# Competing phases of interacting electrons in twisted bilayer graphene and related moiré heterostructures 

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## Magic-angle twisted bilayer graphene

- two graphene layers with small rotational mismatch $\theta$
- long-wavelength moiré pattern
- @ $\theta_{M} \approx 1.05^{\circ}, 1.16^{\circ}: \sim 10,000$ atoms per moiré cell

- correlated insulator and superconductivity



## Outline

- Introduction \& motivation
- twisted bilayer graphene - basics \& experiments
- related moiré heterostructures
- twisted bilayer graphene - models
- Effective lattice models \& many-body approaches
- functional renormalization group approach
- next-to-minimal model and tentative phase diagram
- conclusions \& outlook

Twisted bilayer graphene - basics \& experiments

## Moiré pattern in STM



图Li et al., Nature Physics 6 (2010)

## Correlated magic-angle tBLG - basic mechanism

- for small twist angles $\theta<10^{\circ}$
- moiré pattern $\rightarrow$ superlattice potential $\rightarrow$ reconstruction of low-energy band structure:

- flat band structure at magic angle $\theta \approx I^{\circ}$ :
- $2 \times 2 \times 2=8$ nearly flat bands
- 2 bands crossing at mini-Dirac points
- spin (2 x)
- singlelayer valley ( 2 x )
- vary carrier concentration by gate voltage:

茖Bistritzer \& MacDonald (201I) E[meV]

- between $n= \pm 4 n_{0}$
(relative to charge neutrality)
- $n_{0} \xlongequal{\wedge} \mathrm{I}$ e- per unit cell of superlattice
$\longrightarrow$ angle $\theta$ controls ratio bandwith/interaction: $t / U \sim\left|\theta-\theta_{M}\right|$
$\longrightarrow$ strongly-correlated states!


## Magic-angle tBLG - phase diagram I.0 (2018)



- band insulator at $n= \pm 4 n_{0}$
- correlated insulator at $n= \pm 2 n_{0}$
- superconducting domes at $n / n_{0}=-2 \pm \delta$
- $\mathrm{T}_{\mathrm{c}} \sim 1.7 \mathrm{~K}$
- $\mathrm{T}_{\mathrm{c}} / \mathrm{T}_{\mathrm{F}}$ large
- resemblance to cuprate phase diagram!
- Cao et al., Nature 556, 43 (2018)
( Cao et al., Nature 556, 80 (2018)



## Questions



- Are the integer fillings $n / n_{0}= \pm 2$ special?
- Are there further correlated states in different parameter regimes?



## $\mathbf{2}^{\text {nd }}$ generation of $\mathbf{t B L G}$ experiments (2019)



央Columbia University:Yankowitz et al., Science 363, I059 (2019)

- apply hydrostatic pressure P
[ variation of interlayer tunneling w
$\square$ changes magic angle $\theta_{M} \sim w$
Ein-situ control of $t / U \sim\left|\theta-\theta_{M}\right|$
- pressure increases $\theta_{\mathrm{M}}$
$\square$ reduce moiré lattice constant
$\square$ increase energy scale: $\mathrm{T}_{\mathrm{c}, \mathrm{sc}} \sim 3 \mathrm{~K}$
- correlated insulator also at $n / n_{0}=+3$, superconductor near $n / n_{0}= \pm 2$

图Efetov Lab, Barcelona: Lu et al., arXiv: I 903.065 I3


- very low twist-angle disorder
- reduced modulations of $\theta$ across device
- $\Delta \theta<0.02^{\circ}$
- insulating gaps at $n / n_{0}=-3,-2,-1,0,+1,+2,+3$
- SC domes in between ( $\mathrm{T}_{\mathrm{c}, \mathrm{SC}} \sim 0.14-3 \mathrm{~K}$ )
- more results on finite $B \perp$, role of topology with aligned $h B N$ substrate, Landau fans

