of graphene

reciprocal space



sublattice index $\boldsymbol{\sigma}$
($\sigma^z = \pm 1 = \mathrm{A/B}$)

layer valleys - layer index $\boldsymbol{\tau}$
($\tau^z = \pm 1 =$ top/bottom)

$$\boxed{H_0 = i(\underbrace{\boldsymbol{\sigma} \cdot \partial}_{\text{single-layer graphene}})\tau^0}$$

identical for both layers (for appropriate bases)

in units of

$E_c = 2v_0 K \sin(\theta/2)$

v_0: bare single layer Dirac velocity

spin degeneracy (weak SOC) - spin index $\boldsymbol{\mu}$: discard $\Rightarrow$ four bands

INTERLAYER COUPLING

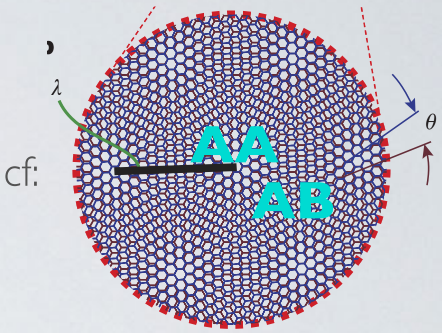
Cao et al 2018

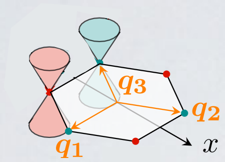
$$\boxed{H_\alpha = \alpha \sum_{j=1}^{3} e^{-i\mathbf{q}_j \cdot \mathbf{r}} T_j^+ + \mathrm{h.c.}}$$

$$T_j^+ = \underbrace{\left(\beta\sigma^0 + e^{\frac{2\pi i}{3}(j-1)}\sigma^+ + e^{-\frac{2\pi i}{3}}\sigma^-\right)}_{\text{sublattice}} \tau^+$$

layer (top/bottom)

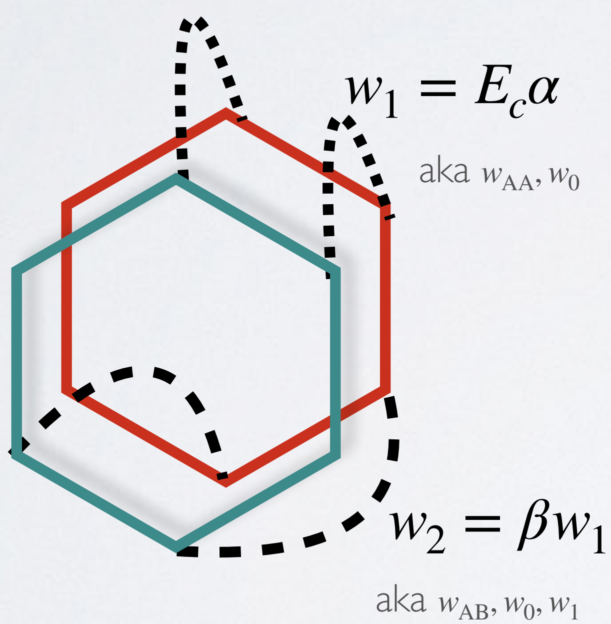
space dependent Hamiltonian ($e^{-i\mathbf{q}_j\cdot\mathbf{r}}$), cf:





in units of $E_c = 2v_0 K \sin(\theta/2)$

real space



Nam-Koshino parameter β:

Bistritzer-MacDonald model:

$w_1 = w_2$ $\quad\beta = 1$

chiral model:

$w_2 = 0$ $\quad\beta = 0$ Tarnopolsky et al 2018

"standard" approach: solve numerically a Schrödinger equation with thousands of bands

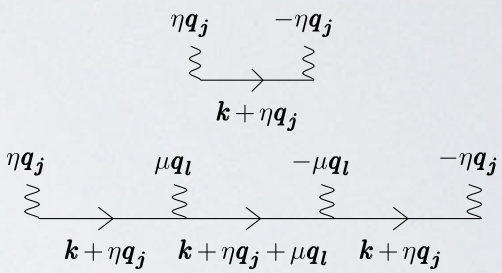
our approach: treat H_α as a perturbation to H_0 $\rightarrow$ obtain analytical results, generalizable to other moiré systems

