The nature of correlations in the insulating states of twisted bilayer graphene

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Pizarro et al, arXiv:1805.07303

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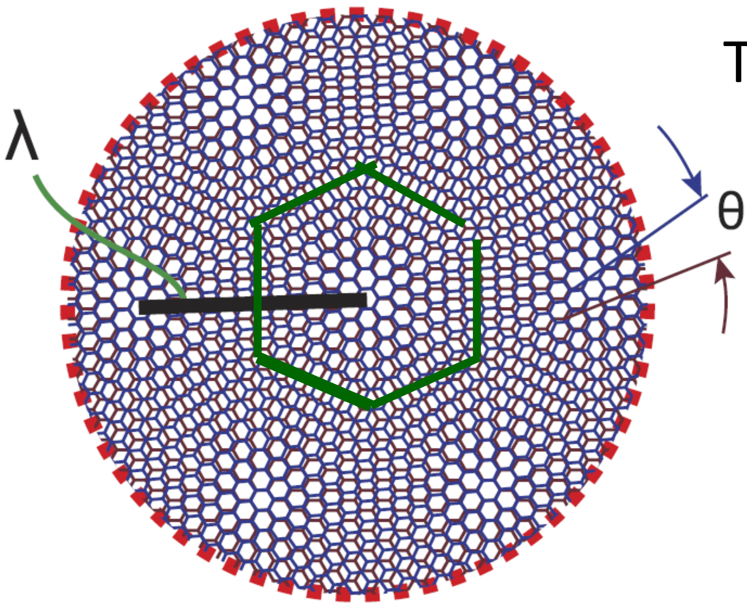
Outline

- ❑ Insulating (Mott?) states and Superconductivity in twisted bilayer graphene (TBG)
- ❑ Mott insulating states
- ❑ Predictions for Mott states in two-orbital Hubbard model for the honeycomb lattice in local approximation:
  - Critical interaction
  - Magnetic field dependendence
  - Temperature dependence
  - Gap size
- ❑ Beyond local approximation
- ❑ Summary

Small angle twisted bilayer graphene (TBG)



Two graphene layers. Rotation angle ~ 1º

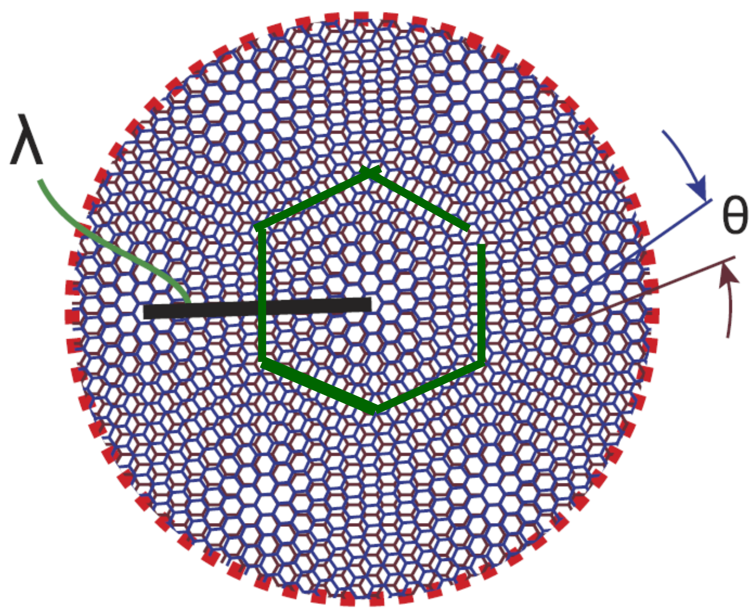
Moiré Pattern

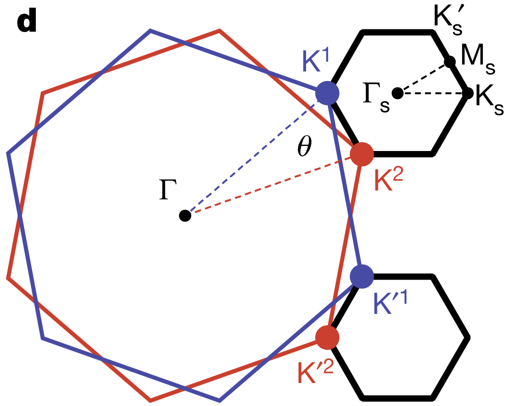
Moiré unit cell ~ thousands of atoms

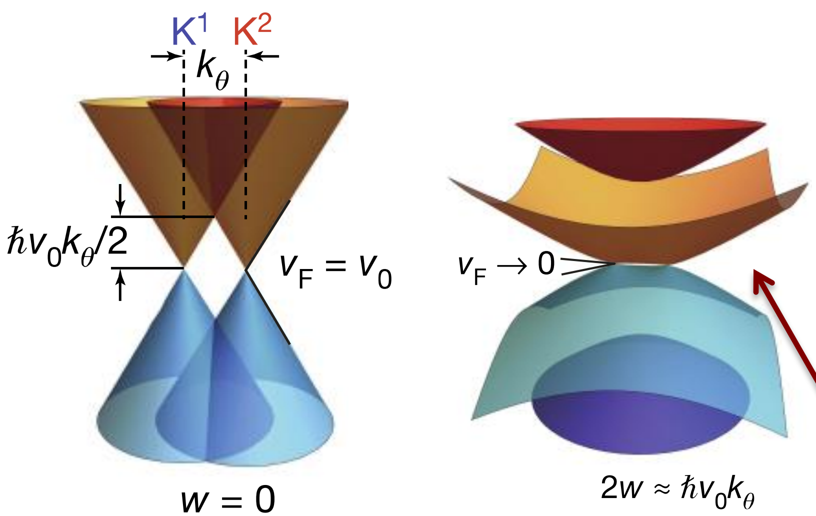
Moiré lattice constant λ~13 nm

Cao et al, Nature 556, 80 (2018)

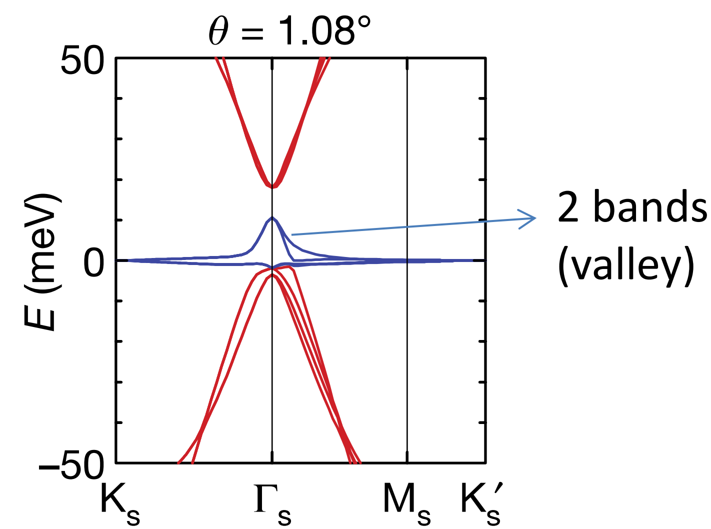
Small angle twisted bilayer graphene (TBG)







Magic angle

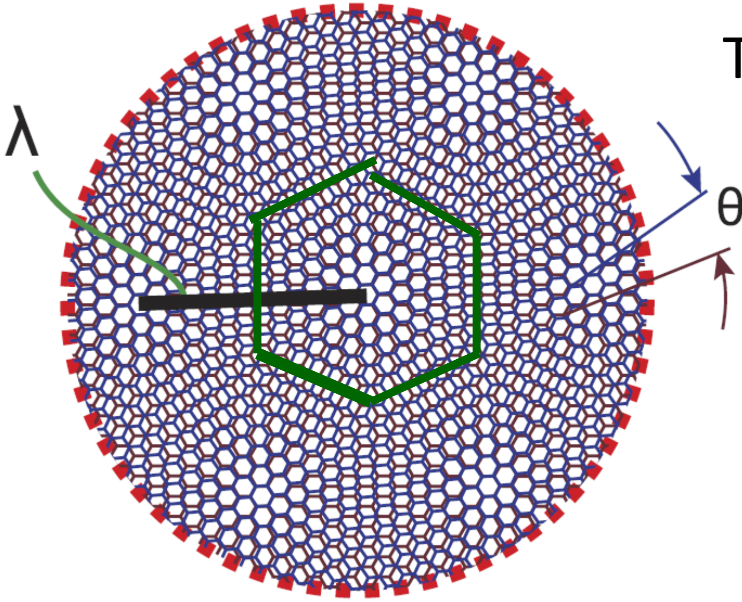


Flat bands
(sensitive to interactions)

Bistritzer & MacDonald, PNAS 108, 12233 (2011)

Cao et al, Nature 556, 80 (2018)

Small angle twisted bilayer graphene (TBG)

