Exploring correlations in twisted bilayer graphene

E. Bascones

Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)

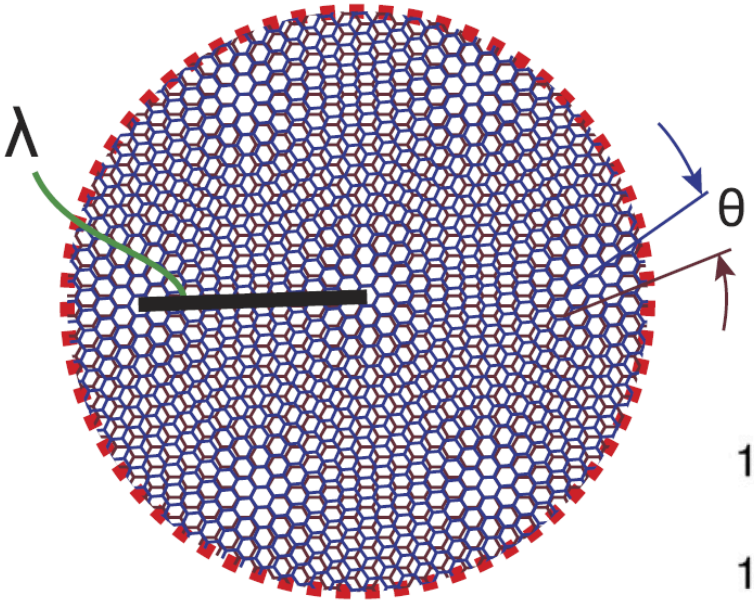
In collaboration with:

M. J. Calderón
(ICMM-CSIC)

P. San José
(ICMM-CSIC)

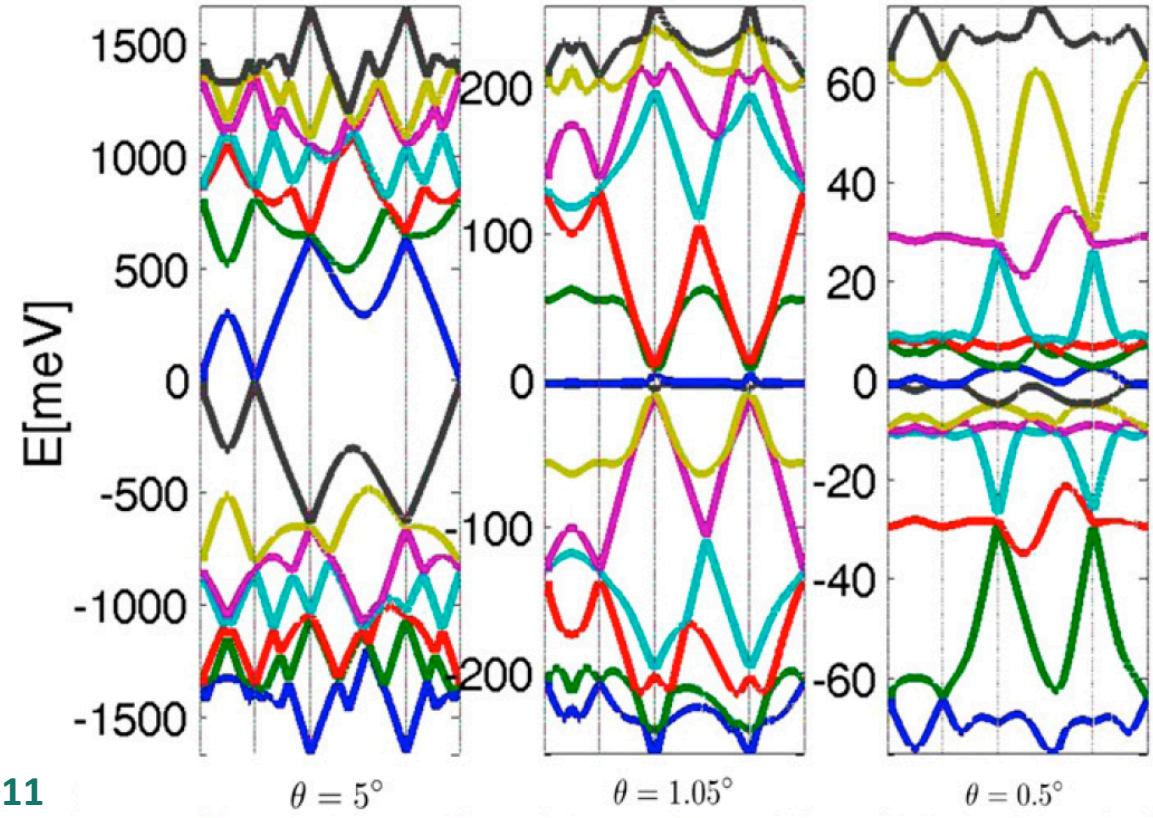
GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD
icmm
CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

Correlated states in twisted bilayer graphene



Two graphene layers rotated

Moiré Pattern

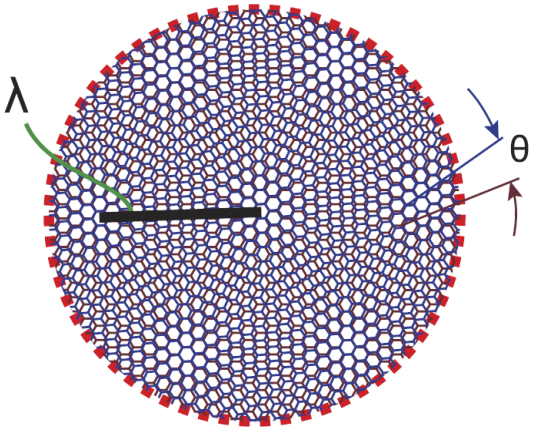


Bistritzer & Macdonald, PNAS 2011

leni@icmm.csic.es

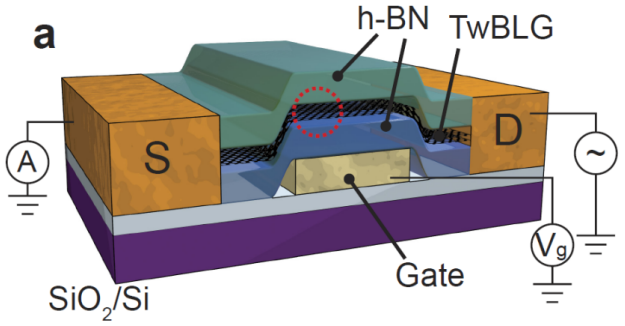
Correlated states in twisted bilayer graphene

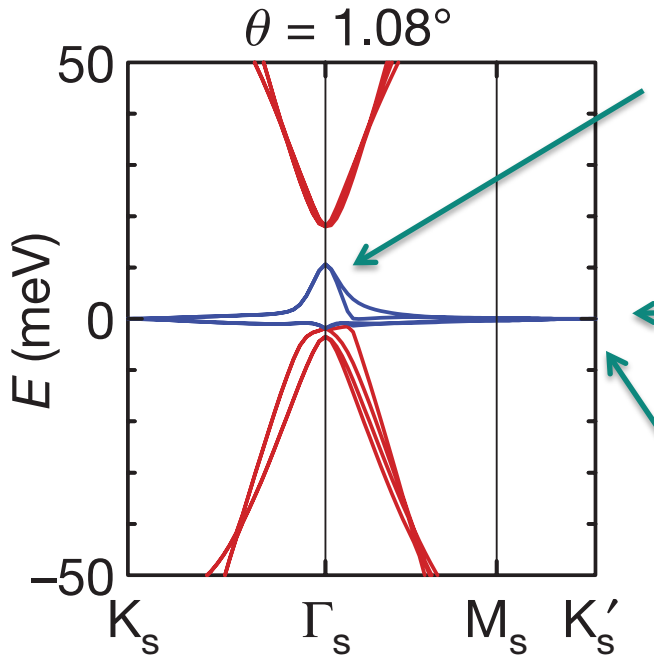
Rotation angle ~ 1º



Moiré unit cell ~ 11000 atoms

Moiré lattice constant λ~13 nm





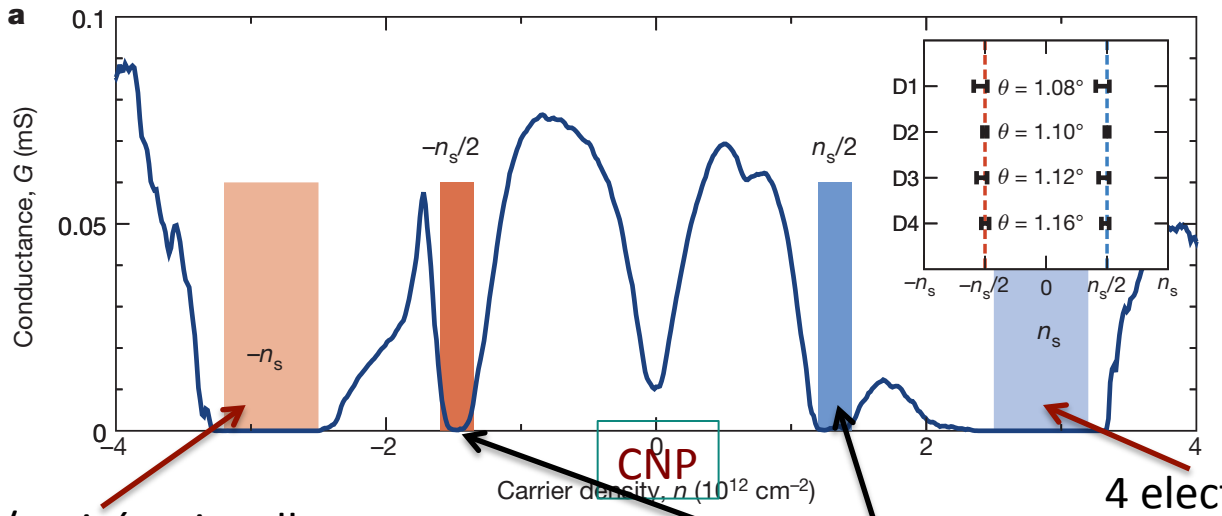
2 valleys:
4 spin degenerate flat bands
(2 upper & 2 lower bands)

CNP. Undoped system

Dirac points at K and K'

Cao et al, Nature 556, 80 (2018)
Cao et al, Nature 556, 43 (2018)

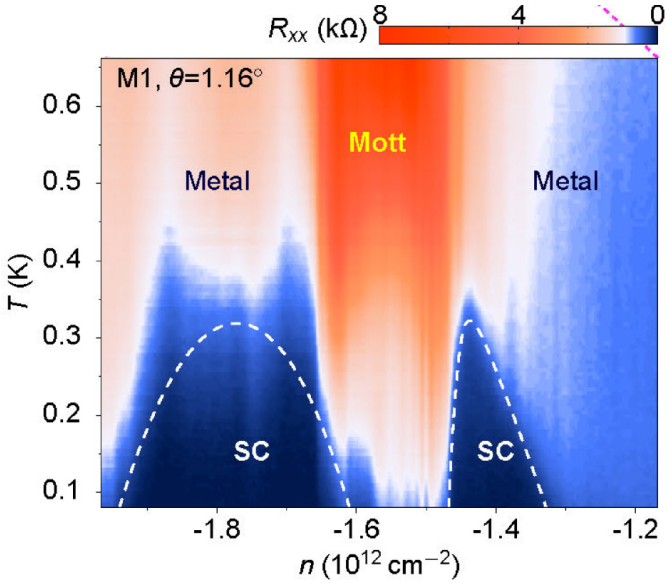
Correlated states in twisted bilayer graphene



4 holes/moiré unit cell
(flat bands empty)

4 electrons/moiré unit cell
(flat bands filled)

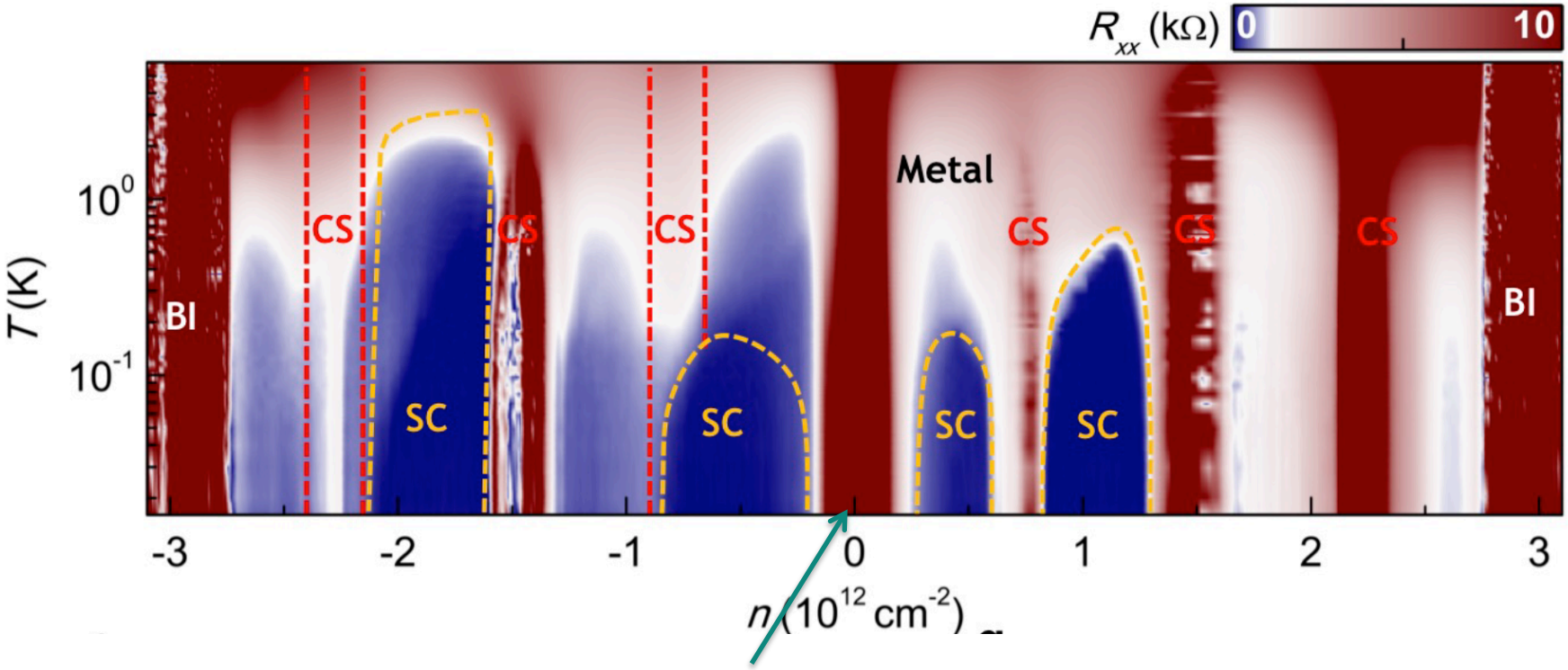
Correlated insulating states:
2 electrons/holes moiré unit cell
(flat bands half-filled)



Cao et al, Nature 556, 80 (2018)
Cao et al, Nature 556, 43 (2018)

Correlated states in twisted bilayer graphene

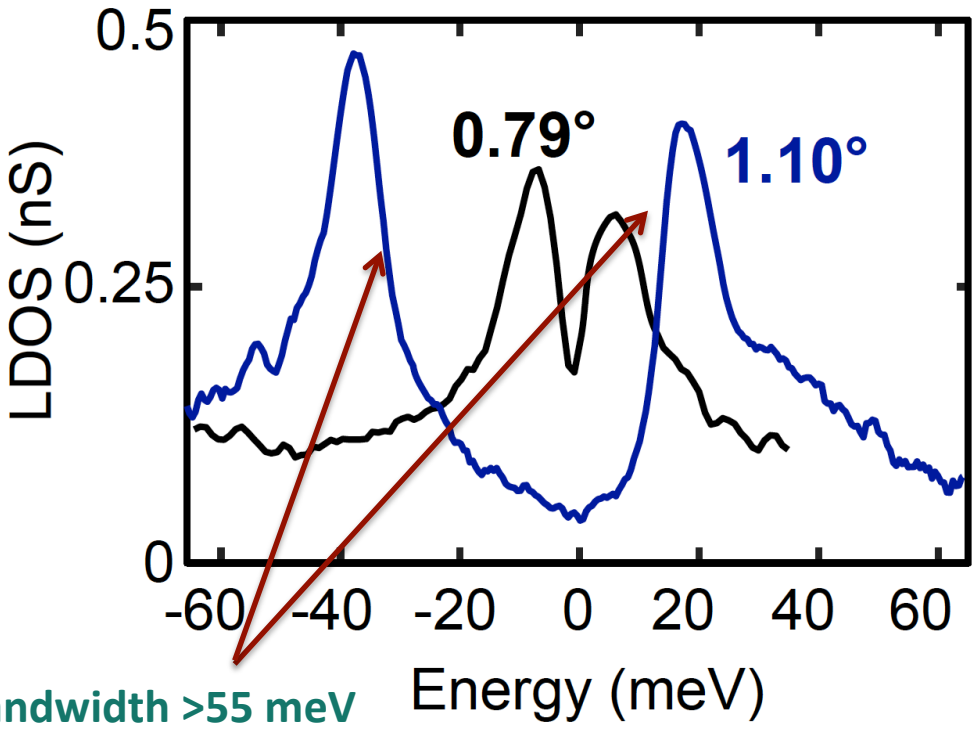
Correlated states at all commensurate fillings
& many superconducting domes



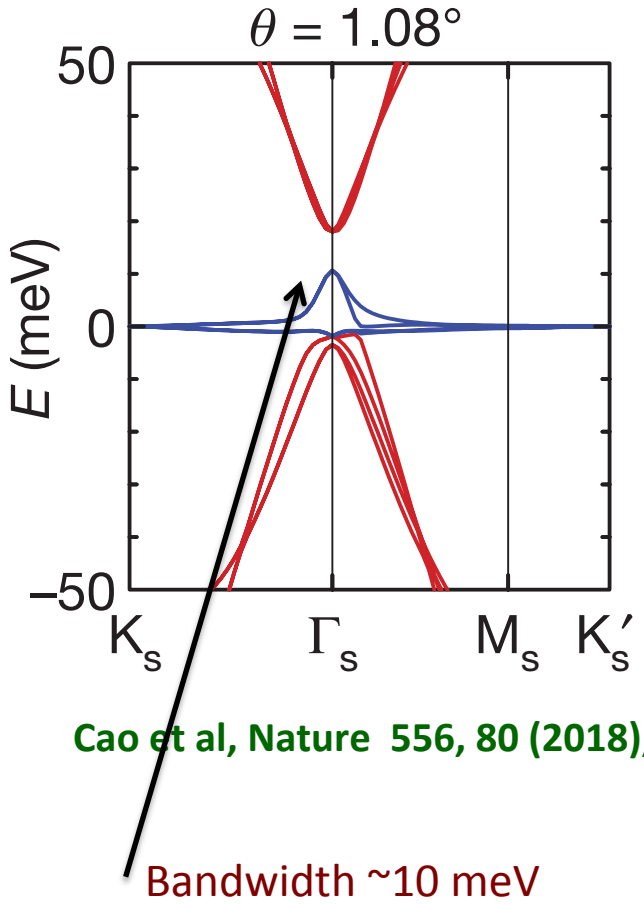
Charge neutrality point (CNP)
Undoped system

Lu, Efetov et al arXiv: 1903.06513

Correlated states in twisted bilayer graphene



Bandwidth >55 meV



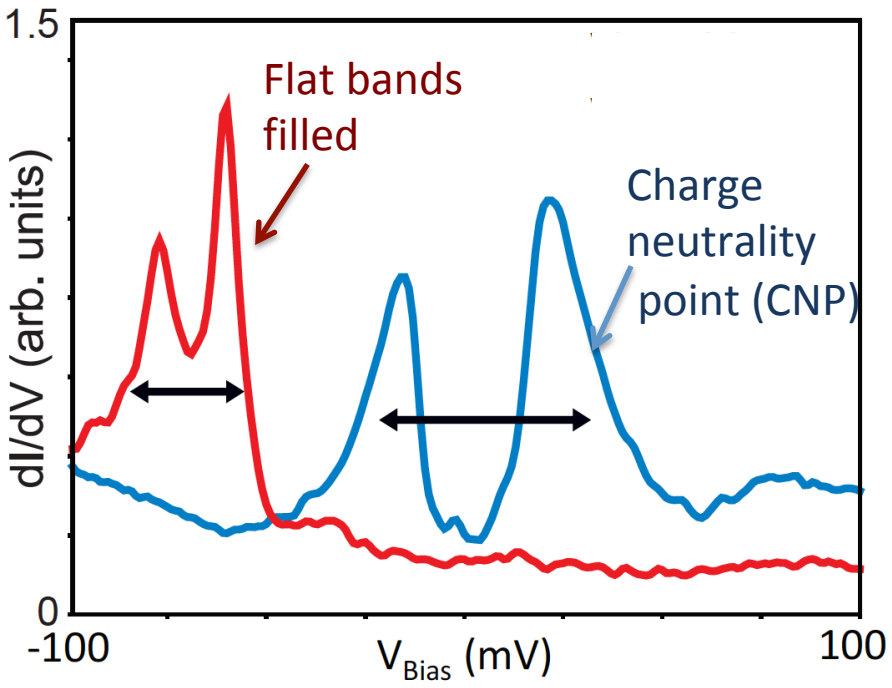
Cao et al, Nature 556, 80 (2018),

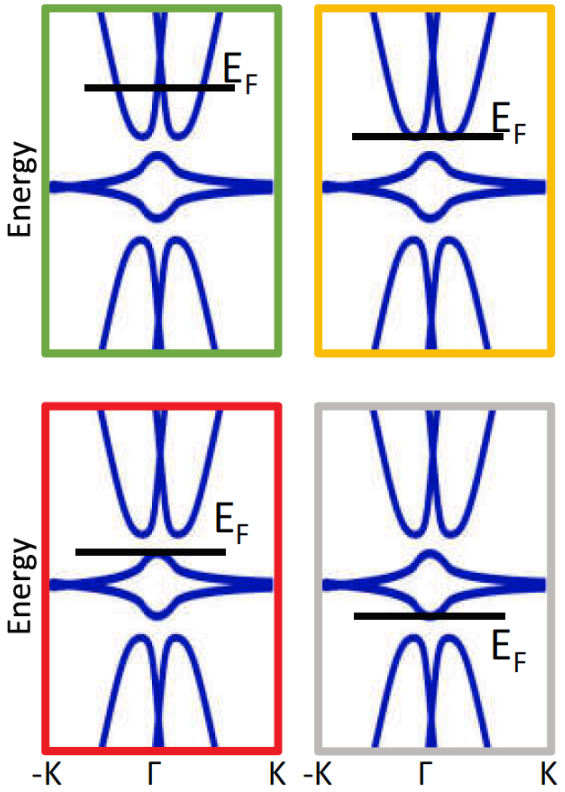
Bandwidth ~10 meV

Kerelsky, Pasupathy, Dean et al, Nature 572, 95-100 (2019)