PERTURBATION BY INTERLAYER COUPLING

$$H_0 = i\,(\boldsymbol{\sigma}\cdot\boldsymbol{\partial})\,\tau_0, \quad H_\alpha = \alpha\sum_{j=1}^{3} e^{-i\boldsymbol{q_j}\cdot\boldsymbol{r}}T_j^+ + \text{h.c.}$$

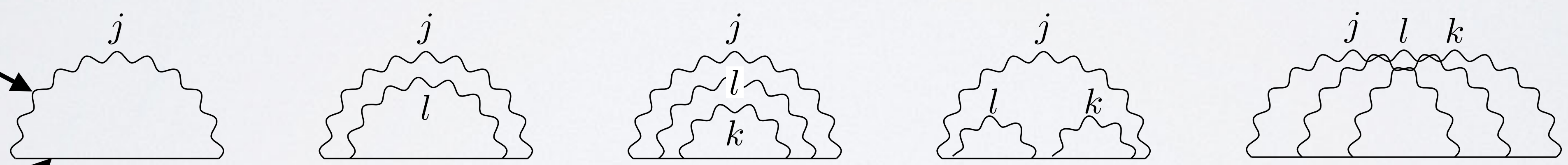
$$T_j^+ = \left(\beta\,\sigma_0 + e^{i(j-1)2\pi/3}\sigma_+ + e^{-i(j-1)2\pi/3}\sigma_-\right)\tau_+$$

$$H_0' = H_0 + H_\alpha$$



sixth order in α, exact in β: $\quad (G_0')^{-1} = H_0 - \partial_\tau - \Sigma \approx N_\psi[v(\alpha,\beta)i(\boldsymbol{\sigma}\cdot\boldsymbol{\partial})\tau_0 - \partial_\tau]$

"momentum insertion" TT



G_0

(a) Σ_α^2 (b) Σ_α^4 (c) $\Sigma_\alpha^{6,\mathrm{nes}}$ (d) $\Sigma_\alpha^{6,\mathrm{row}}$ (e) $\Sigma_\alpha^{6,\mathrm{cro}}$

$$\Sigma_\alpha^2(\boldsymbol{k},\Omega) = \alpha^2\sum_{\eta,j} T_j^{\bar\eta} G_0(\boldsymbol{k}+\eta\boldsymbol{q}_j,\Omega)T_j^\eta$$

technical details:

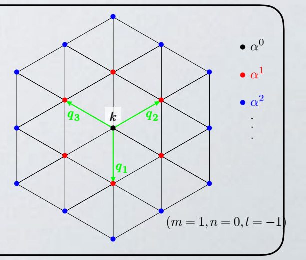
define $G_0'(\boldsymbol{b},\boldsymbol{k},\Omega)$ through $\langle\mathcal{T}\psi_{\boldsymbol{k},\Omega}\psi^\dagger_{\boldsymbol{k}+\boldsymbol{q},\Omega}\rangle_0' = \sum_{\boldsymbol{b}\in\mathcal{R}} G_0'(\boldsymbol{b},\boldsymbol{k},\Omega)\delta(\boldsymbol{b}-\boldsymbol{q})$

focus on

$$G_0'(\boldsymbol{k},\Omega) = G_0'(\boldsymbol{0},\boldsymbol{k},\Omega)$$

give a non-zero contribution to $G_0'(\boldsymbol{k},\Omega)$ if the following conditions are met.

(i) Total momentum is conserved, i.e. $\sum_{r=1}^m \eta_r\boldsymbol{q}_{j_r} = \boldsymbol{0}$.
(ii) Consecutive hopping processes affect different layers, *i.e.* $\eta_{2r} = -\eta_{2r-1}$ for all $r = 1,\dots,n/2$.



