# BIASED TWISTED BILAYER GRAPHENE: MAGNETISM AND GAP

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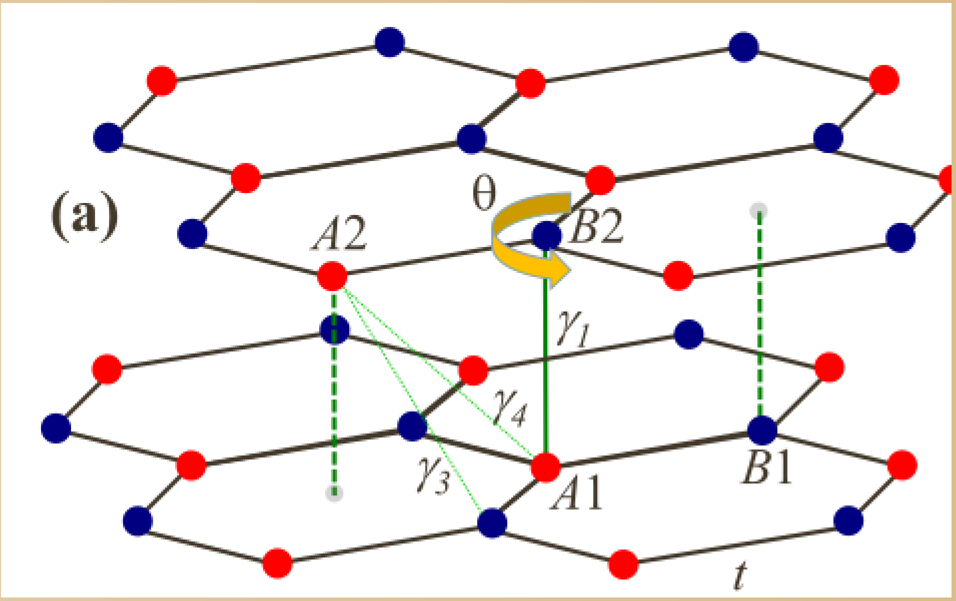
# Presentation outline:

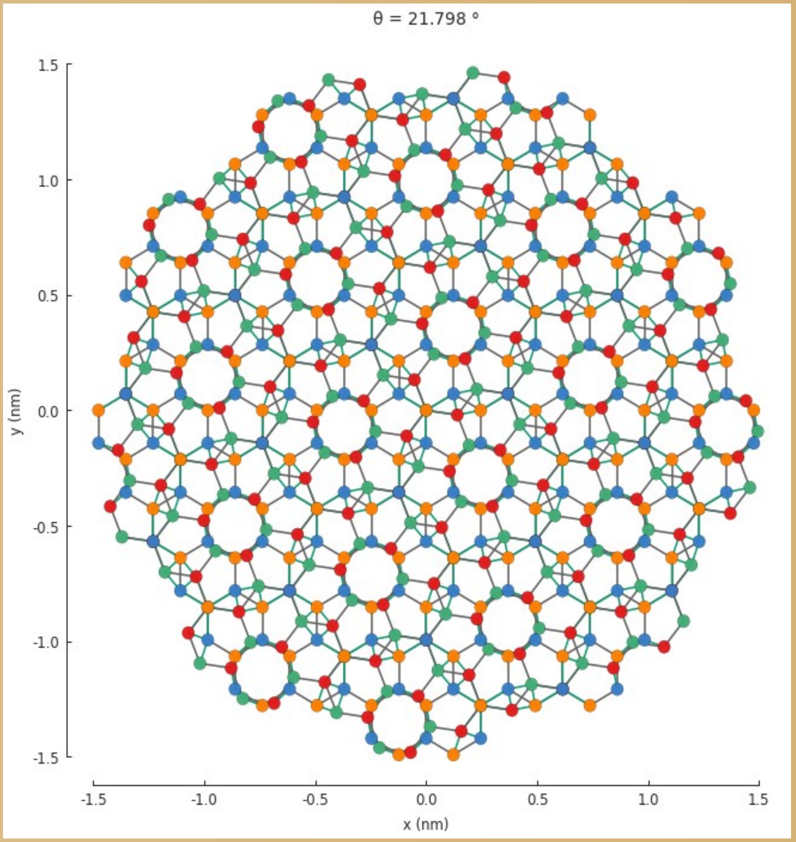
– General properties of twisted bilayers
– Effect of the bias: nested Fermi surface
– Exitonic gap + magnetism

# Twisted bilayer graphene

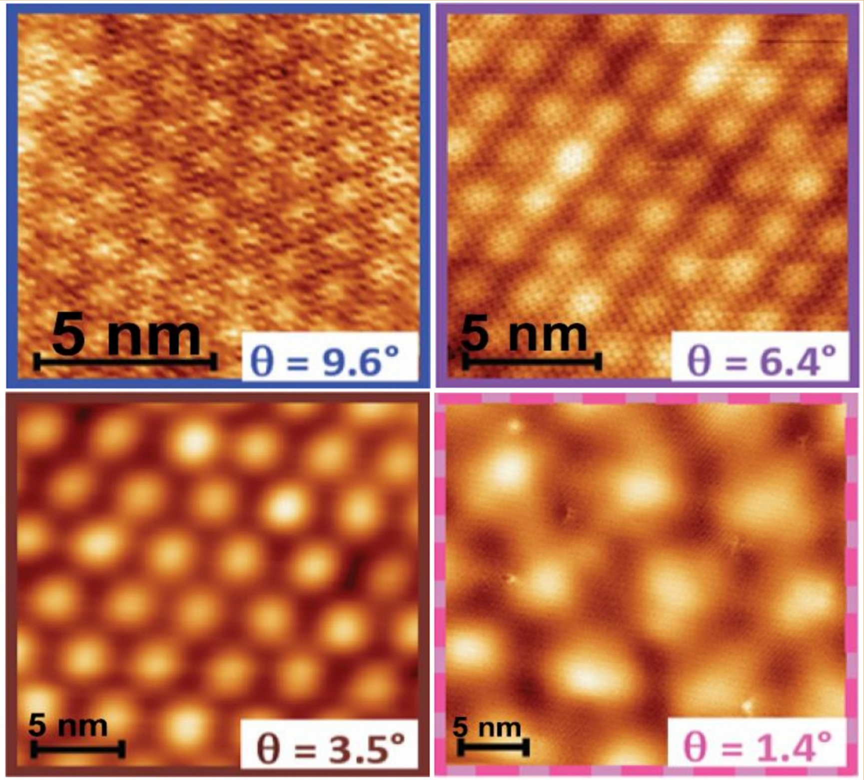
System before rotation: AB bilayer graphene