Stanford: Sharpe et al., arXiv: I 90 I. 03520

new platform established for study of correlated electrons
$\checkmark$ high control of twist angle, low level of disorder, pressure/gate tunable band widths/fillings

## Related 2D van der Waals moiré heterostructures

－magic－angle twisted bilayer graphene $\checkmark$
－$A B C$ trilayer graphene on hexagonal boron nitride
－experiments：tunable insulating and SC behavior
Chen et al．，Nat．Phys．I5， 237 （2019）
（2019）
－twisted double bilayer graphene
－experiments：spin－polarized correlated insulating and SC behavior
Liu et al．，arXiv：I903．08I30（2019）
苜 Cao et al．，arXiv：I903．08596（2019）
－twisted bilayer boron nitride
－theoretical：multi－flat bands and strong correlations
食Xian et al．，arXiv：I8I2．08097（2018）
－transition metal dichalcogenides
－theoretical：flat bands and strong correlations with and without twist．．．

Twisted bilayer graphene - models

## Geometry of twisted honeycomb bilayers

- start from $A B$ stacking
$\vec{a}_{1}=(1 / 2, \sqrt{3} / 2)^{T} a_{0}$
$\vec{a}_{2}=(-1 / 2, \sqrt{3} / 2)^{T} a_{0}$
- commensurate structure when B' rotated to site formely occupied by other B'
- 2D bilayer crystal only at discrete set of commensurate rotation angles


## Geometry of twisted honeycomb bilayers

- start from $A B$ stacking

$$
\begin{aligned}
& \vec{a}_{1}=(1 / 2, \sqrt{3} / 2)^{T} a_{0} \\
& \vec{a}_{2}=(-1 / 2, \sqrt{3} / 2)^{T} a_{0}
\end{aligned}
$$

## Geometry of twisted honeycomb bilayers

- 2D bilayer crystal only at discrete set of commensurate rotation angles

$$
\cos \left(\theta_{i}\right)=\frac{3 i^{2}+3 i+1 / 2}{3 i^{2}+3 i+1}, \quad i \in \mathbb{N}_{0}
$$



- emergent moiré superlattice spanned by real space lattice vectors $t_{1}$ and $t_{2}$



## Geometry of twisted honeycomb bilayers

- example: $\theta \approx 2.6^{\circ}(i=12)$

- local AA, AB and BA stacking regions
- moiré superlattice vectors $t_{1}$ and $t_{2}$


## Mini Brillouin zone



- reciprocal lattice vectors: $\quad \vec{G}_{1}=\frac{4 \pi}{3\left(3 i^{2}+3 i+1\right)}\left[\vec{a}_{1}+(3 i+1) \vec{a}_{2}\right]$

$$
\vec{G}_{2}=\frac{4 \pi}{3\left(3 i^{2}+3 i+1\right)}\left[(3 i+1) \vec{a}_{1}-(3 i+2) \vec{a}_{2}\right]
$$

- Dirac points of single-layer graphene layers: $K_{1}, K_{1}{ }^{\prime}, K_{2}, K_{2}{ }^{\prime}$


## Effective continuum model

- moiré period much larger than atomic scale $\rightarrow$ continuum model
- neglect intervalley mixing (large momentum space separation)

Lopes dos Santos et al., PRL 99, 256802 (2007)
全Bistritzer, MacDonald, PNAS I08, I 2233 (201I)

- independent calculation for each valley $\xi \in \pm$
- I Dirac cone from each layer: interlayer hybridization

- effective $4 \times 4$ Hamiltonian

$$
H^{(\xi)}=\left(\begin{array}{cc}
H_{1} & U^{\dagger} \\
U & H_{2}
\end{array}\right) \quad \text { intralayer Dirac Hamiltonians }
$$



- Dirac cones become nearly flat for magic angles
- dependence on modelling of interlayer coupling (lattice relaxation, corrugation,...)