DIRAC CONE VELOCITY AS A FUNCTION OF THE HOPPING PARAMETERS

$$N_\psi v(\alpha,\beta) = \boxed{1 - 3\alpha^2} + \alpha^4(1-\beta^2)^2 - \frac{3}{49}\alpha^6(37 - 112\beta^2 + 119\beta^4 - 70\beta^6)$$

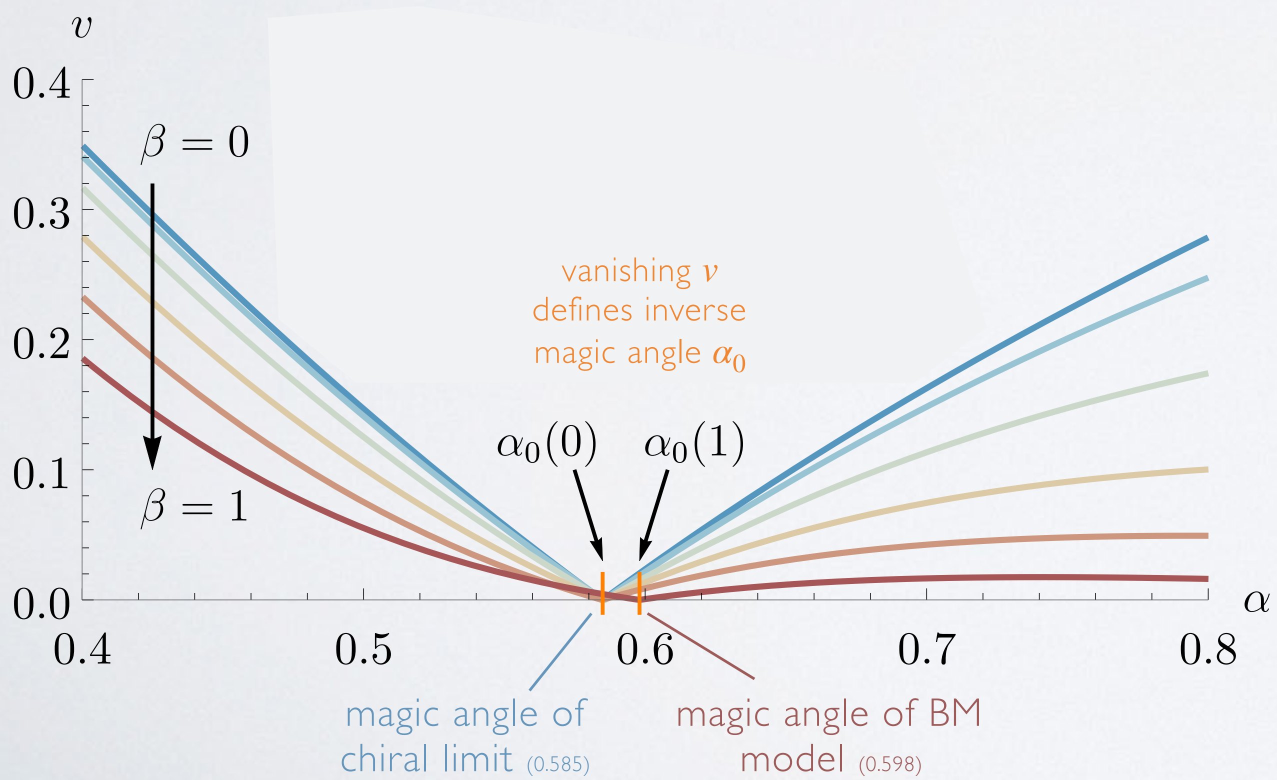
obtained by BM

New! Better! Superbly accurate! Cool numbers!

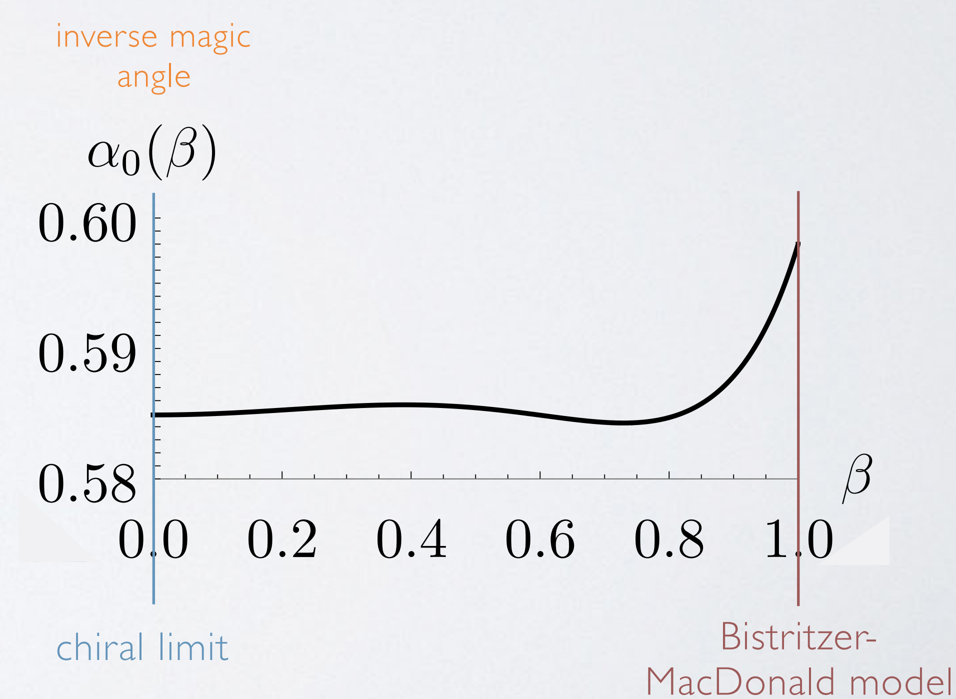
note: expression at $\beta = 0$ obtained by Tarnopolsky et al