“Commensurate” twist angle



# Twisted bilayer graphene as seen on experiment




Scanning spectroscopy of twisted bilayer samples with different twist angles

I. Brihuega et al., Phys. Rev. Lett., **109**, 196802 (2012)

Moire superlattice is clearly seen

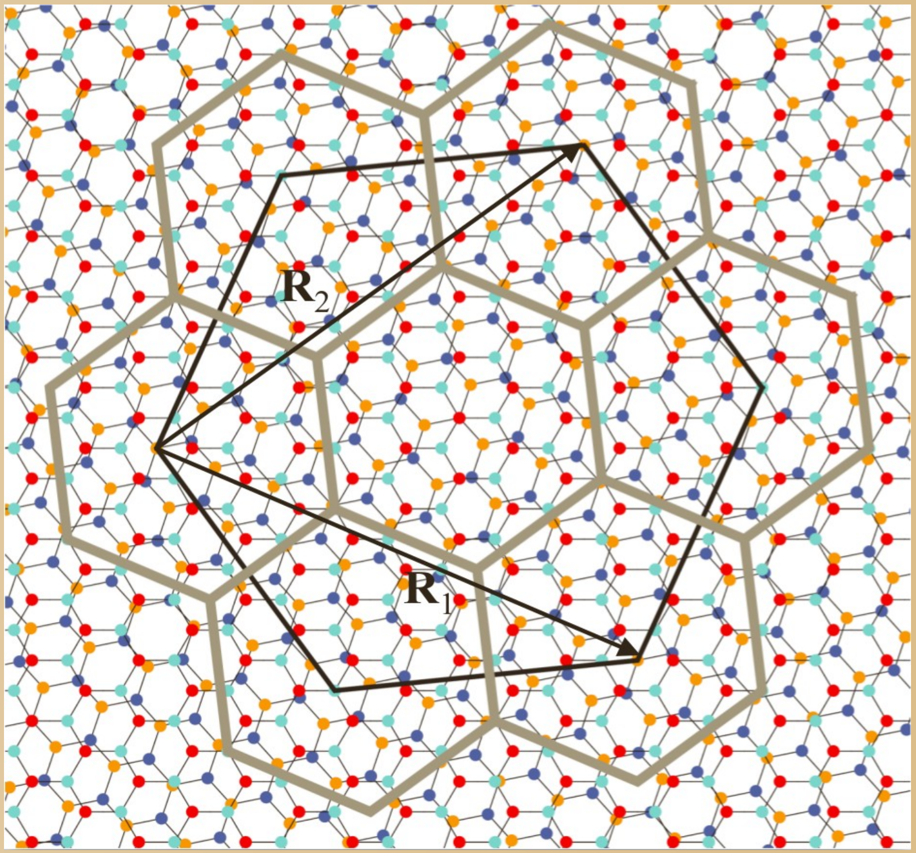
# Theory of the single-electron dispersion for twisted bilayer graphene

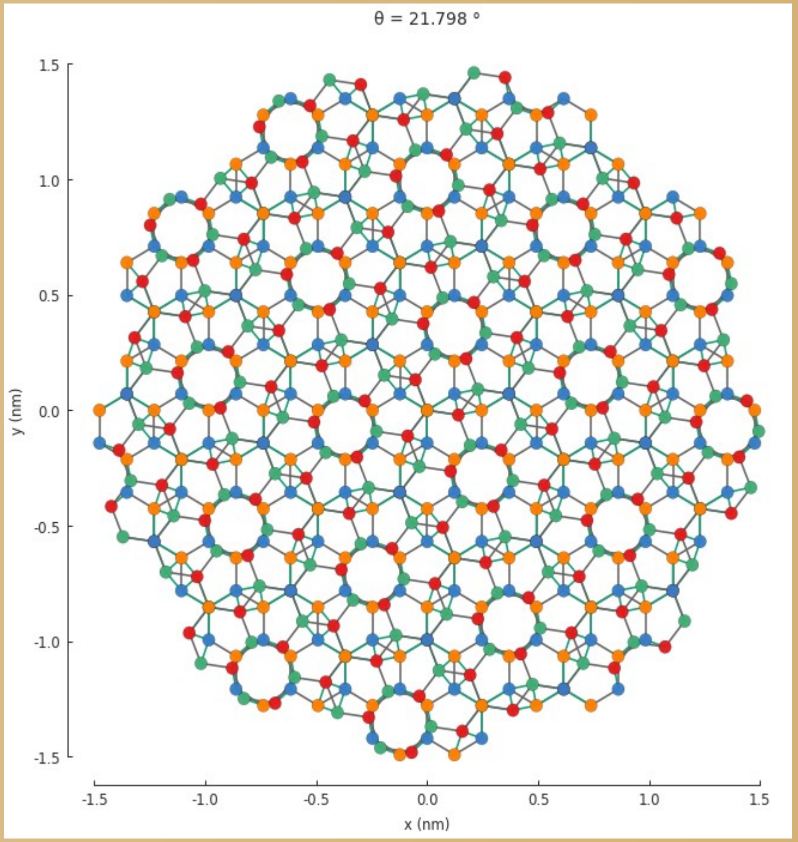
Most of our knowledge about single-electron properties of twisted bilayers comes from calculations at “commensurate” angles