## Effective continuum model

- full calculation of band dispersion in continuum model

- at magic angles $\theta_{M}$ (here: $\theta_{M}=1.05^{\circ}$ )
- emergence of multiple nearly flat bands
- well-separated from other bands
- van Hove singularities in flat bands


Koshino et al, PRX 8, 031087 (2018)

## Wannier orbitals for flat bands \& effective lattice model

- symmetry analysis for tBLG:
- Wannier orbitals centered at nonequivalent AB and BA spots in moiré pattern
- formation of emergent honeycomb lattice

- emergent triangular lattice:ABC trilayer graphene-hBN, twisted double BLG,TMDs


## Wannier orbitals for flat bands \& effective lattice model

- flat band dispersion from continuum model
- construct max-localized Wannier orbitals
- tight-binding + extended Hubbard model


$$
H=\sum_{\xi= \pm} \sum_{i j} t\left(\boldsymbol{r}_{i j}\right) e^{i \xi \phi\left(\boldsymbol{r}_{i j}\right)} c_{i \xi}^{\dagger} c_{j \xi} \quad+\quad \text { extended Hubbard i.a. }
$$

- hopping integrals and electron-electron interaction parameters:

Koshino et al, PRX 8, 031087 (2018)
全Kang \& Vafek, PRX 8, 031088 (2018)
(a) From orbital 1

(b) From orbital 2



## Correlated moiré heterostructures - precis

## Precis

- 2D moiré heterostructures:
- emergent flat bands, small kinetic energy
- enhanced interaction effects


## correlation-driven states!

- construction of effective models on emergent moiré honeycomb/triangular superlattice
- universal features:
- multi-orbital structure inherited from two valleys $\rightarrow$ Hund's couplings
- onsite and sizable further-neighbor interactions
...starting point for application of many-body methods...
- what is the nature of the correlated insulating and SC states?
- Kekulé valence bond solid, (anti)ferromagnet, interaction-induced top. states,...?
- featureless Mott insulator?
- gapped quantum spin liquid with neutral spin-l/2 excitations?
- topological/chiral d+id superconductor, f-wave superconductor,...?


## Functional renormalization group approach

## Effective action

- system of interacting fermions: $\quad \mathcal{S}[\psi, \bar{\psi}]=-\left(\bar{\psi}, G_{0}^{-1} \psi\right)+V[\psi, \bar{\psi}]$ general two-particle i.a.
- bare propagator (translation and spin rotation invariance):

$$
G_{0}\left(k_{0}, \mathbf{k}\right)=\frac{1}{i k_{0}-\xi_{\mathbf{k}}}, \quad \xi_{\mathbf{k}}=\epsilon_{\mathbf{k}}-\mu
$$

- generating functional (for connected Green functions):

$$
\mathcal{G}[\eta, \bar{\eta}]=-\ln \int \mathcal{D} \psi \mathcal{D} \bar{\psi} e^{\mathcal{S}[\psi, \bar{\psi}]} e^{(\bar{\eta}, \psi)+(\bar{\psi}, \eta)}
$$

- effective action: $\quad \Gamma[\phi, \bar{\phi}]=(\bar{\eta}, \phi)+(\bar{\phi}, \eta)+\mathcal{G}[\eta, \bar{\eta}], \quad \phi=-\frac{\partial \mathcal{G}}{\partial \bar{\eta}}, \quad \bar{\phi}=\frac{\partial \mathcal{G}}{\partial \eta}$ (generates one-particle irreducible vertex functions)