note: N is wavefunction normalization factor

Dirac velocity as a function of the inverse twist angle for various values of β:



inverse magic angle as a function of β:



SYMMETRIES

- C_3 rotation around z $C_{3z} = e^{\frac{2i\pi}{3}\sigma^z}\tau^0$
- C_2 rotation around x $M_y = C_{2x} = \sigma^x\tau^x$

D_3

- 2d-inversion x time reversal $C_{2z}T = IT = \sigma^x\tau^0\mathscr{K}$
- (unitary) particle-hole antisymmetry, acts in real space as reflection $x \to -x$, $P = \sigma^x\tau^z$, $\{P, H_0'\} = 0$

lost when:
- keep angular dependence in kinetic energy ($\boldsymbol{\sigma}_{\pm\theta/2}\cdot\boldsymbol{k}$)
- $O(k^2)$ terms included
- intervalley scattering allowed ($K_{t/b}^{(g)} \leftrightarrow {K'_{t/b}}^{(g)}$)

dichromatic magnetic group

find its irreps and multiplication table

GROUP THEORY ANALYSIS OF COUPLINGS

- call Γ the irrep under which the wavefunction transforms (4d irrep)
- find all copies of the trivial irreps in the product $(\Gamma^\dagger \otimes \Gamma) \otimes (\Gamma^\dagger \otimes \Gamma)$ cf. $(\psi^\dagger M \psi)(\psi^\dagger M \psi)$
- those are the products $\rho \otimes \rho$ of the irreps below:

symmetric in sublattices | antisymmetric in sublattices

eight one-dimensional coreps

Corep.	A_1^+	a_1^+	A_2^+	a_2^+	A_1^-	a_1^-	A_2^-	a_2^-
$\hat{R}^{(i)}$	$\sigma_0\tau_0$	$\sigma_0\tau_x$	$\sigma_0\tau_z$	$\sigma_0\tau_y$	$\sigma_z\tau_y$	$\sigma_z\tau_z$	$\sigma_z\tau_x$	$\sigma_z\tau_0$
IT	✓	✓	✓	✓				
C_2	✓	✓			✓	✓		
P		✓		✓		✓		✓

$$\rho^{(i)} = \psi^\dagger \hat{R}^{(i)} \psi$$

four two-dimensional coreps

Corep.	E_2^+	E_4^+	E_2^-	E_4^-
$\sqrt{2}\,\hat{\boldsymbol{M}}^{(j)}$	$\boldsymbol{\sigma}\tau_0$	$\boldsymbol{\sigma}\tau_x$	$\boldsymbol{\sigma}\tau_y$	$\boldsymbol{\sigma}\tau_z$

$$\boldsymbol{J}^{(j)} = \psi^\dagger \hat{\boldsymbol{M}}^{(j)} \psi$$

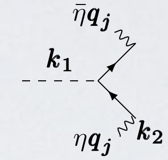
off-diagonal in sublattices

$$S_{\text{int}} = -\sum_{i=1}^{8} g_i \int \mathrm{d}^2 r\, \mathrm{d}\tau\, \rho^{(i)}(\boldsymbol{r})\rho^{(i)}(\boldsymbol{r}) - \sum_{j=1}^{4} \lambda_j \int \mathrm{d}^2 r\, \mathrm{d}\tau\, \boldsymbol{J}^{(j)}(\boldsymbol{r}) \cdot \boldsymbol{J}^{(j)}(\boldsymbol{r})$$

treat all these

RENORMALIZATION GROUP APPROACH

Hubbard-Stratonovich decoupling: $S_{\text{int}}[\psi^\dagger,\psi] \to S_{\text{Hub}}[\psi^\dagger,\psi,\phi]$



