Functional renormalization group and electrons on (twisted) honeycomb bilayers

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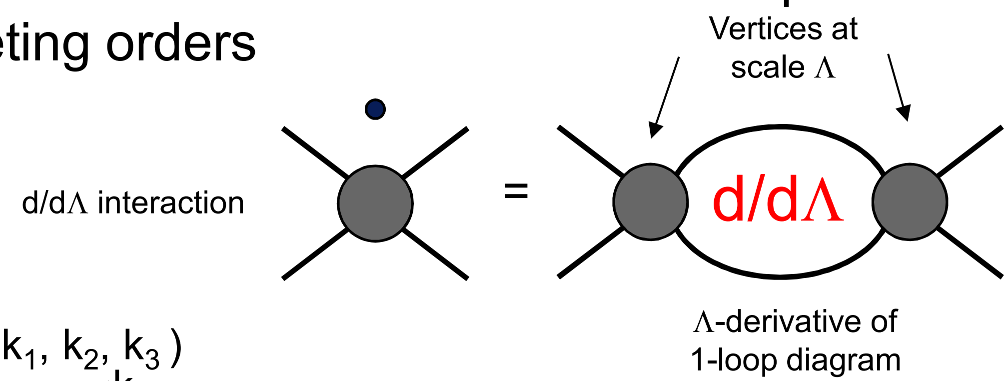
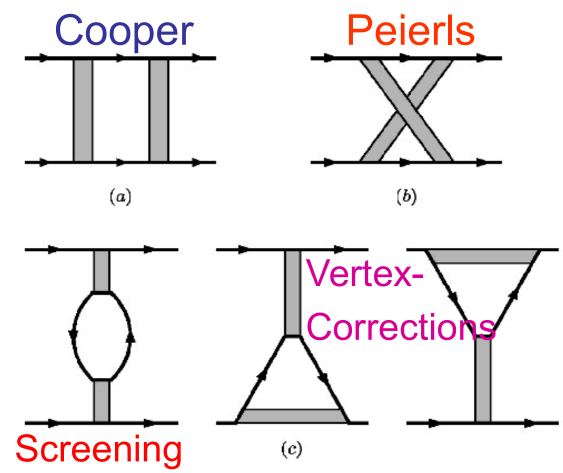
Laura Classen (BNL/UMN), Michael Scherer (Cologne)
Lennart Klebl (RWTH Aachen University)

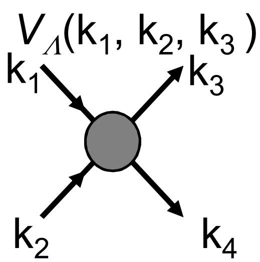
Support DFG Ho2422/x-y

Functional RG for fermions

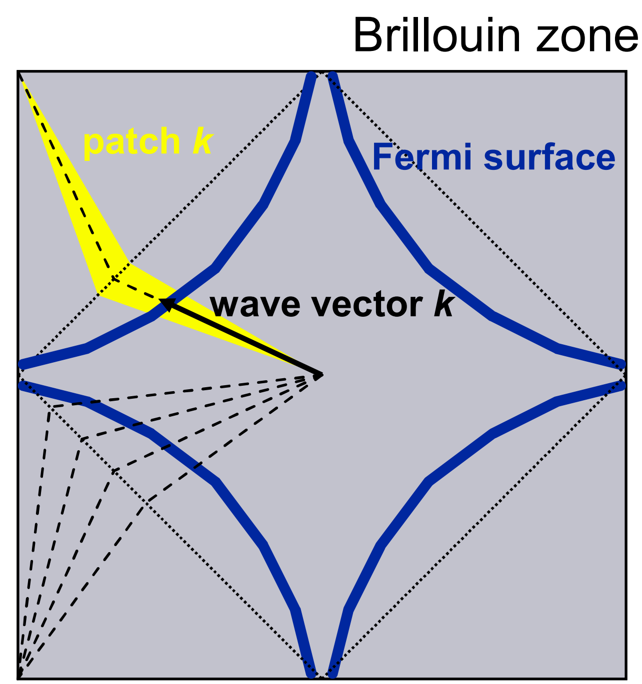
fRG captures all one-loop contributions to **effective interactions**: unbiased description of competing orders







k = wavevector, band, frequency

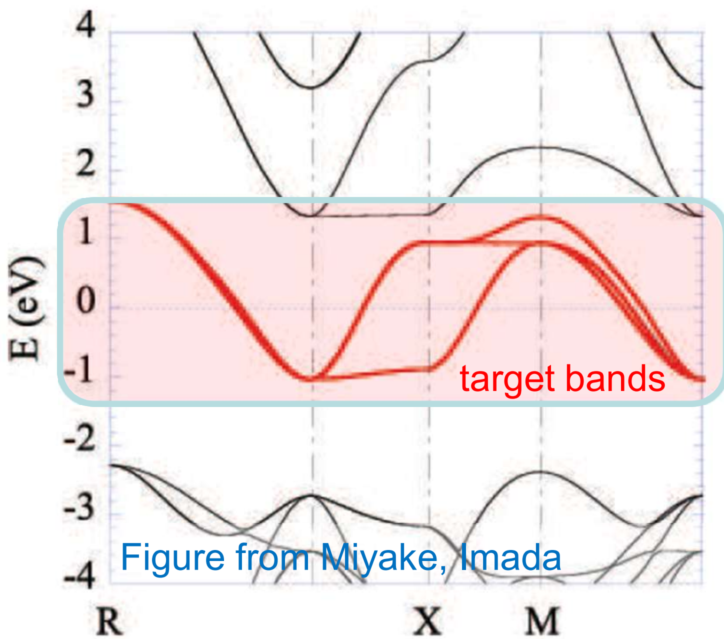


fRG keeps track of wavevector structure:

- ***N*-patch**: discretize Brillouin zone into *N* patches
- More recently: channel decomposition & form factor expansion, frequency dependence, self-energies …

Standard playground: effective low-energy models

fRG usually applied to few bands near Fermi level



Effective target band Hamiltonian

$$H = H_K + H_U \ ,$$

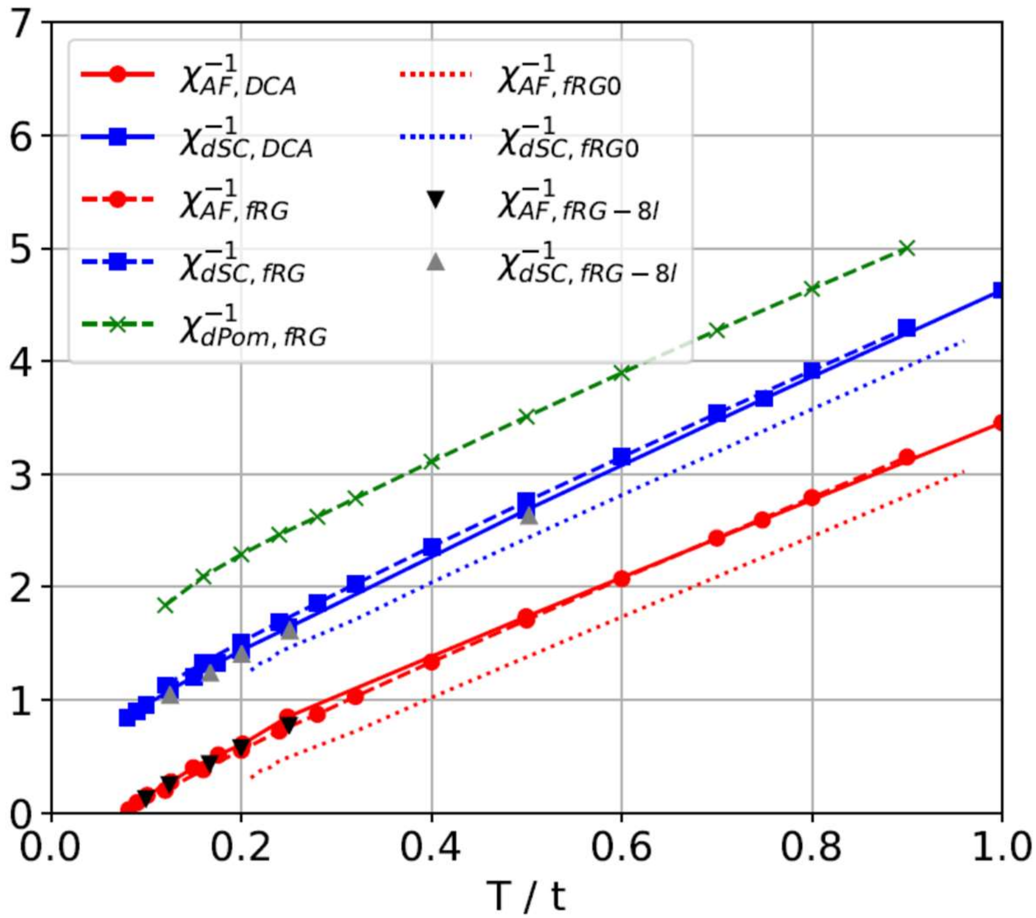
$$H_K = \sum_{Rn,R'n'} c^\dagger_{Rn} t_{Rn,R'n'} c_{R'n'} \ ,$$

$$H_U = \frac{1}{2} \sum_{R,nn',mm'} c^\dagger_{Rn} c_{Rn'} U_{nn'R,mm'R'} c^\dagger_{R'm} c_{R'm}$$

How do interactions change ground state?

Phase transitions? Symmetry breaking?

Quantitative comparison with DCA (dynamical cluster approximation)



2D square lattice Hubbard model, U=2t, with Thomas A. Maier, Douglas J. Scalapino:

Compare

- fRG (*N*=48-patch, 8^3 Matsubara freqs, Katanin 1-loop
- DCA (*N*=32)
- Multi-(8-)loop-fRG (Tagliavini, Hille, CH, et al., Scipost 2019)

fRG agrees quantitatively with non-perturbative numerical approaches!