Correlated states in twisted bilayer graphene

STM experiments

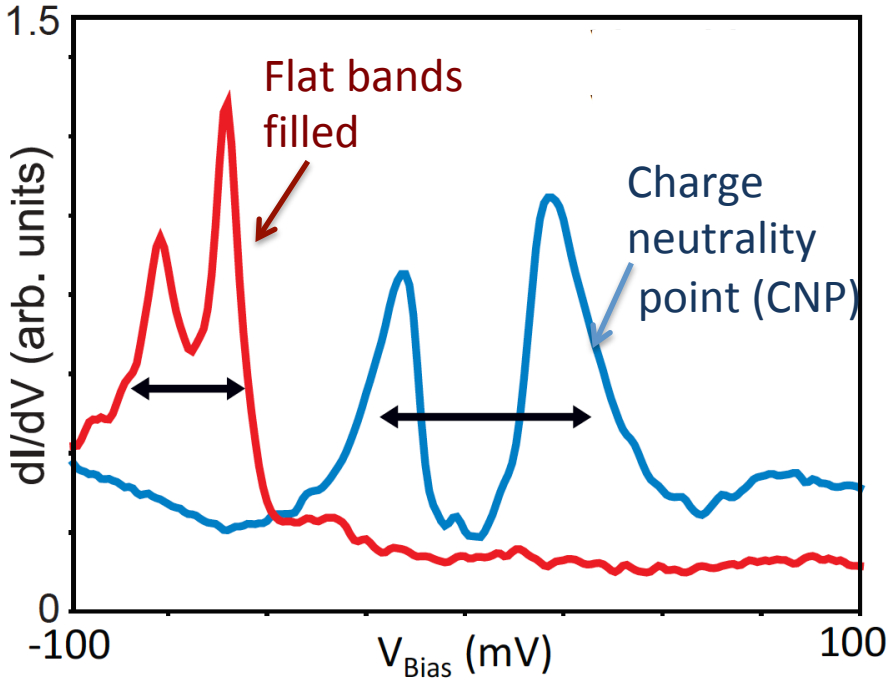




Choi, Nadja-Perge, et al Nature Physics (2019) arXiv:1901.02997

A symmetry breaking state at CNP?

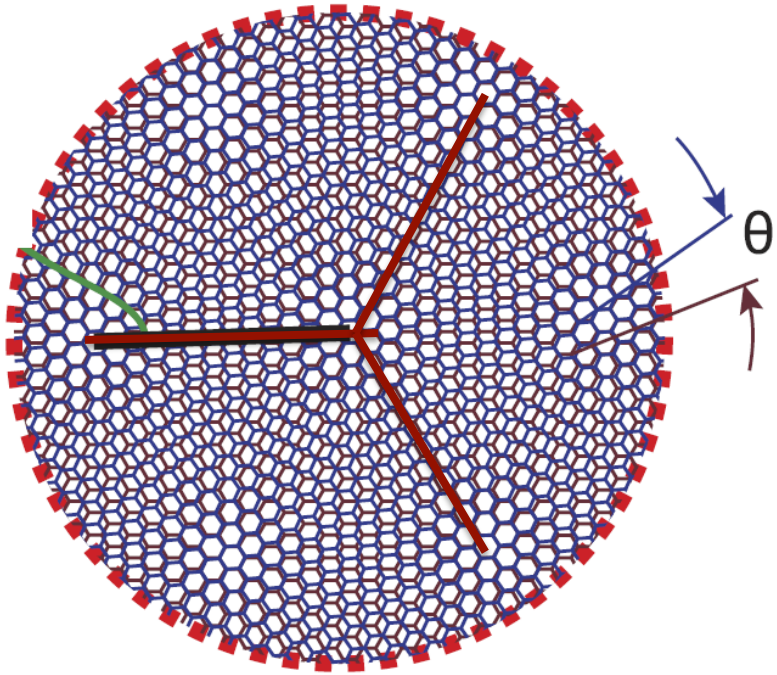
STM experiments



Choi, Nadja-Perge, et al Nature Physics (2019) arXiv:1901.02997

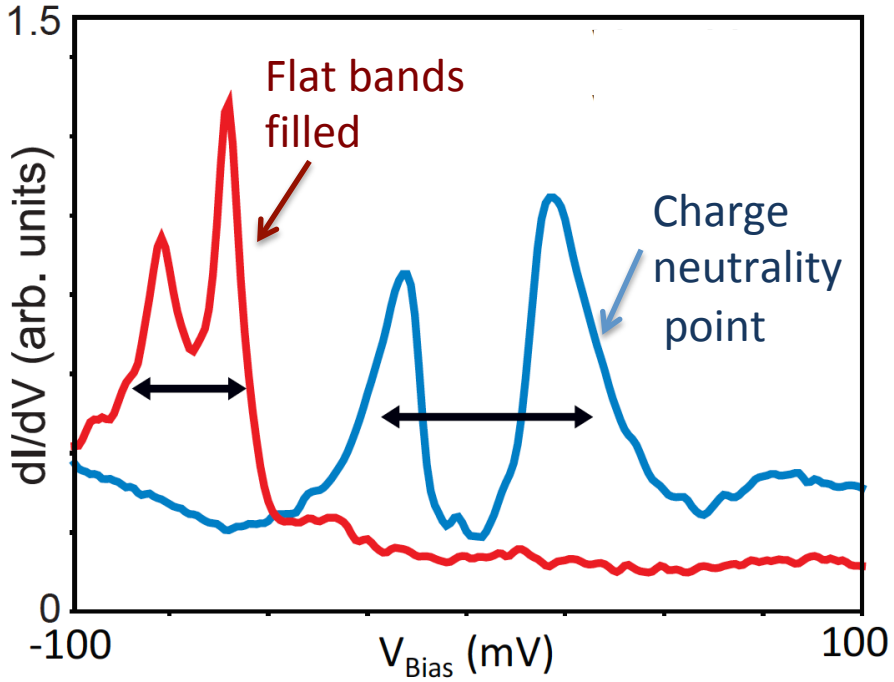
Symmetries in each valley

- C_3 symmetry
- $C_{2z}T$
- M_{2Y}



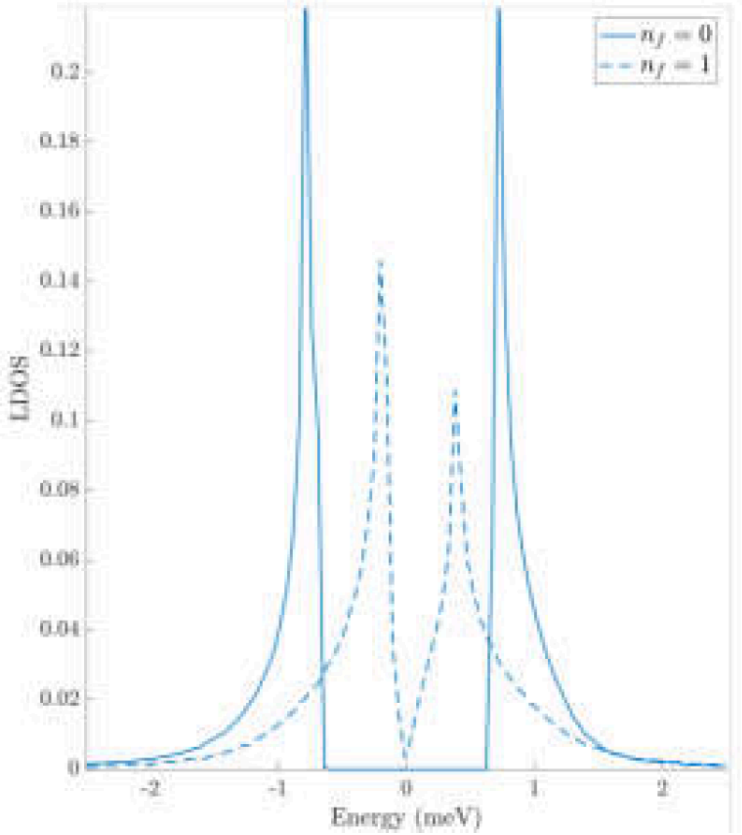
A symmetry breaking state at CNP?

STM experiments



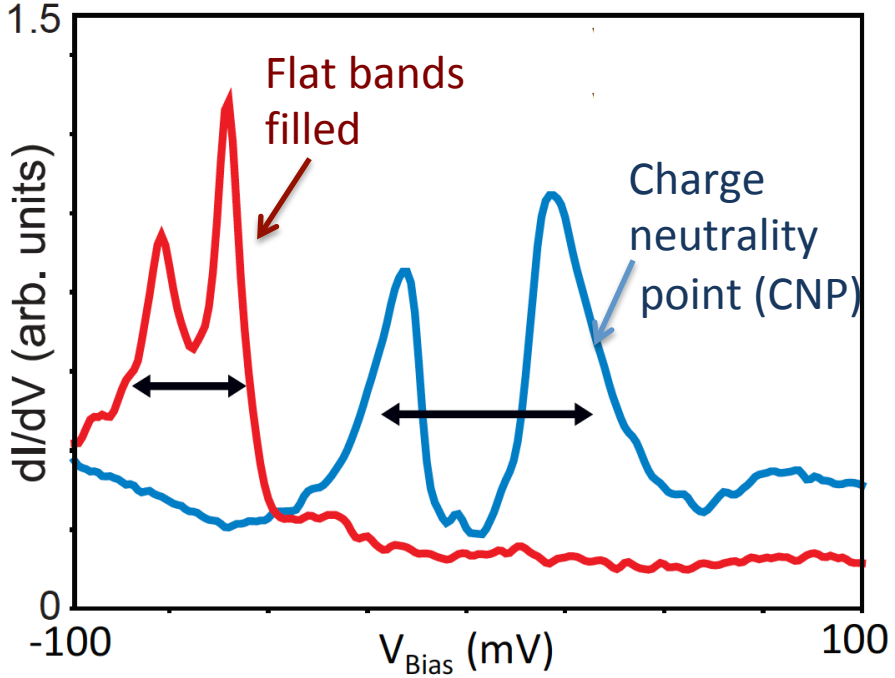
Choi et al, Nature Physics (2019)
arXiv:1901.02997

Breaking of $C_{2z}T$ symmetry?



A symmetry breaking state at CNP?

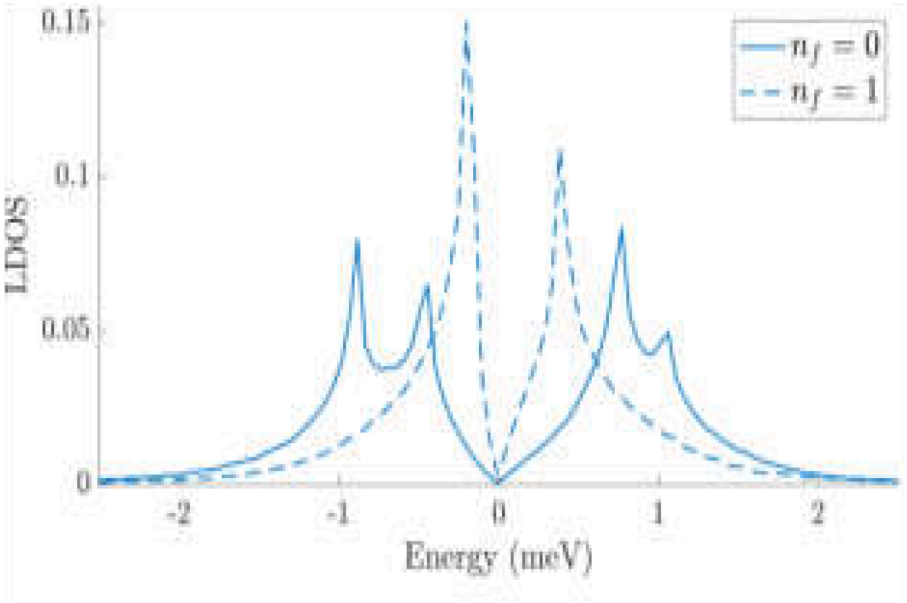
STM experiments



Choi et al, Nature Physics (2019)
arXiv:1901.02997

..

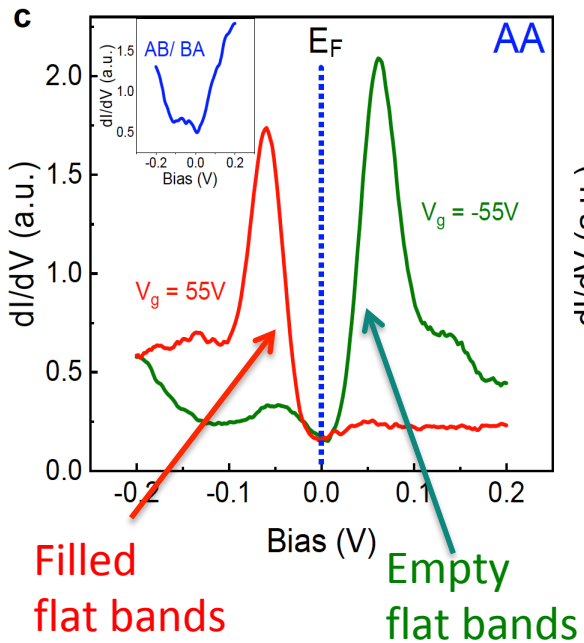
Nematic state?

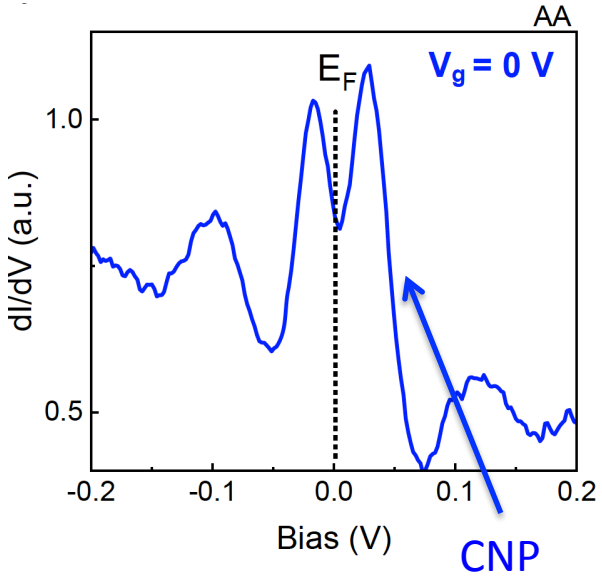


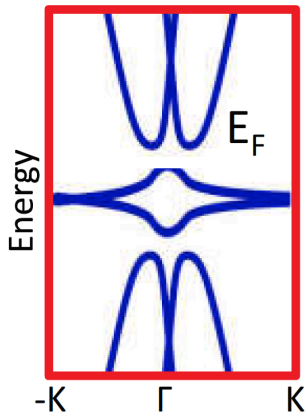
Mean field state which breaks C_3 symmetry of a given valley

A symmetry breaking state at CNP?

STM experiments

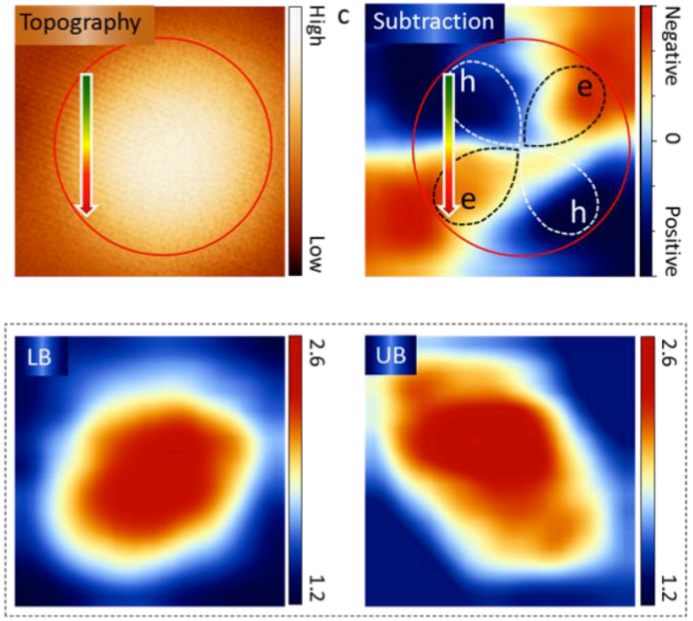






CNP

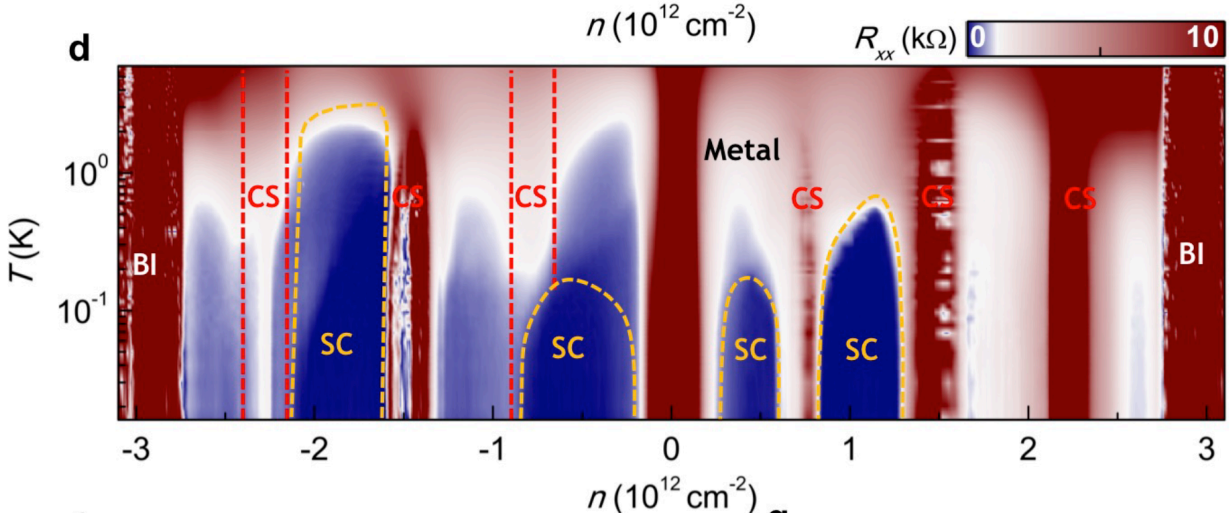
Nematic state?



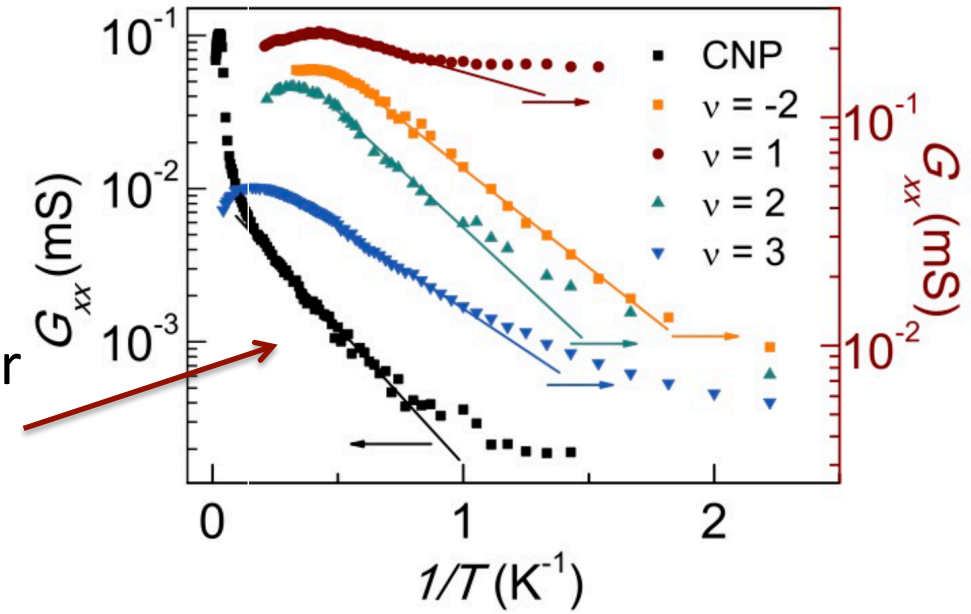
Jiang, Andrei et al, Nature (2019)
1904.10153

Modifications of the band structure whenthe chemical potential is in the flat bands also seen by Xie, Yazdani, Bernevig et al Nature 572, 101 (2019)

A symmetry breaking state at the CNP?