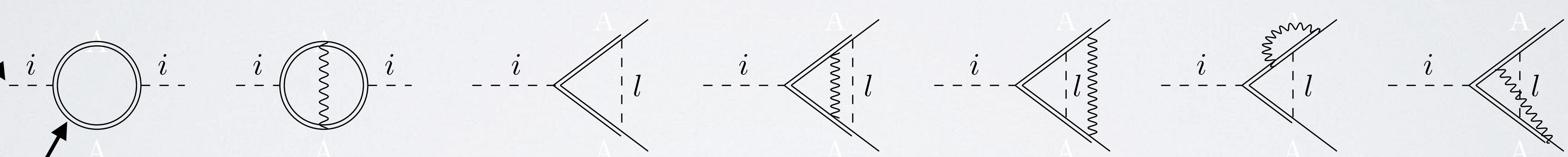
coupling strengths

$$S_{\text{Hub}}[\psi^\dagger,\psi,\phi] = \sum_{i=1}^{8}\int \mathrm{d}^2r\,\mathrm{d}\tau\,\left(\phi_i^2 + 2\sqrt{g_i}\,\psi^\dagger\phi_i R_i\psi\right) + \sum_{j=9}^{12}\int \mathrm{d}^2r\,\mathrm{d}\tau\,\left(\boldsymbol{\varphi}_j^2 + 2\sqrt{\lambda_i}\,\psi^\dagger\boldsymbol{\varphi}_j\cdot\boldsymbol{M}_j\psi\right)$$

1d irreps

2d irreps

ϕ,φ



(a) Π_i^0 (b) Π_i^1 (c) V_{il}^0 (d) $V_{il}^{1,\text{int}}$ (e) $V_{il}^{1,\text{ext}}$ (f) $V_{il}^{1,\text{iso}}$ (g) $V_{il}^{1,\text{cro}}$

G_0'

renormalized

up to α^2

$$-\frac{\partial \log g_i}{\partial \log \mu} = -\epsilon + v^{-1}\sum_{l=1}^{12} f_{il}(\alpha,\beta)g_l$$

RG parameter (momentum scale)

renormalized velocity

epsilon expansion, $d+1 = D = 2+\epsilon$

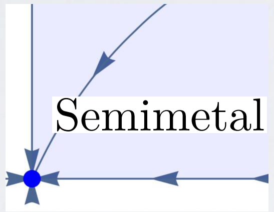
$(\epsilon = 1)$

RENORMALIZATION GROUP APPROACH

- 4 couplings with nonzero divergent corrections (discard others), all diagonal in layers, i.e. τ^0, τ^z

σ^0 sublattice structure → no pole in ϵ
$\tau^\pm$ structure → correction vanishes at low energy

- non-interacting fixed point at origin



- flows controlled by critical points, dominant instabilities are those whose fixed point collapses the fastest towards the origin

Channel	Coupling	$\hat{M}_i$	FP $g_i^*(\alpha,\beta)$
a_2^-	g_0	$\sigma_z\tau_0$	$\pi v\epsilon/\left(4\left[1-12\alpha^2(1-\beta^2)\right]\right)$
a_1^-	g_z	$\sigma_z\tau_z$	$\pi v\epsilon/4$
E_2^+	λ_0	$\boldsymbol{\sigma}\tau_0/\sqrt{2}$	$\pi v\epsilon/\left(4\left[1-3\alpha^2(1-\beta^2)\right]\right)$
E_4^-	λ_z	$\boldsymbol{\sigma}\tau_z/\sqrt{2}$	$\pi v\epsilon/\left(4\left[1+3\alpha^2(1+\beta^2)\right]\right)$

flow equations in two-dimensional parameter space:

a_1^- $$-\mu\frac{\partial g_z}{\partial\mu} = -\epsilon g_z + \frac{4g_z^2}{\pi v} + \frac{4g_z\lambda_z}{\pi v}\left[1-6\alpha^2\left(1-\beta^2\right)\right]$$ 1d irrep