Using fRG one level higher …

… from models to materials

Interaction parameters from first principles

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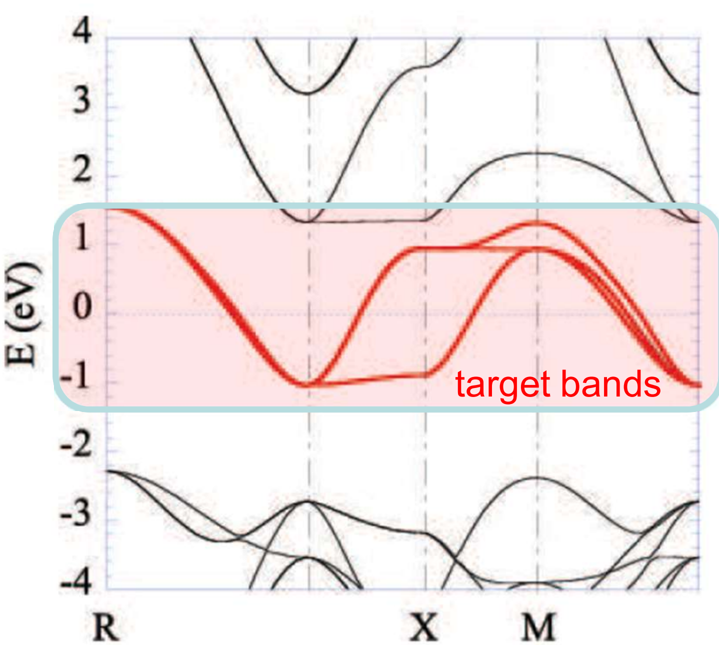
How do we compute effective low-energy interactions and Hubbard-*U*s ab initio?



$$H = H_K + H_U \ ,$$

$$H_K = \sum_{Rn,R'n'} c^\dagger_{Rn} t_{Rn,R'n'} c_{R'n'} \ ,$$

$$H_U = \frac{1}{2} \sum_{R,nn',mm'} c^\dagger_{Rn} c_{Rn'} U_{nn'R,mm'R'} c^\dagger_{R'm} c_{R'm}$$

?

picture from Imada & Miyake

Coulomb integrals in Wannier basis

- Derive localized Wannier state basis from Bloch states

$$w_{n\mathbf{R}}(\mathbf{r}) = \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} \psi_{n\mathbf{k}}(\mathbf{r})$$

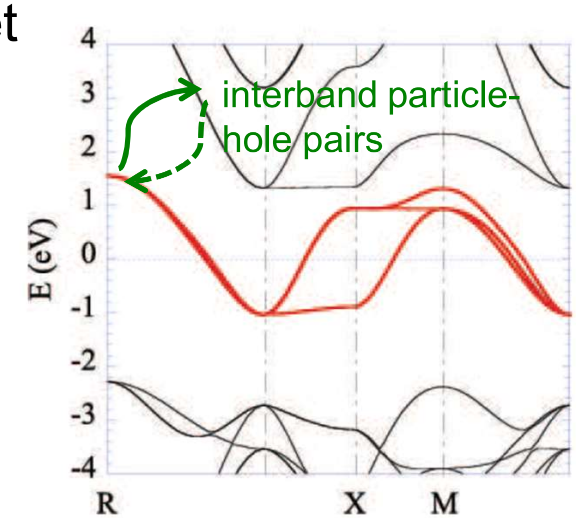
- Compute matrix elements with Coulomb kernel

$$U_{n\mathbf{R},n'\mathbf{R}'} = \langle w_{n\mathbf{R}} w_{n'\mathbf{R}'} | v_0(\mathbf{r}-\mathbf{r}') | w_{n\mathbf{R}} w_{n'\mathbf{R}'} \rangle$$

- Such ***U*s turn out too large** if only few target bands kept

- Needs to be included: screening due to bands not considered further

$$v_0(\mathbf{r}-\mathbf{r}') \quad \rightarrow \quad \frac{v_0(\mathbf{r}-\mathbf{r}')}{\epsilon(\mathbf{r},\mathbf{r}')}$$



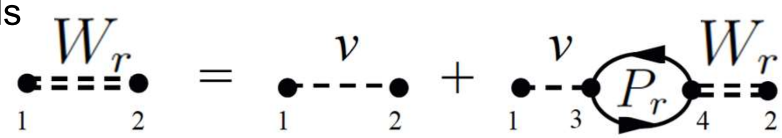
Constrained random phase approximation (cRPA)

- Divide spectrum into high-energy (=*r*) and low-energy (=target, often *d*-bands) part.
- Take only particle-hole screening involving at least one intermediate particle in high-energy band away from Fermi level

Bare Coulomb interaction

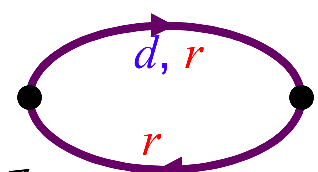
Effective interaction in target bands

$$W_r(\omega) = [1 - vP_r(\omega)]^{-1} v$$

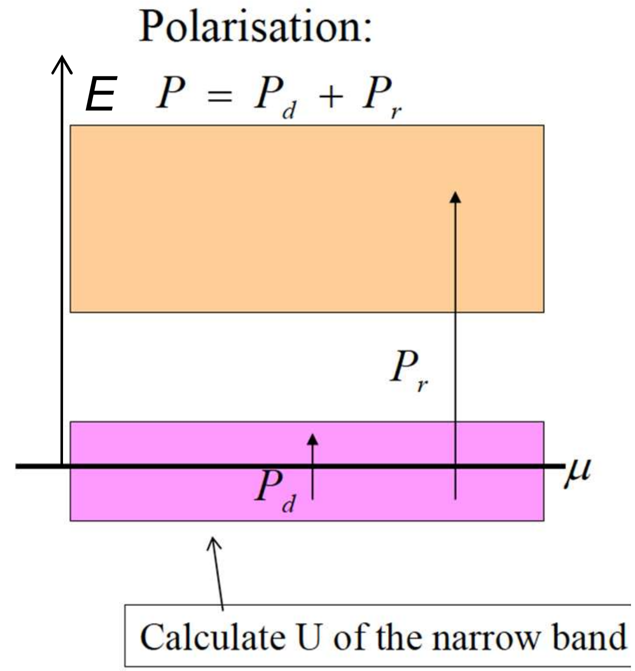


Polarization $P = P_d + P_r$

$P_r =$



at least one high-energy line

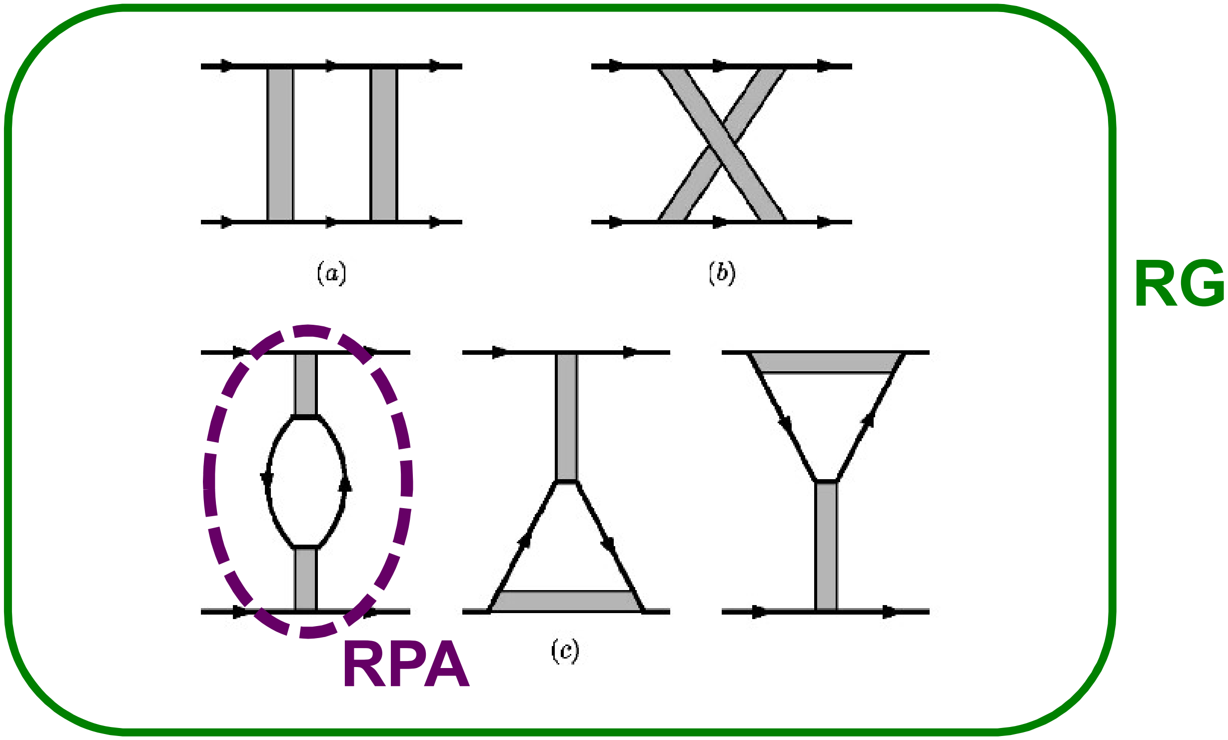


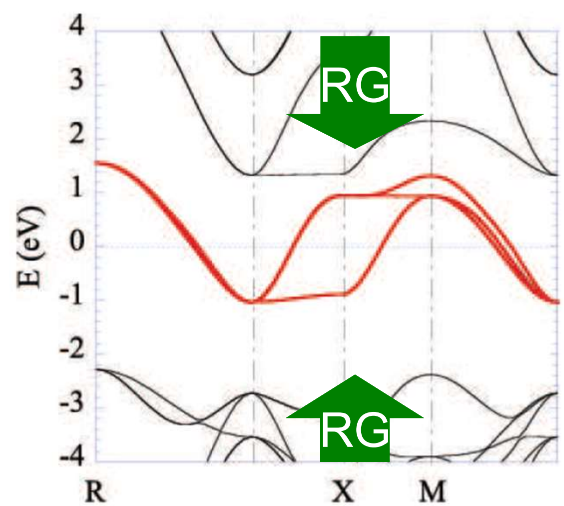
Phys. Rev. B 70, 195104 (2004)