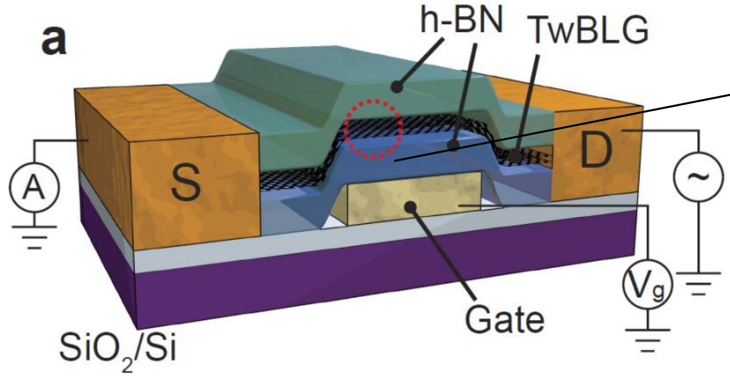


Two graphene layers. Rotation angle ~ 1º

Moiré Pattern: thousands atoms/u.cell

Flat bands

Doping with electrons or holes via a gate voltage

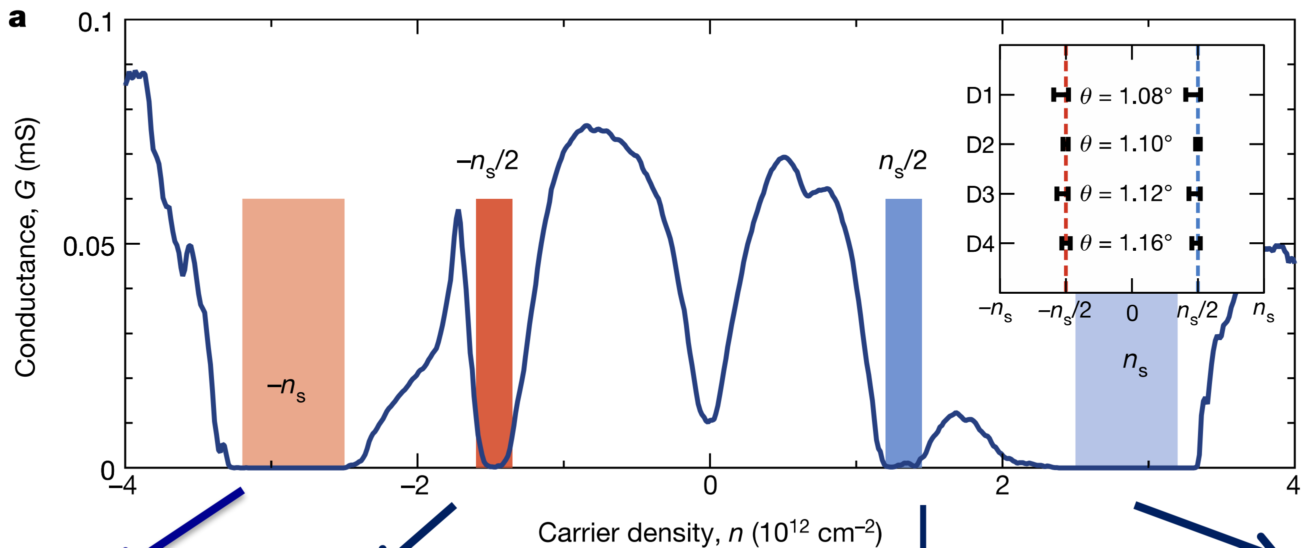


d ~10-30 nm ~ 2 λ

Long-range interaction is screened

Cao et al, Nature 556, 80 (2018)

Insulating states and superconductivity in TBG



Insulating
~2 h$^+$ /3000 C atoms

Insulating
~1 h$^+$ /3000 C atoms

Insulating
~1 e$^-$ /3000 C atoms

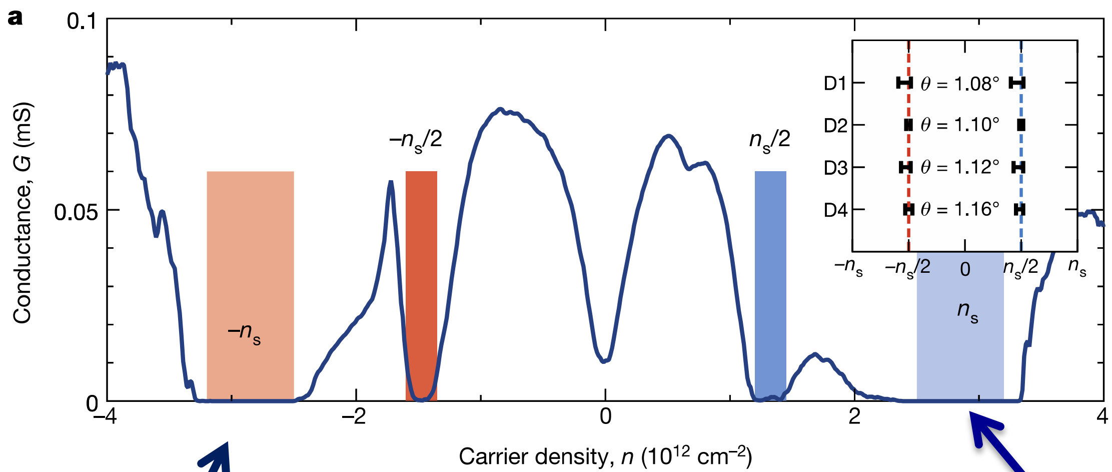
Insulating
~2 e$^-$ /3000 C atoms

Semimetallic
Undoped
(Charge neutrality point)

Cao et al, Nature 556, 80 (2018)

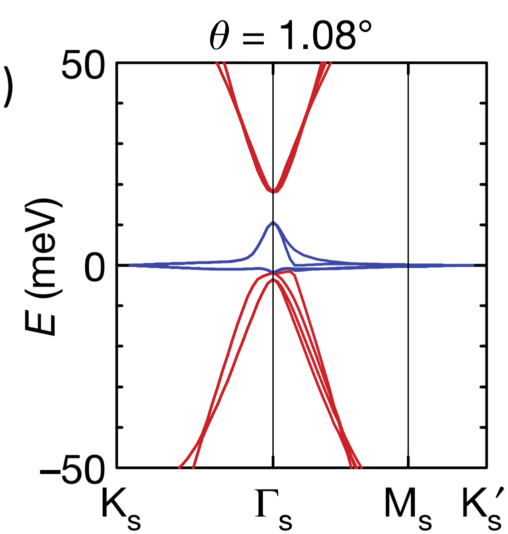
Extreme tunability at very low densities

Insulating states and superconductivity in TBG



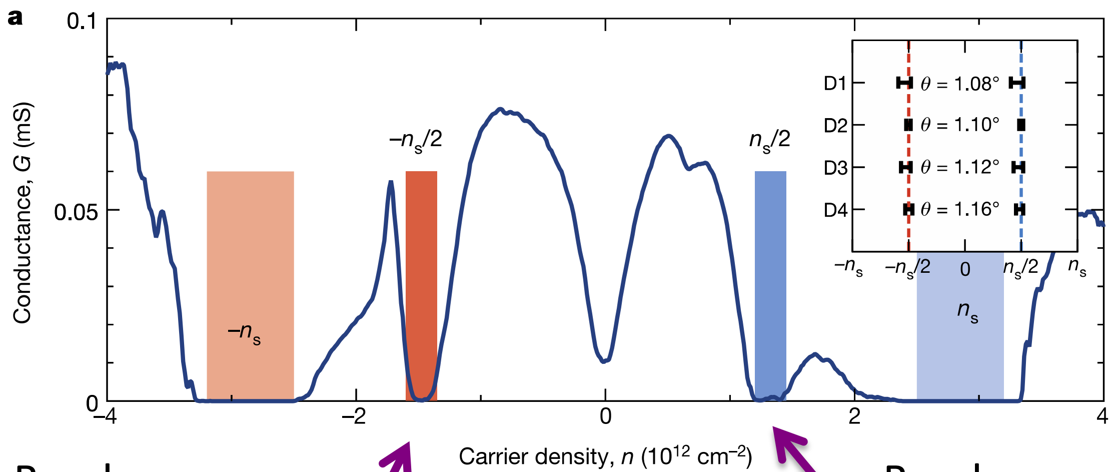
Band gap
(4 holes per
Moiré unit cell)

Band gap
(4 electrons per
Moiré unit cell)



Cao et al, Nature 556, 80 (2018)

Insulating states and superconductivity in TBG

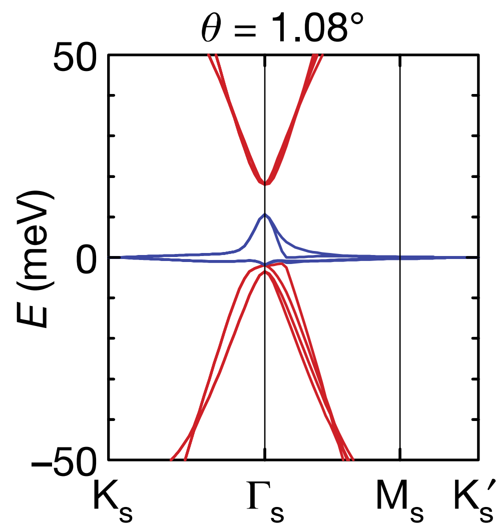


Cao et al, Nature 556, 80 (2018)

Band gap (2 holes per Moiré unit cell)

Band gap (2 electrons per Moiré unit cell)

Gaps sensitive to temperature and magnetic field

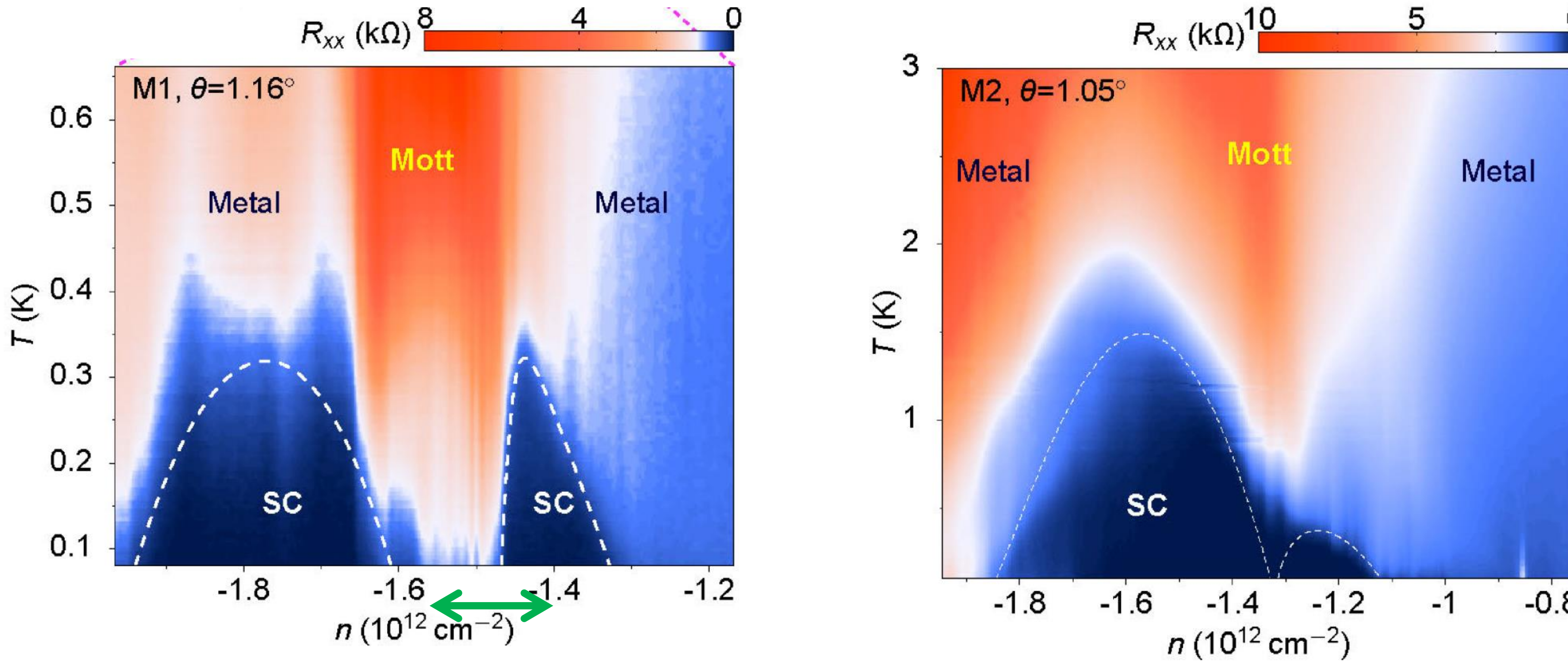


Flat band (strongly affected by interactions)

Mott insulating states?