E_4^- $$-\mu\frac{\partial \lambda_z}{\partial\mu} = -\epsilon \lambda_z + \frac{4\lambda_z^2}{\pi v}\left[1+3\alpha^2\left(1+\beta^2\right)\right] + \frac{2\lambda_z g_z}{\pi v}\left[1-6\alpha^2\left(1-\beta^2\right)\right]$$ 2d irrep

ORDER PARAMETERS

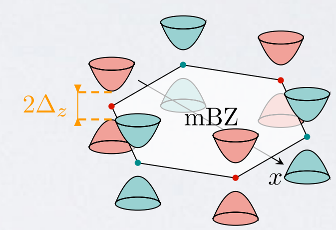
- mean-field associated with four of the couplings (important in the RG)

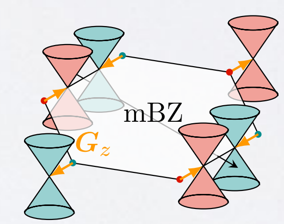
real space density

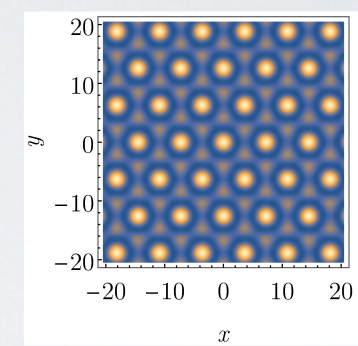
$$\Delta_{0/z} = -2g_{0/z} \int \mathrm{d}\omega \int_{\Lambda} \frac{\mathrm{d}^2 q}{(2\pi)^3} \langle \psi^{\dagger}_{q,\omega} \sigma_z \tau_{0/z} \psi_{q,\omega} \rangle$$

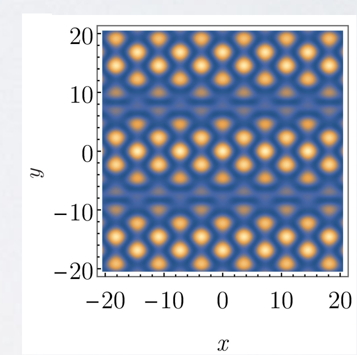
$$\boldsymbol{\mathcal{G}}_{0/z} = -2\lambda_{0/z} \int \mathrm{d}\omega \int_{\Lambda} \frac{\mathrm{d}^2 q}{(2\pi)^3} \langle \psi^{\dagger}_{q,\omega} \boldsymbol{\sigma} \tau_{0/z} \psi_{q,\omega} \rangle.$$