Aryasetiawan, Imada, et al., PRB 70, 195104 (2004), ...
Imada, Miyake, 2010
Wehling

cfRG: going beyond cRPA

- Renormalization group can integrate out modes & sum one-loop diagrams beyond RPA
- 'Functional' RG keeps track of dependences of interactions on **3 momenta and frequencies** 😬😟





cfRG framework:
Honerkamp, PRB 2012

PHYSICAL REVIEW B **98**, 235151 (2018)

Limitations of constrained random phase approximation downfolding

Carsten Honerkamp,[1] Hiroshi Shinaoka,[2] Fakher F. Assaad,[3] and Philipp Werner[4]
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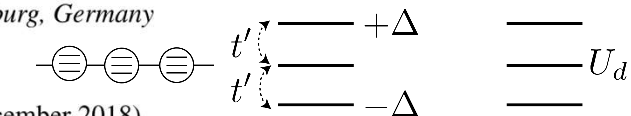
[2]*Department of Physics, Saitama University, Saitama 338-8570, Japan*
[3]*Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany*
[4]*Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland*

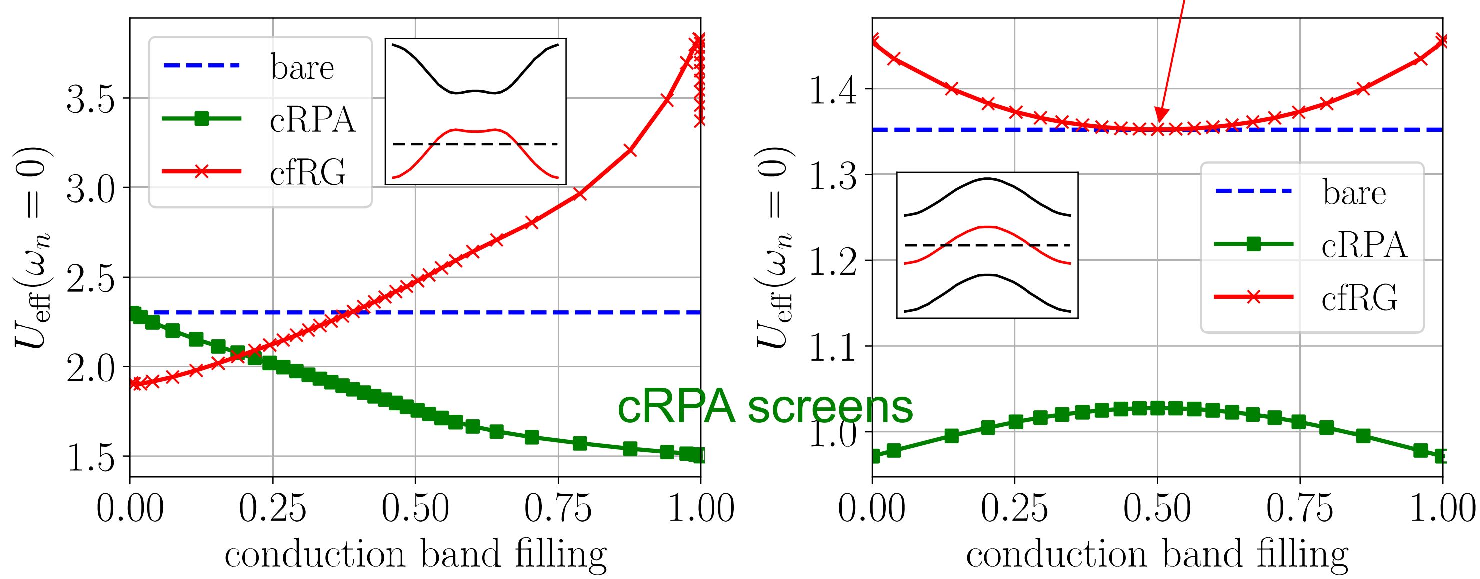


(Received 11 September 2018; revised manuscript received 3 December 2018; published 26 December 2018)

We check the accuracy of the constrained random phase approximation (cRPA) downfolding scheme by considering one-dimensional two- and three-orbital Hubbard models with a target band at the Fermi level and one or two screening bands away from the Fermi level. Using numerically exact quantum Monte Carlo simulations of the full and downfolded model, we demonstrate that depending on filling, the effective interaction in the low-energy theory is either barely screened or antiscreened, in contrast to the cRPA prediction. This observation is explained by a functional renormalization group analysis, which shows that the cRPA contribution to the screening is to a large extent canceled by other diagrams in the direct particle-hole channel. We comment on the implications of this finding for the *ab initio* estimation of interaction parameters in low-energy descriptions of solids.

renormalizations vanish

U_{eff}: Effective onsite repulsion in conduction band



Cancellation of loop corrections

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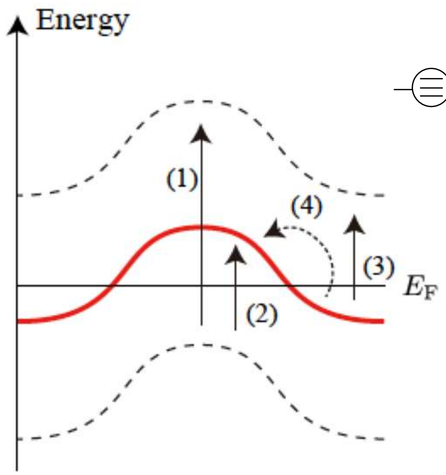
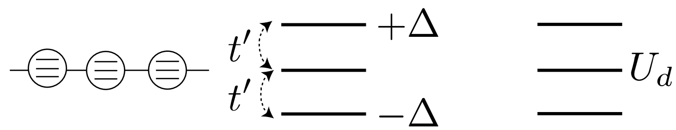
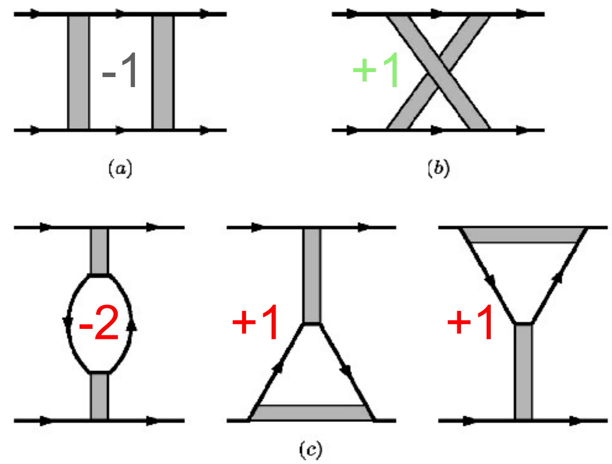




With Shinaoka, Werner, Assaad PRB 2018



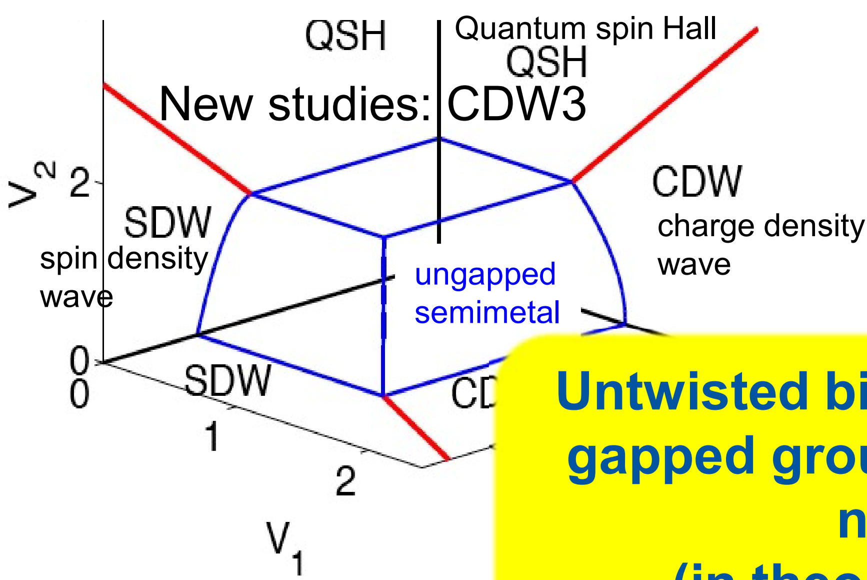
- Insights from fRG/diagrammatics (note *k*-independent hybridization *t'*):
  - → Direct PH channel drops out in 2nd order just as in single-band Hubbard model
  - → Crossed PH and PP loops have same absolute value, but sign-reversed, due to band symmetry.
- Cancellation of renormalization for instantaneous (frequency-averaged) vertices

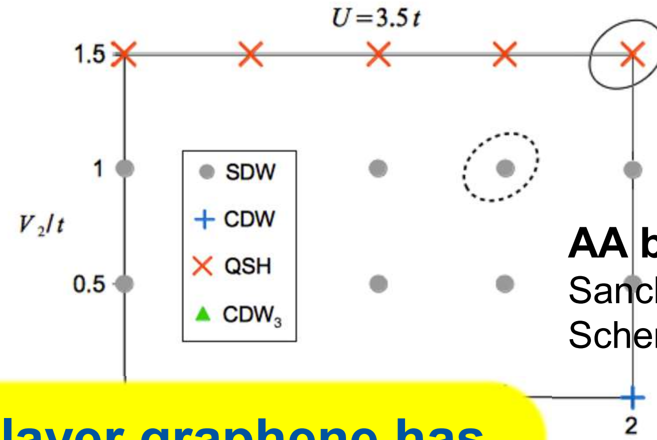
fRG for untwisted graphene bilayers

N-Layer graphene @ charge neutrality

see also Vafek et al., MacDonald et al., Nandkishore, Levitov

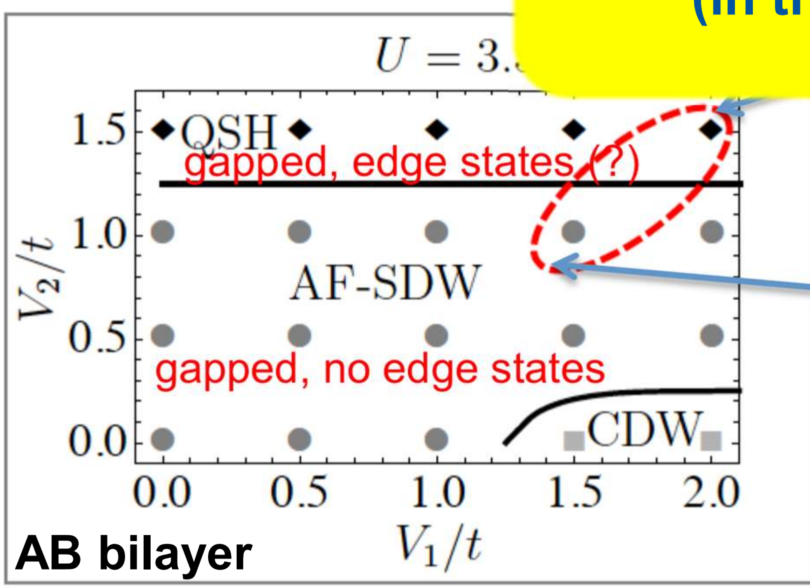
Single layer: Raghu, Scherer[0], CH et al., PRL 2008