Lu, Efetov, et al arXiv: 1903.06513



Activated behavior at CNP-> gap

$C_{2z}T$ broken?

leni@icmm.csic.es

Correlated states in twisted bilayer graphene

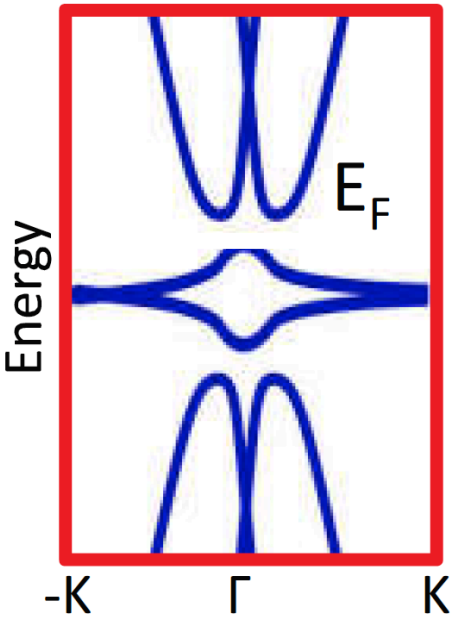
- Nature of insulating and superconducting states?
- Are the modifications of the DOS at CNP due to a symmetry breaking state? Which symmetry is broken?
- Is the observed lack of symmetry at the CNP (C3, C2zT) due to electronic ordering or the coupling to the substrate/ lattice strain?
- Are other bands beyond the flat bands affected by the correlated states?

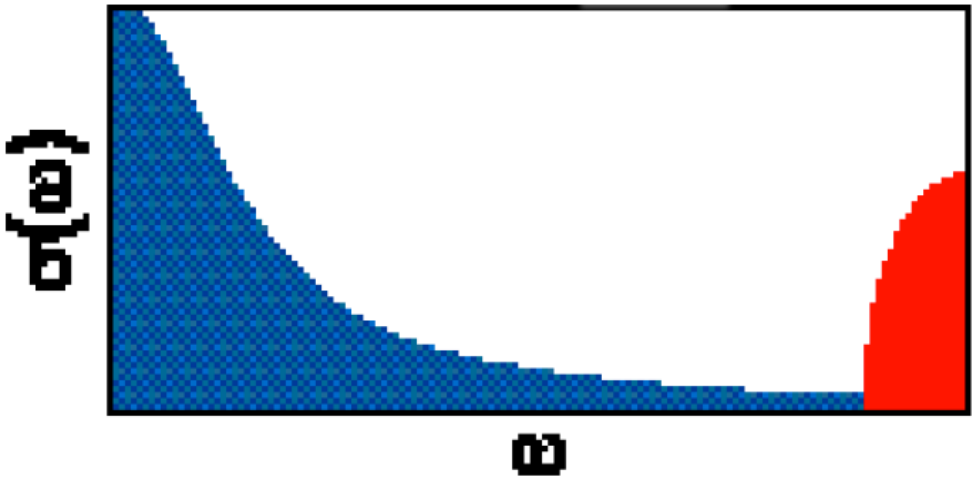
More experiments needed

Optical conductivity to study the state at CNP

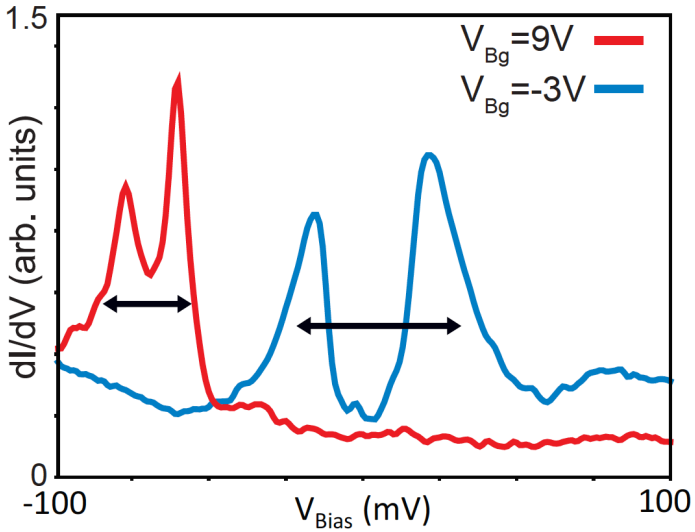
Changes in the optical conductivity due to correlated states (nematic or other kind) introduced phenomenologically.

Focus on changes due to modification of the band structure (possible incoherent states or scatering rate effects not included)





Basov et al, RMP 83, 471 (2011)



leni@icmm.csic.es

Models to study twisted bilayer graphene

Tight binding models for pz-carbon orbitals (~11000 atoms per unit cell)

Continuum model (starts from continuum description of each graphene layer and couples them)

Tight-binding Model with effective orbitals for the Moiré unit cell (not carbon pz orbitals) centered at symmetry points of the Moiré unit cell which mimic the bands from

Models to study twisted bilayer graphene

Tight binding models for pz-carbon orbitals (~11000 atoms per unit cell)

Continuum model (starts from continuum description of each graphene layer and couples them)

Tight-binding Model with effective orbitals for the Moiré unit cell (not carbon pz orbitals) centered at symmetry points of the Moiré unit cell which mimic the bands from

Only flat bands included (2 orbitals per spin & valley)

A few bands beyond flat bands included (4, 5,6, 8,10 bands per Spin & valley)

10 band model Focus on single valley

Po, Zhou, Senthil, Vishwanath, PRB 99, 195455 (2019)

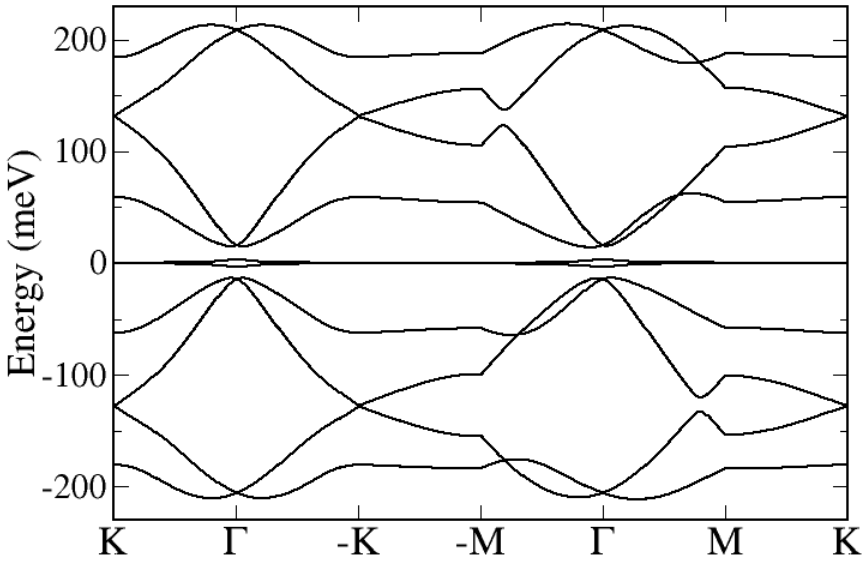
leni@icmm.csic.es

Effective 10 band model for twisted bilayer graphene

Unrelaxed model

Fitting to "unrelaxed" band structure from continum model but with V_{AA}/V_{AB}=0.82

1.05º

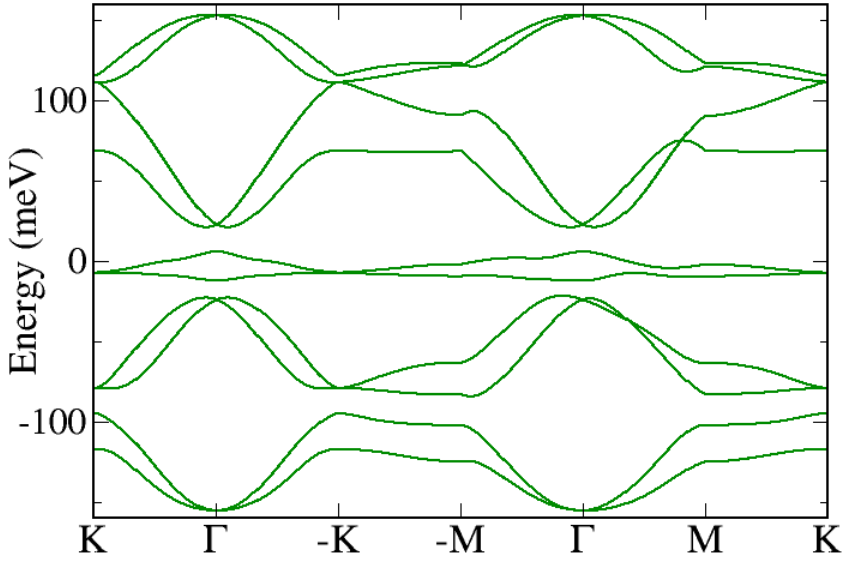


Po, Zhou, Senthil, Vishwanath, PRB 99, 195455 (2019)

Relaxed model

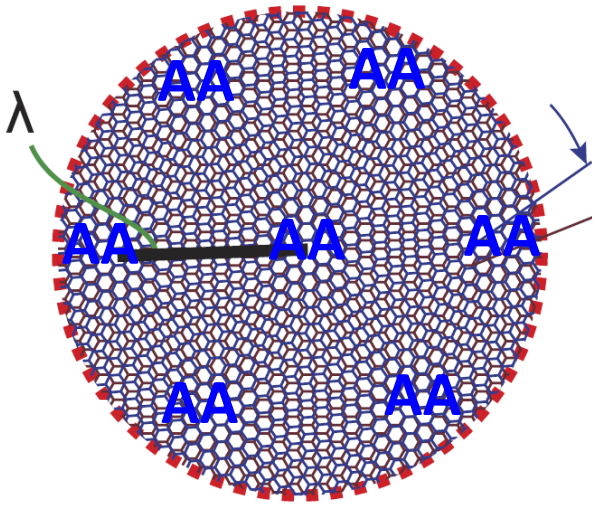
Fitting to relaxed band structure

0.90º



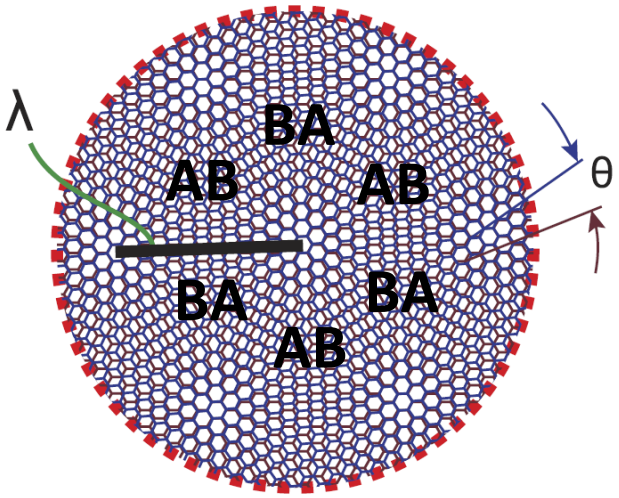
Carr, Kaxiras et al, arXiv:1901.03420

Effective 10 band model for twisted bilayer graphene



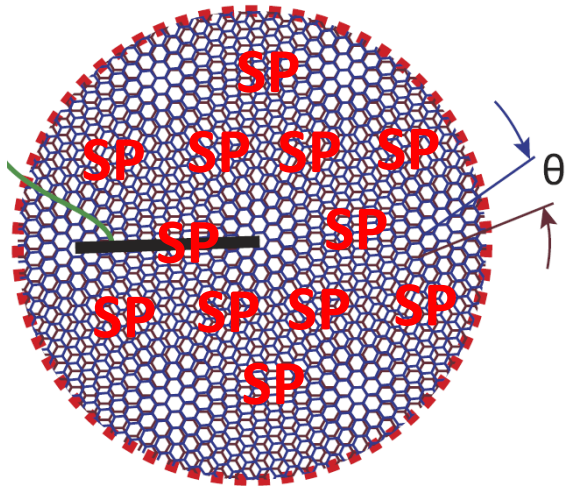
AA Centers
(moiré unit cell center):
Triangular lattice

3 orbitals:
pz, **p+** & **p-**



AB/BA Points :
Hexagonal lattice

4 orbitals:
2 orbitals per site
(p+ & p-)



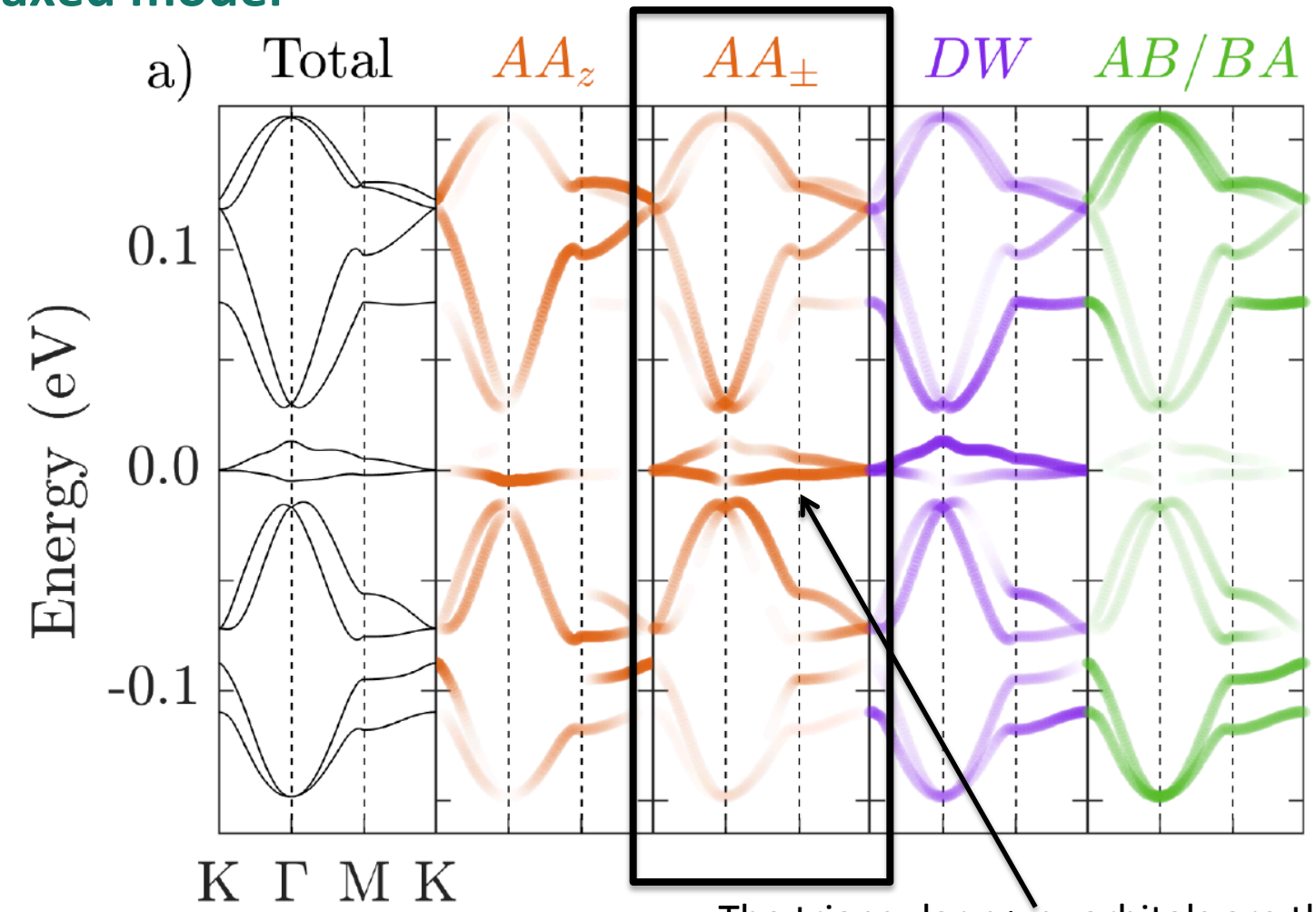
SP Points :
Kagome lattice

3 orbitals:
1 s orbital per site,

Po, Zhou, Senthil, Vishwanath, PRB 99, 195455 (2019)

Effective 10 band model for twisted bilayer graphene

Relaxed model

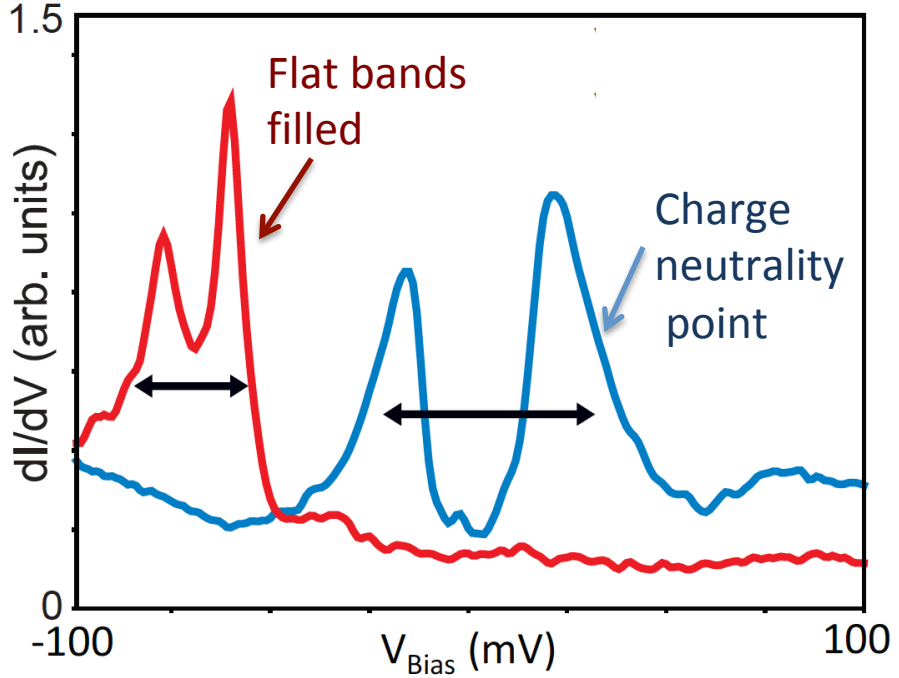


The triangular p+,p- orbitals are the ones which contribute the most to the flat bands and the ones expected to be more affected by the correlated state

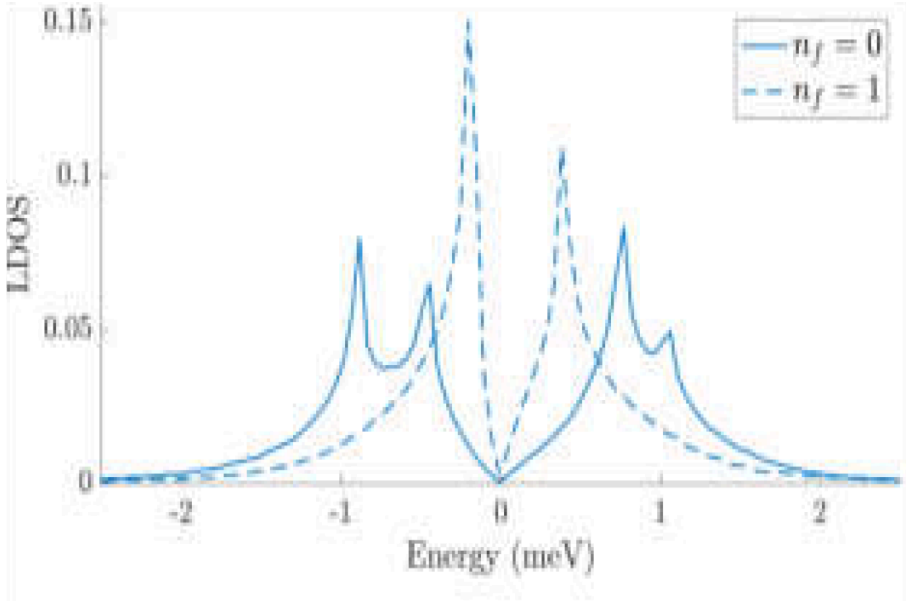
Carr, Kaxiras et al, arXiv:1901.03420

Nematic correlated state in the 10 band model for TBG

STM experiments



Nematic state?



$$\mathcal{O}_{C_3} = \sum_{\boldsymbol{r}} \left(\tau^{\dagger}_{+,\boldsymbol{r}+\boldsymbol{a}_2} + \tau^{\dagger}_{+,\boldsymbol{r}-\boldsymbol{a}_1-\boldsymbol{a}_2} + \tau^{\dagger}_{+,\boldsymbol{r}+\boldsymbol{a}_1} \right) \tau_{-,\boldsymbol{r}} + h.c.$$

$$= \sum_{\boldsymbol{k}} \left(\phi_{01} + \phi_{10} + \phi^{*}_{11} \right) \tau^{\dagger}_{+,\boldsymbol{k}} \tau_{-,\boldsymbol{k}} + h.c.$$