## Functional flow equations

- modify bare propagator by introduction of flow parameter $(\mathbb{R}$ cutoff, cuts out soft modes $<\Lambda): \quad G_{0}^{\Lambda}\left(k_{0}, \mathbf{k}\right)=\frac{\Theta_{\epsilon}\left(\left|\xi_{\mathbf{k}}\right|-\Lambda\right)}{i k_{0}-\xi_{\mathbf{k}}}$
- define all the above quantities with modified bare propagator
$\rightarrow$ variation w.r.t to scale provides exact RGequation:

$$
\frac{\partial}{\partial \Lambda} \Gamma^{\Lambda}[\phi, \bar{\phi}]=\operatorname{Tr}\left[G_{0}^{\Lambda} \frac{\partial\left(G_{0}^{\Lambda}\right)^{-1}}{\partial \Lambda}\right]-\operatorname{Tr}\left[\left(\frac{\delta^{2} \Gamma^{\Lambda}[\phi, \bar{\phi}]}{\delta \phi \delta \bar{\phi}}+\left(G_{0}^{\Lambda}\right)^{-1}\right)^{-1} \frac{\partial\left(G_{0}^{\Lambda}\right)^{-1}}{\partial \Lambda}\right]
$$

图 Wetterich (1993)
Salmhofer \& Honerkamp (2001)

- exact RG equation has one-loop structure
- removing cutoff $(\Lambda \rightarrow 0)$ yields the full effective action
- lowering cutoff corresponds to momentum-shell integration



## Truncation and approximations

- exact RG equation cannot be solved exactly!
- starting point for systematic approximations (vertex expansion)

... infinite hierarchy of flow equations!


## Symmetries and approximations

- system with spin-rotational invariance:
- RG flow of general 4-point function $\Gamma(4) \Lambda: \quad \Gamma_{\sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4}}^{(4) \Lambda}=V^{\Lambda} \delta_{\sigma_{1} \sigma_{3}} \delta_{\sigma_{2} \sigma_{4}}-V^{\Lambda} \delta_{\sigma_{1} \sigma_{4}} \delta_{\sigma_{2} \sigma_{3}}$
$\square$ interaction vertex $V$ :


$$
V_{\Lambda}\left(k_{1}, k_{2}, k_{3}, k_{4}\right)
$$

- momentum arguments include frequency, wavevector and orbital indices
- ground-state properties: neglect frequency dependence, set external frequencies to zero


## Symmetries and approximations

- system with spin-rotational invariance:
- RG flow of general 4-point function $\Gamma^{(4) \Lambda:} \Gamma_{\sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4}}^{(4) \Lambda}=V^{\Lambda} \delta_{\sigma_{1} \sigma_{3}} \delta_{\sigma_{2} \sigma_{4}}-V^{\Lambda} \delta_{\sigma_{1} \sigma_{4}} \delta_{\sigma_{2} \sigma_{3}}$
$\square$ flow of spin-independent interaction vertex $\boldsymbol{V}^{\boldsymbol{\wedge}}$ :

$$
\begin{aligned}
& \frac{d}{d \Lambda} V^{\Lambda}\left(K_{1}, K_{2} ; K_{3}, K_{4}\right)= \int d K V^{\Lambda}\left(K_{1}, K_{2}, K\right) L^{\Lambda}\left(K,-K+K_{1}+K_{2}\right) V^{\Lambda}\left(K,-K+K_{1}+K_{2}, K_{3}\right), \\
&+\int d K\left[-2 V^{\Lambda}\left(K_{1}, K, K_{3}\right) L^{\Lambda}\left(K, K+K_{1}-K_{3}\right) V^{\Lambda}\left(K+K_{1}-K_{3}, K_{2}, K\right)\right. \\
&+V^{\Lambda}\left(K_{1}, K, K+K_{1}-K_{3}\right) L^{\Lambda}\left(K, K+K_{1}-K_{3}\right) V^{\Lambda}\left(K+K_{1}-K_{3}, K_{2}, K\right), \\
&\left.+V^{\Lambda}\left(K_{1}, K, K_{3}\right) L^{\Lambda}\left(K, K+K_{1}-K_{3}\right) V^{\Lambda}\left(K_{2}, K+K_{1}-K_{3}, K\right)\right], \\
&+\int d K V^{\Lambda}\left(K_{1}, K+K_{2}-K_{3}, K\right) L^{\Lambda}\left(K, K+K_{2}-K_{3}\right) V^{\Lambda}\left(K, K_{2}, K_{3}\right) . \\
& \text { - where } L^{\Lambda}\left(K, K^{\prime}\right)=\frac{d}{d \Lambda}\left[G_{0}^{\Lambda}(K) G_{0}^{\Lambda}\left(K^{\prime}\right)\right]
\end{aligned}
$$