Insulating states and superconductivity in TBG

Superconductivity emerges from the insulating (Mott?) state with two holes/electrons per Moiré unit cell

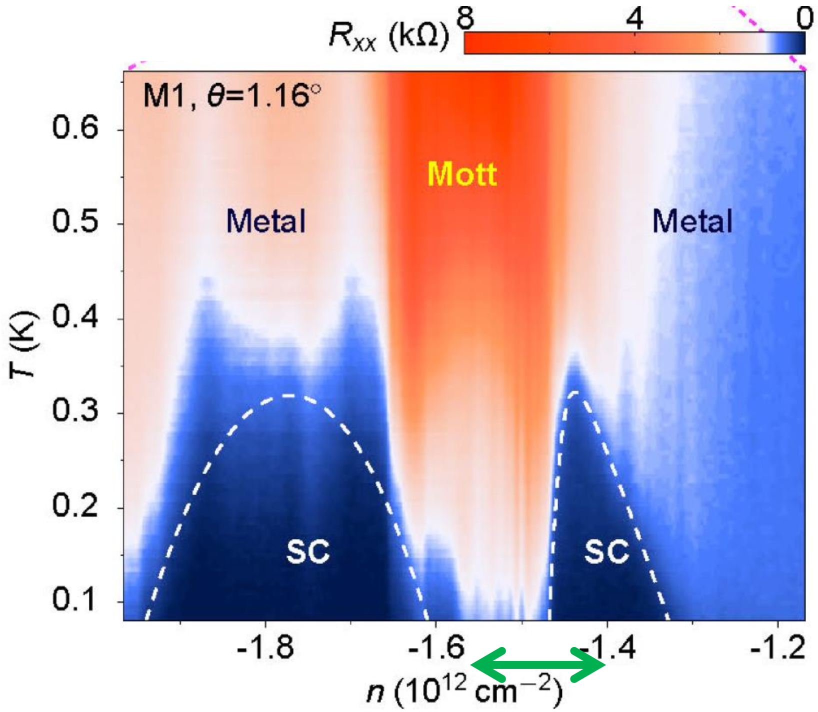


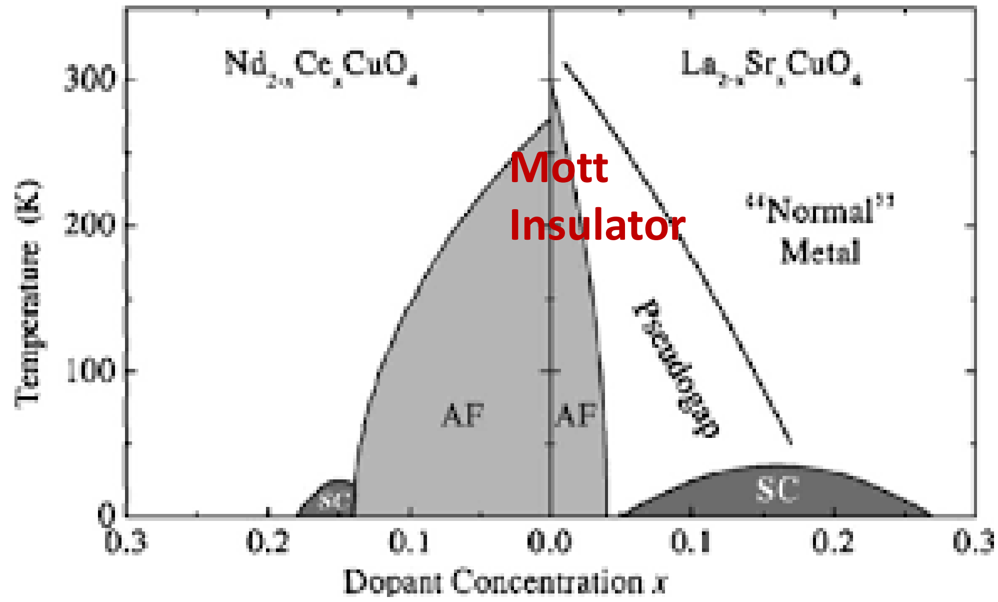
1 electron per 30 thousand C atoms
(0.2 e- per Moiré unit cell)

Most probably unconventional superconductivity

Cao et al, Nature 556, 43 (2018)

Insulating states and superconductivity in TBG





Similarity with cuprates phase diagram

Most probably unconventional superconductivity → Understanding the insulating state is the key to unveil the origin of the superconductivity

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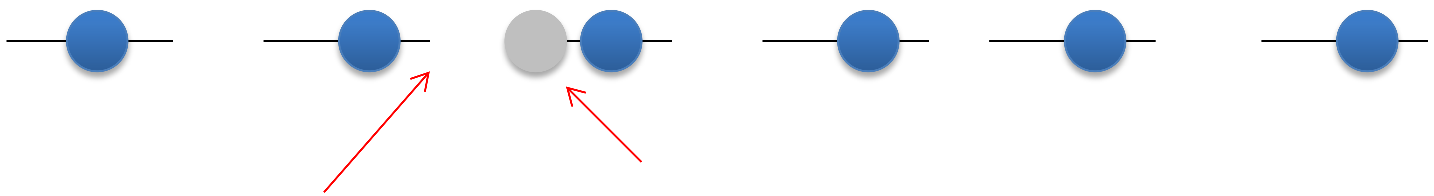
Mott insulating states

Atomic lattice with a **single orbital** per site and average occupancy 1 (**half filling**)

Kinetic energy (t) **+** **Interaction between electrons in the same site U**



Kinetic energy
(hopping)
saves energy t

Double occupancy
costs energy U

For U >> t **electrons localize:** **Mott insulator**
Mott transition at Uc

Repulsion can drive
the system into
an insulating state

The system is metallic away from half-filling but correlated
to minimize double occupancies

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Mott insulating states

Atomic lattice with a **single orbital** per site and average occupancy 1 (**half filling**)

Kinetic energy (t) **+** **Interaction between electrons in the same site U**

- Electrons localized in real space (delocalized in momentum space)
- The system is insulating due to local (on-site) interactions
- The insulating behavior linked to the filling not to details of the Fermi surface
- No symmetry breaking is required (but local electrons have tendency to order AF)

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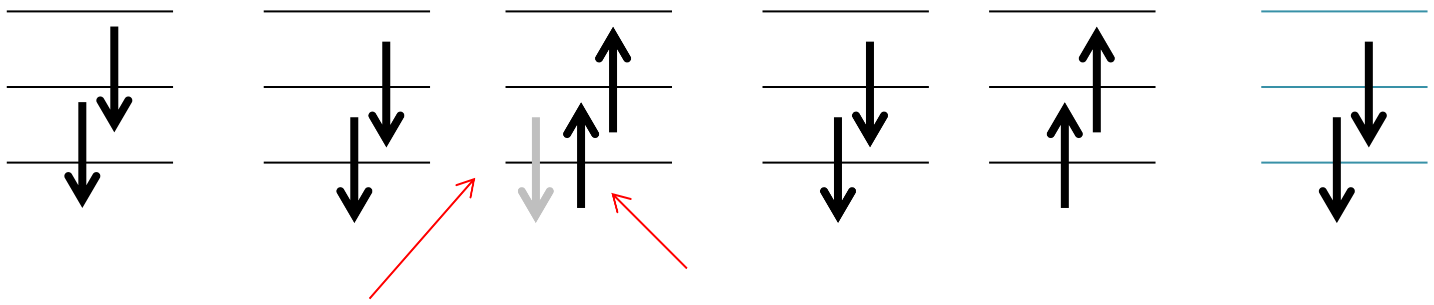
Mott insulating states. Multi-orbital systems

- Mott transition when the average number of electrons per site is an integer **n**

Filling=n/2N **N:** number of orbitals



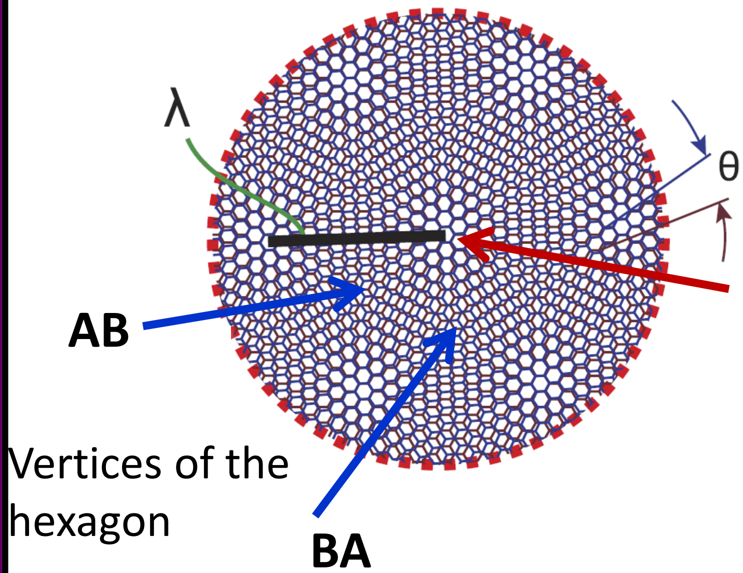
Hopping saves kinetic energy

Look for charging energy cost & compare with kinetic energy

$$\Delta_U = E(n+1) - E(n-1) - 2E(n)$$

Depends on U, Hund's coupling …

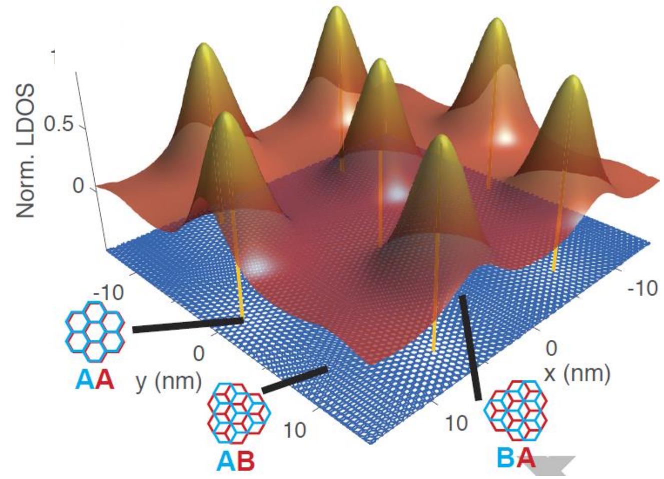
Local model for TBG. Original proposal



AA (center of the unit cell)