$$\cos\theta = \frac{3m^2 + 3mr + r^2/2}{3m^2 + 3mr + r^2}$$

Here *m* and *r* are co-prime natural numbers

# Commensurate angles: superstructure



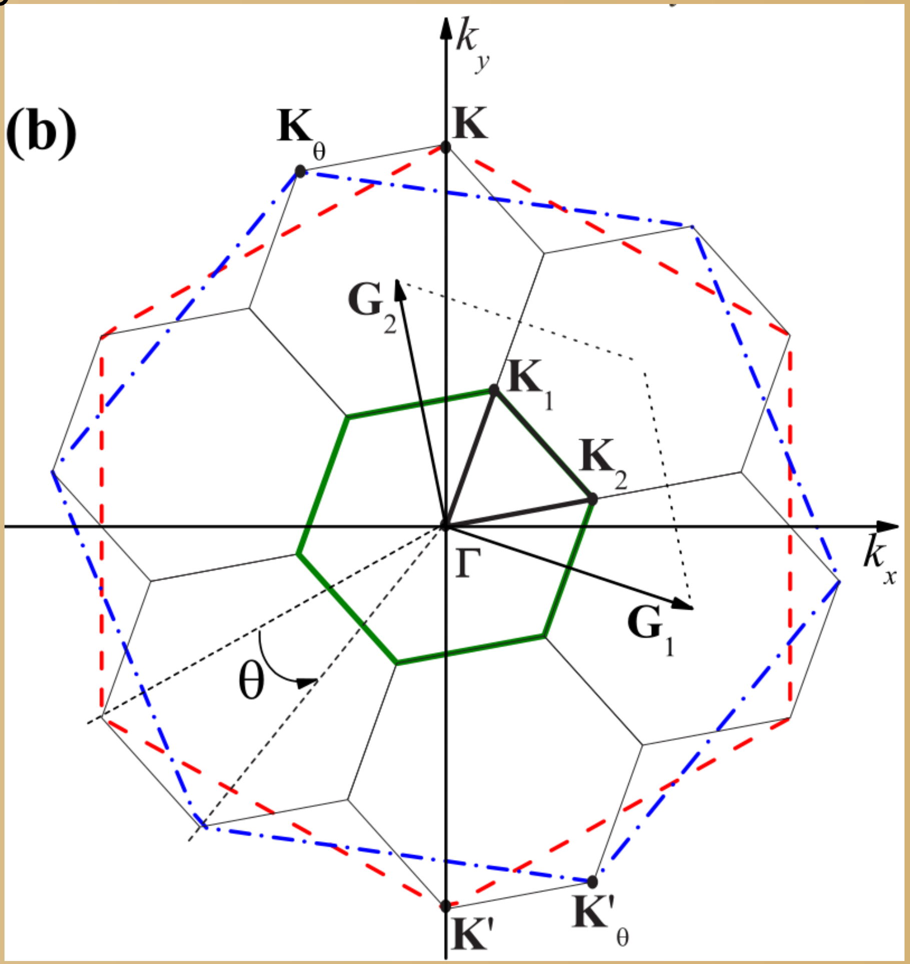



# Commensurate angles: superstructure in the reciprocal space

Red dashed line – Brillouin zone of the unrotated layer

Blue dashed line – Brillouin zone of the rotated layer

Green solid line – Brillouin zone of the superstructure.



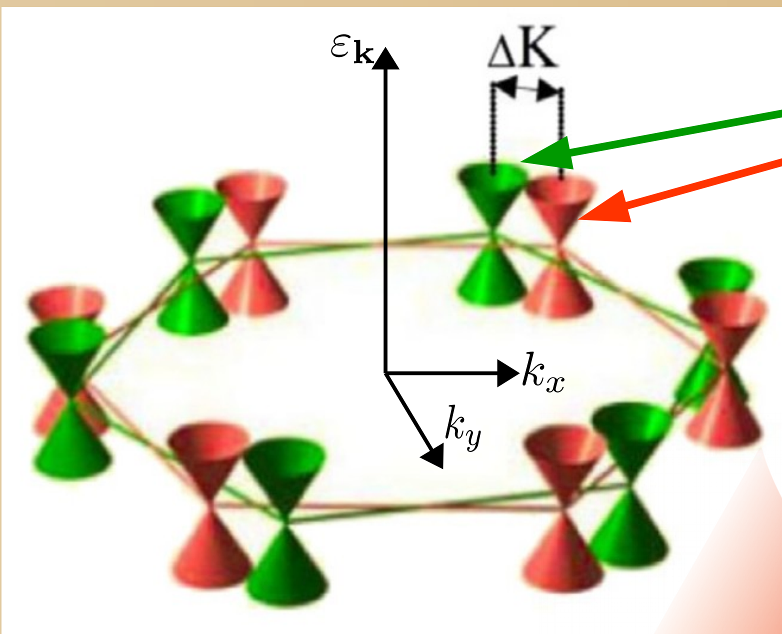
# Why theorists like commensurate angles?

**Advantages**

1. Periodic structure emerges (one can study finite supercells)

2. Arbitrary incommensurate angle can be approximated

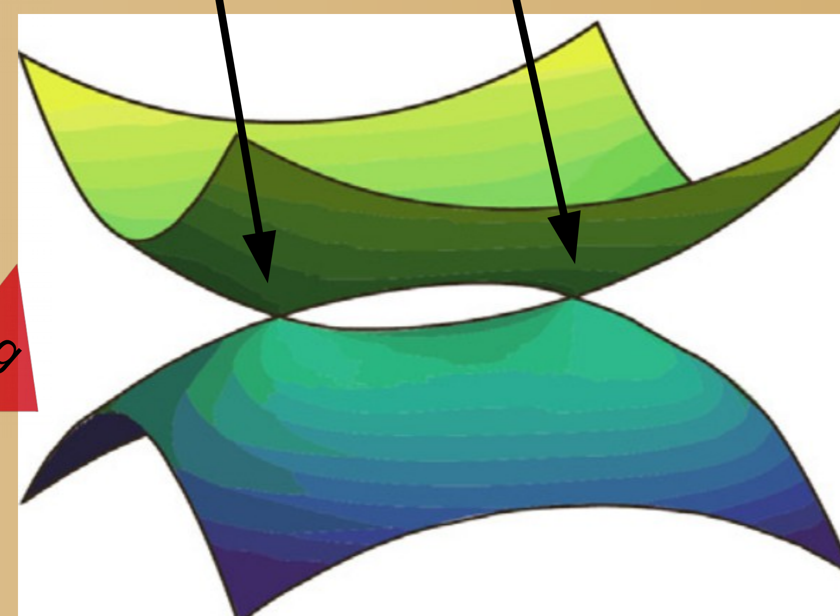
# Calculation at a commensurate angle: single-particle dispersion