## Symmetries and approximations

- system with spin-rotational invariance:
- RG flow of general 4-point function $\Gamma^{(4) \Lambda:} \Gamma_{\sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4}}^{(4) \Lambda}=V^{\Lambda} \delta_{\sigma_{1} \sigma_{3}} \delta_{\sigma_{2} \sigma_{4}}-V^{\Lambda} \delta_{\sigma_{1} \sigma_{4}} \delta_{\sigma_{2} \sigma_{3}}$
$\square$ flow of spin-independent interaction vertex $V^{\wedge}$ :

- corresponds to infinite order summation of one-loop pp and ph terms
- unbiased investigation of competition between various correlations
- flow to strong coupling indicates ordering transition: analyze components of ${ }^{\wedge}$ ^


## Multi-orbital models

## - orbital degrees of freedom:

- valley d.o.f. in tBLG, d-orbitals of iron pnictides and transition-metal oxides
- sublattice index of bipartite/multi-layer lattice (e.g., graphene's honeycomb lattice)
- general non-interacting part of multi-orbital model: $H_{0}=\sum_{\vec{k}, s} \sum_{o, o^{\prime}} c_{o, s, \vec{k}}^{\dagger} K_{o, o^{\prime}}(\vec{k}) c_{o^{\prime}, s, \vec{k}}$
- unitary transformation to energy band representation:

$$
\begin{aligned}
& c_{b, s, \vec{k}}=\sum_{o} u_{b o, \vec{k}} c_{o, s, \vec{k}} \\
& c_{b, s, \vec{k}}^{\dagger}=\sum_{o} u_{b o, \vec{k}}^{*} c_{o, s, \vec{k}}^{\dagger}
\end{aligned} \quad H_{0}=\sum_{\vec{k}, s, b} E_{b}(\vec{k}) c_{b, s, \vec{k}}^{\dagger} c_{b, s, \vec{k}}
$$

- interaction part of Hamiltonian has to be transformed accordingly
$\square$ adds momentum dependence to interaction vertex at bare level - orbital makeup


## Fermi-surface patching scheme



- wavevector dependence of Fermi surface from discretization in $\mathbf{N}$ patches:

- interaction constant within one patch
- representative momenta lie at Fermi level
- finite set of coupled flow equations for components of $V^{\wedge}$
- facilitates numerical implementation
- example:
- $t-t^{\prime}-\mu$-Hubbard model on the square lattice: vertex has $N^{3}$ components
- generally: $\boldsymbol{V}^{\boldsymbol{\wedge}}$ has $\mathbf{N}_{\mathbf{b}}^{\mathbf{4}} \mathbf{N}^{\mathbf{3}}$ components


## fRG: from bare to effective interaction

- excitations at intermediate scales generate momentum structure in low-energy interaction

- low-energy effective action \& momentum structure
$\Rightarrow$ two-particle interaction vertex $V\left(\vec{p}, \vec{p}^{\prime}, \vec{p}+\vec{q}\right)$
$\square$ flow to strong coupling: singularity for $\Lambda \rightarrow \Lambda^{*}$
5 read off dominant interactions and e.g. extract form factors of order parameters


## fRG: from bare to effective interaction



- sharp momentum structures in the interaction vertex emerge
- e.g., onsite interaction ( $U=3.0 t$ ), typical pattern ( $k_{3}$ fixed at point 1 ):

- mean-field decoupling $\rightarrow$ antiferromagnetic SDW (AF-SDW) or d-wave SC


## fermion fRG approach - Precis

- fermion fRG: discovery tool for leading many-body instabilities

- treats all fermionic fluctuation channels on equal footing
- infinite-order resummation of all fermionic I-loop diagrams
- can deal with multi-orbital band structures, non-local i.a. \& competing correlations
- due to truncations/approximations: qualitative (not quantitative) tool
- prediction of different types of magnetism / superconductivity / bond order states / ...