TBG: Triangular lattice of Hexagonal Moiré unit cells centered at the AA sites

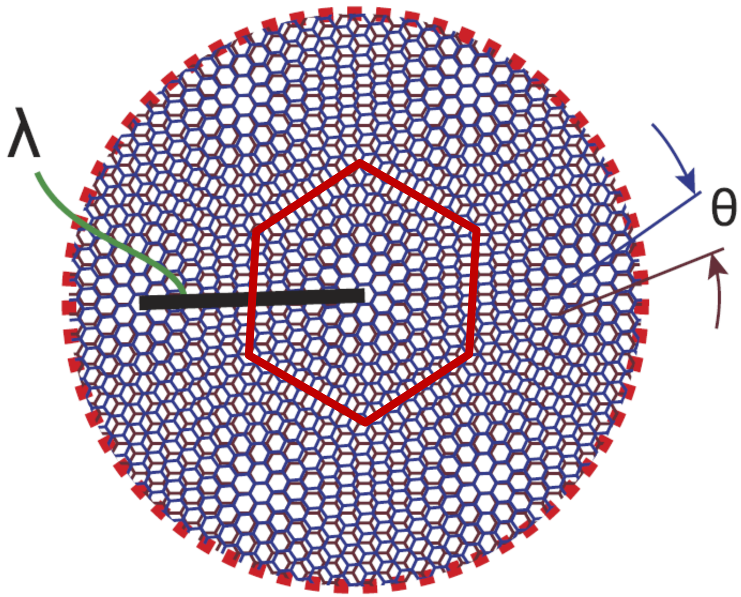
Close to the charge neutrality point (Dirac points) the electronic states are localized in the AA regions



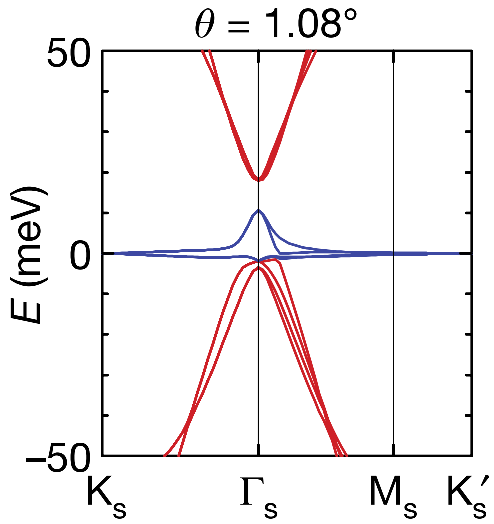
Originally proposed:
Effective triangular lattice model for the Moiré pattern

Cao et al, Nature 556, 80 (2018)

Mott insulating states in TBG? Original proposal



TBG: Triangular lattice of Hexagonal Moiré unit cells centered at the AA sites



- Two bands (valley) for E>0
- Two bands (valley) for E<0

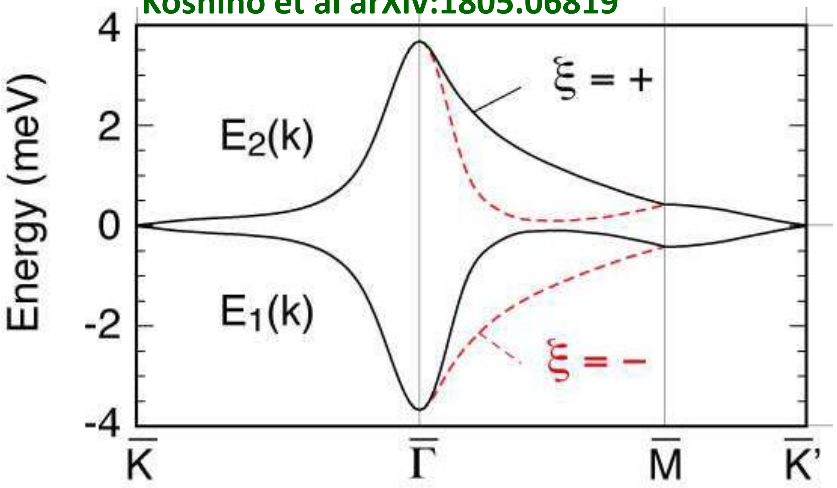
Two-orbital model
in a triangular lattice

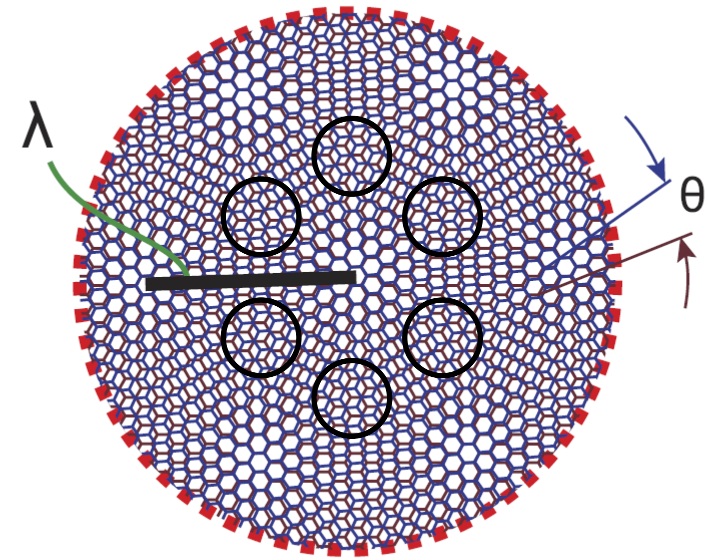
Insulating states with ±2 electrons
per Moiré unit cell correspond
to half-filling the E>0 and the E<0 bands

Originally proposed: Mott insulating state at half-filling in a triangular lattice

Mott insulating states in TBG? The honeycomb lattice

Effective **honeycomb lattice two-orbital model** for the Moiré superlattice:





- It accounts for both E>0 and E<0.
- Two orbitals (valley degree of freedom)
- t~2 meV, W~10 meV, U ~20 meV
- Half-filling x=1/2 (4 electrons per Moiré unit cell) corresponds to the undoped system

  Insulating states: x=1/4 and x=3/4 (1 and 3 electrons/site, 2 and 6/Moiré unit cell)

Yuan & Fu, PRB 98, 045103 (2018), H.C. Po et al, 1803.09742, Liu et al: arXiv:1804.10009, Kang & Vafek:1805.04918

A Hubbard model for the Moiré honeycomb lattice

Hubbard: Only on-site interactions. U ~20 meV

$$U\sum_{m}\hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U'\sum_{m\neq m'}\hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U' - J_H)\sum_{m<m',\sigma}\hat{n}_{m\sigma}\hat{n}_{m'\sigma}$$

Intraorbital interaction U

Interorbital interaction U'

Hund's coupling

spin

Assume $U'=U-2J_H$ → Two independent interactions **U, J_H**

No assumption on the sign of J_H

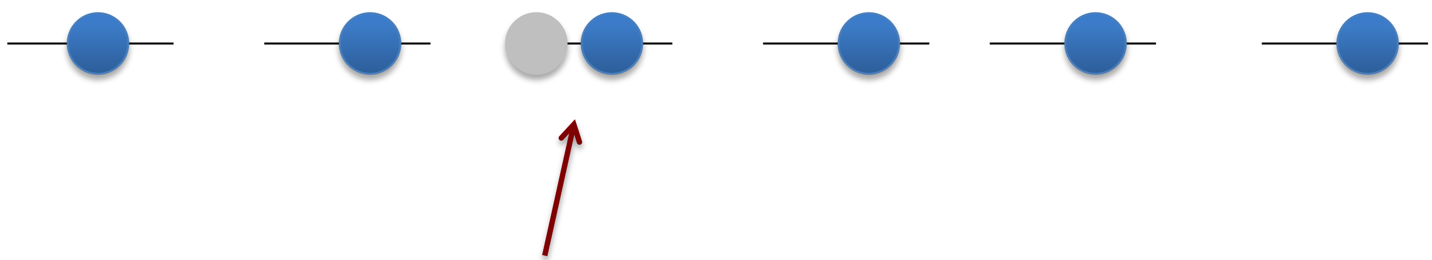
J_H ~0 (Yuan & Fu, arXiv:1803.09699)

J_H <0 due to phonons (Dodaro et al, arXiv:1804.03164)

Hopping t restricted to first nearest neighbors

A Hubbard model for the Moiré honeycomb lattice

Calculations using **single site** slave-spin technique & comparison with known results from DMFT in other lattices/#orbitals



Only local correlations included

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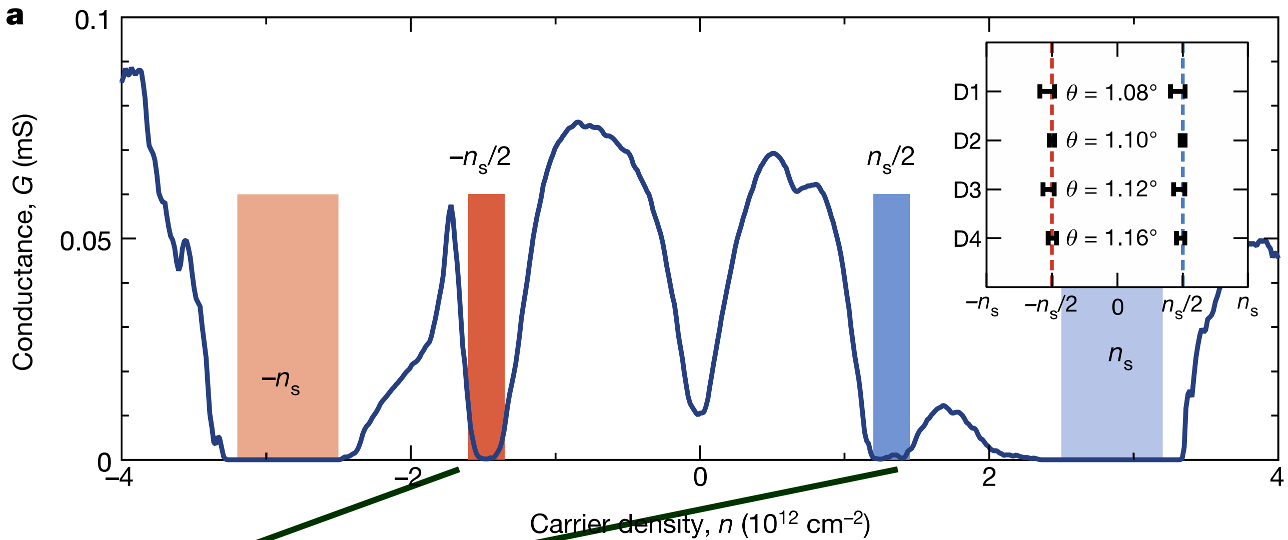
Mott insulating states in the honeycomb 2-orbital model