sym/antisym in layers



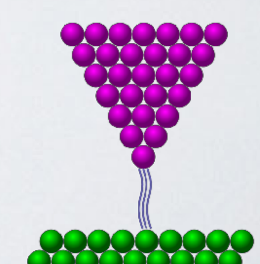






$|\psi_t + \psi_b r|^2$

asymmetry factor for STM between top and bottom layers



top

bottom

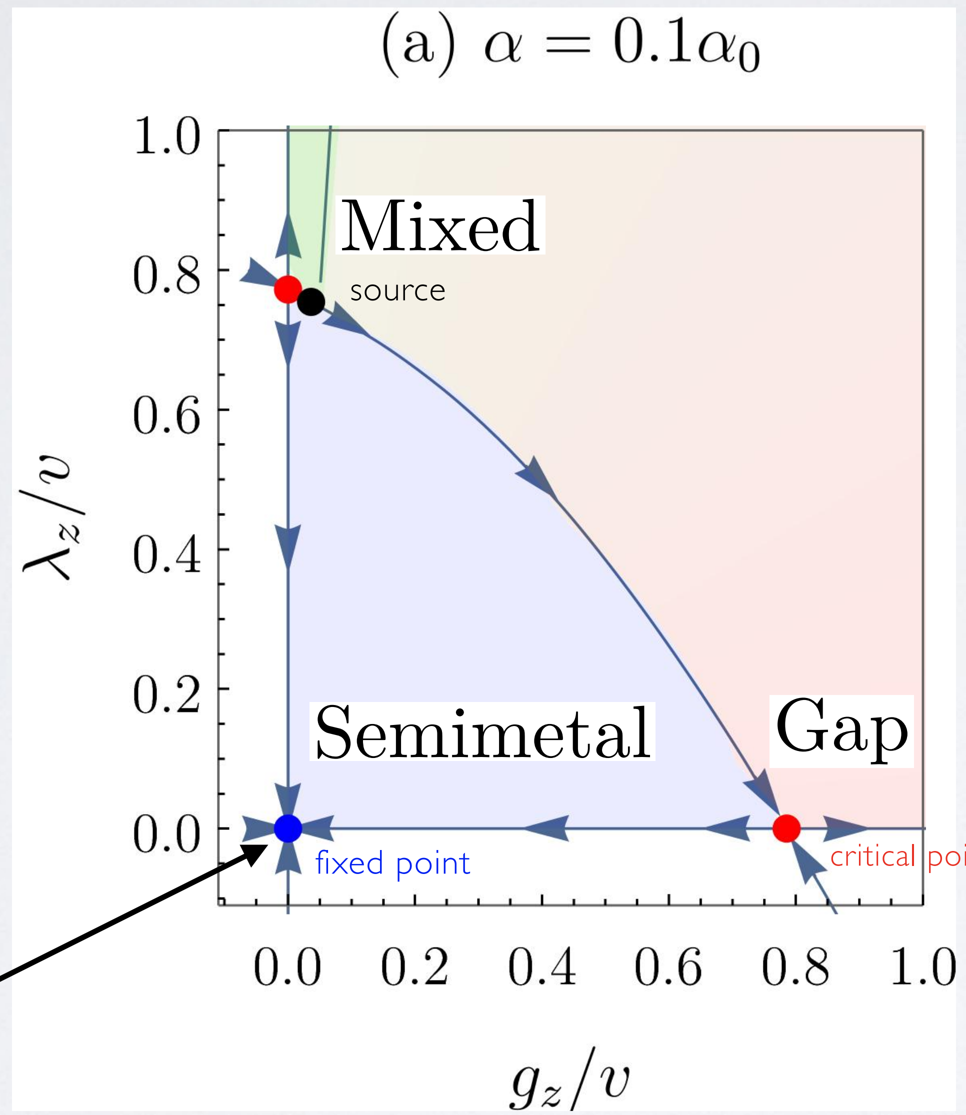
$$H'_{\mathrm{MF}} = H'_0 + \boldsymbol{\sigma} \cdot \left(\boldsymbol{\mathcal{G}}_0 \tau^0 + \boldsymbol{\mathcal{G}}_z \tau^z \right) + \sigma^z (\Delta_0 \tau^0 + \Delta_z \tau^z)$$

FLOW DIAGRAMS

almost-decoupled layers ("far" from magic angle)

v big

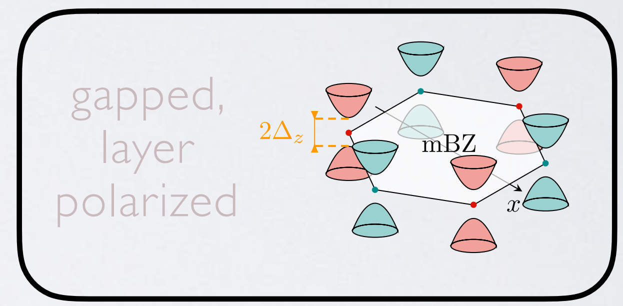
$\boldsymbol{\sigma\tau}^z$



~ "chiral symmetry breaking" transition of Dirac fermions

noninteracting phase

$\sigma^z\tau^z$



$I\mathscr{T}$-breaking

layer polarized

couplings rescaled by v (here v still big)