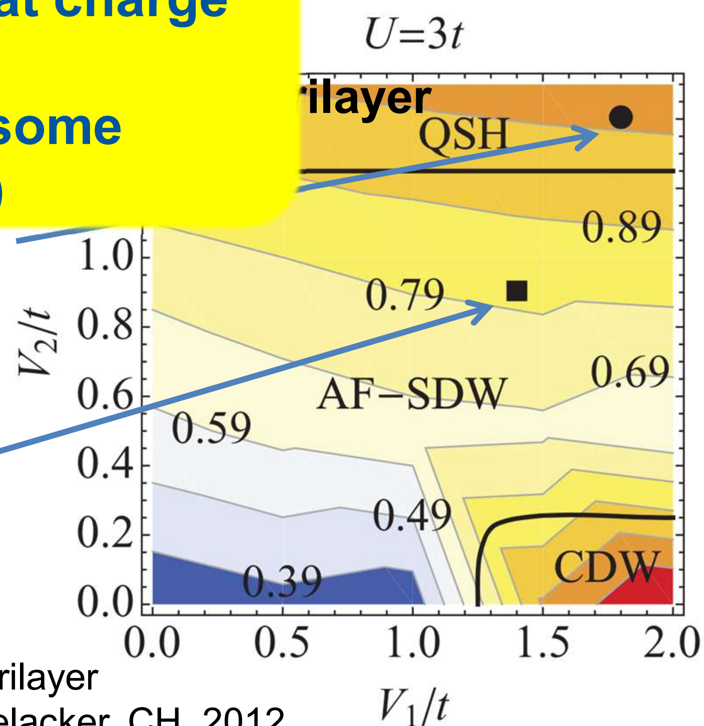


AA bilayer, Sanchez de la Pena, Scherer, CH, 2014

Untwisted bilayer graphene has gapped ground state at charge neutraliy!
(in theory and in some experiments)



Graphite cRPA parameters



cRPA parameters

Graphite cRPA parameters

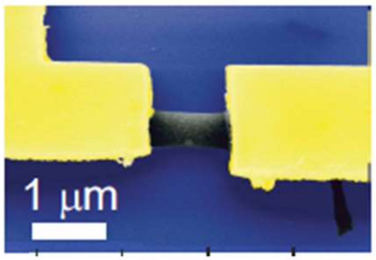
AB bilayer, ABC trilayer
Scherer[(N-1)], Uebelacker, CH, 2012

Bi- & trilayer graphene: Antiferromagnetic order?

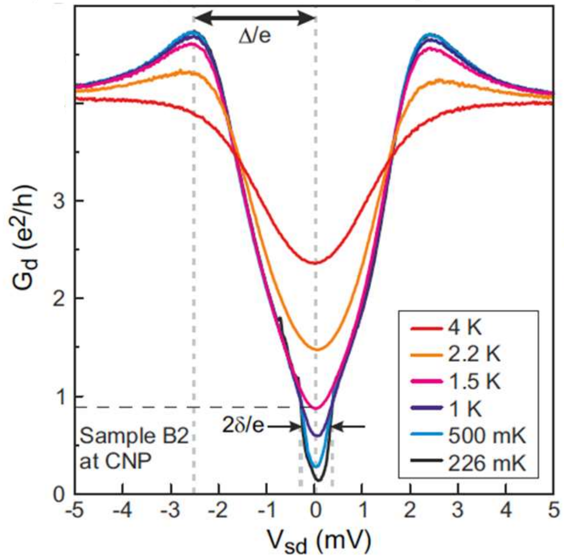
Spontaneously gapped ground state in suspended bilayer graphene

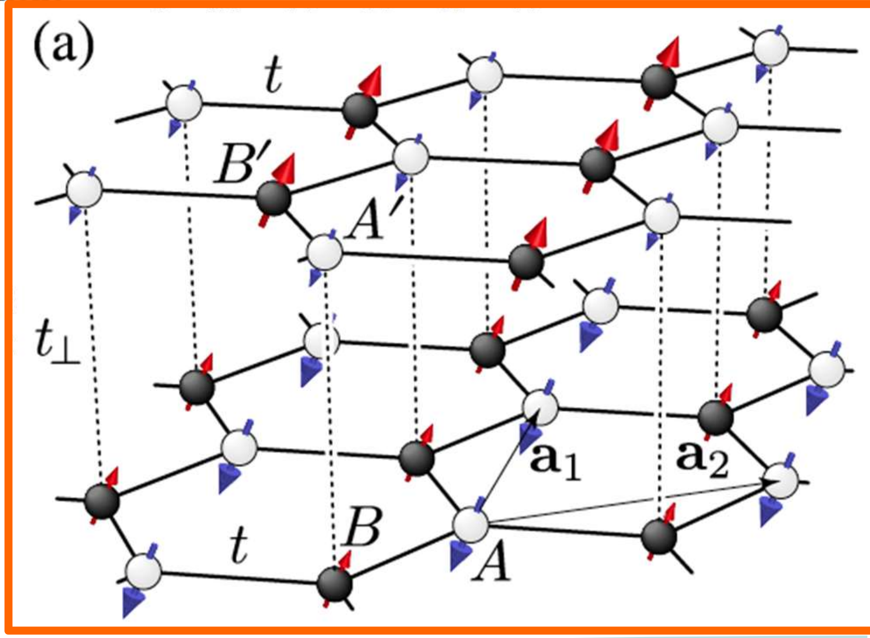
F. Freitag,[1] J. Trbovic,[1] M. Weiss,[1] and C. Schönenberger[1,*]

Phys. Rev. Lett. 108, 076602 (2012)



Clean current-annealed suspendend BLG



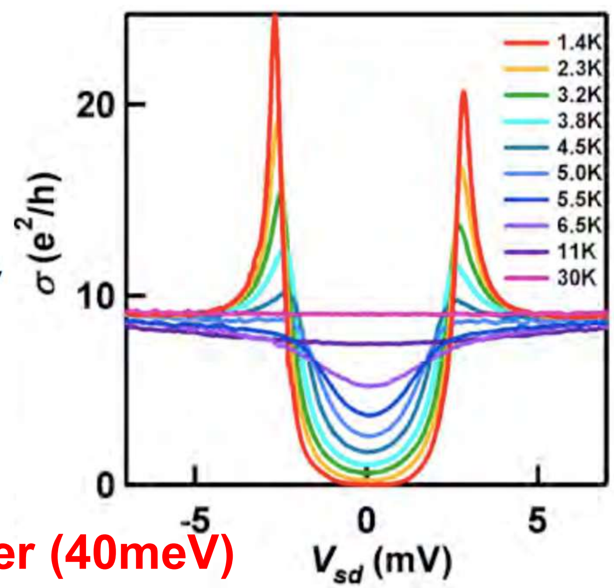


Evidence for a spontaneous gapped state in ultraclean bilayer graphene

Wenzhong Bao[a,b,1], Jairo Velasco, Jr.[a,1], Fan Zhang[c,d,1], Lei Jing[a], Brian Standley[e], Dmitry Smirnov[f], Marc Bockrath[a], Allan H. MacDonald[c,2], and Chun Ning Lau[a,2]

Proc. Nat. Acad. Sci., 109, 10802 (2012)
Trilayer: Nature Physics, 7, 948 (2011),
Lee, C.N. Lau et al. 2014

Gap scale ≈ 2-3meV
***T_c* ≈ 5K in bilayer,**



Also: Nijmegen (Maan) group

Even larger in trilayer (40meV)

fRG for twisted honeycomb bilayers in low-energy model (qualitative studies)

Strong correlations and $d + id$ superconductivity in twisted bilayer graphene

Dante M. Kennes,[1] Johannes Lischner,[2] and Christoph Karrasch[1]
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$$H = -t \sum_{\langle i,j \rangle} \sum_{\substack{\sigma=\uparrow,\downarrow \\ p=x,y}} (c^{\dagger}_{i,\sigma,p} c_{j,\sigma,p} + \mathrm{H.c.}) + U \sum_{i} n_i n_i$$

Yuan-Fu SU(4)-symmetric model, honeycomb lattice for twofold-degenerate Wannier states