2-orbital model: Mott states at **x=1/4, 1/2, 3/4** (1, 2 or 3 electrons per site)



X=1/4 and x=3/4 insulating

X=1/2 Semi-metallic (not insulating)

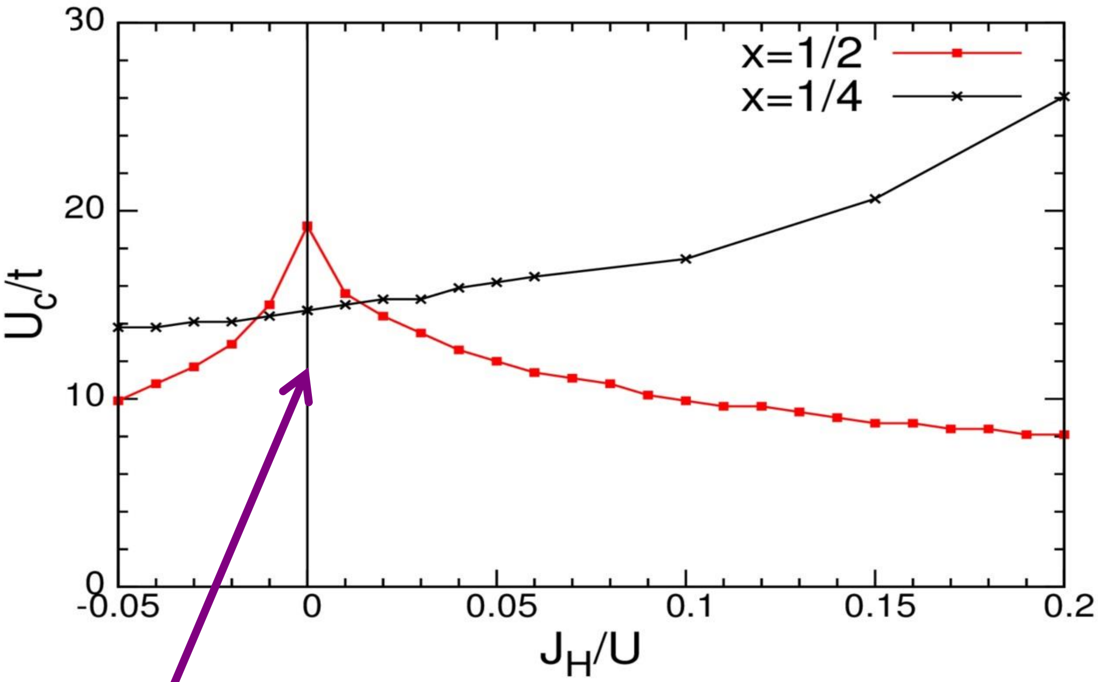
$$U^c_{1/4} < U_{TBG} < U^c_{1/2}$$

OK for J_H~0

Pizarro et al, arXiv:1805.07303

Yuan & Fu, PRB 98, 045103 (2018)

Mott insulating states in the honeycomb 2-orbital model



Away from J_H~0 the charging energy cost $\Delta^U_{1/2}>\Delta^U_{1/4}$

with Δ^U_x=E(n+1)-E(n-1)-2E(n)

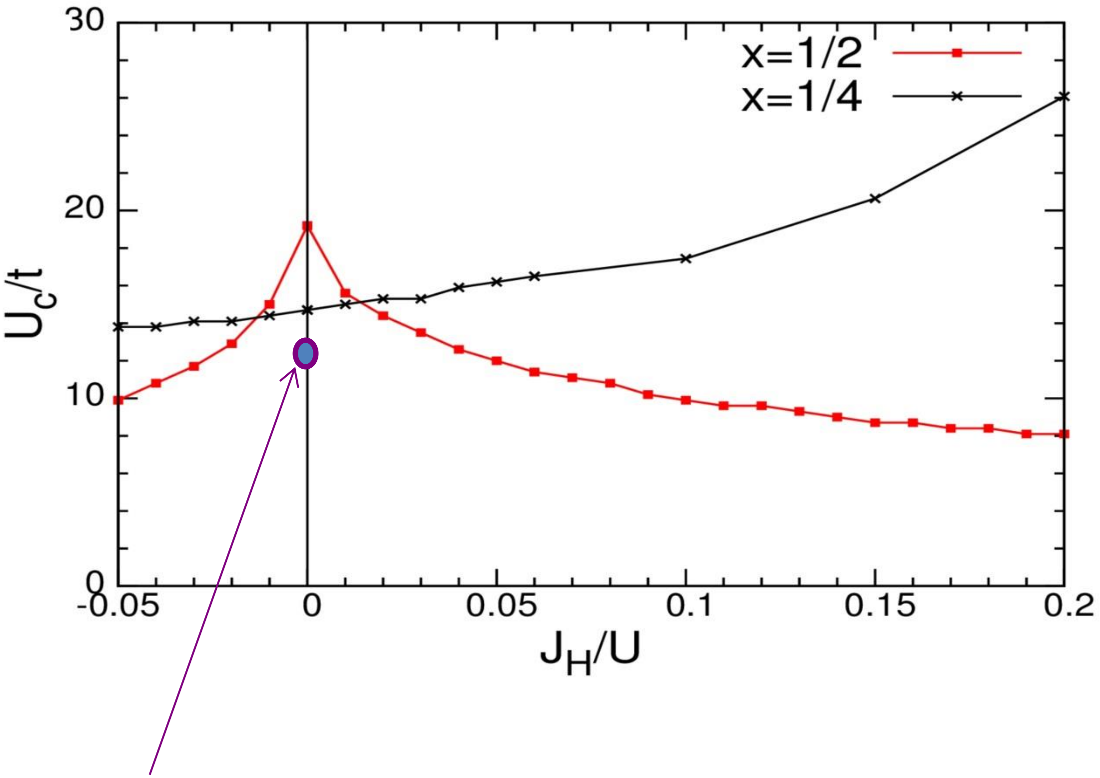
Insulating state promoted at x=1/2

$U^c_{1/4} < U^c_{1/2}$ satisfied in a small region close to J_H~0

Single-site slave spin calculation
on the two-orbital honeycomb lattice

Pizarro et al, arXiv:1805.07303

Mott insulating states in the honeycomb 2-orbital model



At J_H~0 the charging energy cost $\Delta^U_{1/2}=\Delta^U_{1/4}=U$

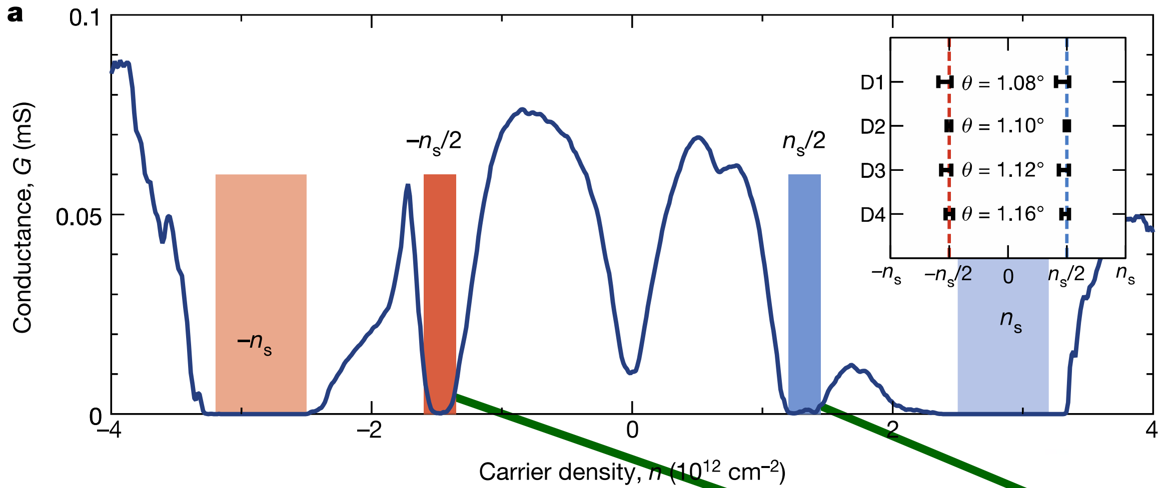
$$\frac{U^c_{1/2}}{U^c_{1/4}}(J_H=0)=1.28$$