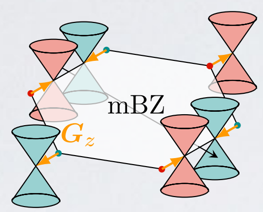
FLOW DIAGRAMS

~AT the magic angle

C_3-breaking

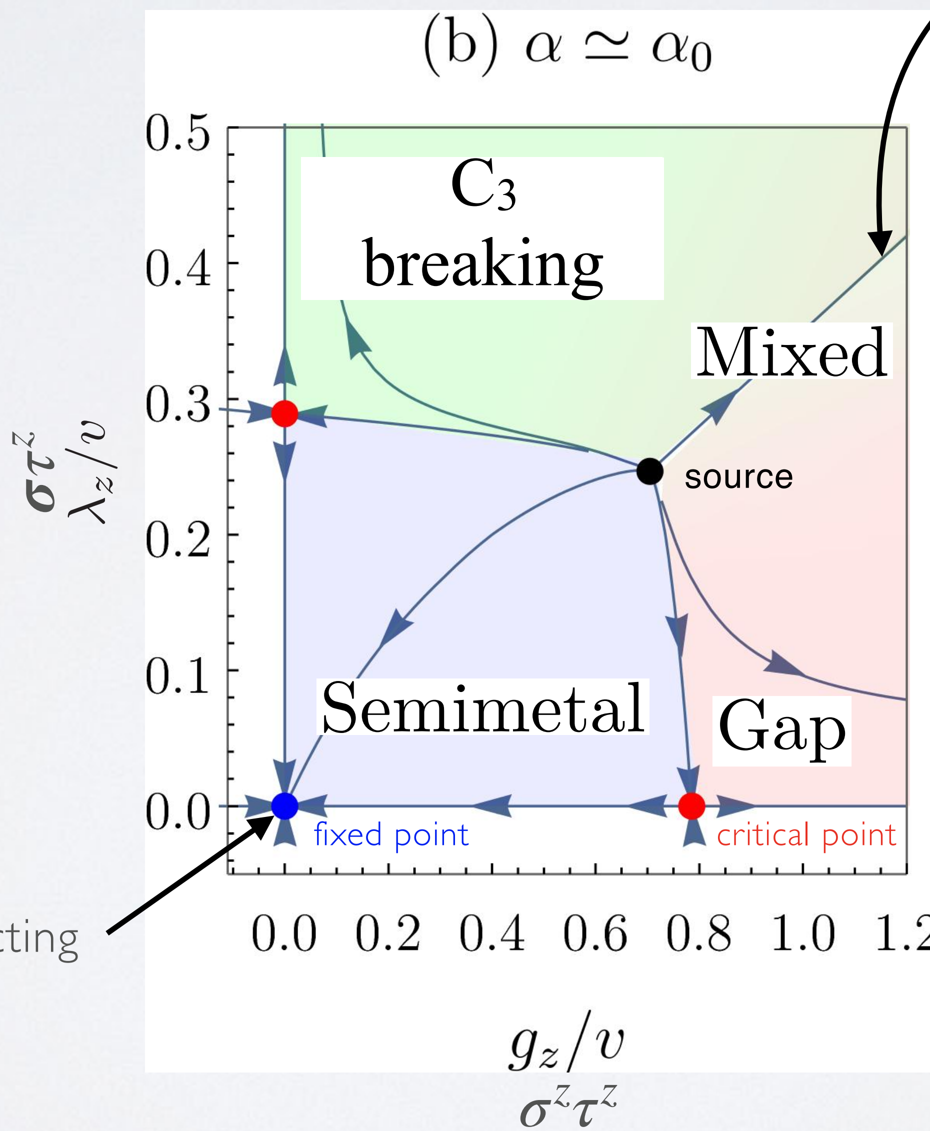
"nematic"

density-modulated (intra moiré unit cell)



see also: Andrei, Pasupathi, Fernandes, Venderbos, Chubukov, Zaletel, Vishwanath etc.

$$\lambda_z = g_z \frac{1+6\alpha^2(1-\beta^2)}{6\alpha^2(3-\beta^2)}$$



crossover region

coexistence of both order parameters, possibly first order transition, or critical point at strong coupling

layer polarized

noninteracting phase

couplings rescaled by $v \to 0$

CONCLUSIONS

- RG procedure which is **perturbative in interlayer coupling**, rather than using band basis.
  - advantage: can **analytically obtain everything**, including magic angle
  - find very **weak dependence on w_{AB} (β)** parameter, esp. below $\beta \sim 0.8$, so chiral model may contain all needed ingredients to recover the physics
- Main result: **dominant new instability at magic angle is the C₃-symmetry-breaking**, i.e. "nematic"
- **Technique development**:
  - diagrammatic approach to velocity renormalization, alternate to band basis
  - new RG approach to dominant instability when all are important (vanishing kinetic energy)