Use N-patch fRG to analyze leading instabilities for weak to moderate couplings

Strong correlations and $d + id$ superconductivity in twisted bilayer graphene

Dante M. Kennes,[1] Johannes Lischner,[2] and Christoph Karrasch[1]
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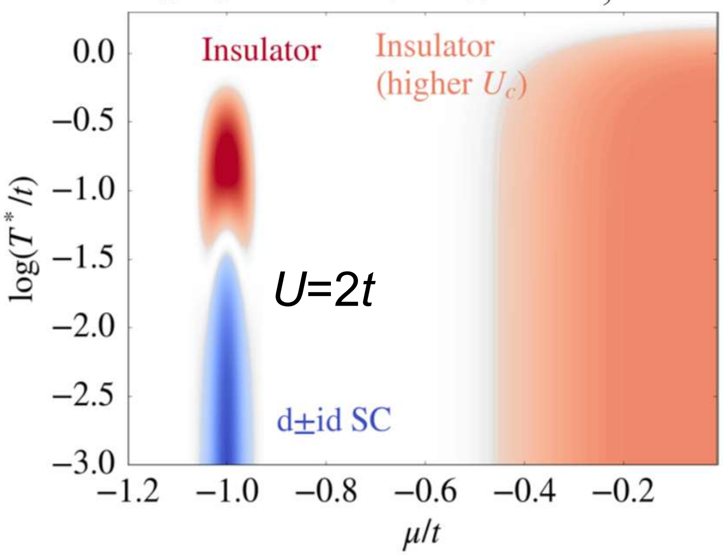
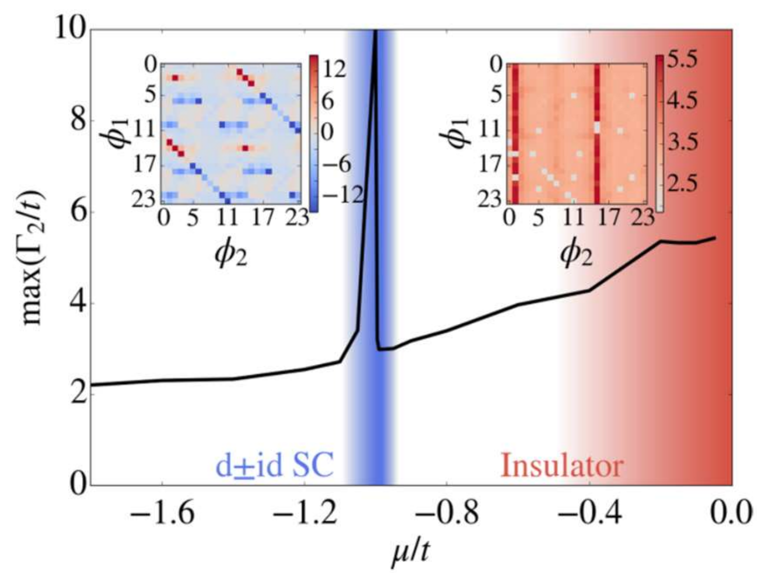
PHYSICAL REVIEW B **98**, 241407(R) (2018)



Yuan-Fu
SU(4)-symmetric model, honeycomb lattice for twofold-degenerate Wannier states



Near van Hove filling: SU(4)-& sublattice-symmetry breaking insulator + *d+id* pairing
(compare Nadkishore, Levitov, Chubukov 2012, SU(2)-case)

Near charge neutrality: only SU(4)-&sublattice-symmetry breaking for larger *U*

Beyond Hubbard & breaking SU(4) symmetry

Unconventional pairing and quantum anomalous Hall state in a minimal model for Moiré flatbands

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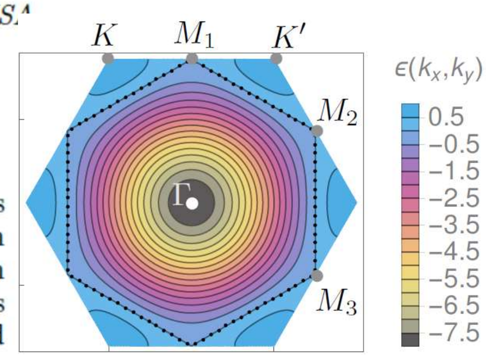
[2] Institut für Theoretische Festkörperphysik, RWTH Aachen University, and JARA Fundamentals of Future Information Technology, Germany
[3] Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany
(Dated: January 8, 2019)

We study the quantum many-body instabilities of a minimal model for Moiré flatband structures as recently proposed to be relevant to twisted bilayer boron nitride and trilayer graphene-boron nitride. To that end we employ a functional renormalization group approach for the interaction vertex with SU(2)×SU(2) symmetry. In particular, we identify in detail the emergent form factors of various leading pairing instabilities. Moreover, we predict the appearance of a unprecedented QAH instability at van-Hove filling.



Triangular lattice, twofold-degenerate Wannier states
Near van Hove filing

$$H_I = \frac{U}{2}\sum_{i,\nu,\nu'} n_{i\nu}n_{i\nu'} + J\sum_{\langle ij\rangle}\sum_{a=1}^{15}\hat{T}_i^a\hat{T}_j^a$$

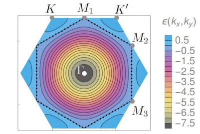
SU(4)-symmetric onsite & n.n. exchange interaction

$$H_I' = -V\sum_i \boldsymbol{S}_i^2 - K\sum_i \boldsymbol{L}_i^2$$

SU(2) spin x SU(2) orbital onsite interaction

$$\boldsymbol{S}_i = \tfrac{1}{2}c^\dagger_{i\sigma o}\boldsymbol{\sigma}_{\sigma\sigma'}c_{i\sigma' o} \qquad \boldsymbol{L}_i = \tfrac{1}{2}c^\dagger_{i\sigma o}\boldsymbol{\tau}_{oo'}c_{i\sigma o'}$$

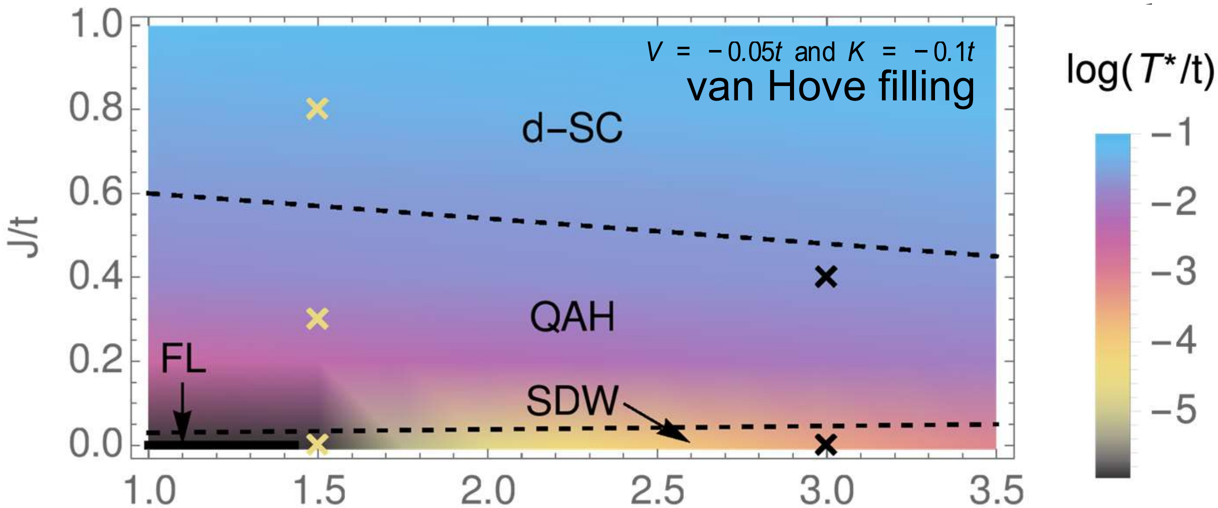
Beyond Hubbard, breaking SU(4) symmetry

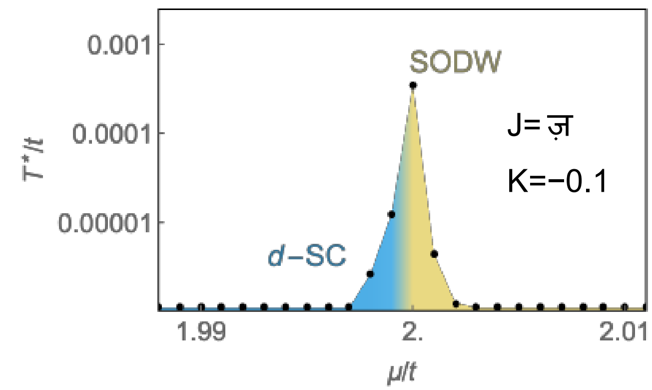


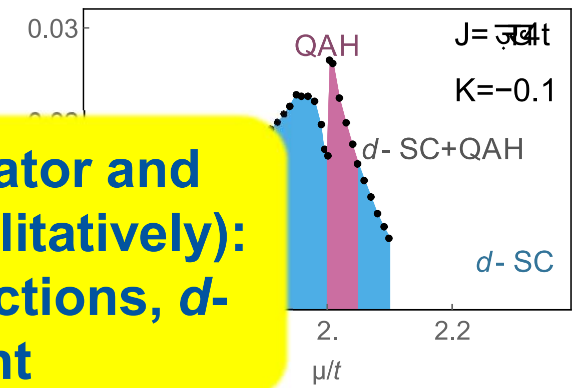
$$H_I = \frac{U}{2}\sum_{i,\nu,\nu'} n_{i\nu}n_{i\nu'} + J\sum_{\langle ij\rangle}\sum_{a=1}^{15}\hat{T}_i^a\hat{T}_j^a$$

$$H_I' = -V\sum_i \boldsymbol{S}_i^2 - K\sum_i \boldsymbol{L}_i^2$$

$$\boldsymbol{S}_i = \tfrac{1}{2}c^\dagger_{i\sigma o}\boldsymbol{\sigma}_{\sigma\sigma'}c_{i\sigma' o} \qquad \boldsymbol{L}_i = \tfrac{1}{2}c^\dagger_{i\sigma o}\boldsymbol{\tau}_{oo'}c_{i\sigma o'}$$

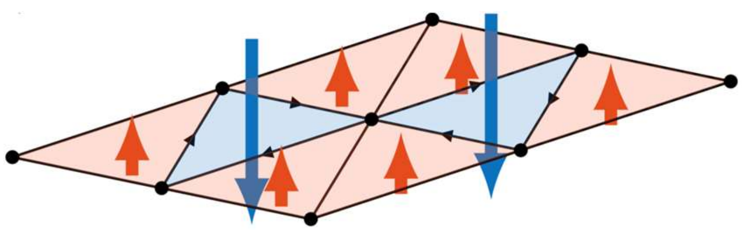






Van Hove scenario for insulator and superconductor in fRG (qualitatively): insulator depends on interactions, *d*-wave pairing most prominent

New possibility:
Quantum anomalous 3Q-loop order
(also Venderbos 2018,



Depending on *J*, the insulator might be QAH!