## Minimal phenomenological model for tDBLG

I. triangular lattice near van-Hove filling (twisted double bilayer graphene)
2. weak tunnelling between nearest-neighbor unit supercells dominates kinetic energy
3. each cell hosts two degenerate orbitals from original valleys +/-
4. no mixing of orbitals due to large momentum space separation
5. spin-independent hopping of electrons
$\longrightarrow$ two-orbital tight-binding model $H_{\text {kin }}=-t \sum_{\langle i j\rangle} \sum_{\sigma=\uparrow, \downarrow} \sum_{o= \pm}\left(c_{i \sigma o}^{\dagger} c_{j \sigma o}+\right.$ h.c. $)$

- 4 flavours: $a \in\{(\uparrow,+),(\downarrow,+),(\uparrow,-),(\downarrow,-)\} \rightarrow$ effective $S U(4)$ symmetry
- add $\operatorname{SU}(4)$ symmetric Hubbard interaction as minimal interaction

$$
H_{\mathrm{int}}=U \sum_{i}\left(\sum_{\alpha=1}^{4} n_{i \alpha}\right)^{2}
$$

- dominant interaction depends only on total charge of site


## Next-to-minimal model

- Include Hund's couplings: $\quad H_{h}=-V_{h} \sum_{i} \vec{S}_{i} \cdot \vec{S}_{i}$
- with $\vec{S}_{i}=\frac{1}{2} c_{i \sigma o}^{\dagger} \vec{\sigma}_{\sigma \sigma^{\prime}} c_{i \sigma^{\prime} o}$

全 Xu \& Balents
Dodaro, Kivelson, Schattner, Sun, Wang Yuan \& Fu
(Po, Zou,Vishwanath, Senthil

- breaks SU(4)
- alternatively "orbital" Hund's coupling (anti-Hund):

$$
H_{K}=-K \sum_{i} \vec{L}_{i} \cdot \vec{L}_{i} \quad \text { with } \quad \vec{L}_{i}=\frac{1}{2} c_{i \sigma o}^{\dagger} \vec{\tau}_{o o^{\prime}} c_{i \sigma o^{\prime}}
$$

- also add $\operatorname{SU}(4)$ exchange coupling J
- hierarchy of model parameters:
- strong onsite interaction $U>J, V_{h}$,
- approximate $\operatorname{SU}(4): U>V_{h}, K$
- tune filling by chemical potential $\mu$

EfRG phase diagram...


## Next-to-minimal models - functional RG approach

- phase diagram:


- interaction-induced quantum anomalous Hall state:
- robust near van-Hove filling, fully gapped spectrum
- breaks time-reversal symmetry
- Chern insulator: Haldane-like loop current

- d $\pm$ id superconductivity:
- SC form factor superposition of $d_{x y}(k)$ and $d_{x^{2}-y^{2}}{ }^{2}(k)$
- expect lowest energy for full gap $\rightarrow d_{x y} \pm i d_{x^{2}-y^{2}}$ superposition
- for $V_{h}>K$ : (spin-singlet) $\times$ (orbital-triblet) pairing function
 ...next: implementation of realistic lattice models...

Conclusions \& Outlook

## Conclusions and Outlook

- Superlattice modulation of moiré heterostructures
- flat bands, strongly-correlated physics, "high-Tc" phase diagrams, highly tunable
- Open questions
- appropriate models and characterization of correlated states
- weak-coupling vs. strong coupling perspective
- Competing orders/instabilities $\rightarrow$ fermion fRG (for tdBLG)
- next-to-minimal triangular $\mathrm{SU}(2) \mathrm{xSU}(2)$
- main phases:
* Chern insulating QAH state
* d $\pm$ id superconductivity