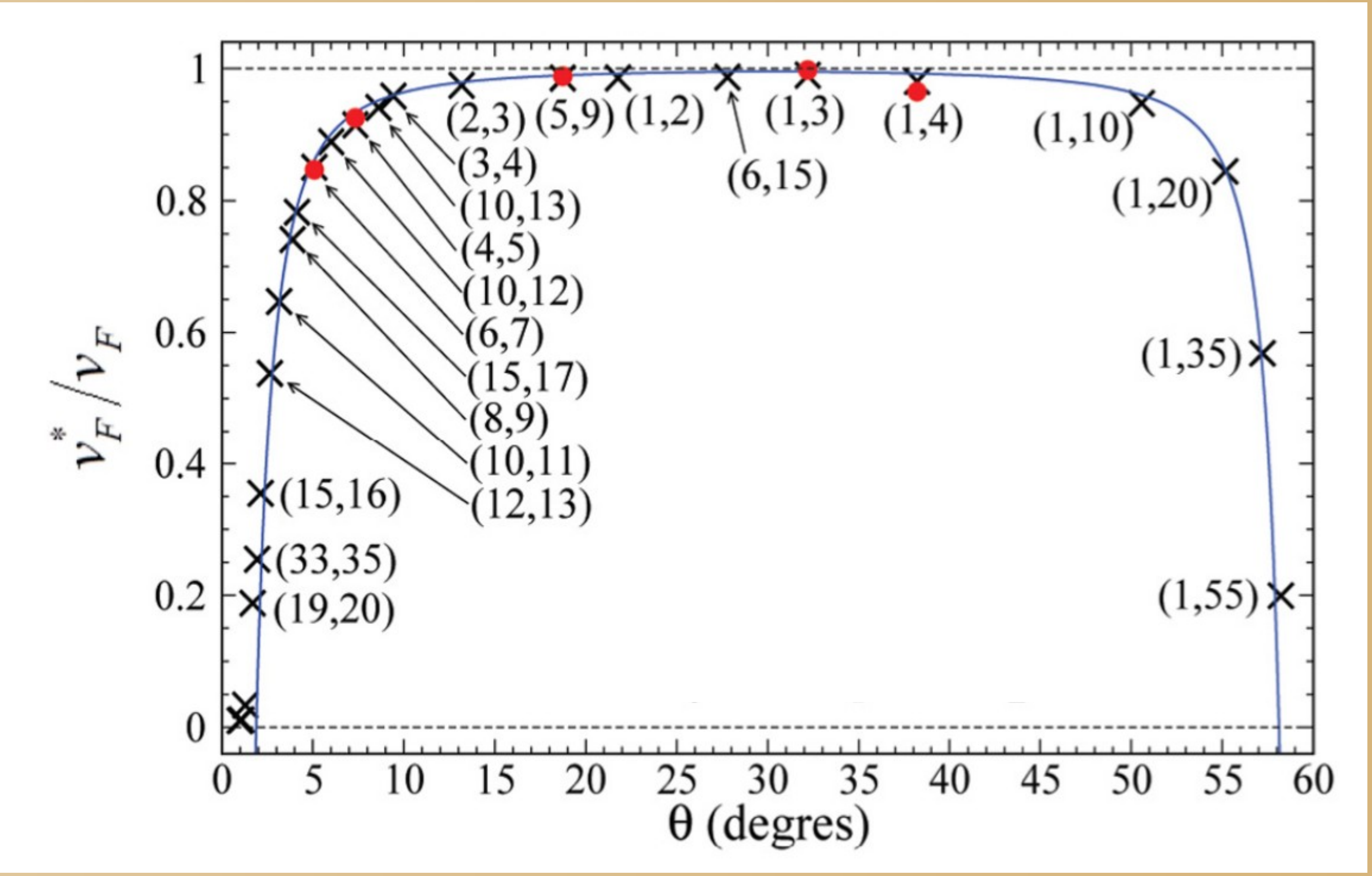

"Monolayer" Dirac cones

Renormalized Dirac cones at the corners of the supercell Brillouin zone

Inter-layer tunneling



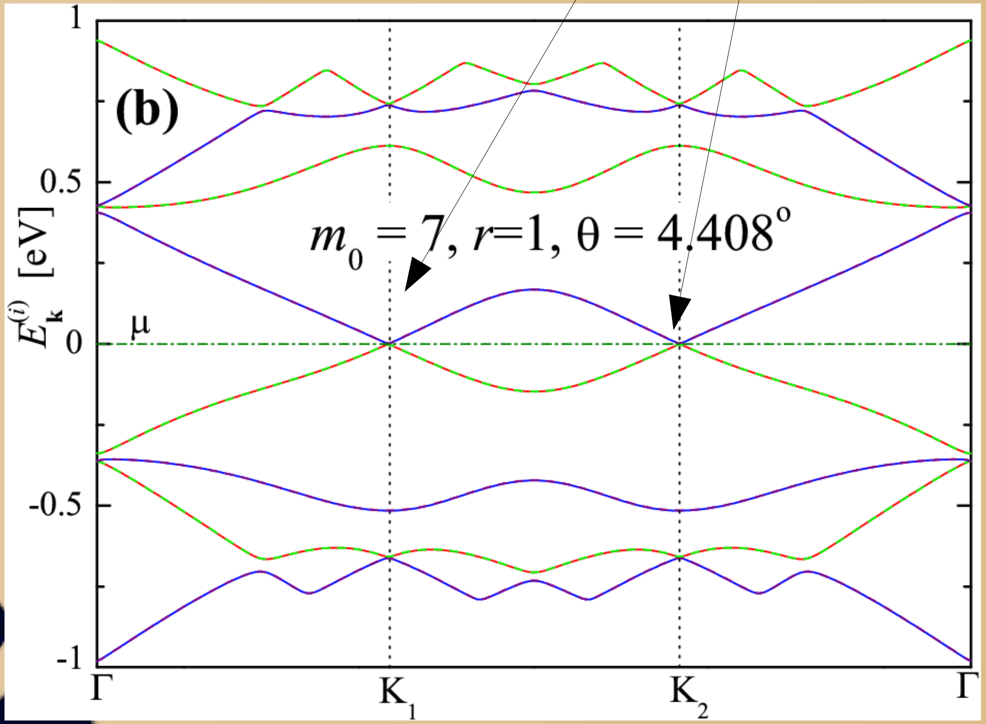
# Fermi velocity renormalization

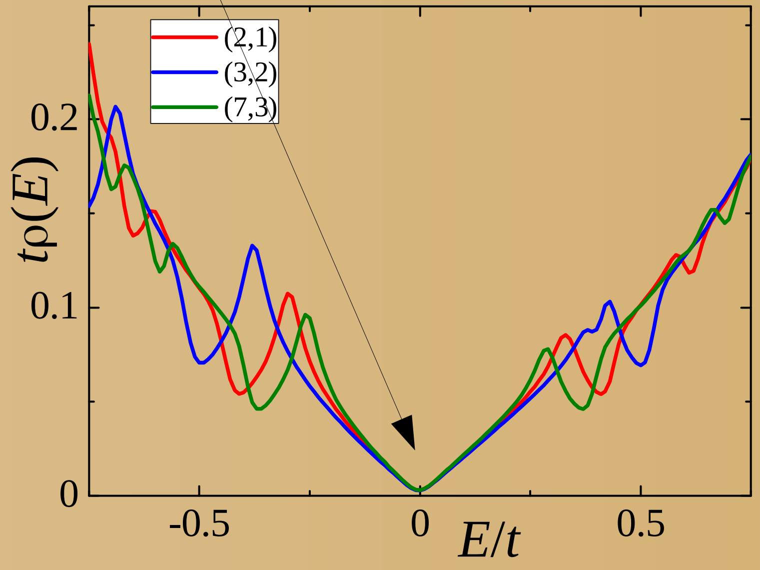