… so far the effective flat-band models

What about the 99.9% rest of the spectrum?

Screening of flat-band interactions?

$$V_{\mathbf{R}'m',\mathbf{R}m} = \sum_{XX'} \iint d\mathbf{r} d\mathbf{r}' |\psi^{X'}_{\mathbf{R}'m'}(\mathbf{r}')|^2 \frac{e^2}{\epsilon|\mathbf{r}-\mathbf{r}'|} |\psi^{X}_{\mathbf{R}m}(\mathbf{r})|^2$$

?

TABLE I. Direct interaction V_n and the exchange interaction J_n for the Wannier orbitals in units of $e^2/(\epsilon L_{\mathrm{M}})$. The definition of $V_0, V_1 \cdots$ is presented in Fig. 6(a). $V_n^{(\mathrm{approx})}$ is the direct interaction terms estimated by the point-charge approximation (see the text).

n	0	1	2	3	4	5
V_n	1.857	1.533	1.145	1.068	0.697	0.614
$V_n^{(\mathrm{approx})}$	1.857	1.524	1.136	1.081	0.679	0.610
J_n	N/A	0.376	0.0645	0.010	0.014	0.001

Koshino, L. Fu, PRX 2018

What about the 99.9% rest of the spectrum? Screening?

- Untwisted graphene: screening due to σ-bands well understood by cRPA (Wehling et al., 2011, 2015)

Freely suspended:

	Graphene	
	Bare	cRPA
$U_{00}^{A \text{ or } B}$ (eV)	17.0	9.3
U_{01} (eV)	8.5	5.5
$U_{02}^{A \text{ or } B}$ (eV)	5.4	4.1
U_{03} (eV)	4.7	3.6

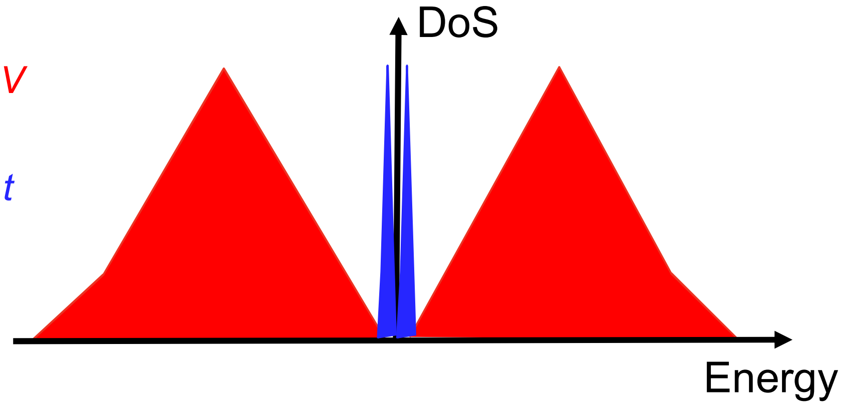
Sandwiched between ε_1 and ε_3:

ε_2	ε_3	U_0	U_1	U_2	U_3
1	1	9.2/ 9.3	4.7	3.3/ 3.2	3.0
1	5	8.2/ 8.3	3.7	2.3/ 2.3	2.0
1	∞	7.6/ 7.7	3.1	1.7/ 1.7	1.4
∞	∞	7.3/ 7.4	2.9	1.5/ 1.5	1.2

- 4 flat bands represent tiny portion of whole π-band spectrum:

  → Full bandwidth π-bands $6t = 16eV$

  → Flat-band window $20meV \approx 0.01t$

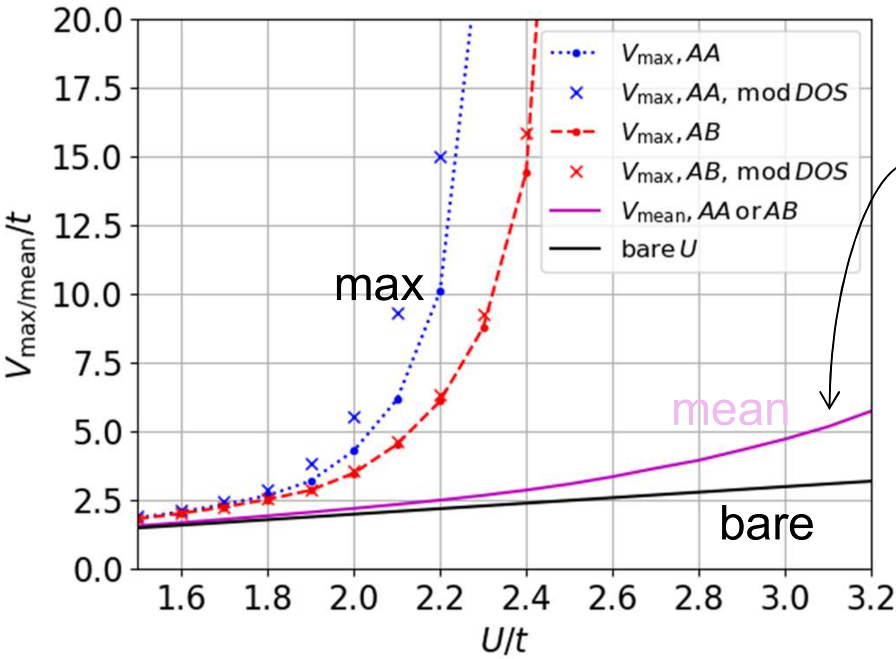


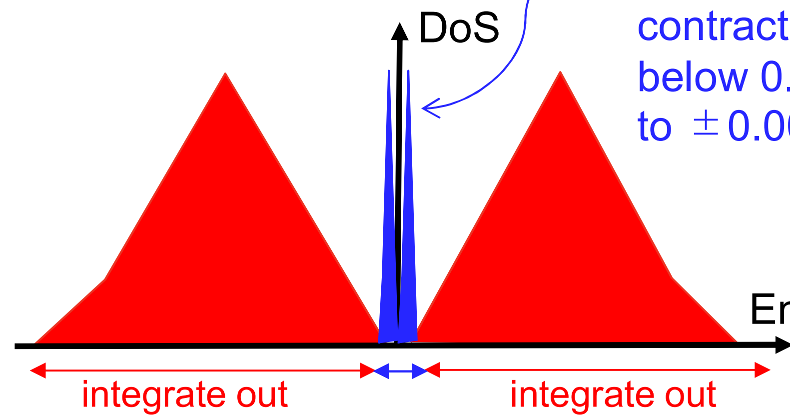
Integrate out the 99.9% rest of the spectrum … screening?

Use cfRG to integrate out spectrum above 0.01t (~20meV) for untwisted system, here only onsite repulsion *U*, gives **strongly momentum-dependent effective interaction:**

Maximal couplings get large, mainly in spin channel (AF-SDW tendency)

Momentum averaged coupling (=effective U), antiscreening rather than screening





Modified DoS in target bands: contract DoS below 0.01*t* to ±0.001*t*

Momentum structure of effective low-energy interactions

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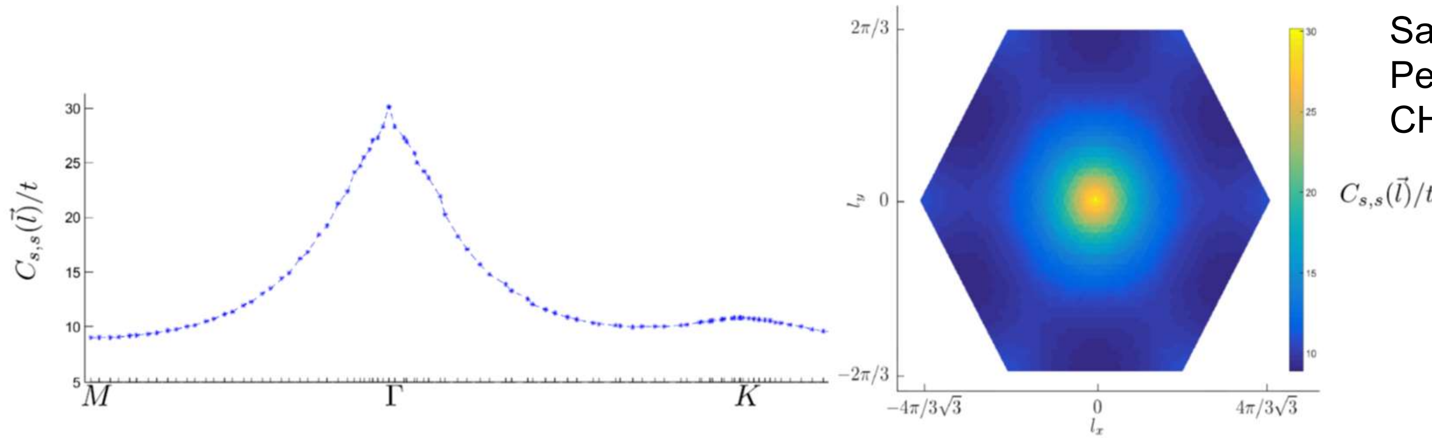
Effective interactions: mainly q=0 peak in effective intersublattice spin interaction: staggered interaction on real lattice



Sanchez de la Pena, Lichtenstein, CH, PRB 2017

Effective interactions on Angström-scale have more structure than bare Coulomb interaction!
Role for effective flat band interaction needs to be determined (not done yet)!