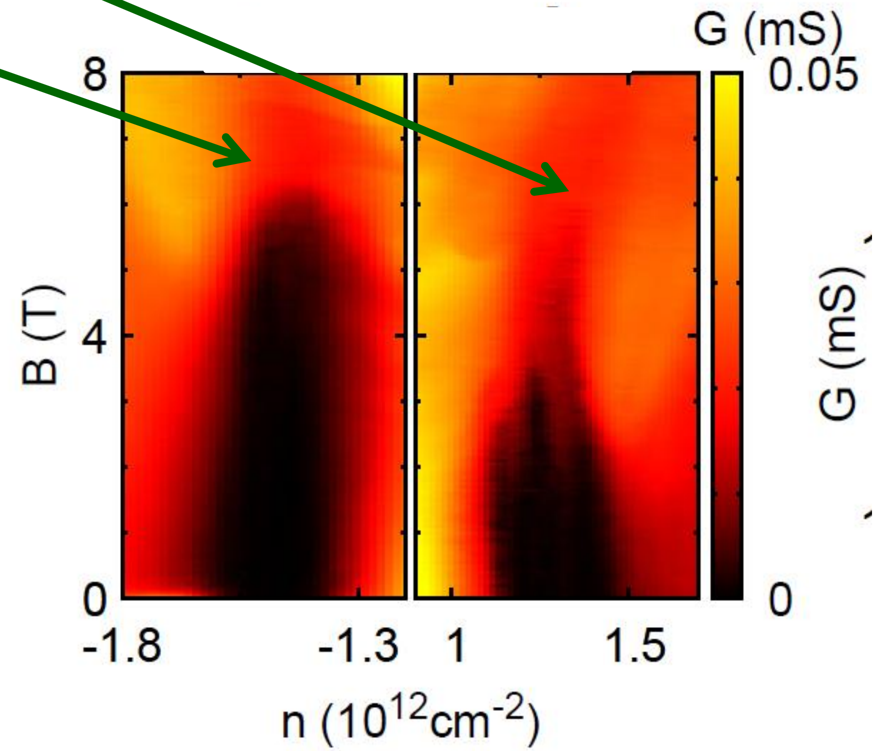
U_c for a single orbital model at half-filling with $\Delta^{1orb}_{1/2}=U$

At J_H~0 orbital fluctuations stabilize the metallic state up to larger interactions for x=1/2 but the metallic state is strongly correlated

Pizarro et al, arXiv:1805.07303

Insulating states and superconductivity in TBG





The insulating character disappears if a perpendicular or parallel magnetic field is applied (Zeeman)

No evidence of AF ordering

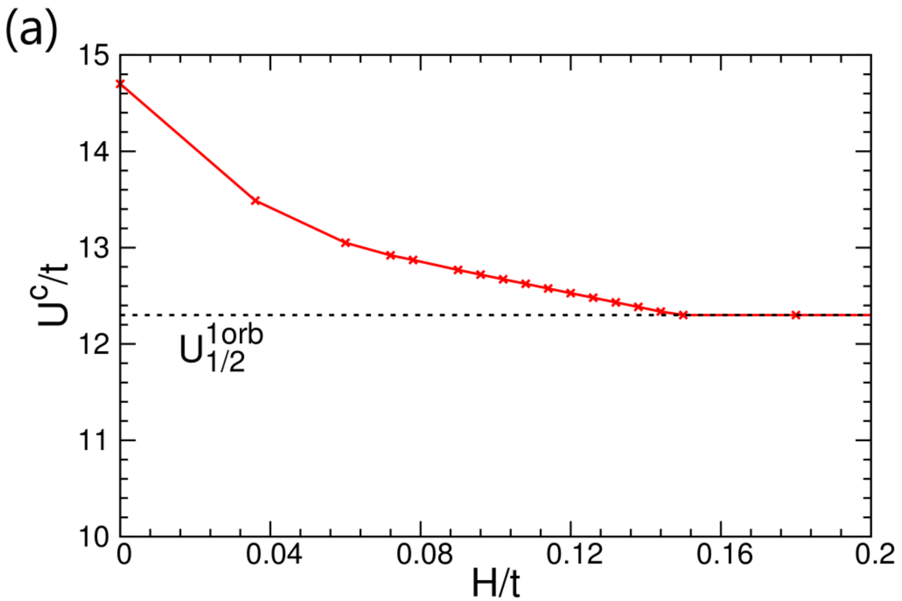
Cao et al, Nature 556, 80 (2018)

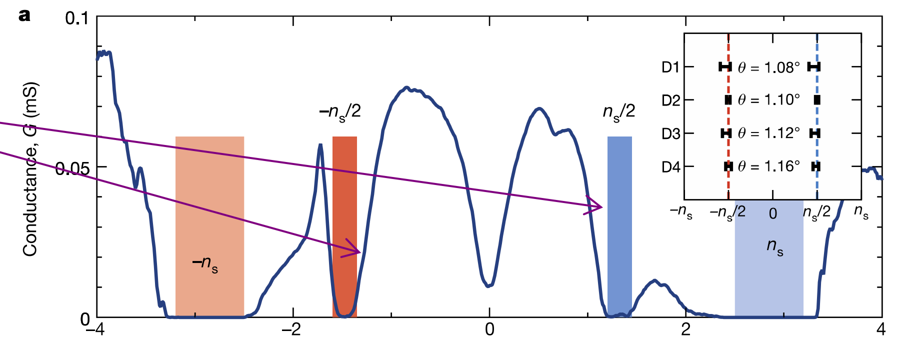
Mott insulating states in the magnetic field

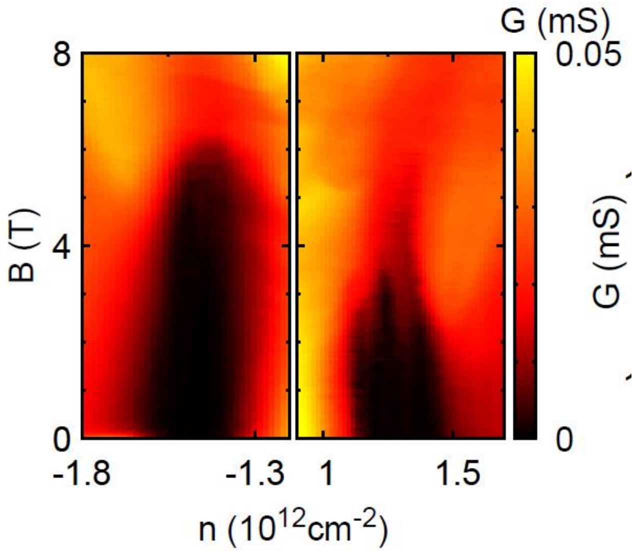
Focus on x=1/4 and J_H=0

Zeeman term

$$H \sum_{j\gamma} (n_{j\gamma\uparrow} - n_{j\gamma\downarrow})$$







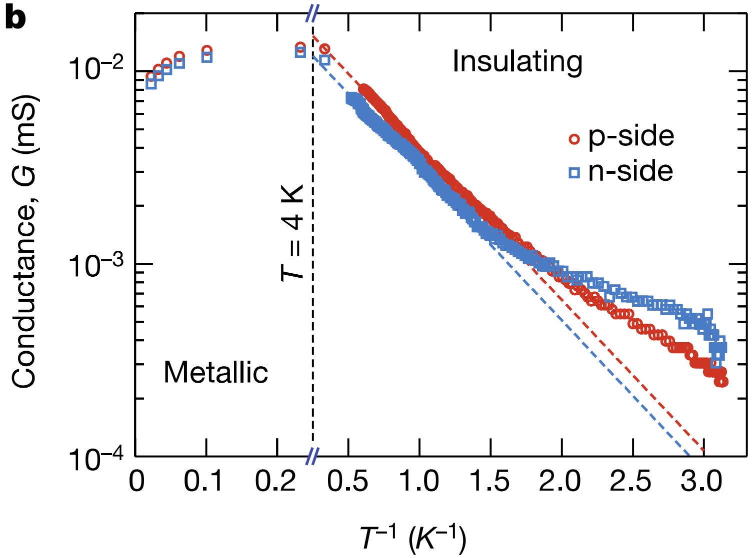
The magnetic field decreases the critical interaction for the Mott transition

Contrary to the experimental results
the magnetic field enhances the insulating tendencies

Pizarro et al, arXiv:1805.07303

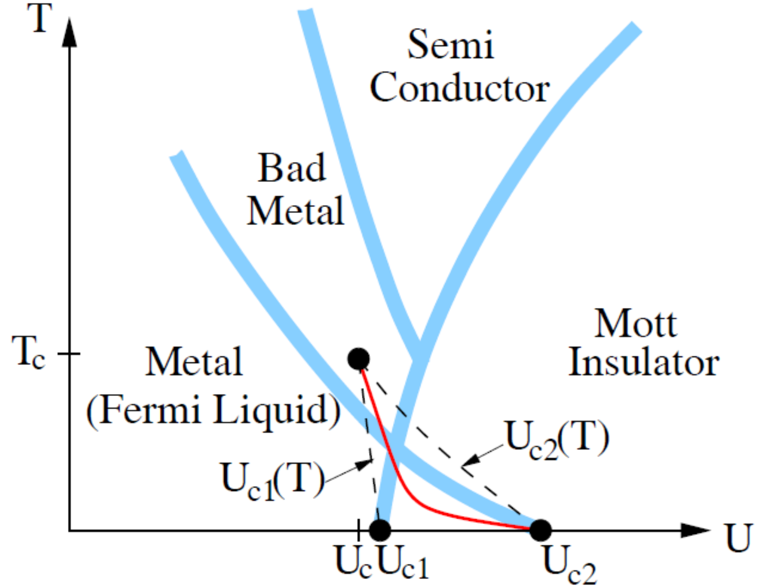
Mott insulating states. Temperature dependence

EXPERIMENT



Experimentally the insulating state is suppressed with increasing temperature

Single orbital. Half-filling. Single-site DMFT (Bethe lattice)



Georges et al, J. de Physique IV 114, 165 (2004)

Contrary to the experimental results
increasing the temperature enhances the insulating tendencies

Pizarro et al, arXiv:1805.07303

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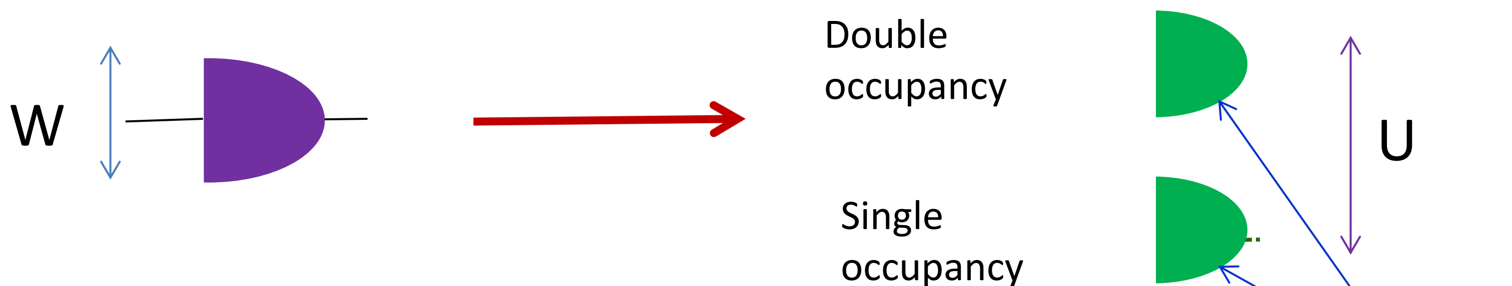
Mott insulating states. Size of the gap (local correlations)