G. Trambly de Laissardière et al., Nano Letters, **10**, 804 (2010)

# Interaction effects: phase transitions?

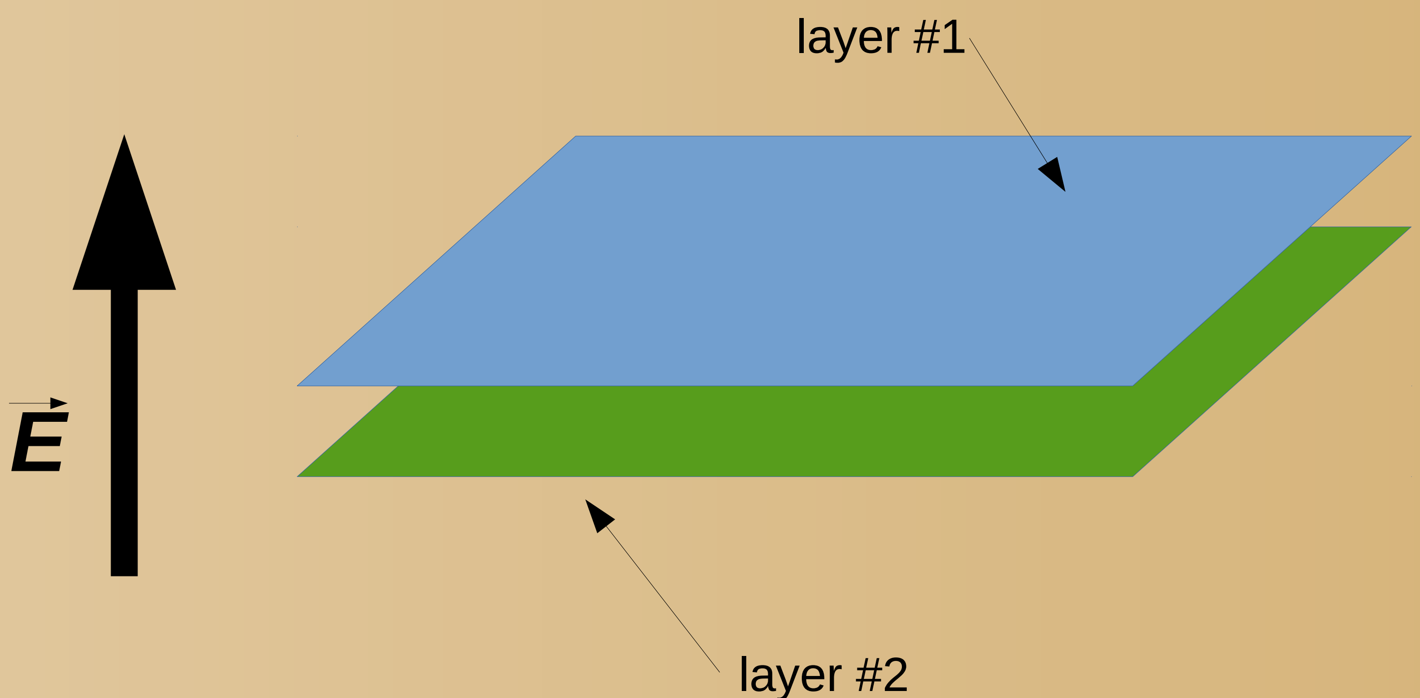
Bad new for phase transition: Dirac cones => vanishing DOS => no mean-field instability




$$T_c \sim \exp(-1/\rho(0)g)$$

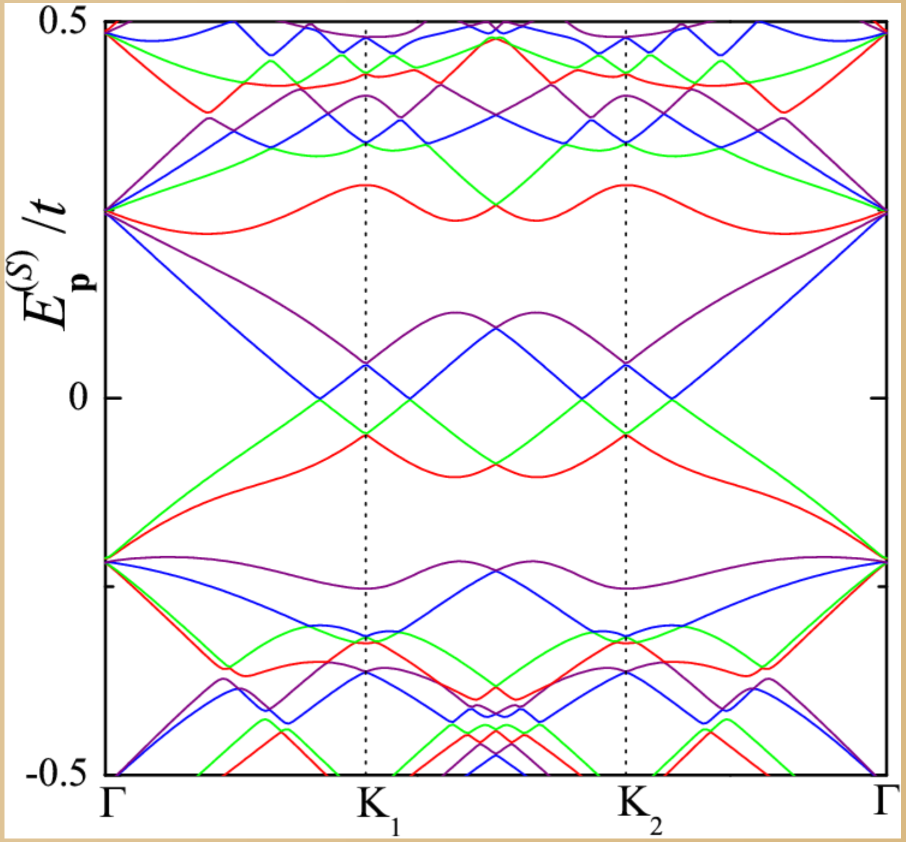
# Biased twisted bilayer?