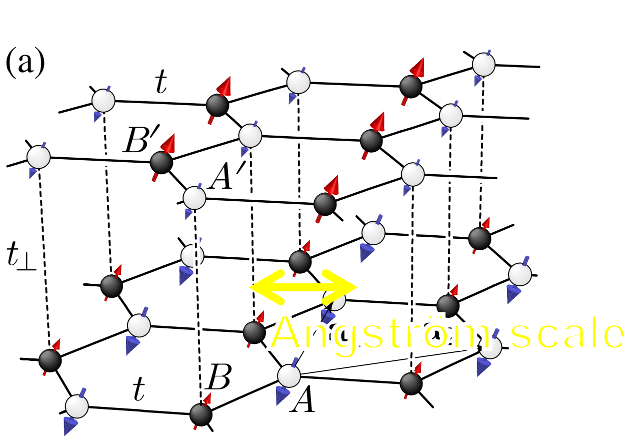
$$V_{\mathbf{R}'m',\mathbf{R}m} = \sum_{XX'} \iint d\mathbf{r}d\mathbf{r}' |\psi^{X'}_{\mathbf{R}'m'}(\mathbf{r}')|^2 \frac{e^2}{\epsilon|\mathbf{r}-\mathbf{r}'|} |\psi^{X}_{\mathbf{R}m}(\mathbf{r})|^2$$

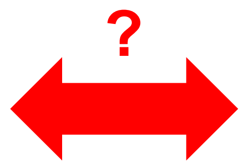
Rather anti-screening than screening

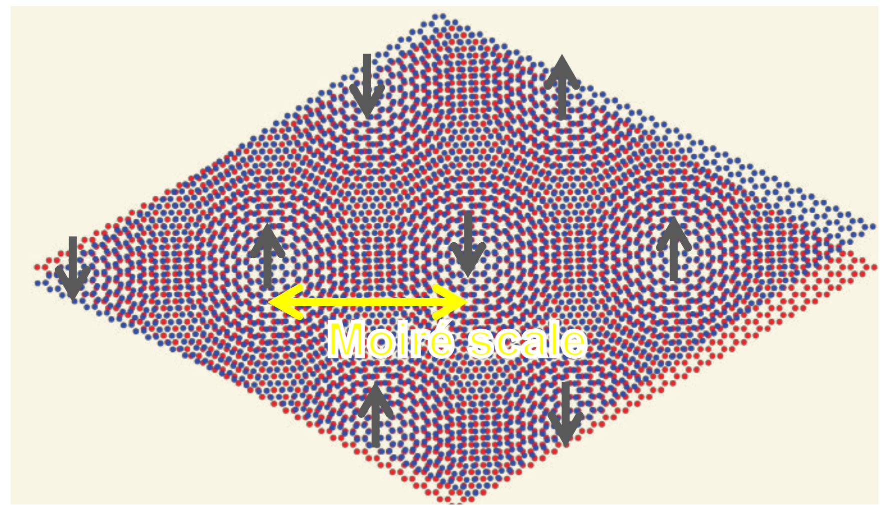
Staggered component in distance dependence

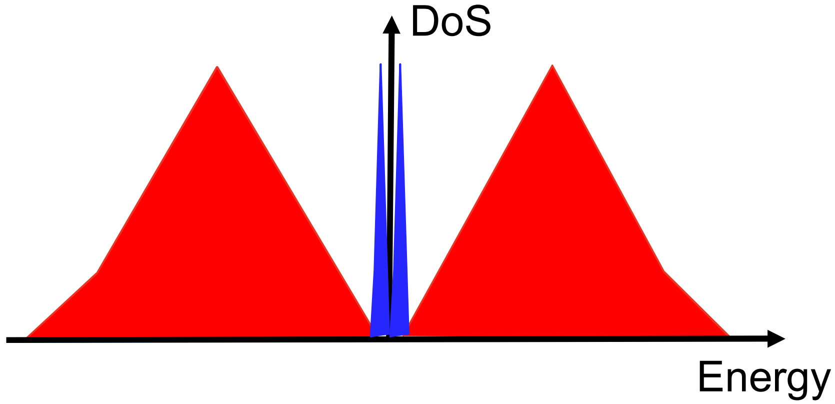
Speculation: What if instabilities of spectrum above 20meV outweigh flat-band physics?

On which length scale does order occur?









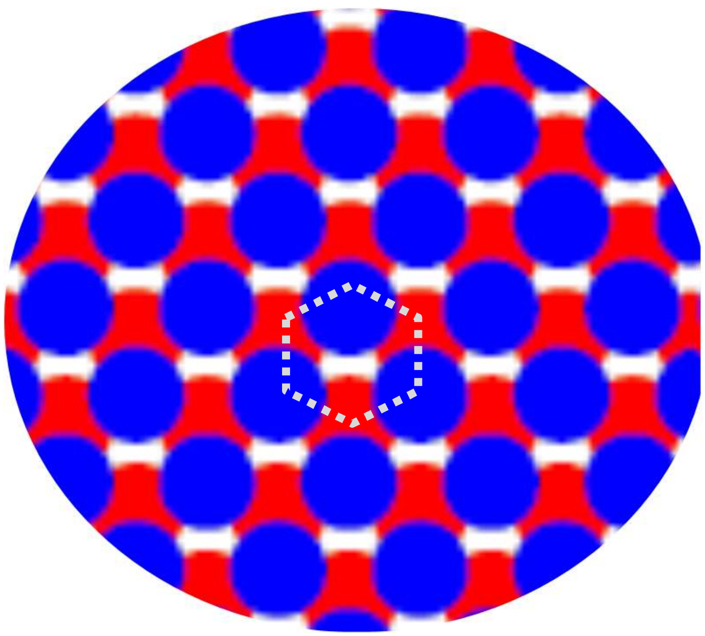
Interband transitions versus intra-flat-band physics

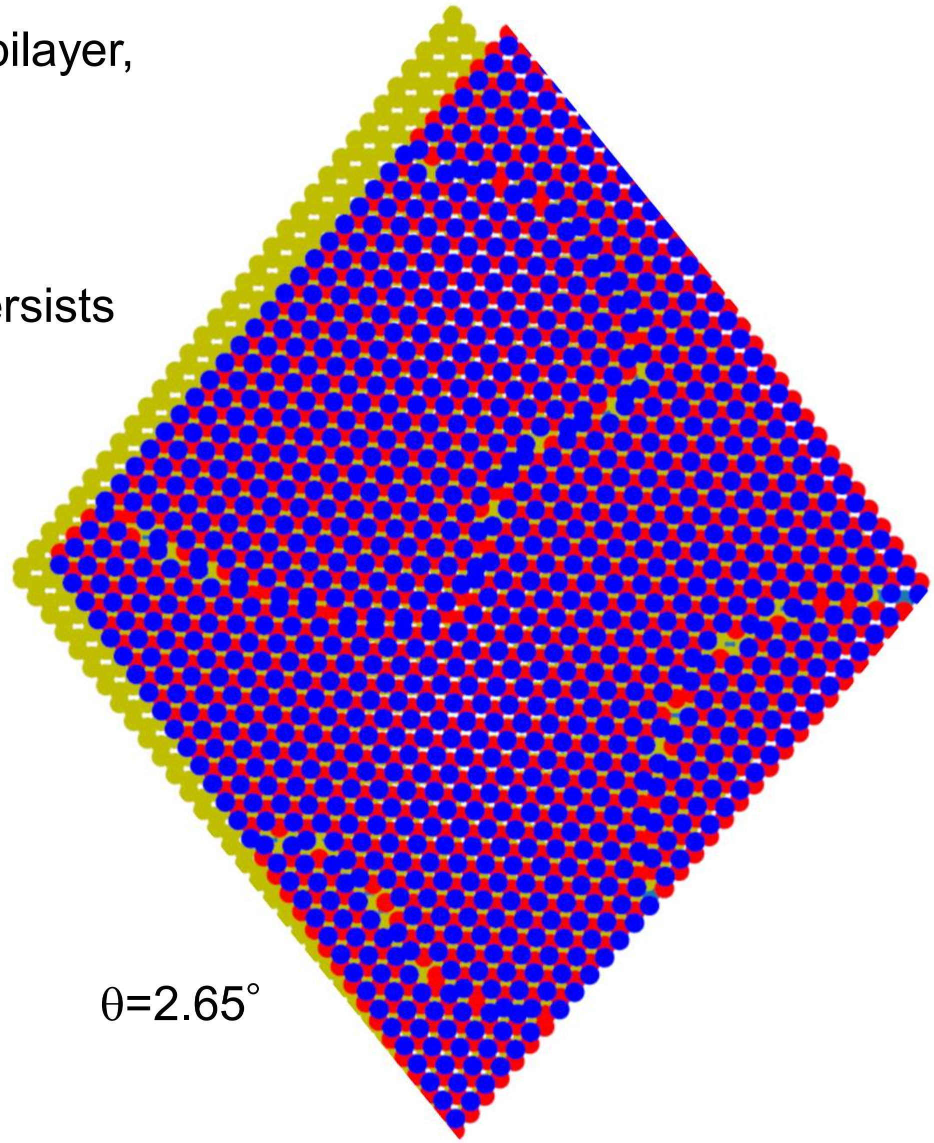
Real-space CDW meanfield for twisted bilayer

Spinless toy model: Charge density selfconsistent meanfield for twisted bilayer, finite size

(with hoppings à la Koshino-Fu):