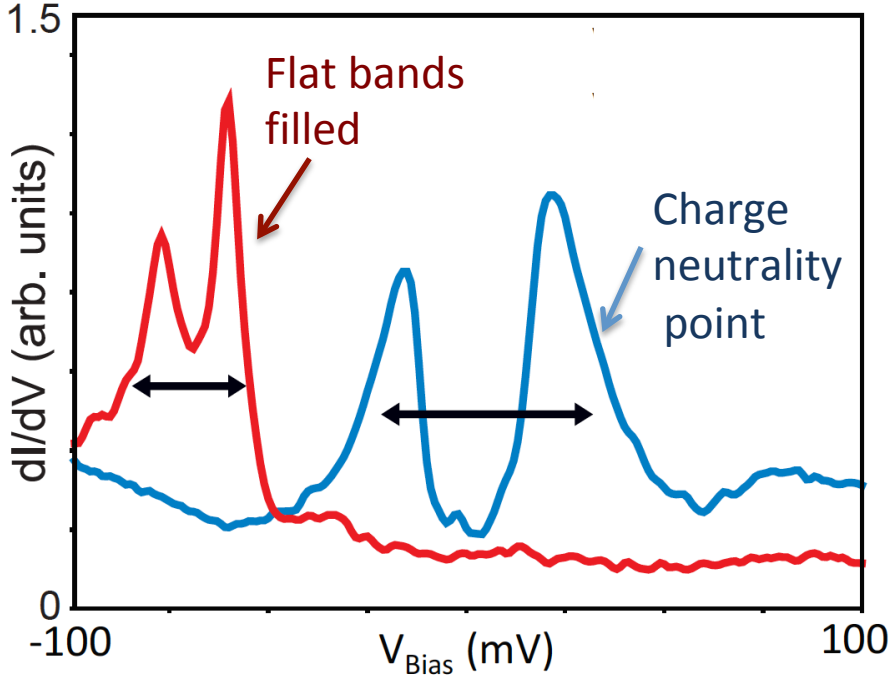
$$\phi_{\ell m} = e^{-i(\ell k_1 + m k_2)}$$

C_3 symmetry breaking introduced in the mixing of p+ and p- orbitals

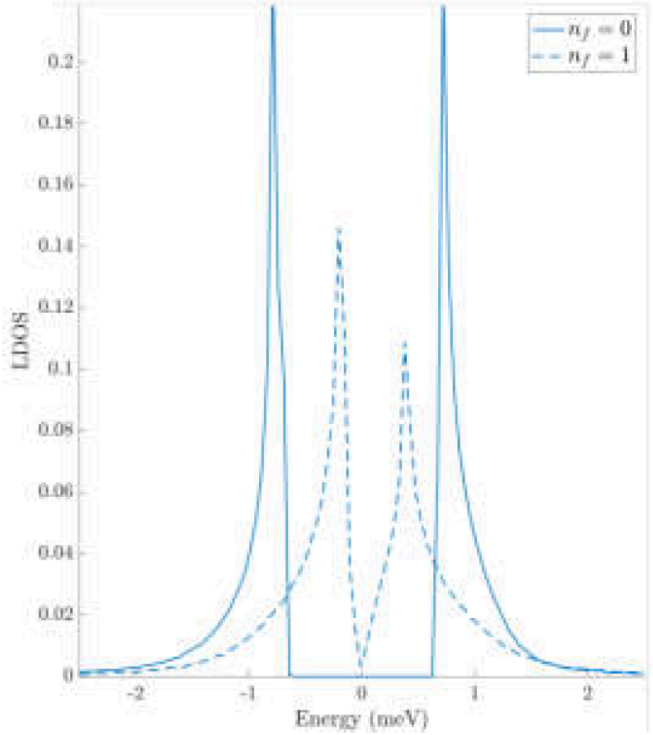
Choi, Nadja-Perge et al, Nature Physics (2019) arXiv:1901.02997

Nematic correlated state in the 10 band model for TBG

STM experiments



Breaking of $C_{2z}T$ symmetry?



$$\mathcal{O}_{C_2\mathcal{T}\cdot M_{2y}} = \sum_{\boldsymbol{r}} \left(\tau^\dagger_{+,\boldsymbol{r}} \tau_{+,\boldsymbol{r}} - \tau^\dagger_{-,\boldsymbol{r}} \tau_{-,\boldsymbol{r}} \right) = \sum_{\boldsymbol{k}} \left(\tau^\dagger_{+,\boldsymbol{k}} \tau_{+,\boldsymbol{k}} - \tau^\dagger_{-,\boldsymbol{k}} \tau_{-,\boldsymbol{k}} \right),$$

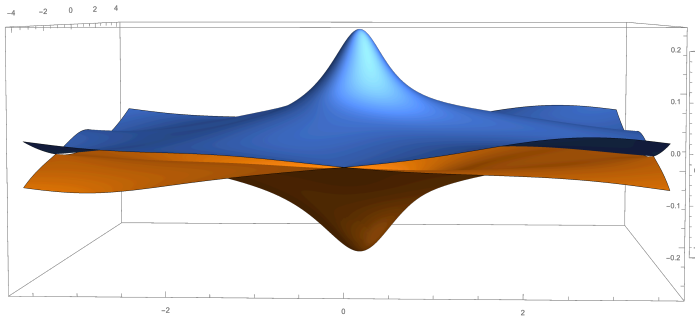
C_2T symmetry breaking introduced as an onsite term for p+ and p- orbitals

Choi et al, Nature Physics arXiv:1901.02997

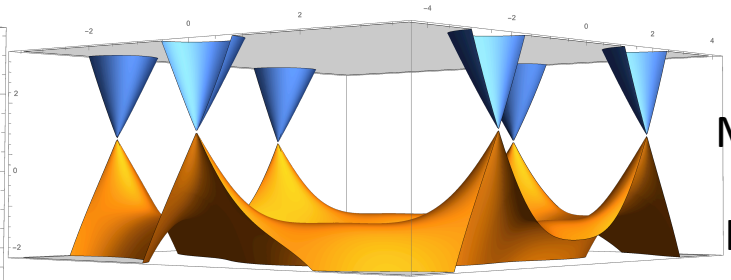
leni@icmm.csic.es

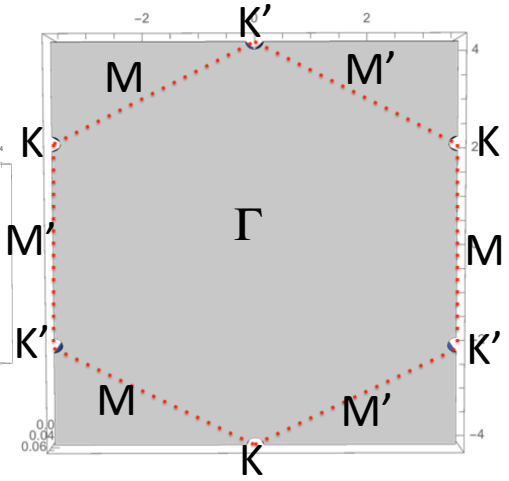
Band structure, DOS & Drude weight: Non-correlated state

Flat bands



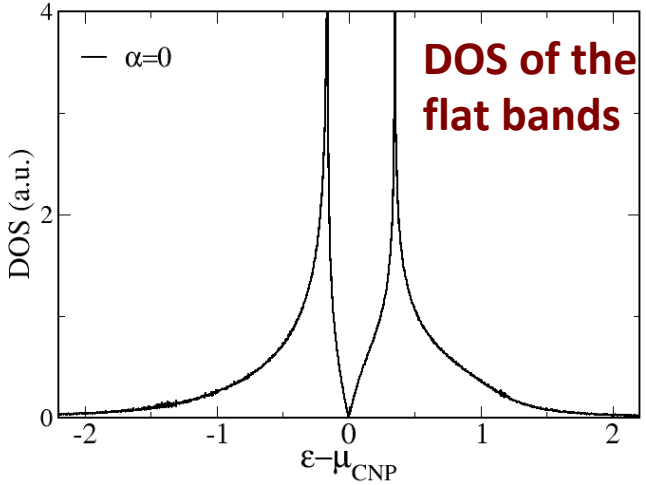
C_3 symmetry





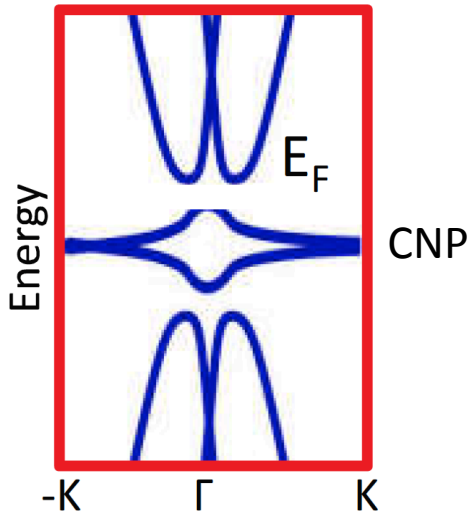
Van Hove singularities (M and M' points)

Dirac points at K and K'

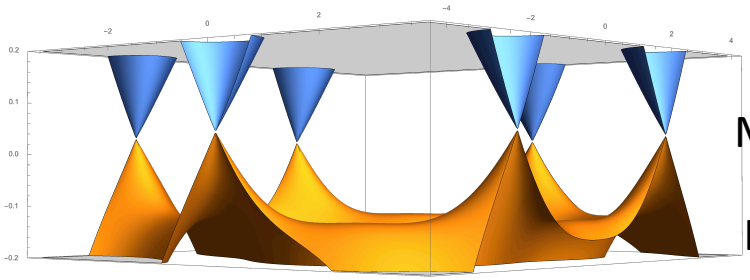


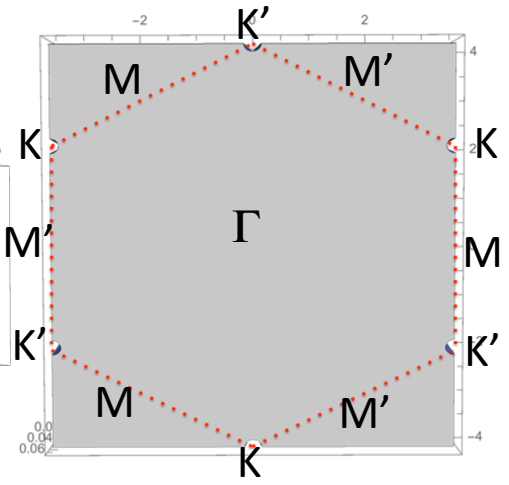
Vanishing density of states @ CNP

Band structure, DOS & Drude weight: Non-correlated state



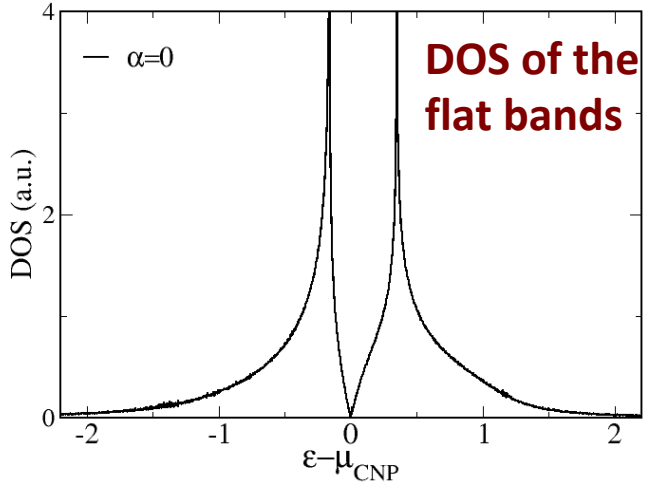
C_3 symmetry



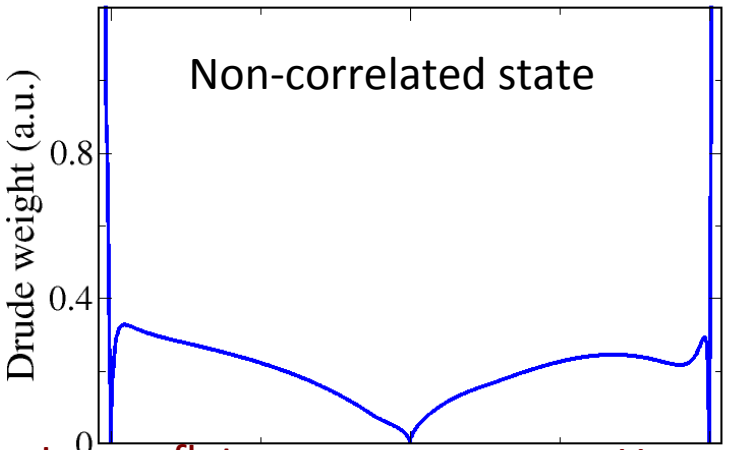


Van Hove singularities (M and M' points)

Dirac points at K and K'



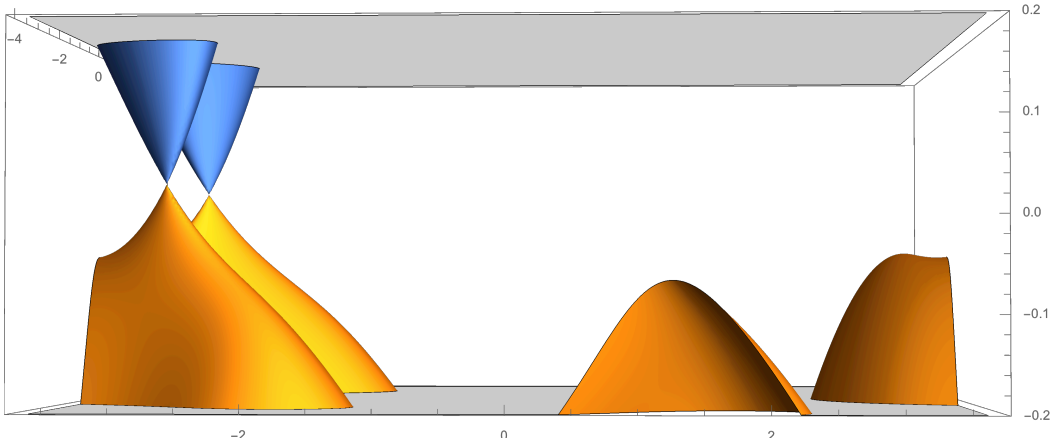
Vanishing density of states @ CNP

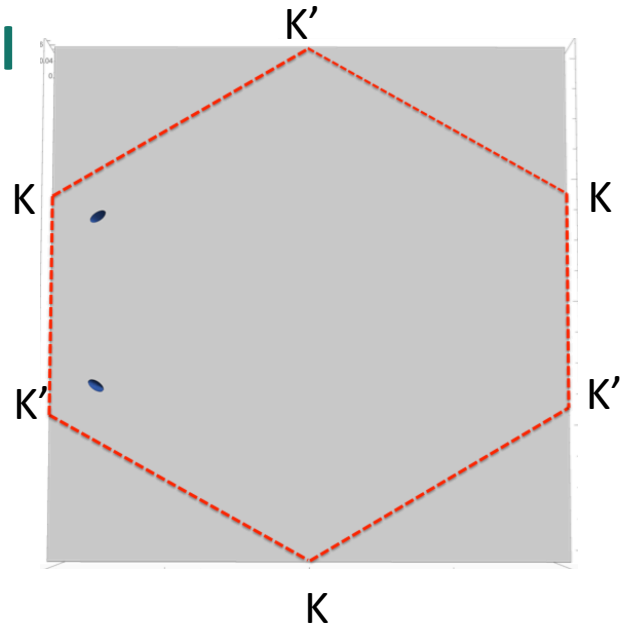


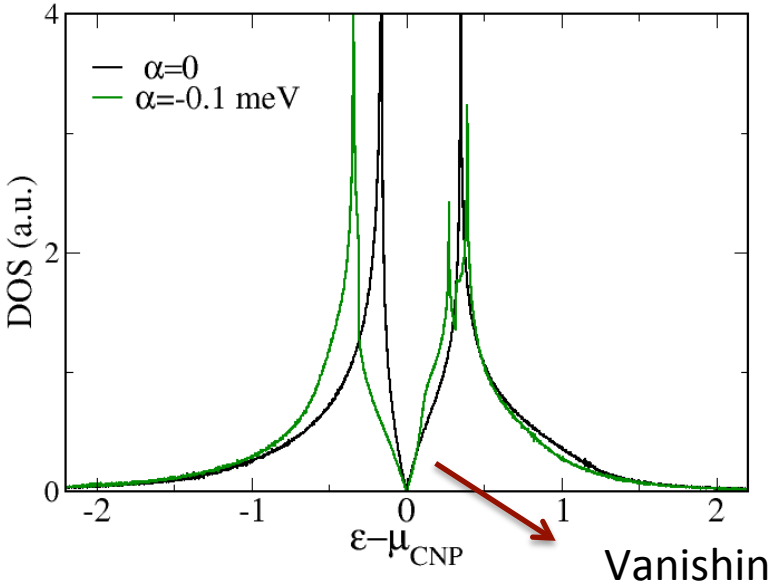
Band structure, DOS & Drude weight: Nematic state

α=0.1 meV

Unrelaxed model







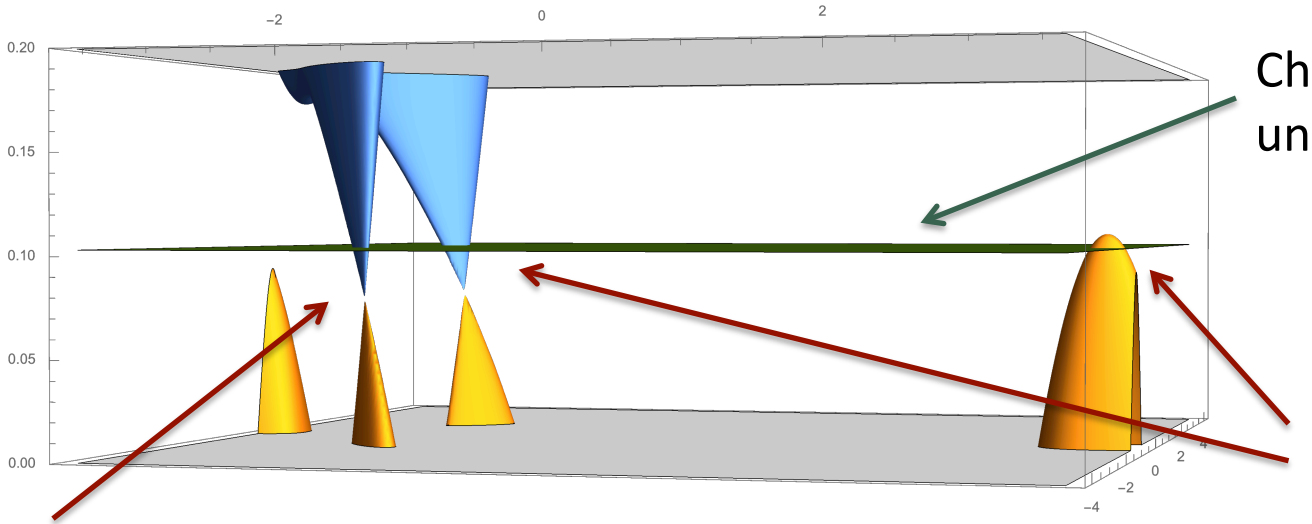
Vanishing Drude at CNP

Dirac points still present but away from K, K'

Band structure, DOS & Drude weight: Nematic state

α=0.25 meV

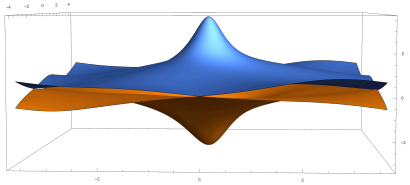
Unrelaxed model



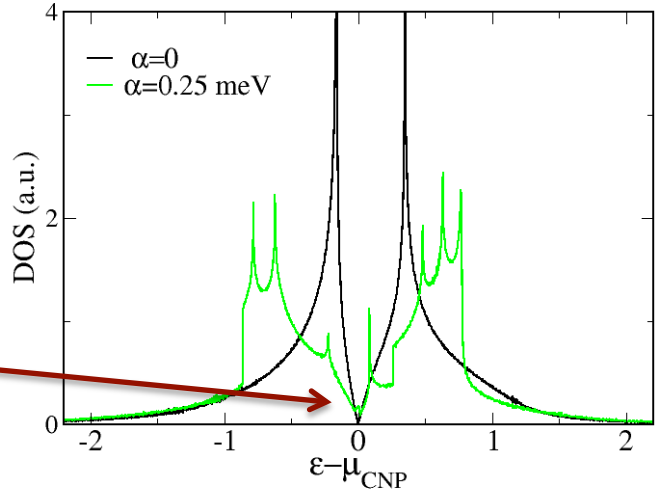
Chemical potential of undoped system (CNP)