Kinetic energy (hopping) saves energy t

Double occupancy costs energy U

Small U/t — Increasing U/t → Large U/t

Metal — Mott transition — Insulator



States broadened by hopping t : incoherent bands

Hubbard bands

Mott insulating states. Size of the gap

Expected size of the gap

$\Delta \sim W,U$

Experiment **Cao et al, Nature 556, 80 (2018)**

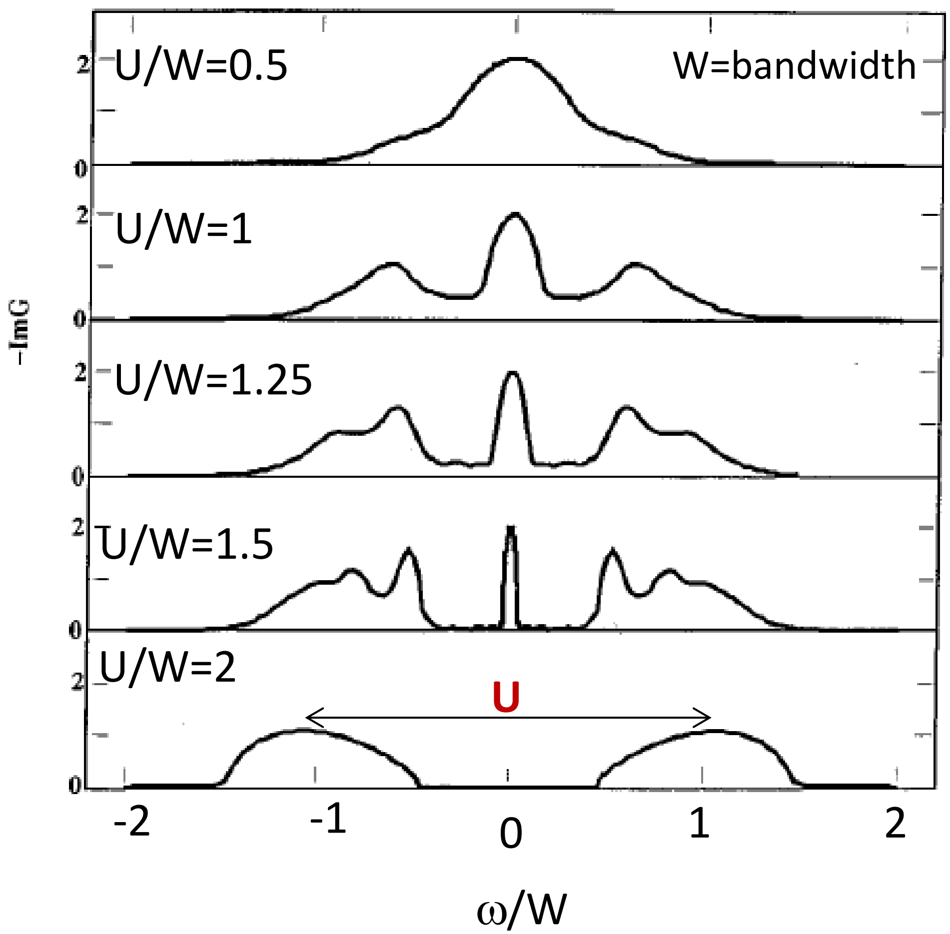
Small gap
$\Delta \sim 0.3$ meV << W,U (10-20 meV)

Dodaro et al, arXiv:1804.03162

Liu et al: arXiv:1804.10009

Experimental gap too small for a Mott insulator

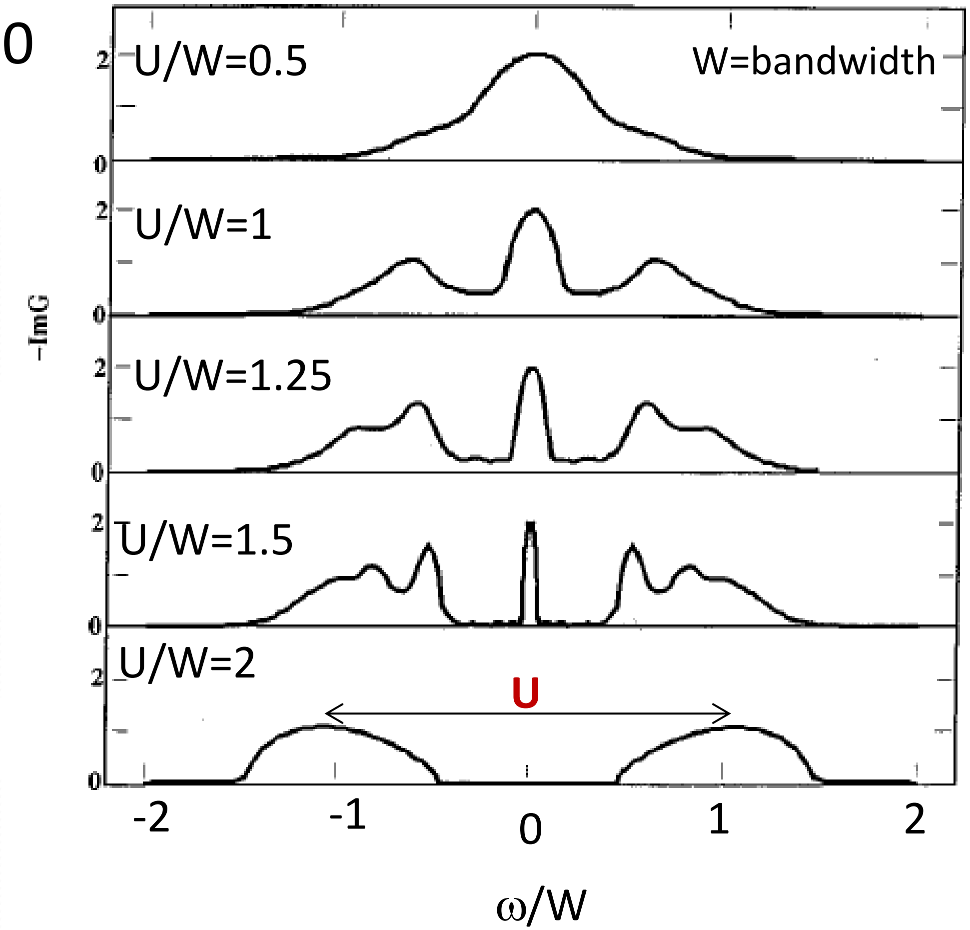
Single orbital. Half-filling.
Single-site DMFT (Bethe lattice)



Georges et al, RMP 68, 13 (1996)

Mott states (local correlations) & the experiment in TBG

Experiment	**Local correlations**
• $U^{c}_{1/4} < U_{TBG} < U^{c}_{1/2}$	OK if $J_H \sim 0$
• Insulating behavior disappears in a magnetic field	
• Insulating behavior disappears with increasing temperature	
• Gap << U,W	



Pizarro et al, arXiv:1805.07303

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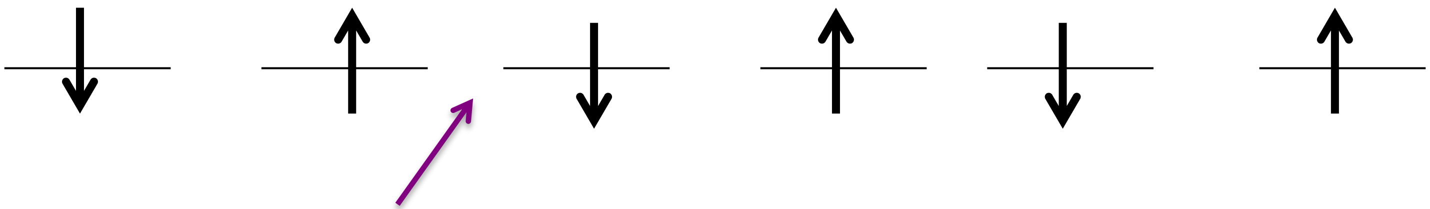
Mott insulating states. Non-local correlations

Intersite-magnetic/orbital correlations



$J \sim t^2/U$

- Correlated insulator (decreases critical interaction) even in the absence of long-range magnetic ordering.
- Lattice dependent. Important in low dimensions and low temperatures (cuprates).
- Cluster techniques (CDMFT, DCA, …). Technically challenging in multi-orbital systems

Pizarro et al, arXiv:1805.07303

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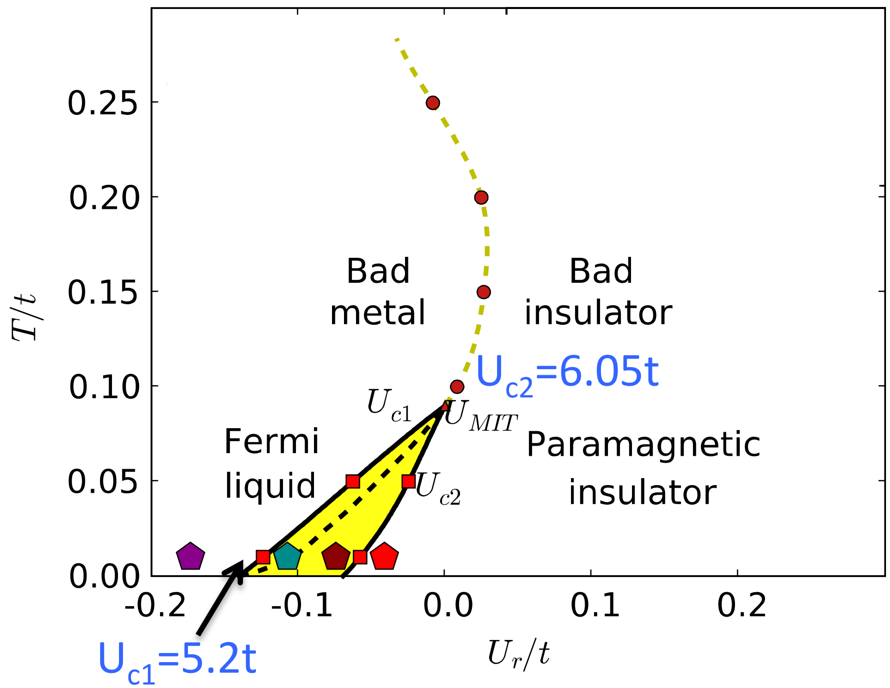
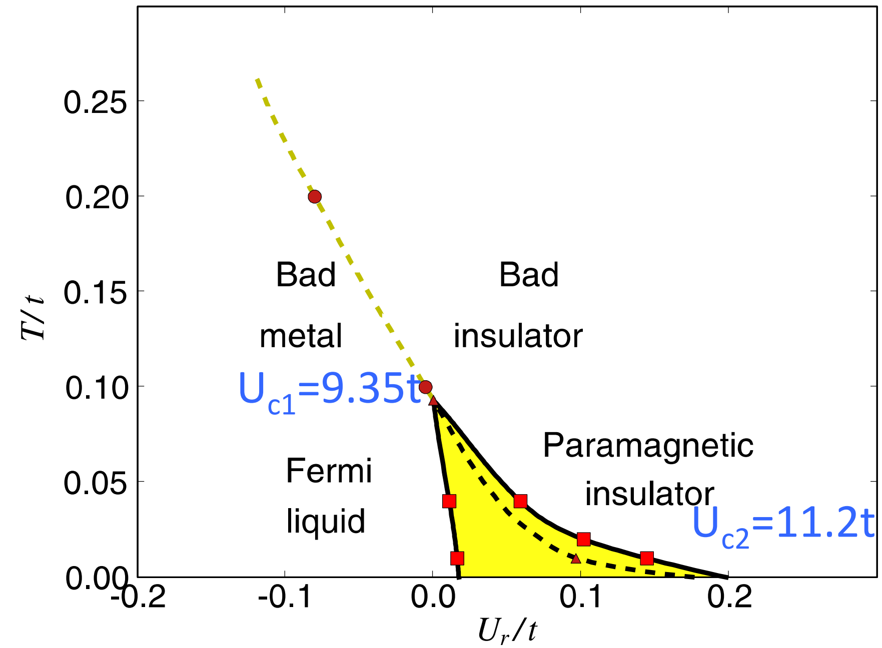
The role of non-local correlations in Mott insulators