$E$ is transverse electric field

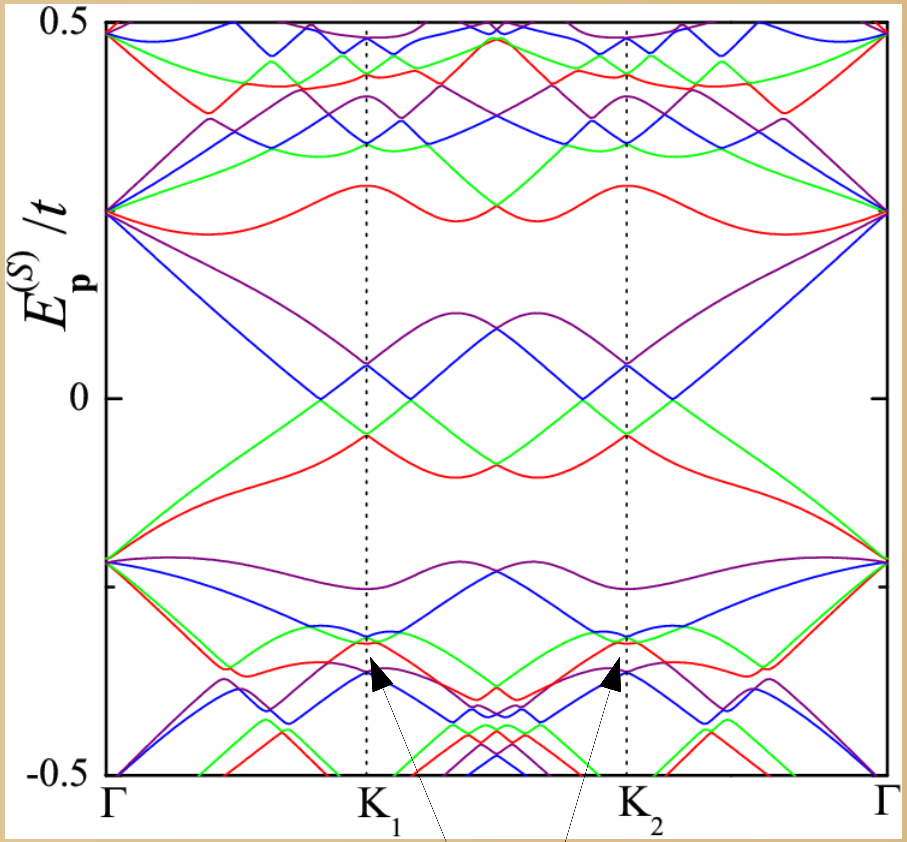
# Biased twisted bilayer?