- red: $n>0.5$, blue $n<0.5$
- CDW order on Angström-scale persists





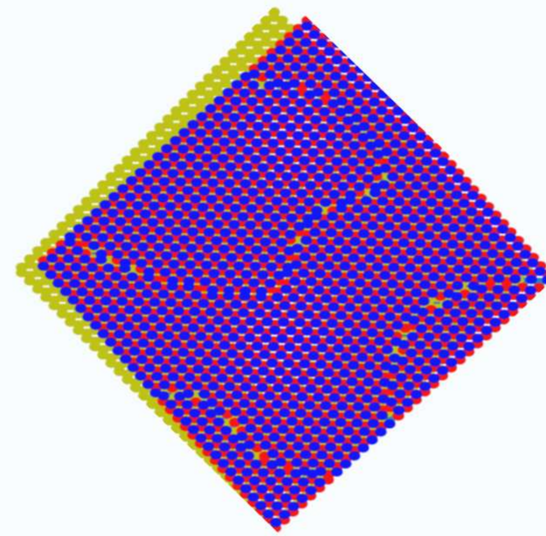
$\theta=2.65^\circ$

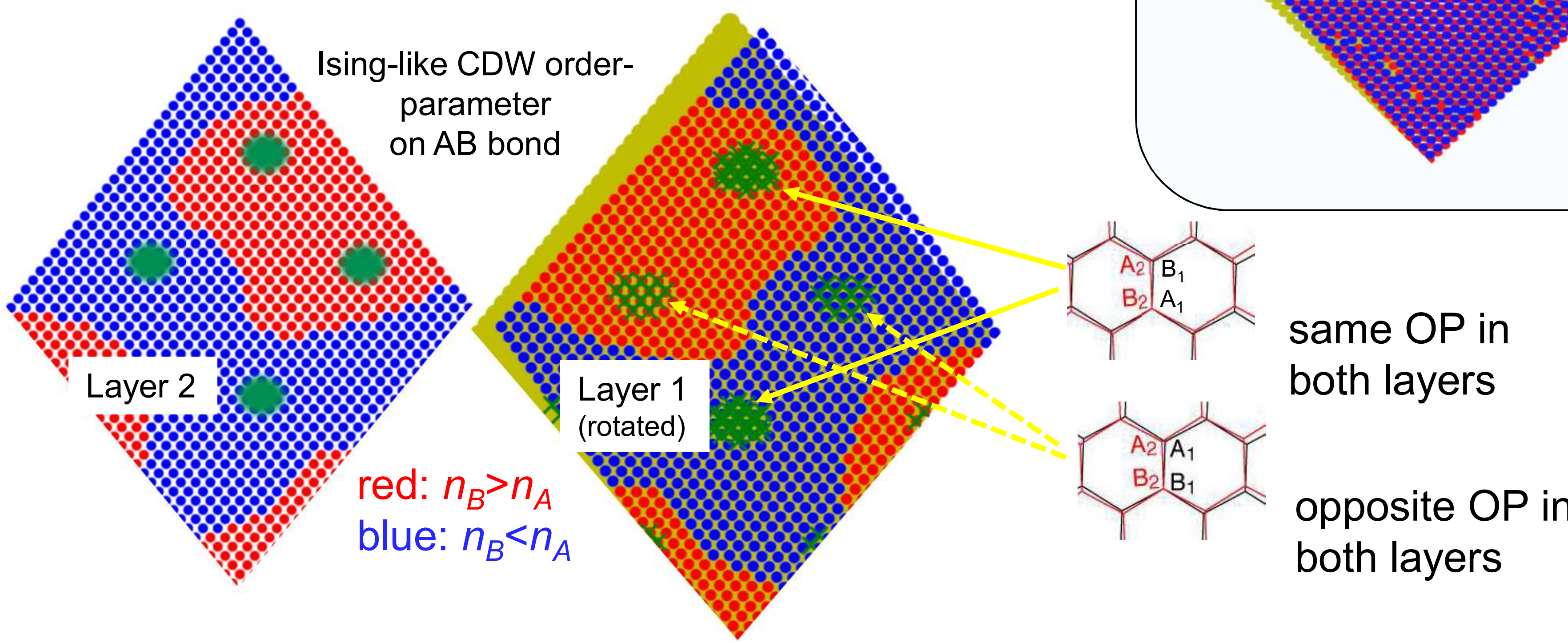
Real space CDW meanfield for twisted bilayer

Charge density meanfield for spinless twisted bilayer model, (with hoppings à la Koshino-Fu):
Plot Ising CDW order parameter, red: $n_B > n_A$
blue: $n_B < n_A$

→ Twisting causes **domain formation** due to registry change of ‘AA‘ regions

Densities in layer 1: red: $n > 0.5$, blue $n < 0.5$

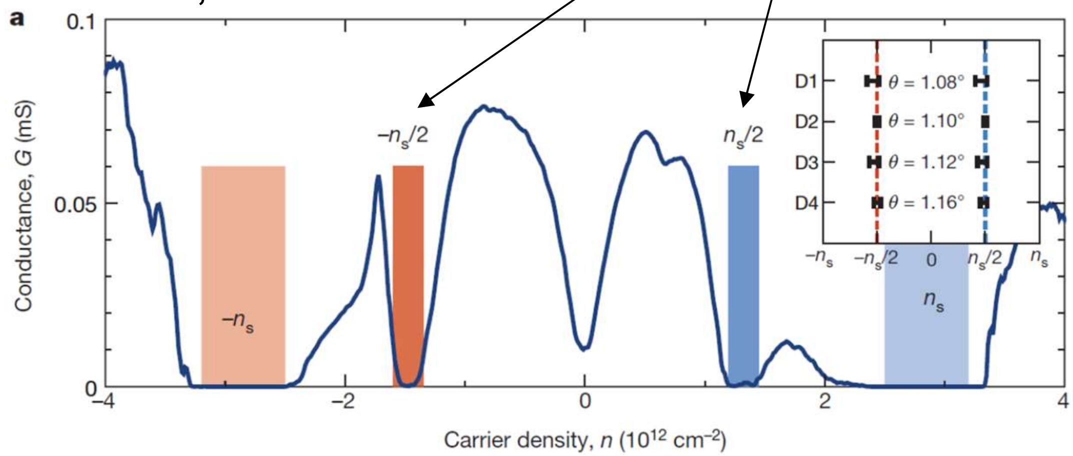


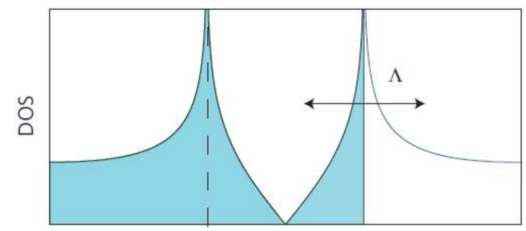


How to understand density dependence?

associated with van Hove fillings (?)

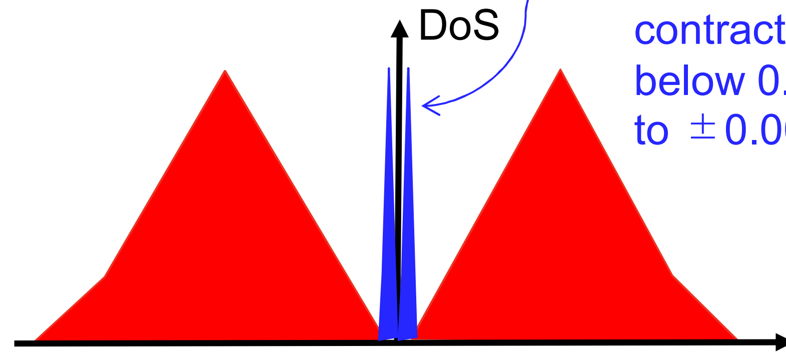
Cao et al, 2018





How does this density dependence work if instability does not arise from flat bands?

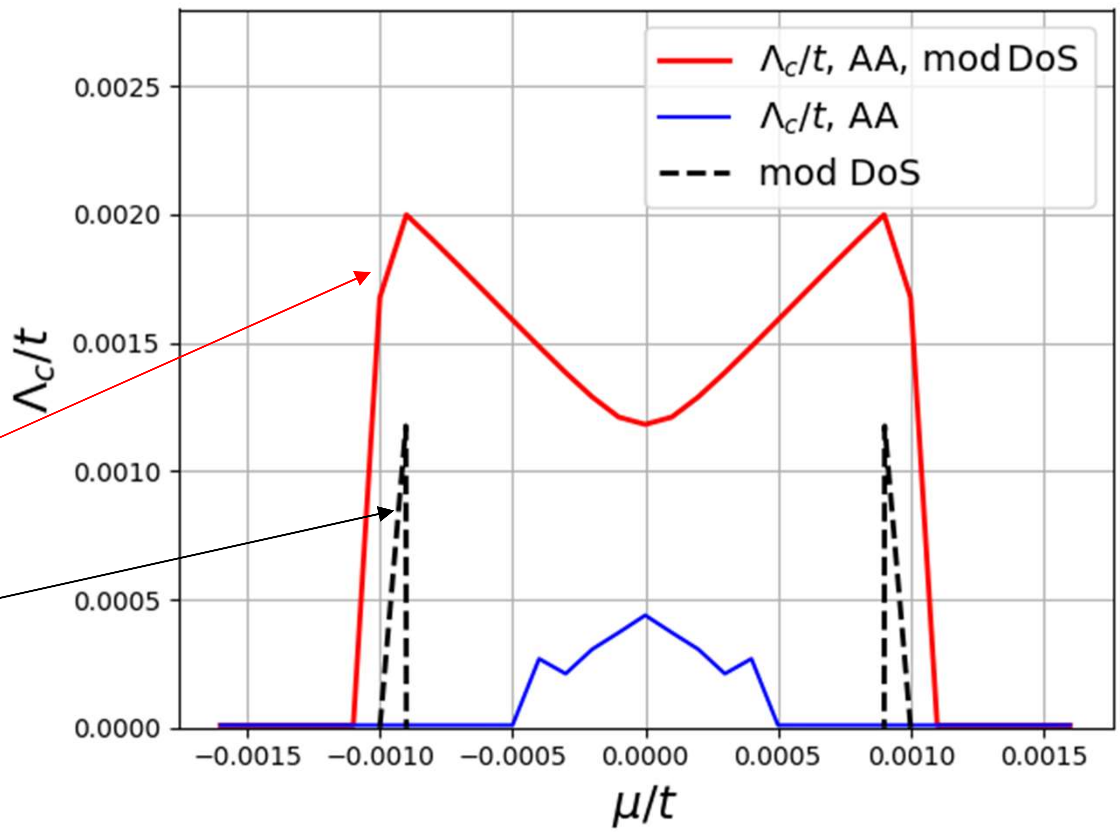
→ 'Poor man's fRG study': Compute density–dependence of instability of untwisted system (simpler …) with modified DoS that has two low-energy peaks at ±0.2meV



Details of low-energy spectrum enter instability scale

Density(μ)–dependence of instability scale Λ_c of untwisted BLG with modified DoS with two low-energy peaks:

System most unstable for Fermi energy near DoS peak



Even though instability is driven by full band width, density of states of flat bands decides about occurrence and energy scale of insulating state!

Conclusions

Functional RG can describe qualitative physics of flat bands:

- Insulating state at van Hove filling depends on parameters (nn exchange-*J* drives QAH)
- *d+id* most prominent pairing state

Constrained functional RG can (potentially) describe renormalization of effective low-energy interactions by higher-energy bands

- Renormalization causes visible momentum and real space structure
- Onsite terms rather anti-screened than screened

Fate/role of intrinsic ordering instabilities on original honeycomb lattice needs to be understood