Small Fermi pockets

Dirac points not at the CNP



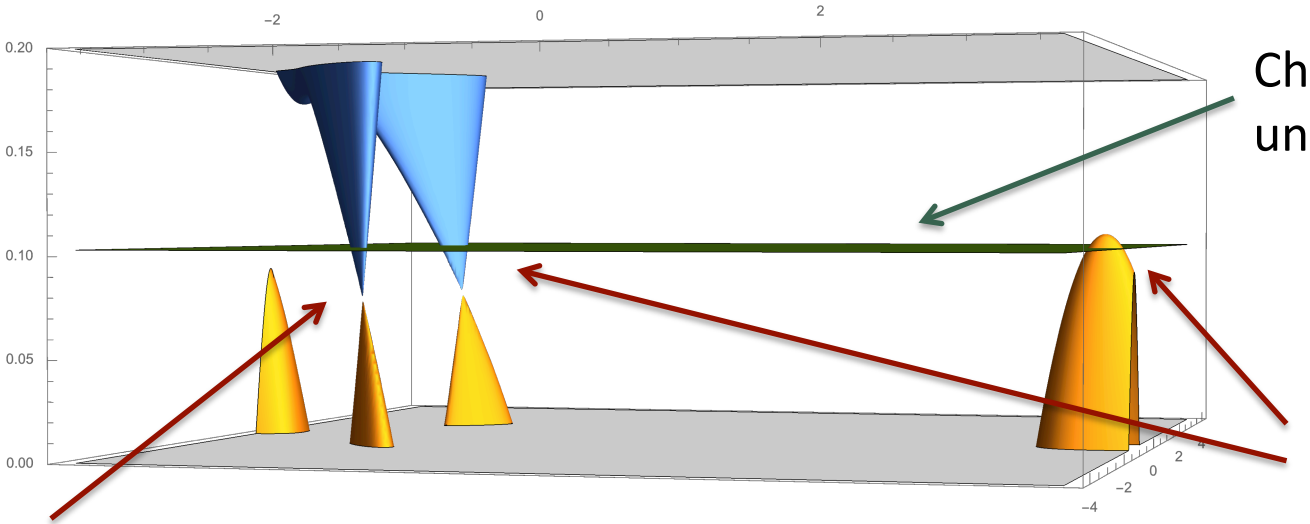
Small but finite density of states @CNP



Band structure, DOS & Drude weight: Nematic state

α=0.25 meV

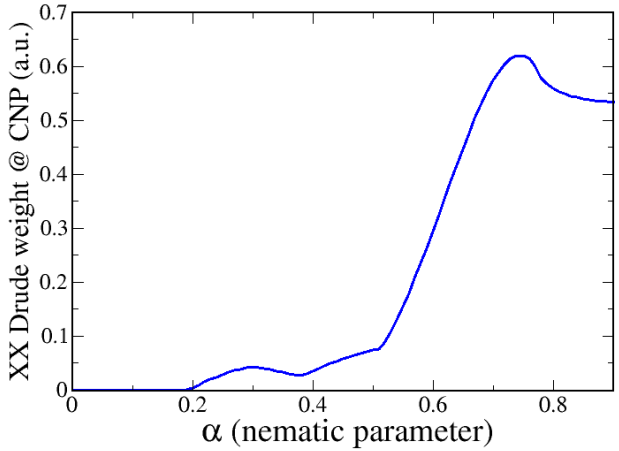
Unrelaxed model

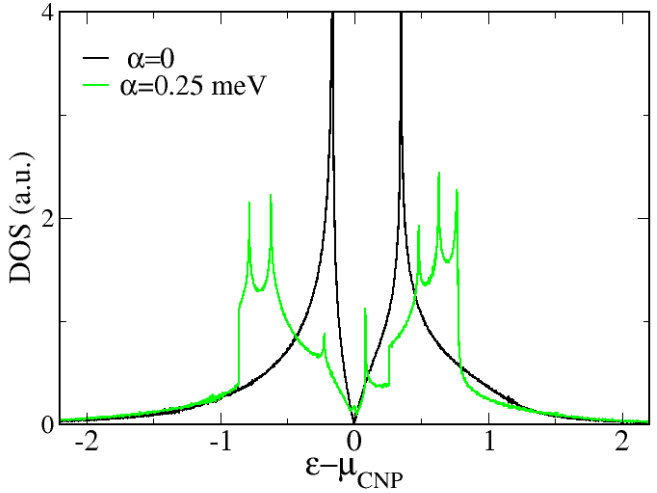


Chemical potential of undoped system (CNP)

Small Fermi pockets

Dirac points not at the CNP



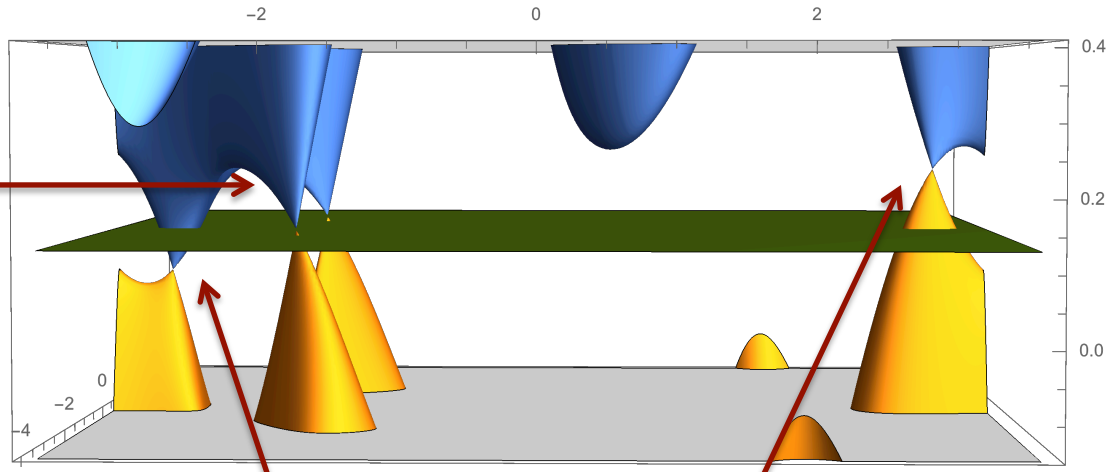


Band structure, DOS & Drude weight: Nematic state

α=0.40 meV

Unrelaxed model

Original
Dirac points



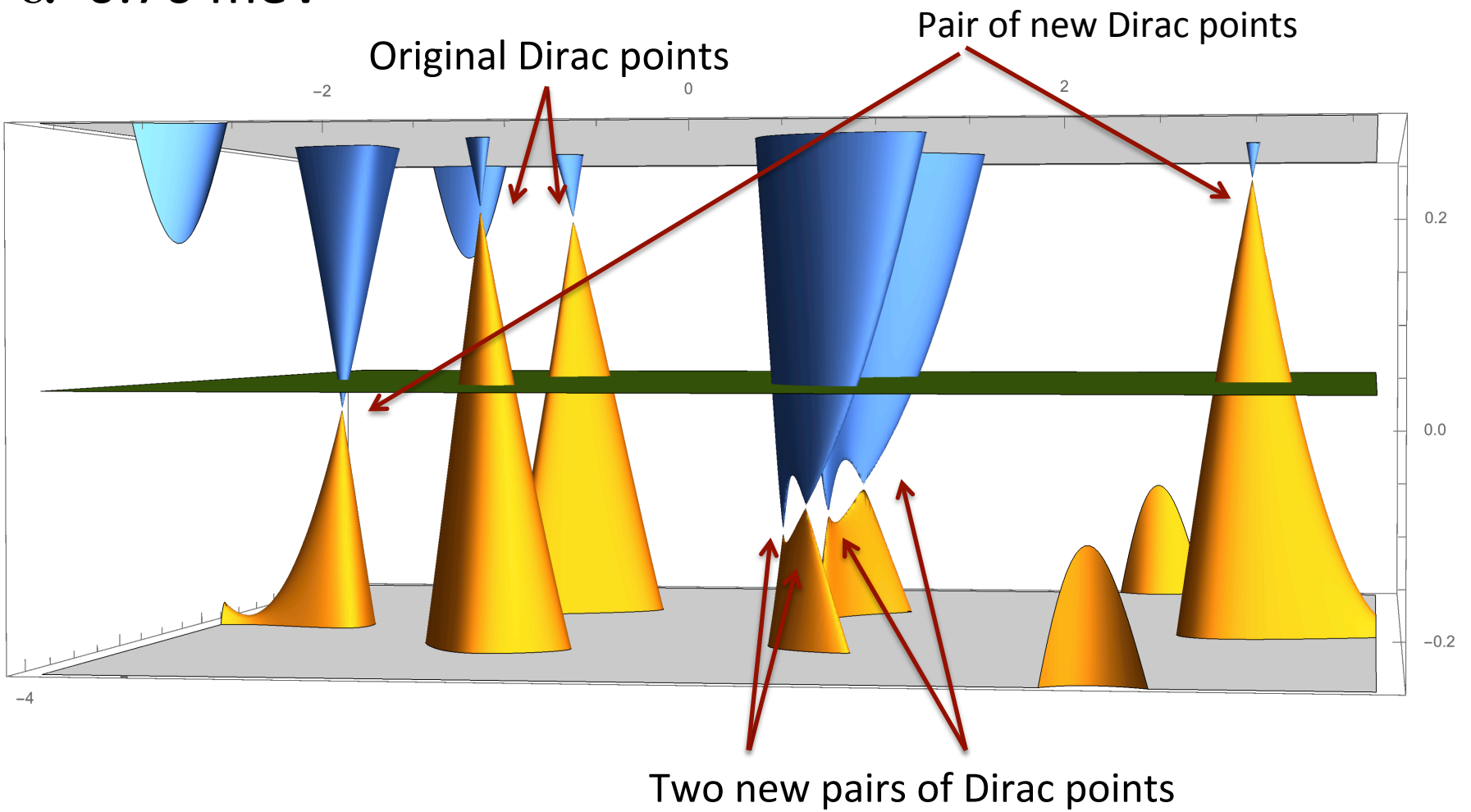
New Dirac points
between the flat bands
For α>0.3 meV

Dirac points of the other valley related by inversion

Band structure, DOS & Drude weight: Nematic state

α=0.70 meV

Unrelaxed model

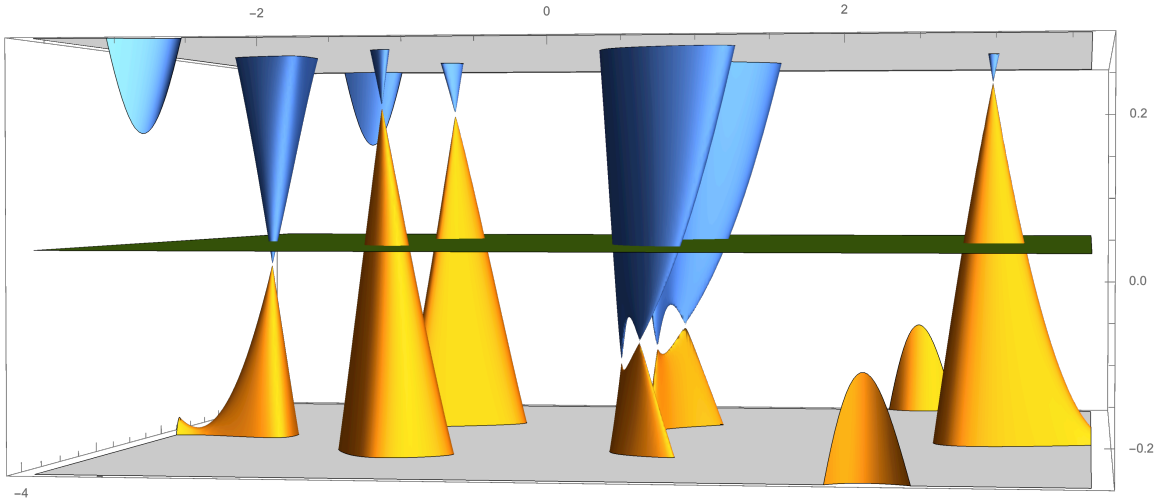


Many Dirac points close to CNP and several Fermi pockets

Nematic state: 1st take-home message

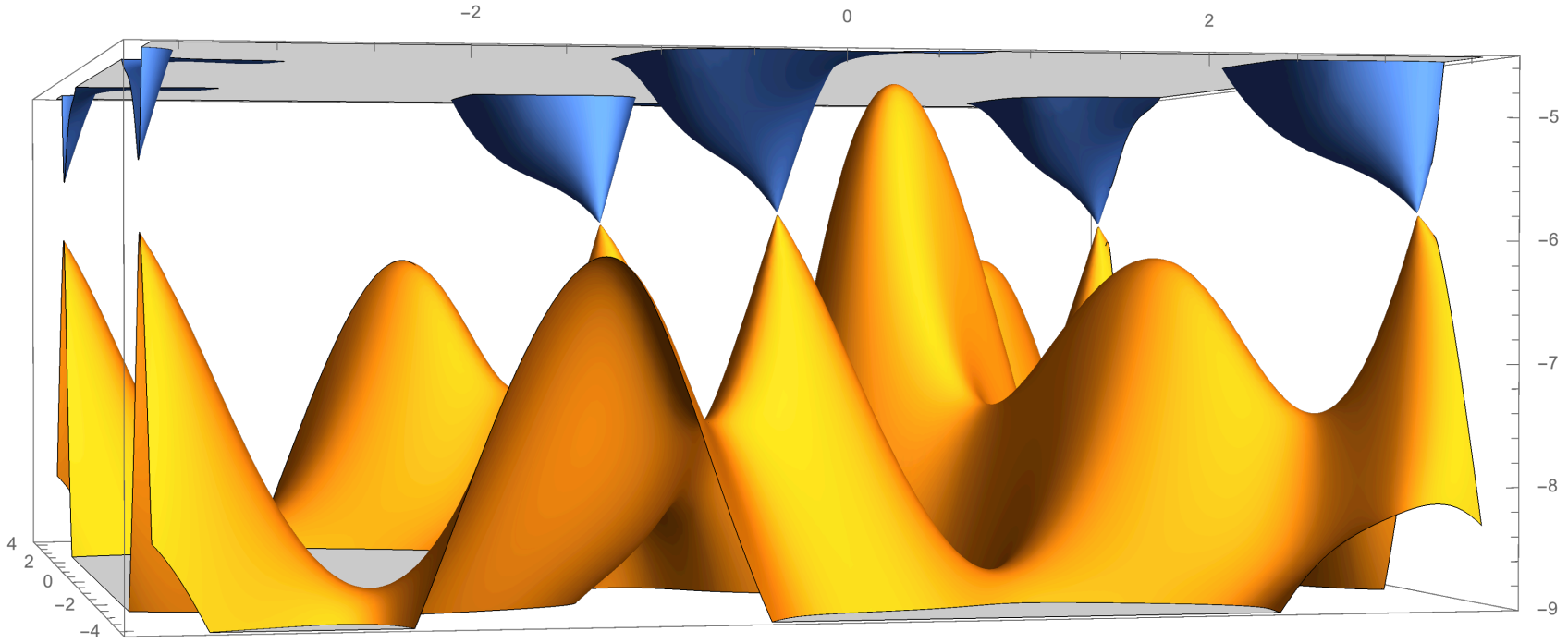
- Effect of nematicity in the band structure close to CNP beyond displacing Dirac points

It may appear {
  - Small Fermi pockets, finite density of states & Drude weight
  - New Dirac points



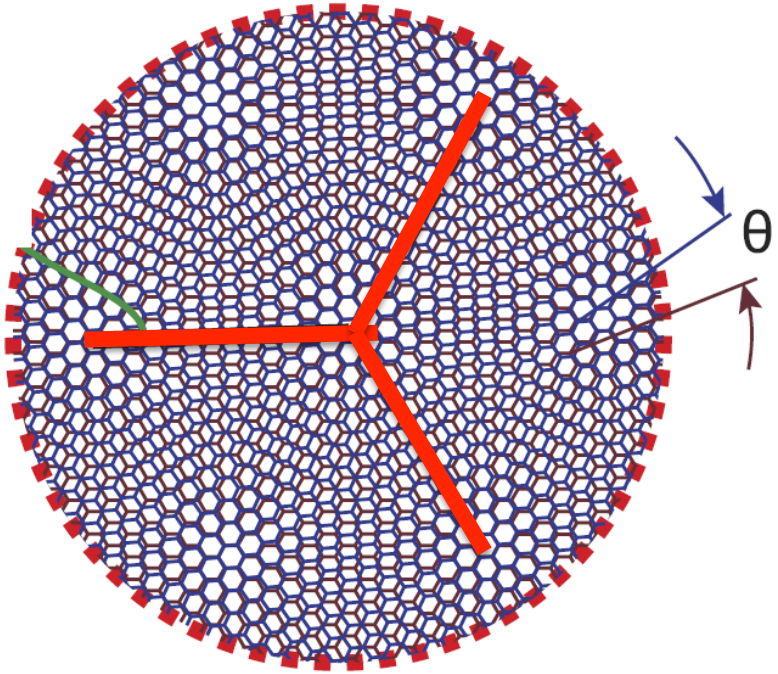
Band structure, DOS & Drude weight: Nematic state

Relaxed tight binding model



- Fermi pockets at CNP starting with very small nematicity.
- No extra new Dirac points in the range of nematic parameters studied

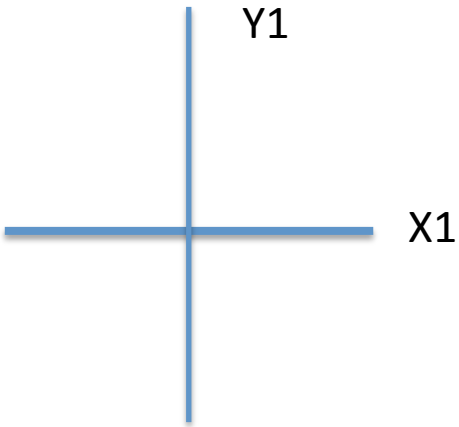
Nematic state: Anisotropy in the optical conductivity

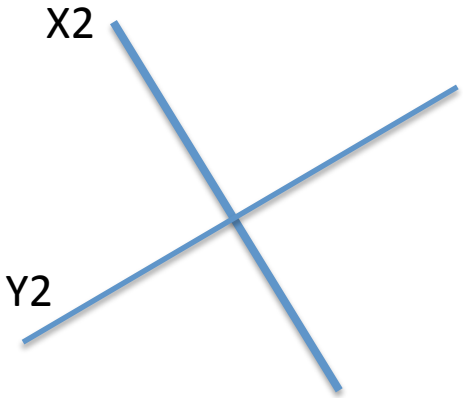


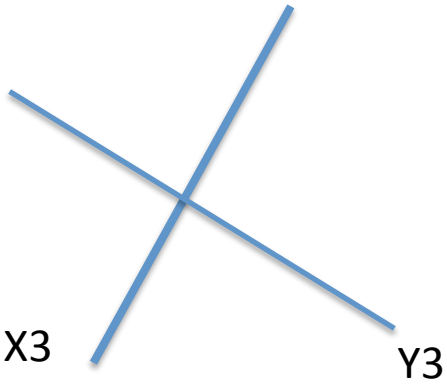
C_3 symmetry

$$\sigma_{x1x1} = \sigma_{x2x2} = \sigma_{x3x3}$$

$$\sigma_{xx} = \sigma_{yy}$$

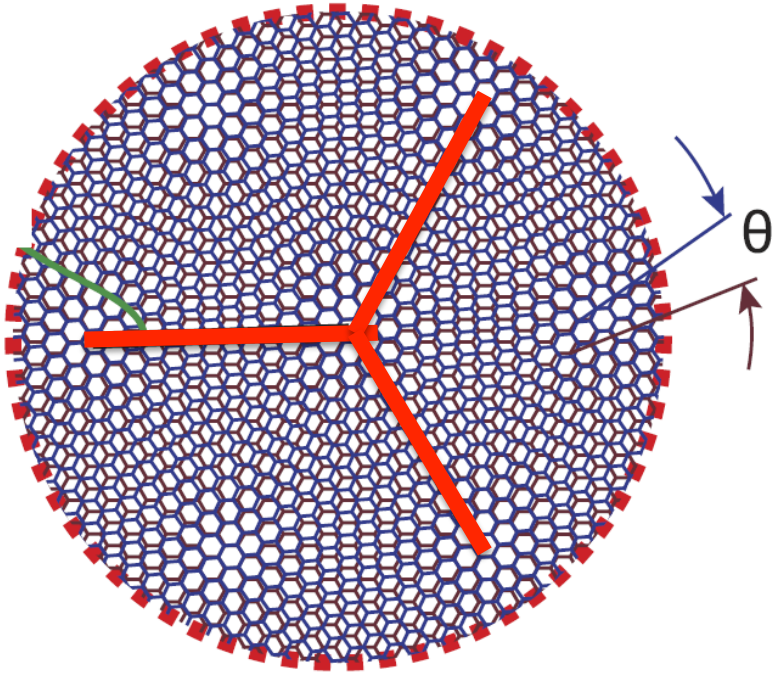






leni@icmm.csic.es

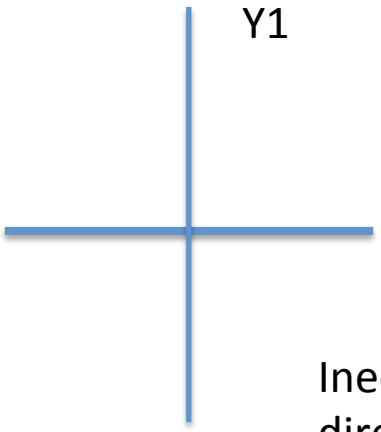
Nematic state: Anisotropy in the optical conductivity