Bilayer spectrum at finite bias



# Biased twisted bilayer?

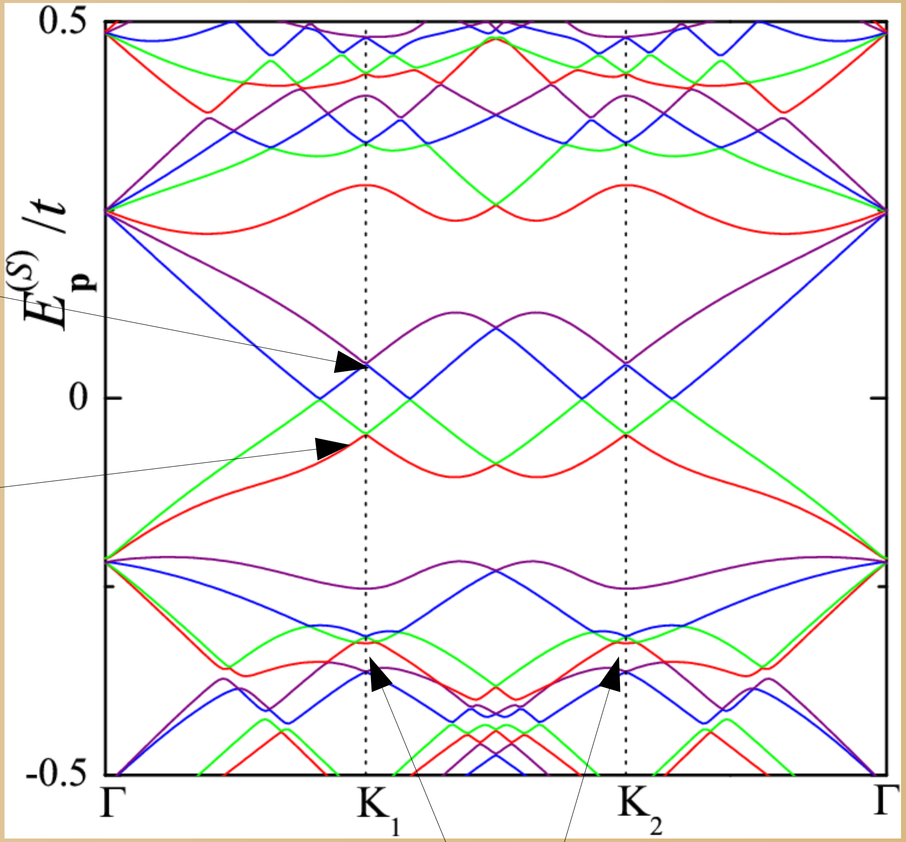
Bilayer spectrum at finite bias




This is where Dirac cones are

# Biased twisted bilayer?

Bilayer spectrum at finite bias




One Dirac cone

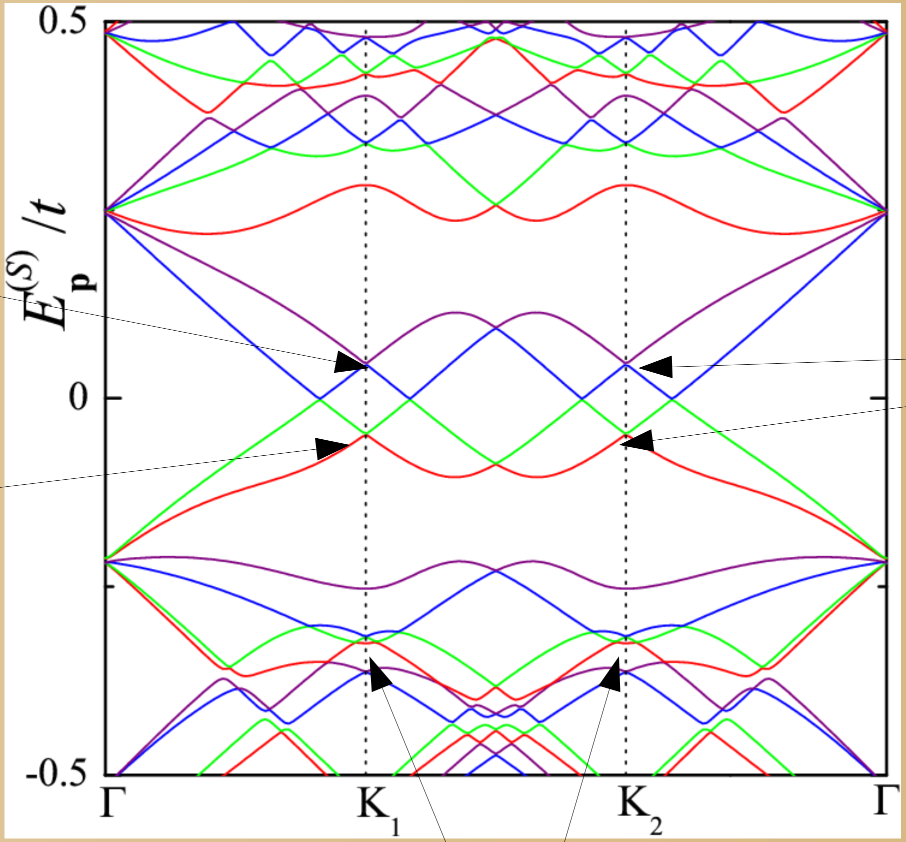
Another Dirac cone

This is where Dirac cones are

# Biased twisted bilayer?

Bilayer spectrum at finite bias

One Dirac cone