Square lattice, single-orbital

With non-local correlations (cluster DMFT, **in the non-magnetic state**)



Without non-local correlations (single-site DMFT)



Park et al, PRL 101, 186403 (2008)

The inclusion of non local correlations:

- Reduces the critical interaction
- Reverses the temperature dependence

Close to Uc the insulating behavior disappears with increasing temperature in agreement with the experiment

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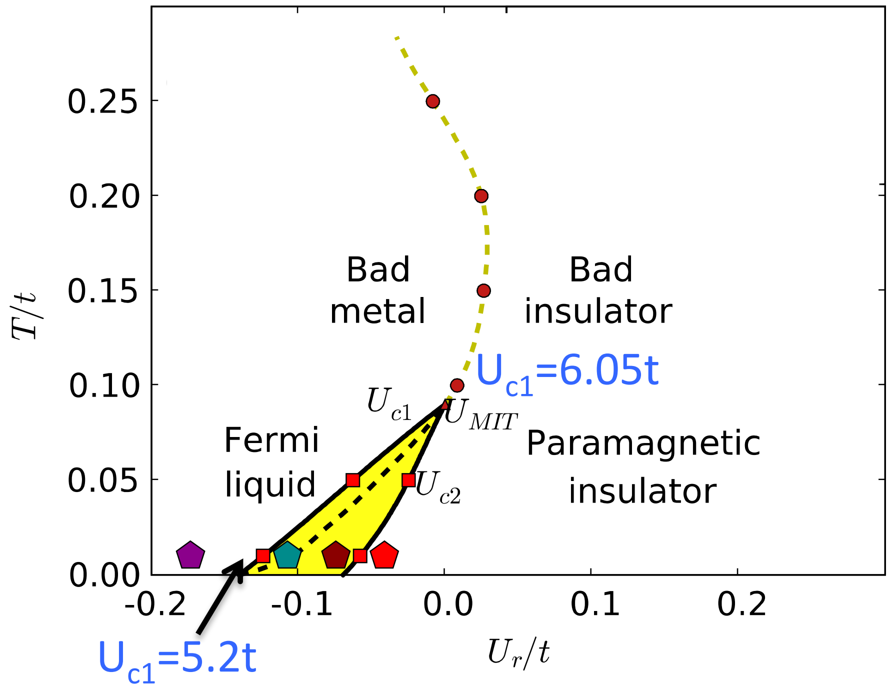
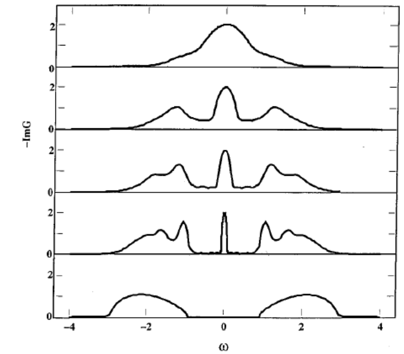
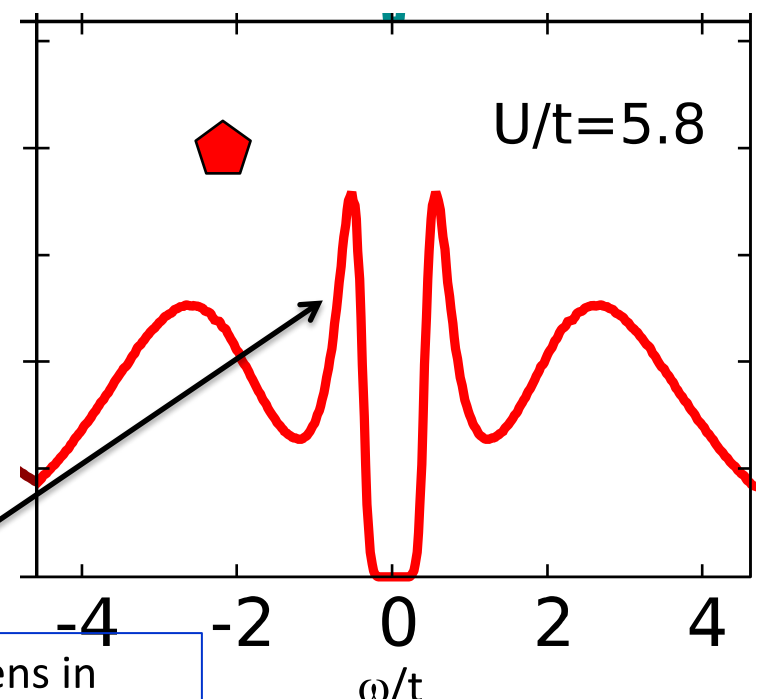
The role of non-local correlations in Mott insulators

Square lattice, single-orbital

With non-local correlations
(cluster DMFT, **in the non-magnetic state**)







Small gap close to Uc
Δ~0.02 W

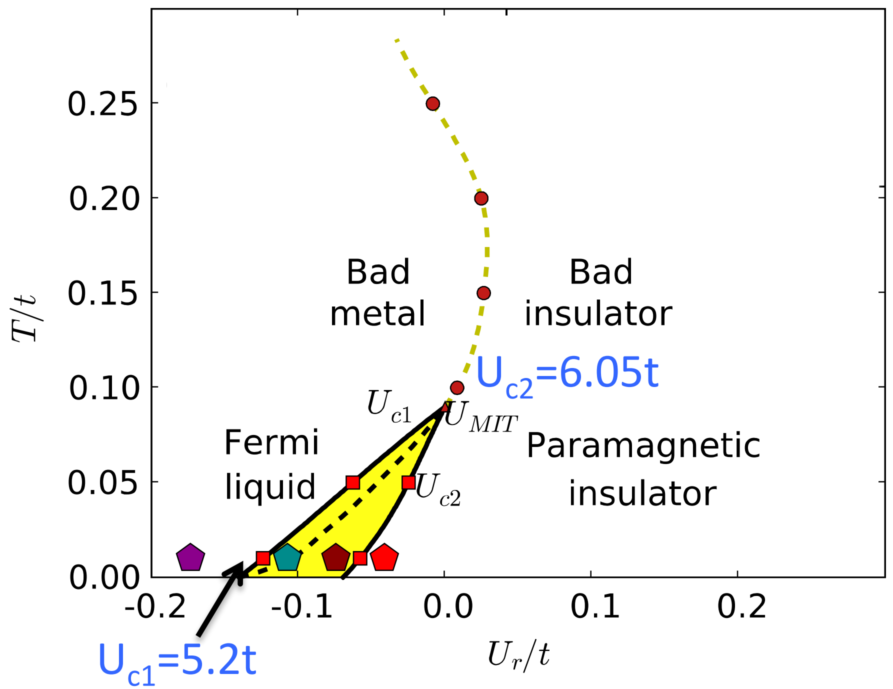
Close to the critical interaction a small gap opens in the quasiparticle peak.
Small gap expected (in agreement with experiment)

Park et al, PRL 101, 186403 (2008)

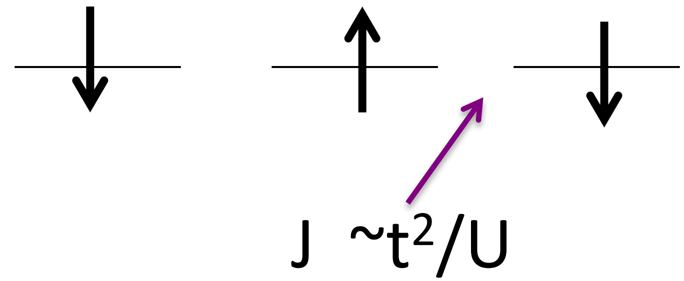
The role of non-local correlations in Mott insulators

Square lattice, single-orbital

With non-local correlations
(cluster DMFT, **in the non-magnetic state**)



Park et al, PRL 101, 186403 (2008)



Hexagonal lattice, two-orbital:
Intersite antiferromagnetic correlations **if Hund's coupling is zero or negative**

A magnetic field will suppress the inter-site magnetic correlations in agreement with the experiment

Key role of short-range Antiferromagnetic Correlations
in the Metal-Insulator Transition even if long-range AF order is not present

Summary: Mott states & the experiment in TBG

Experiment	Local correlations	Non-local correlations
• Insulating behavior disappears with increasing temperature		
• Gap << U,W		
• Insulating behavior disappears in a magnetic field		If $J_H \leq 0$  AF correlations key role in MIT
• $U^c_{1/4} < U_{TBG} < U^c_{1/2}$	 if $J_H \sim 0$	?

• Possibility to find pseudogap physics

Pizarro et al, arXiv:1805.07303

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