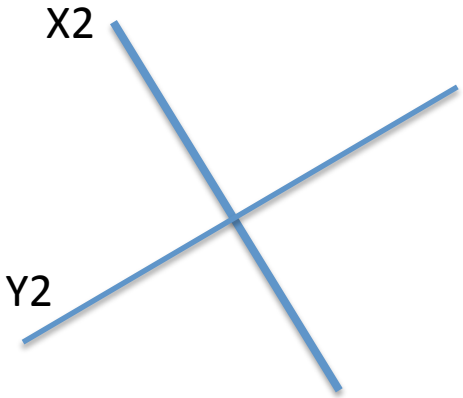
C_3 breaking of the symmetry

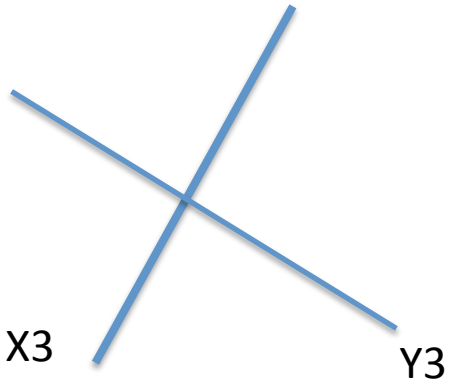
$$\sigma_{x1x1} \neq \sigma_{x2x2} = \sigma_{x3x3}$$

$$\sigma_{xx} \neq \sigma_{yy}$$



Inequivalent direction

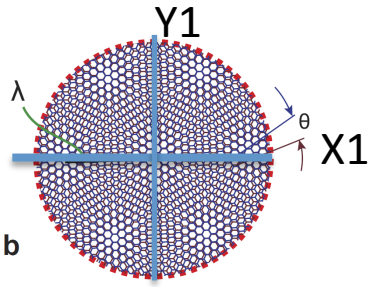




leni@icmm.csic.es

Nematic state: Anisotropy in the Drude weight

Anisotropy=(D_{Y1Y1}/D_{X1X1}-1)

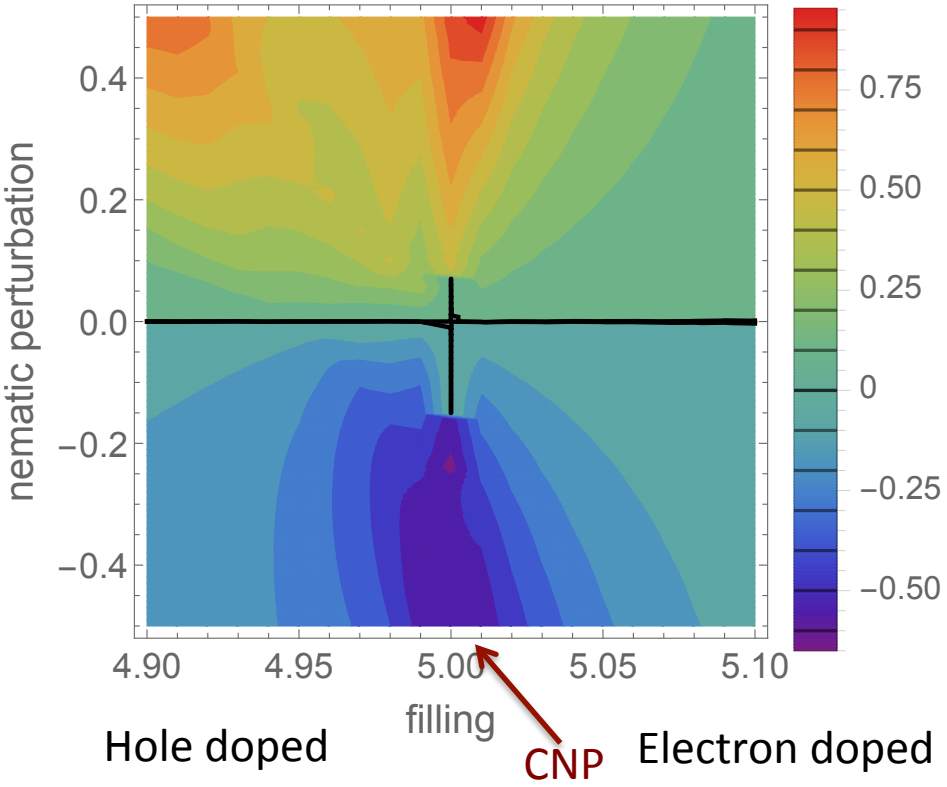


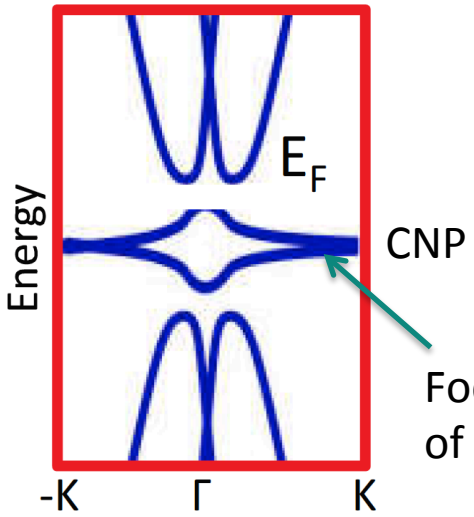
With C3 symmetry

$D_{xx} = D_{yy}$

Relaxed model

(The sign of the nematicity and the sign of the anisotropy directly related)



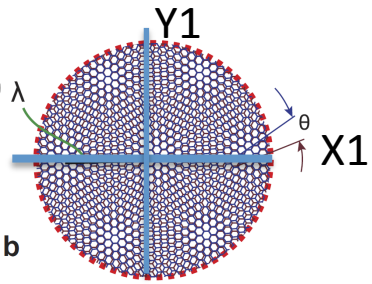


Focus on small region of doping close to CNP

leni@icmm.csic.es

Nematic state: Anisotropy in the Drude weight

Y_1X_1 Anisotropy=$(D_{Y1Y1}/D_{X1X1}-1)$

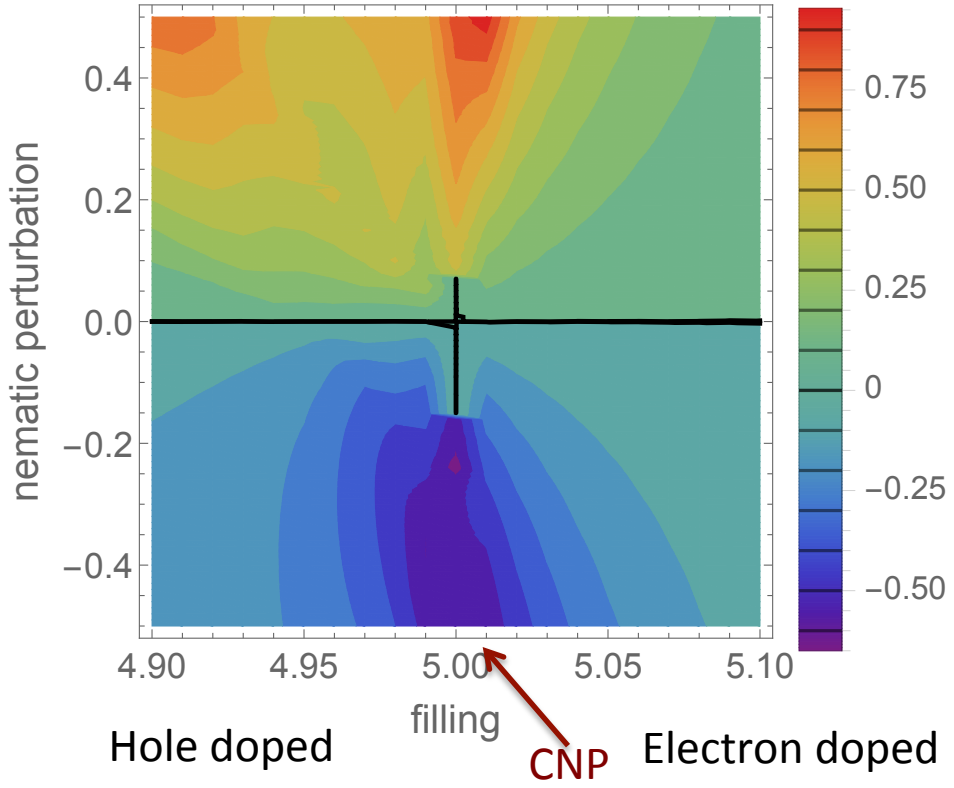


With C3 symmetry

$D_{xx} = D_{yy}$

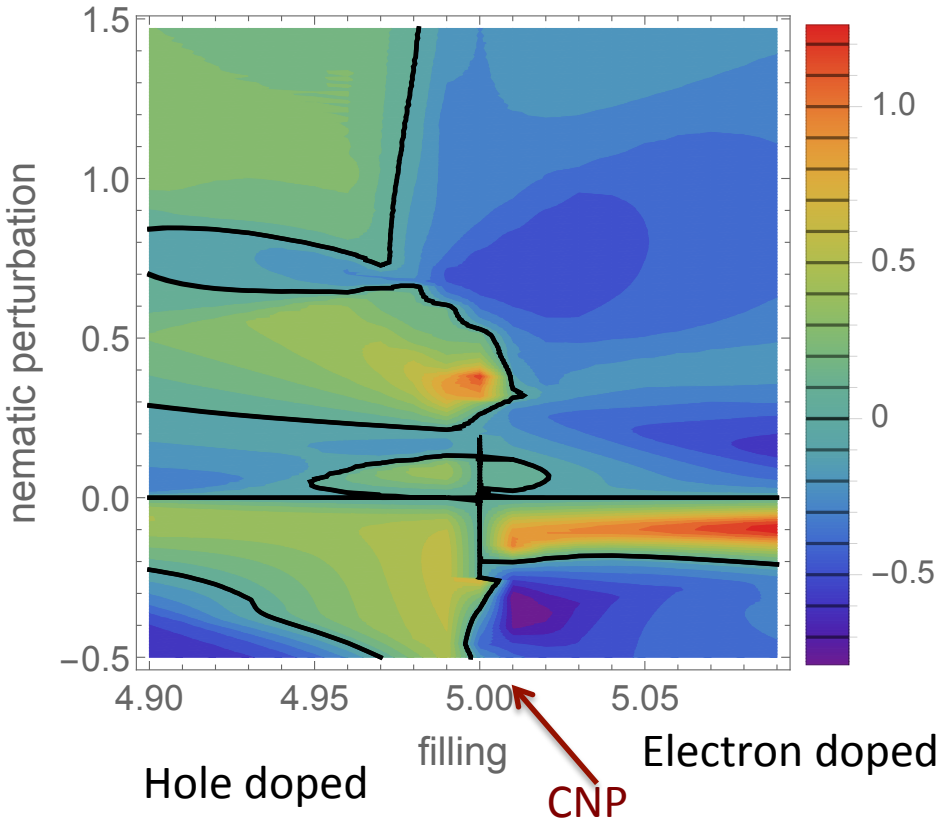
Relaxed model

(The sign of the nematicity and the sign of the anisotropy directly related)



Unrelaxed model

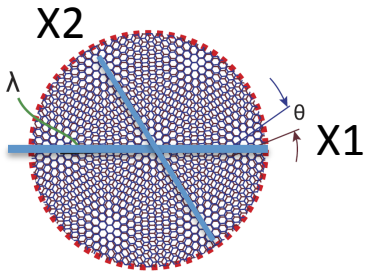
(The sign of the nematicity and the sign of the anisotropy NOT directly related)



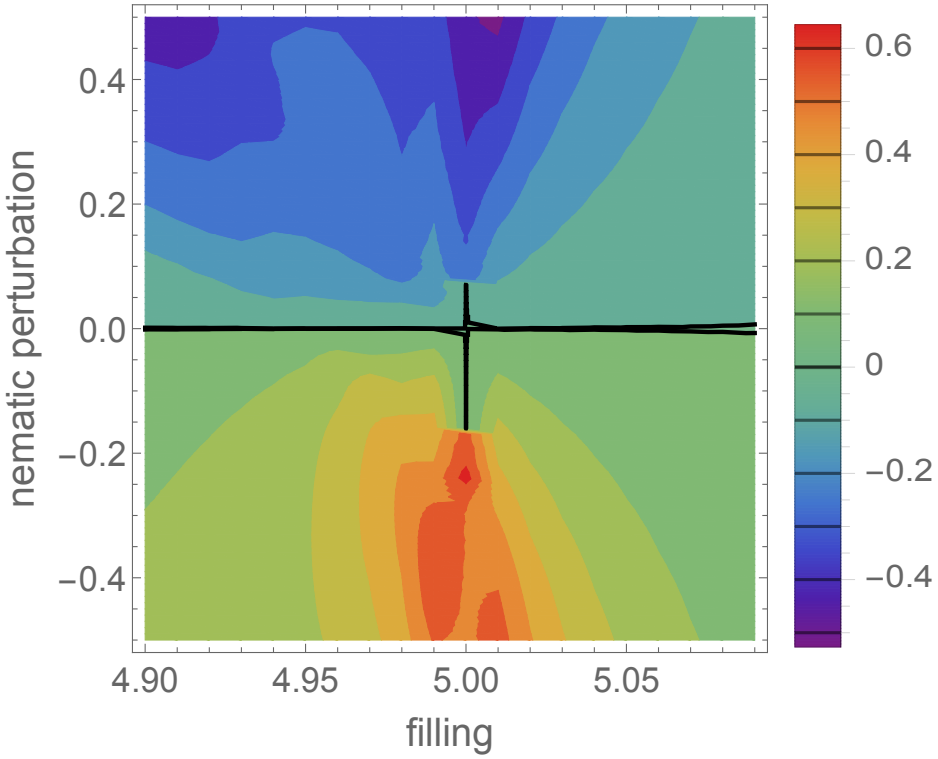
leni@icmm.csic.es

Nematic state: Anisotropy in the Drude weight

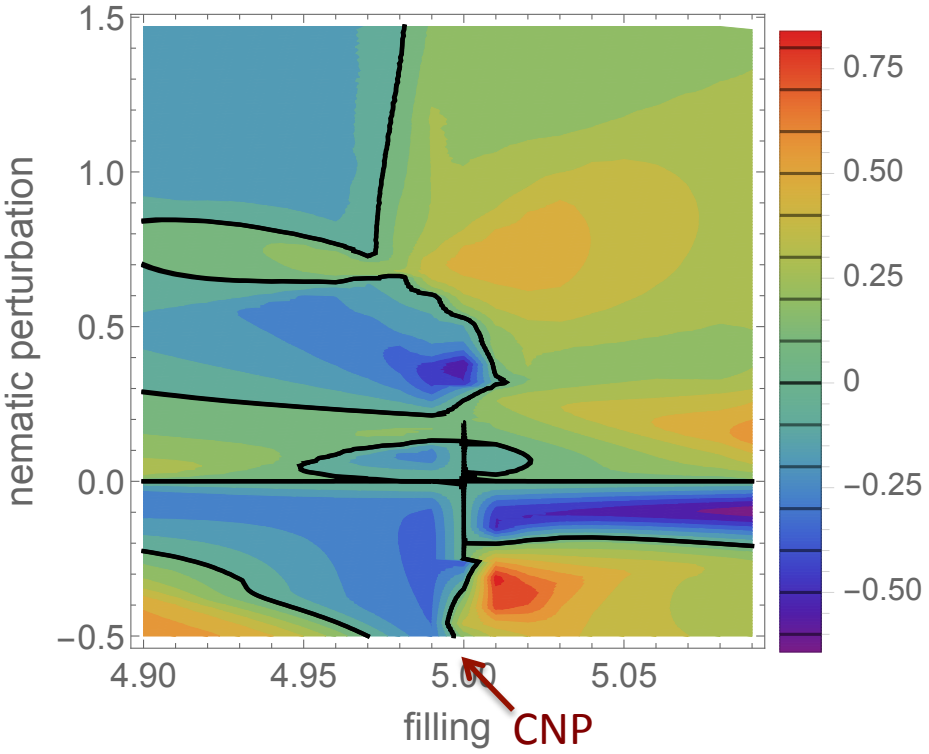
X_2X_1 Anisotropy=(D_{X2X2}/D_{X1X1}-1)



Relaxed model



Unrelaxed model

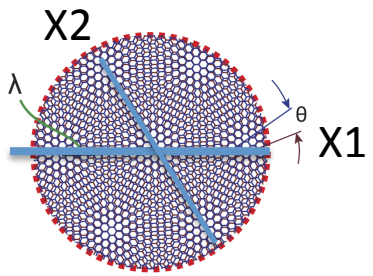


The relation between the sign of the XX Drude anisotropy and the nematicity depends on the underlying band structure

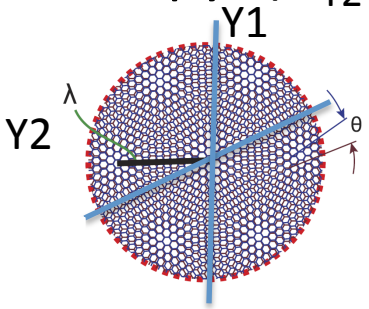
leni@icmm.csic.es

Nematic state: Anisotropy in the Drude weight

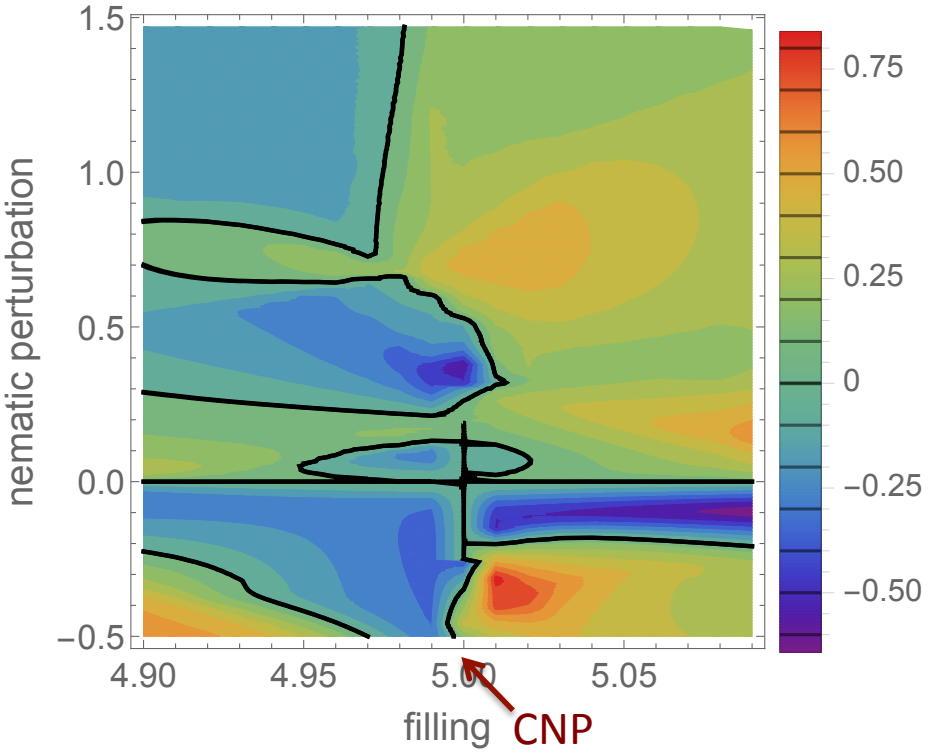
X_2X_1 Anisotropy=(D_{X2X2}/D_{X1X1}-1)

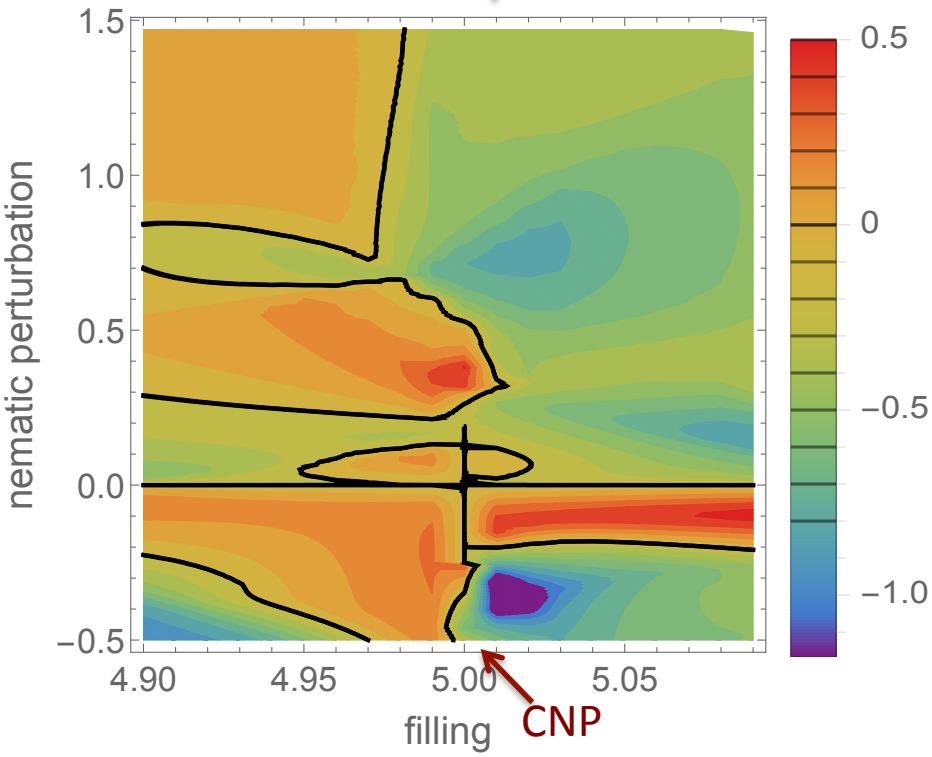


Y_2Y_1 Anisotropy=(D_{Y2Y2}/D_{Y1Y1}-1)



Unrelaxed model





Opposite sign of the Drude anisotropy in XX and YY directions (also true in relaxed model)

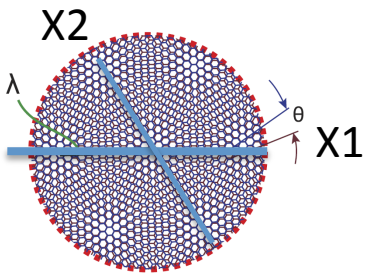
leni@icmm.csic.es

Nematic state: 2nd take-home message

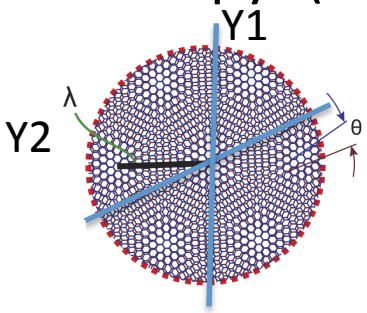
The sign of the XY, XX, YY anisotropy of the Drude weight in the nematic state depends on the underlying TBG band structure

Opposite sign of X_2X_1 and Y_2Y_1 anisotropy seems to be a robust feature

X_2X_1 Anisotropy=(D_{X2X2}/D_{X1X1}-1)

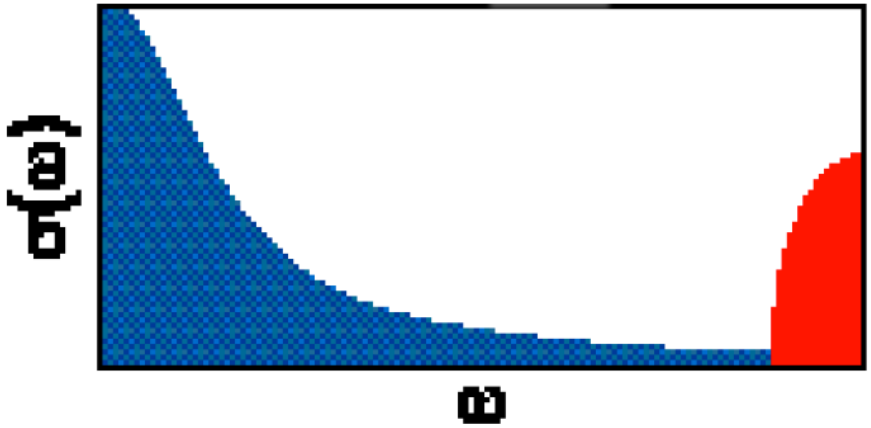


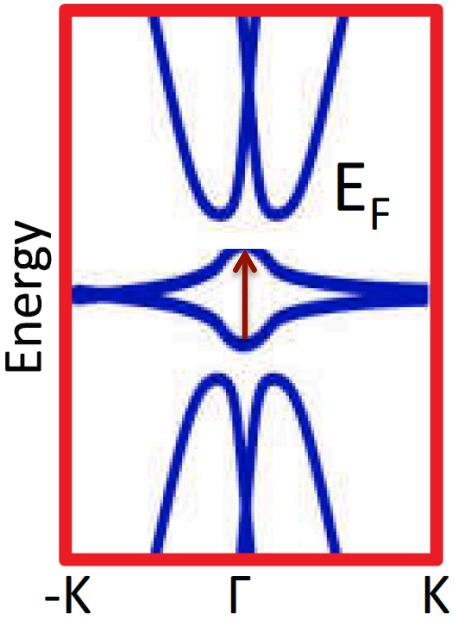
Y_2Y_1 Anisotropy=(D_{Y2Y2}/D_{Y1Y1}-1)

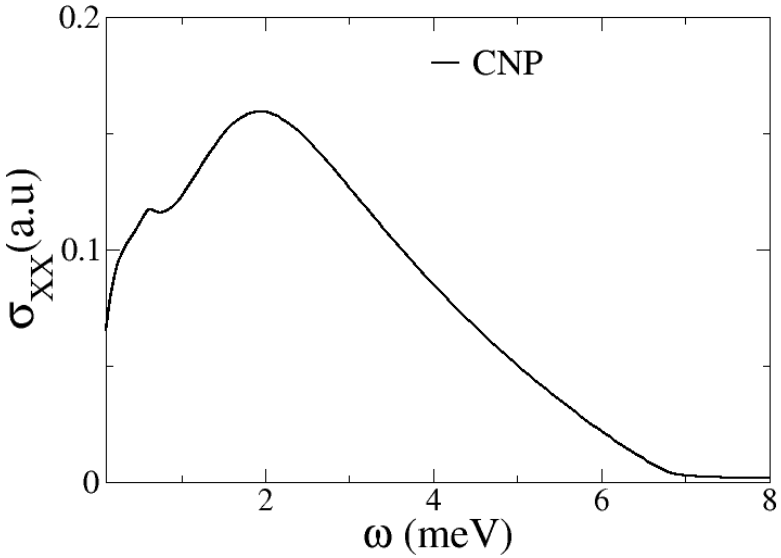


leni@icmm.csic.es

Interband transitions

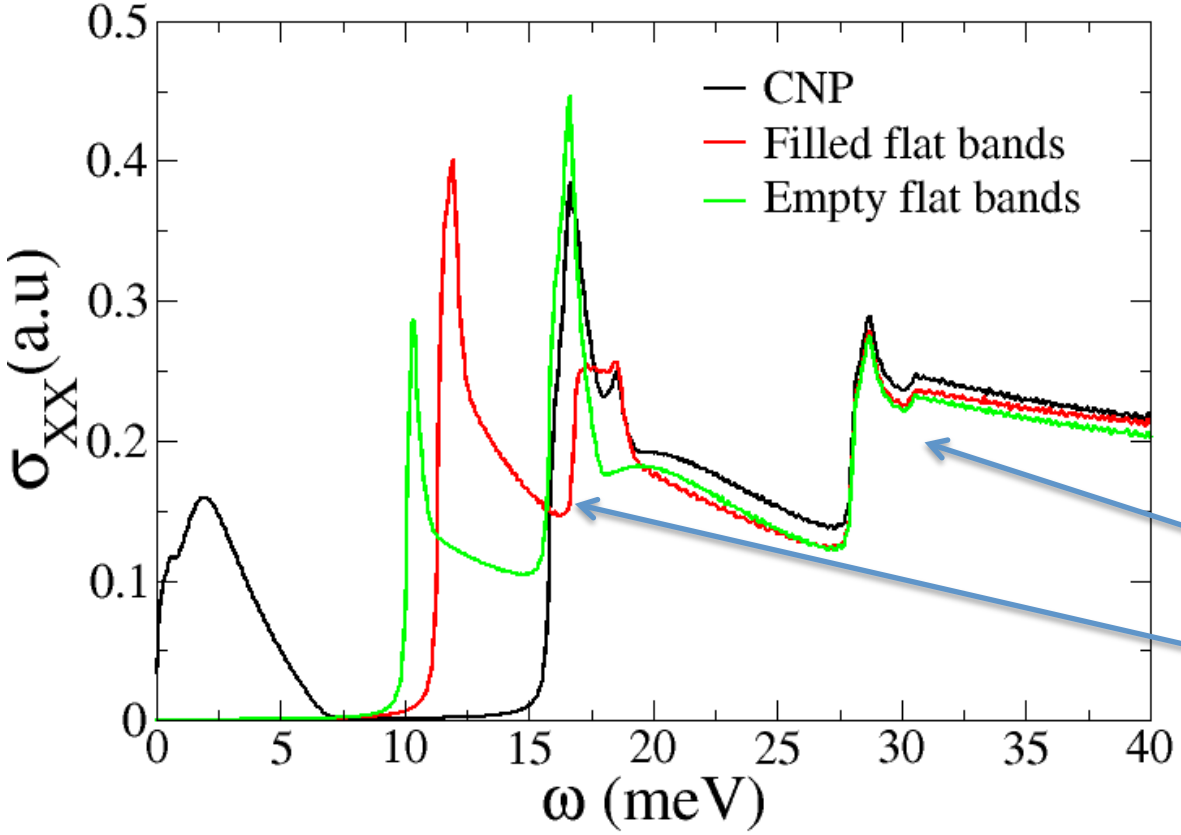


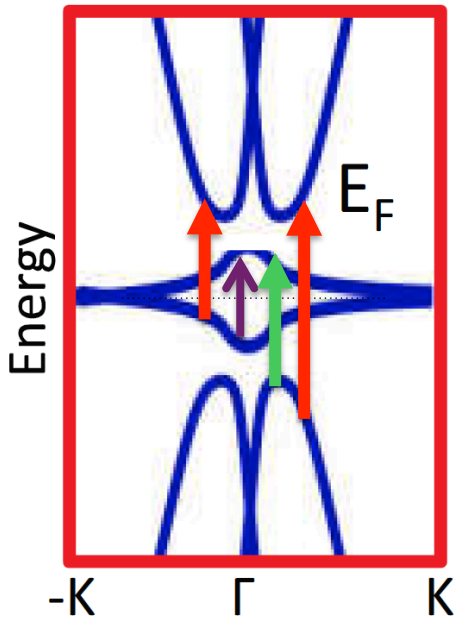




Interband transitions

Focus on interband transitions

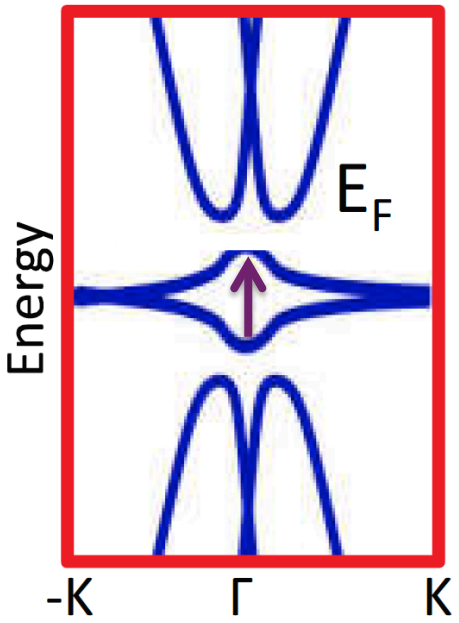


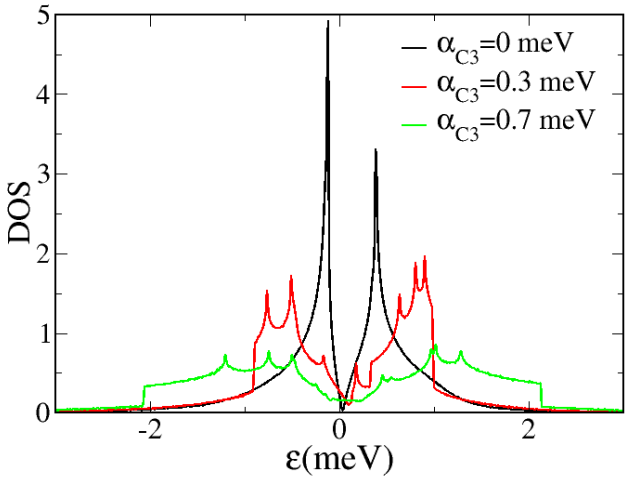


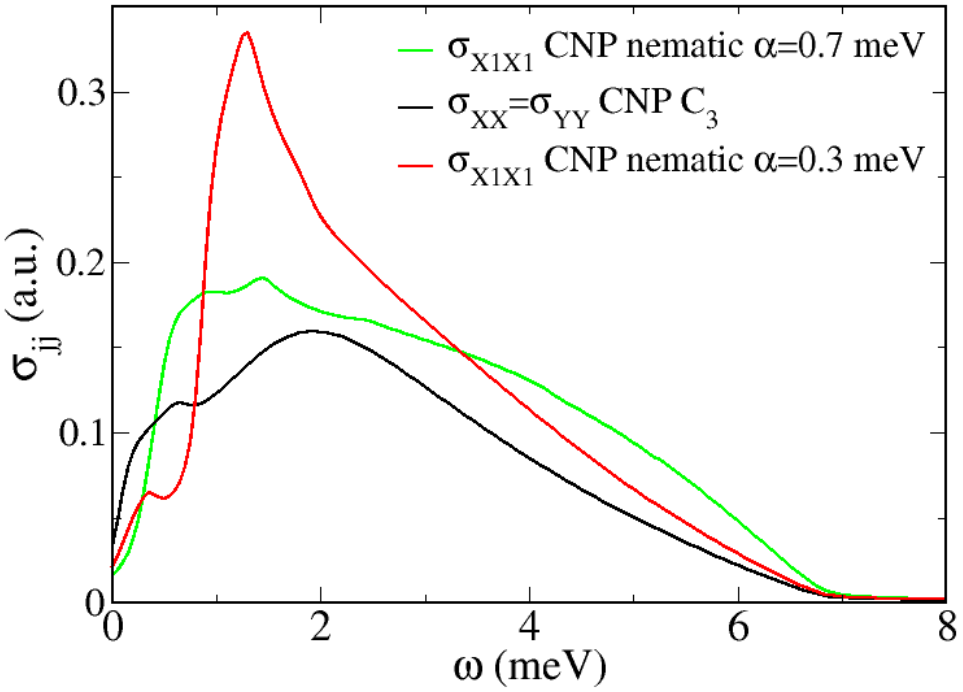
Also follow changes in frequency of these transitions with doping

Only the interband transitions are plotted

Interband transitions in the nematic state



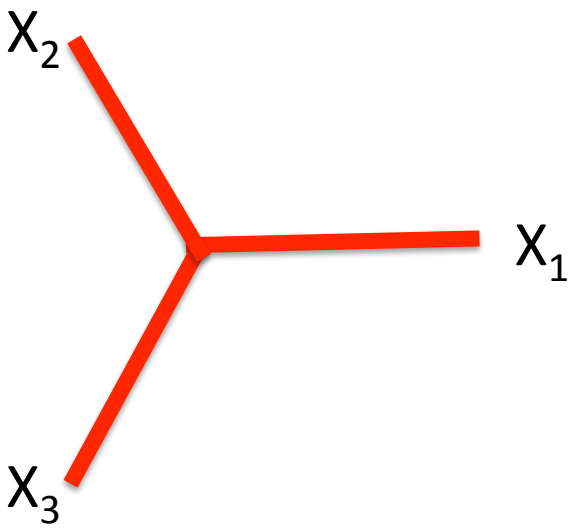




Only the interband transitions are plotted

Interband transitions in the nematic state

Unrelaxed model

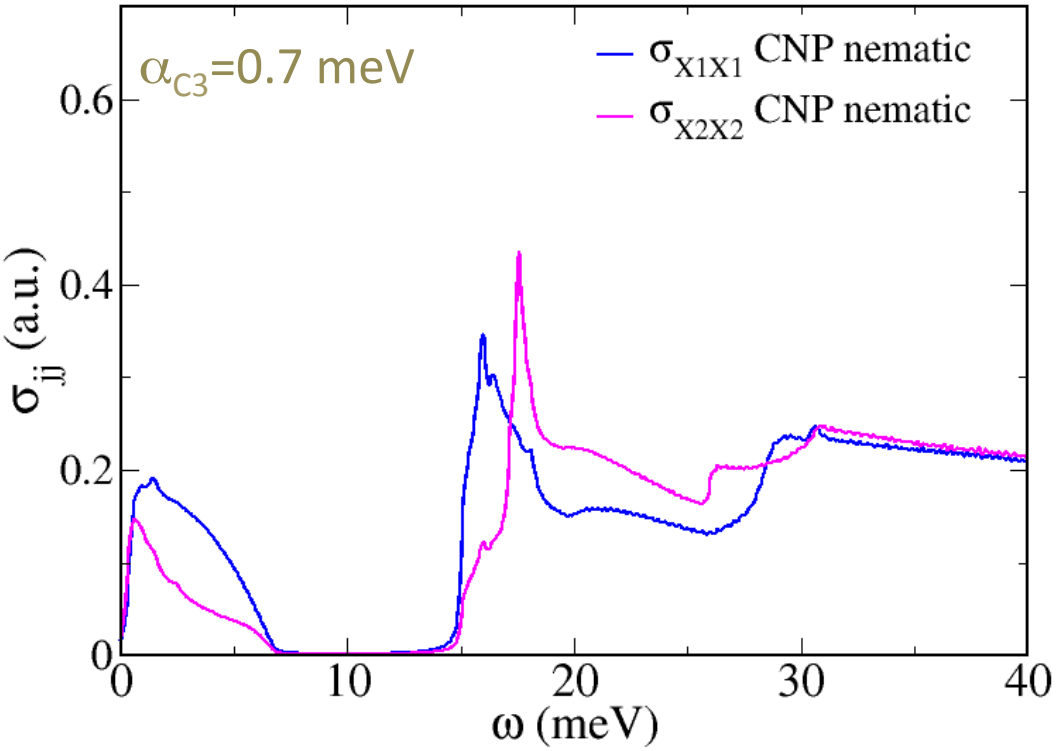


In the nematic state

$\sigma_{x1x1} \neq \sigma_{x2x2} = \sigma_{x3x3}$

With C_3 symmetry

$\sigma_{x1x1} = \sigma_{x2x2} = \sigma_{x3x3}$

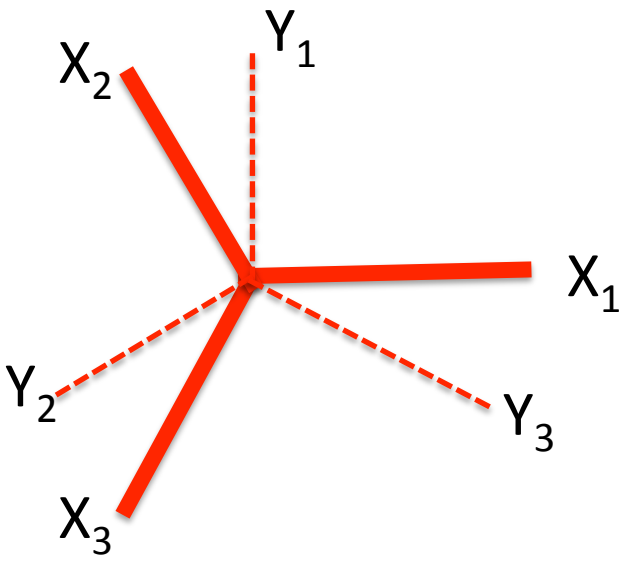


Only the interband transitions are plotted

leni@icmm.csic.es

Interband transitions in the nematic state

Unrelaxed model



In the nematic state

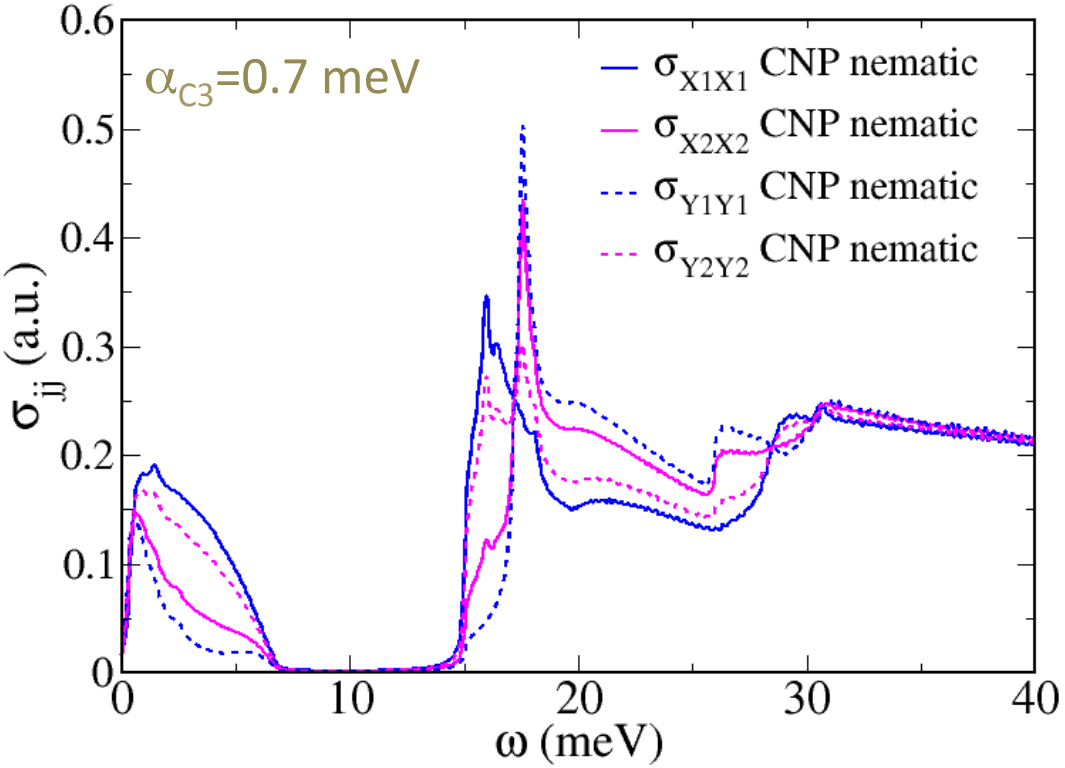
$\sigma_{x1x1} \neq \sigma_{x2x2} = \sigma_{x3x3}$

$\sigma_{xx} \neq \sigma_{yy}$

With C_3 symmetry

$\sigma_{x1x1} = \sigma_{x2x2} = \sigma_{x3x3}$

$\sigma_{xx} = \sigma_{yy}$

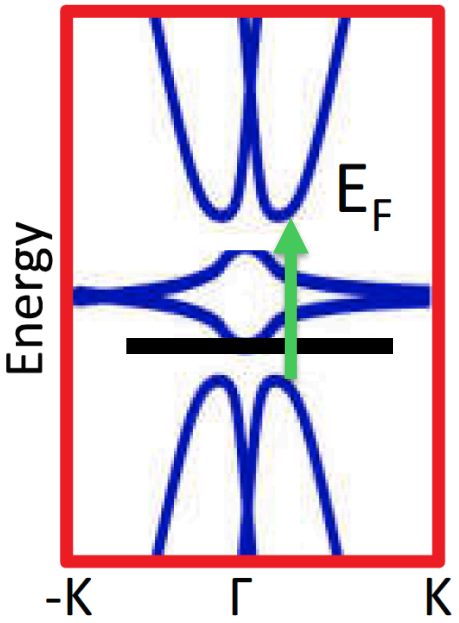


Only the interband transitions are plotted

leni@icmm.csic.es

Interband transitions in the nematic state

Unrelaxed model

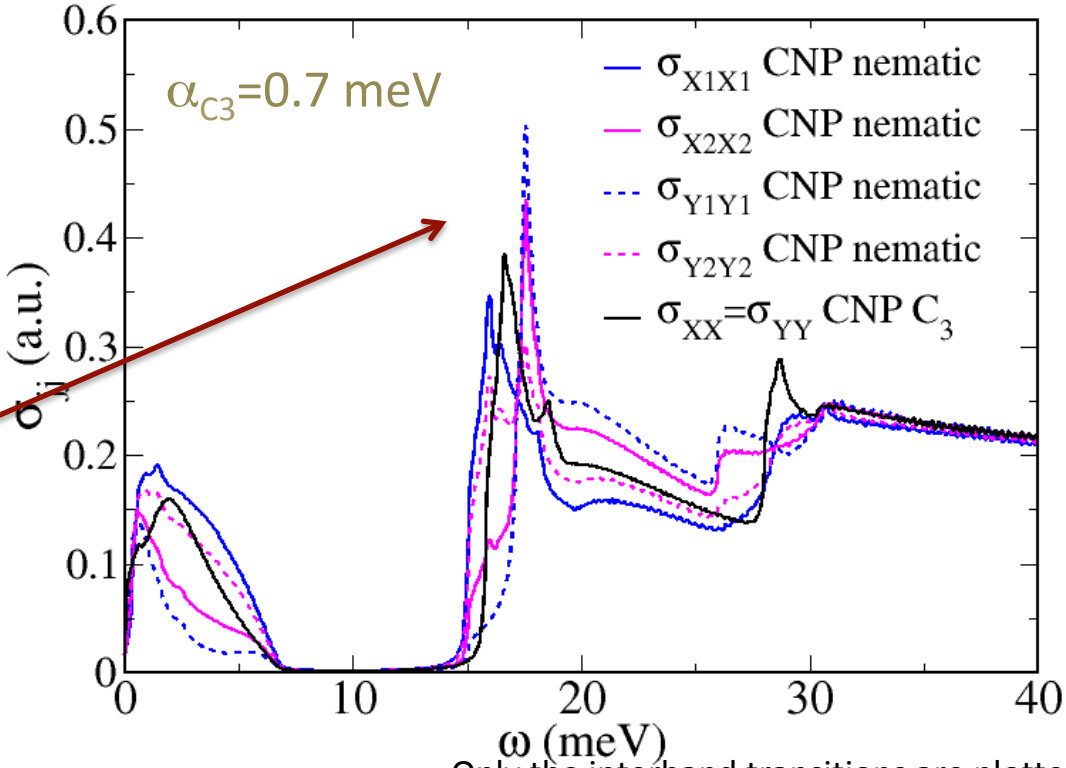


In this nematic state

$\sigma_{x1x1} \neq \sigma_{x2x2} = \sigma_{x3x3}$

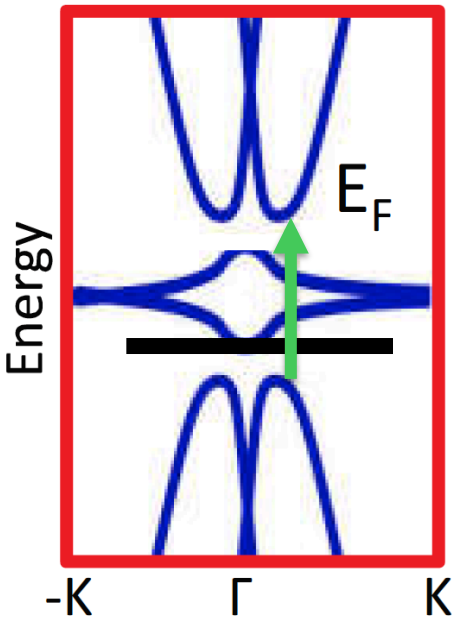
$\sigma_{xx} \neq \sigma_{yy}$

These transitions can be studied as a function of doping



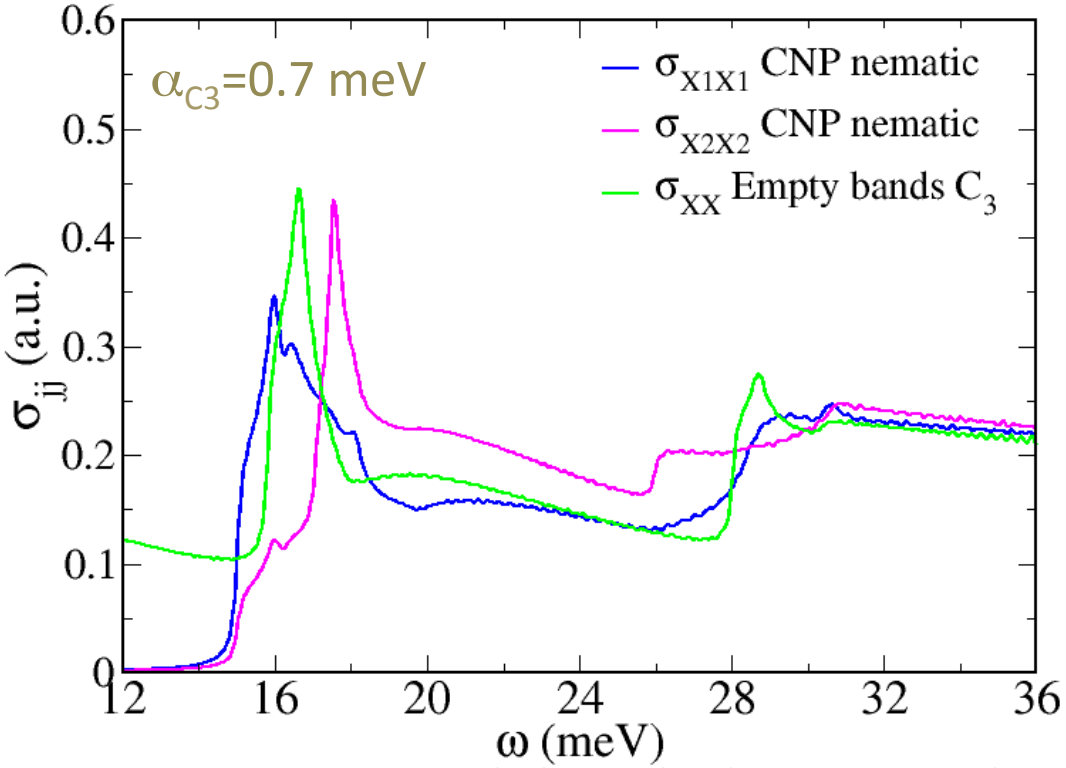
Only the interband transitions are plotted

Interband transitions in the nematic state



In this nematic state

Transitions affected by the nematic state
not restricted to those involving the flat bands

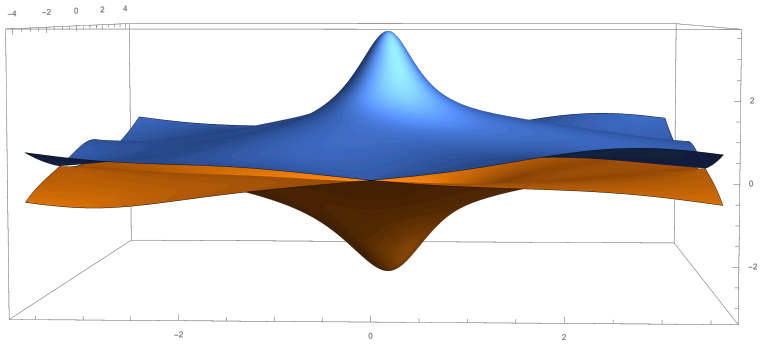


Only the interband transitions are plotted

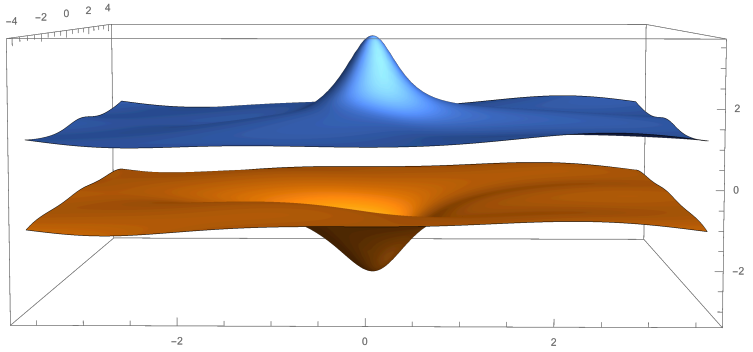
Optical conductivity in the $C_{2z}T$ broken symmetry state

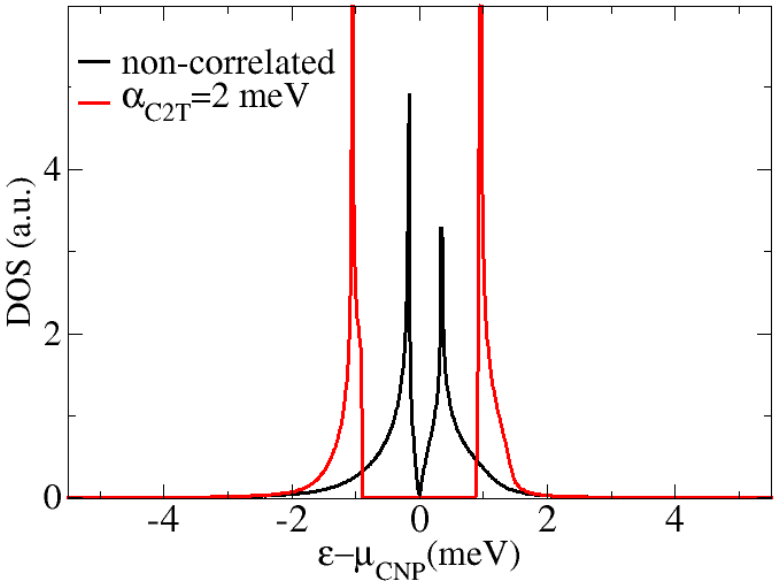
Unrelaxed model

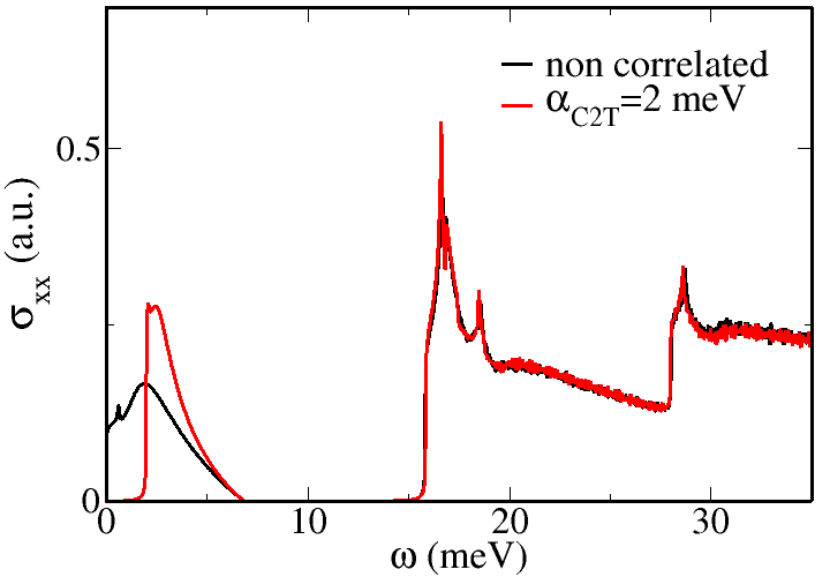
Flat bands non correlated state



Flat bands C2zT Broken symmetry



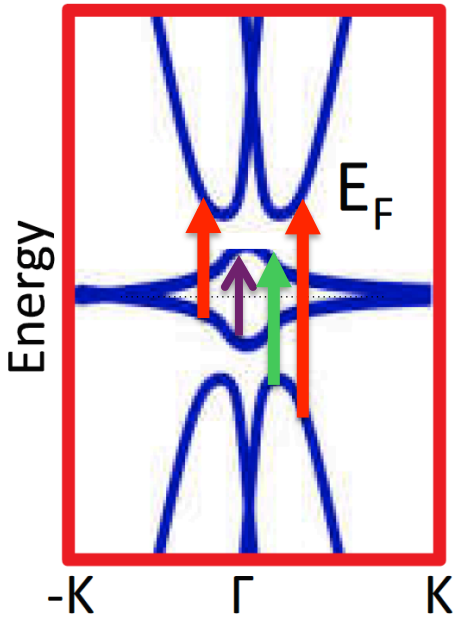




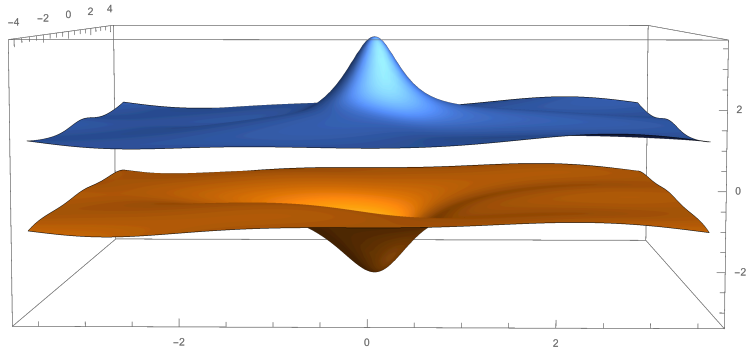
leni@icmm.csic.es

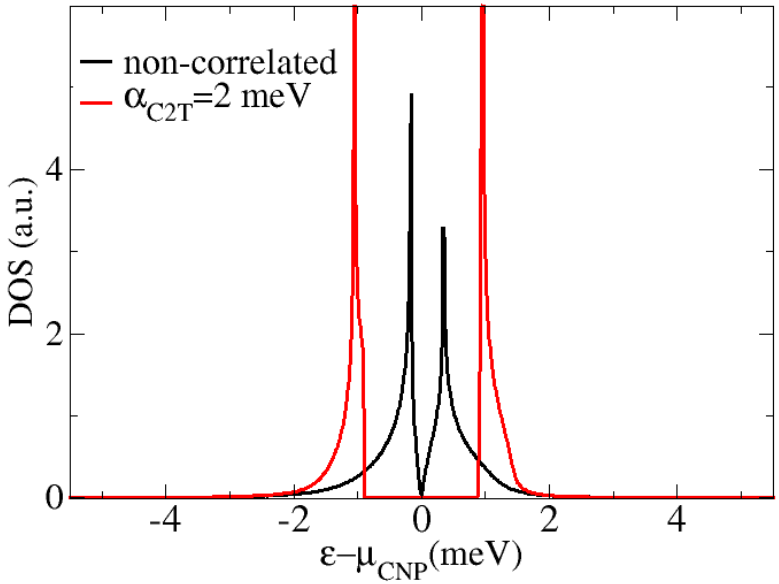
Optical conductivity in the $C_{2z}T$ broken symmetry state

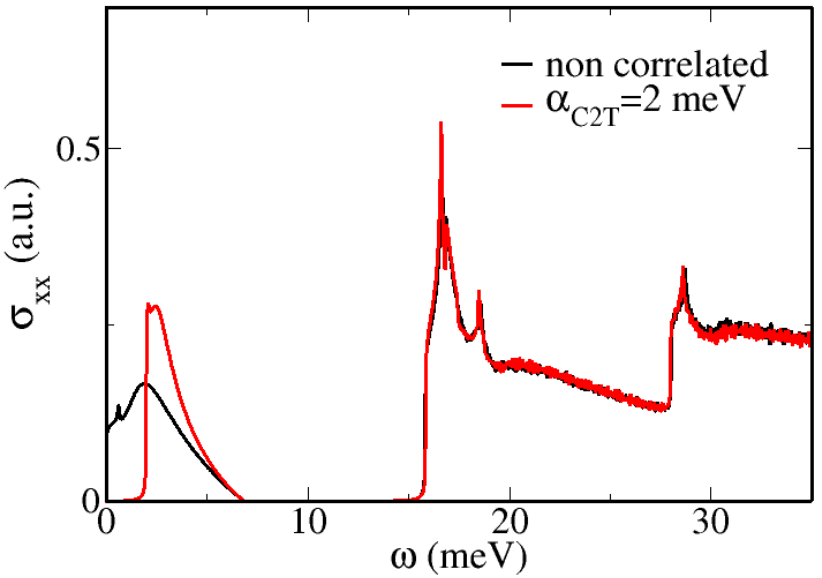
Unrelaxed model



Flat bands C2zT Broken symmetry



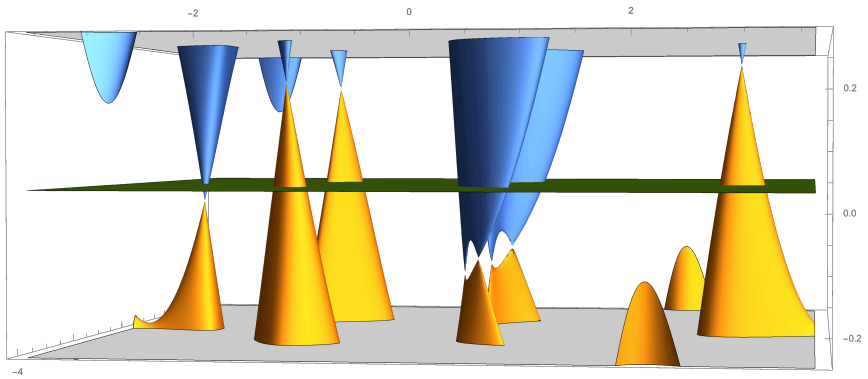


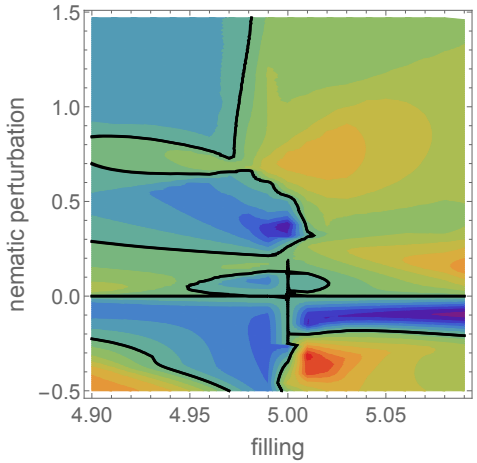


leni@icmm.csic.es

Summary

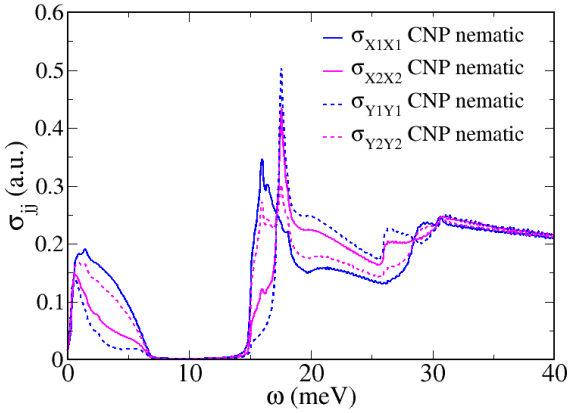
Small Fermi pockets and new Dirac points may appear in the presence of nematicity. The original Dirac points may be away from charge neutrality.

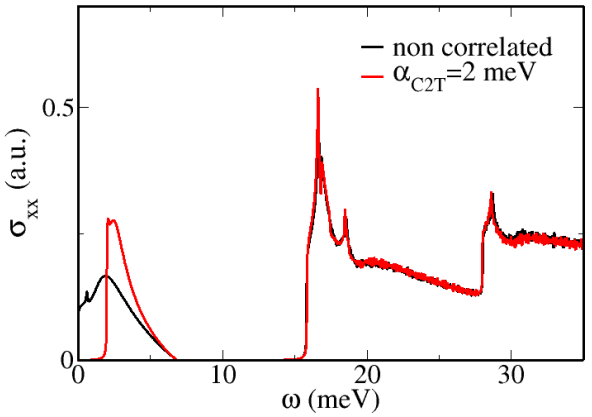




The sign of the anisotropy of the Drude weight depends on the underlying band structure. We find opposite sign for the Drude anisotropy along the XX and YY directions.

Optical conductivity may help identifying the nature of the correlated state





leni@icmm.csic.es