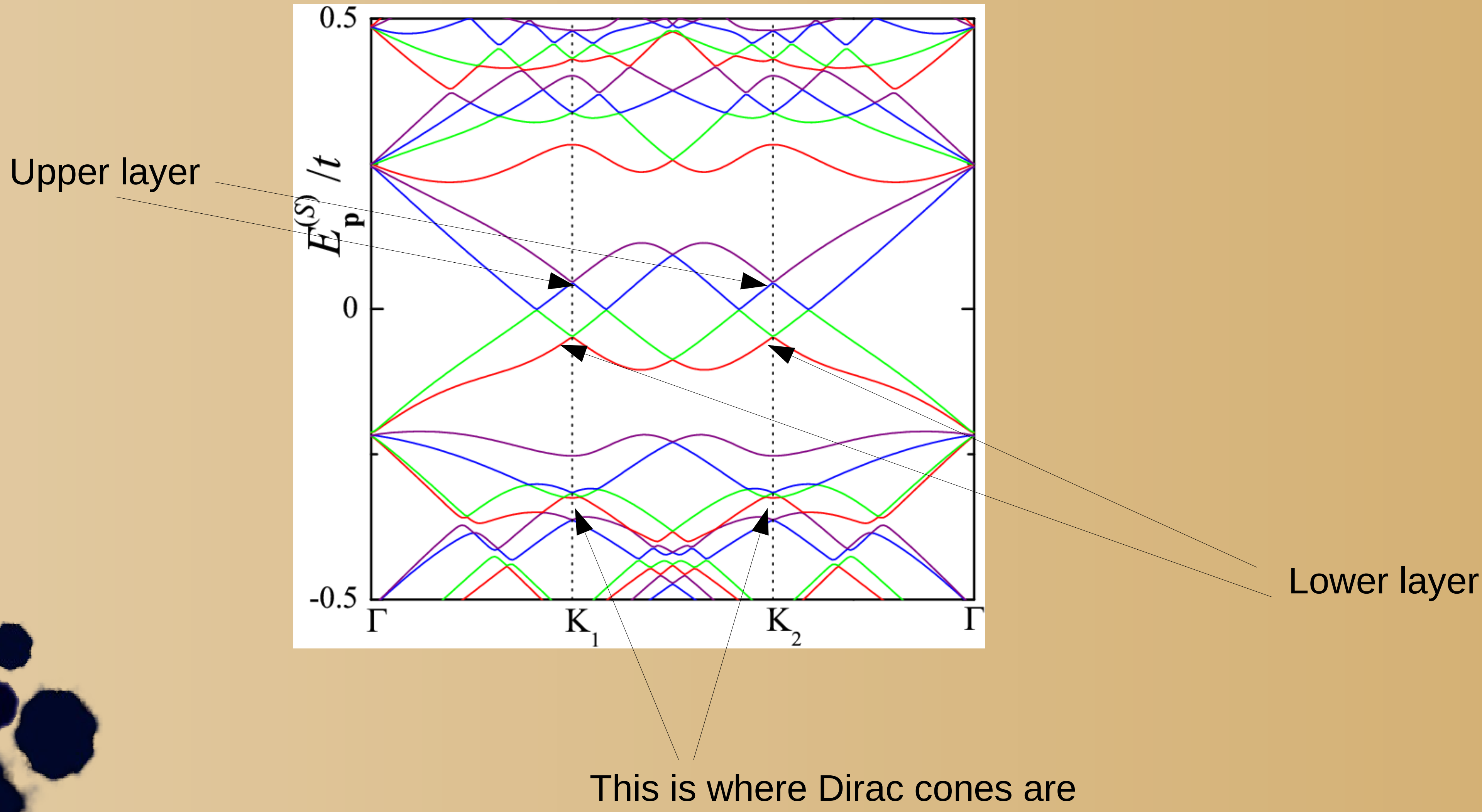

Two more Dirac cones

Another Dirac cone

This is where Dirac cones are

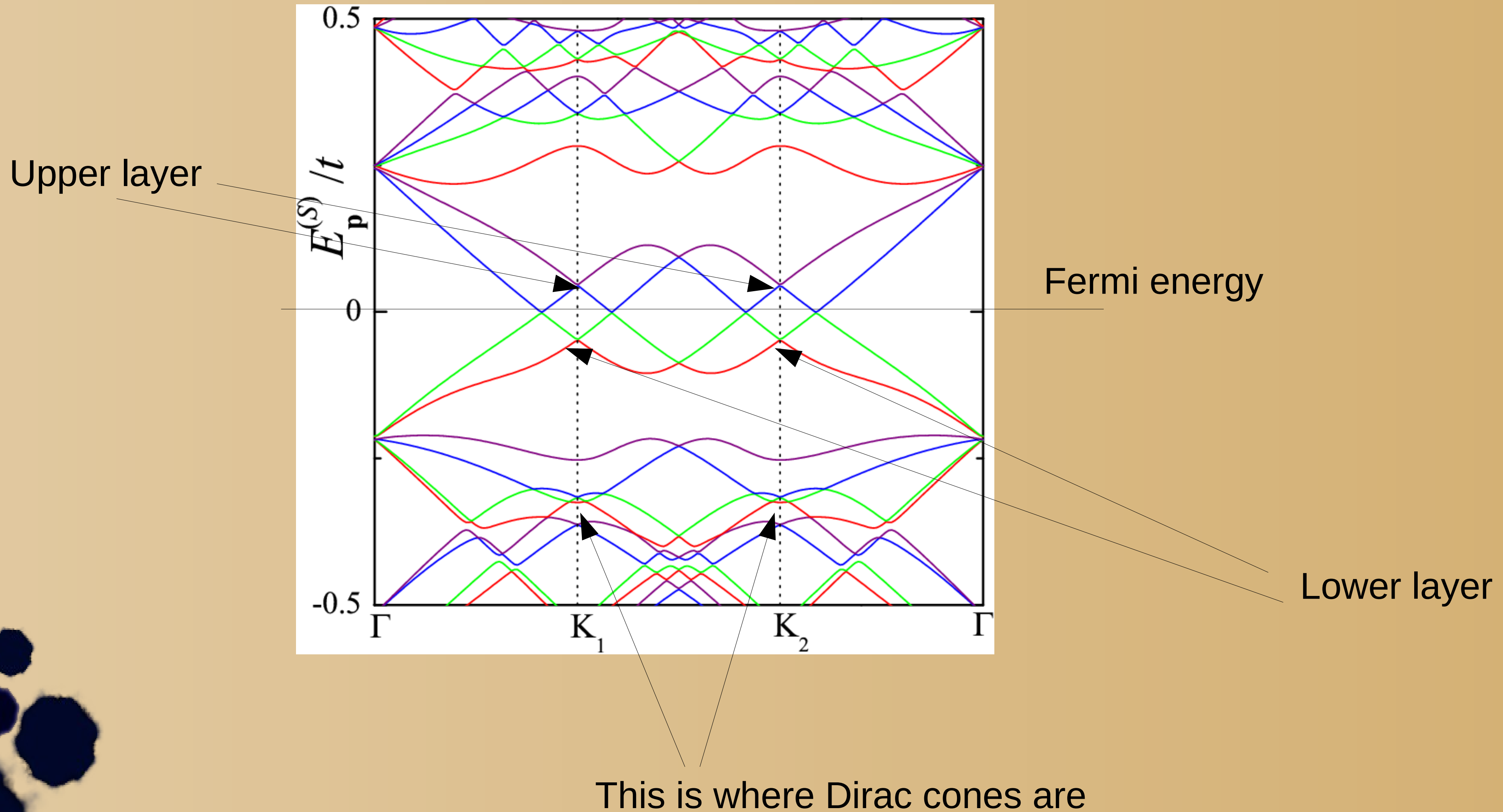
# Biased twisted bilayer?

Bilayer spectrum at finite bias



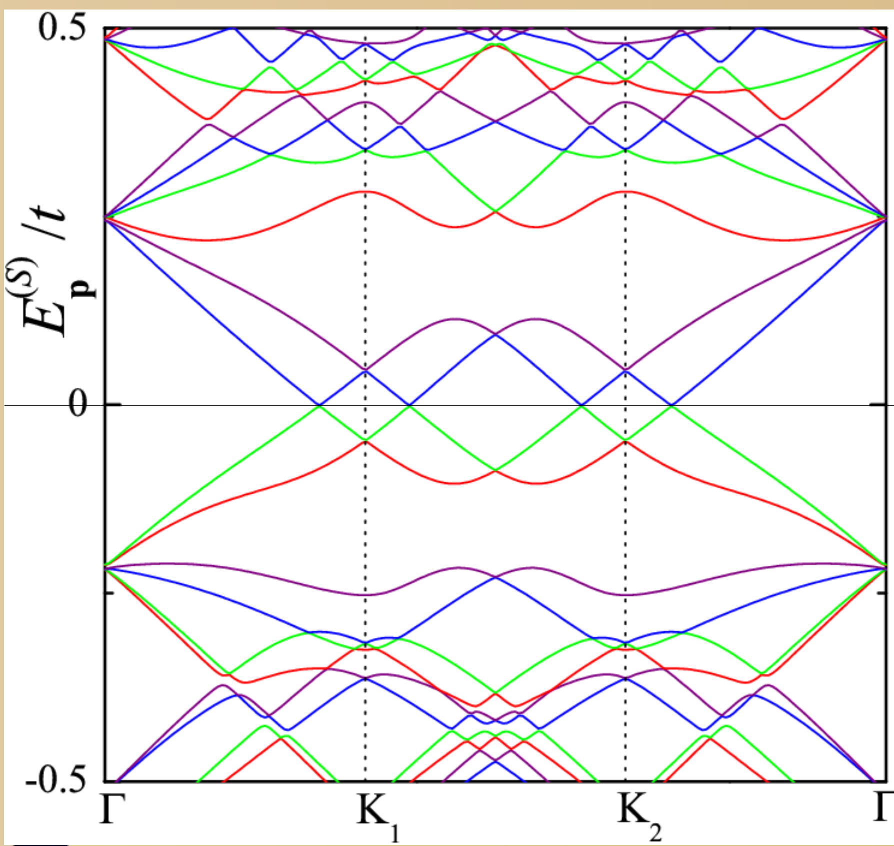
# Biased twisted bilayer?

Bilayer spectrum at finite bias



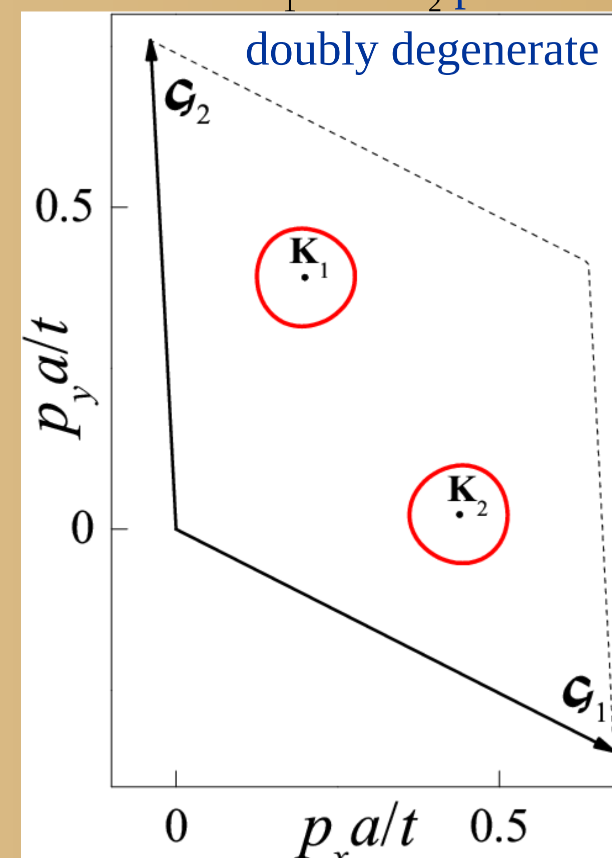
# Fermi surface (Fermi curve)

Spectrum



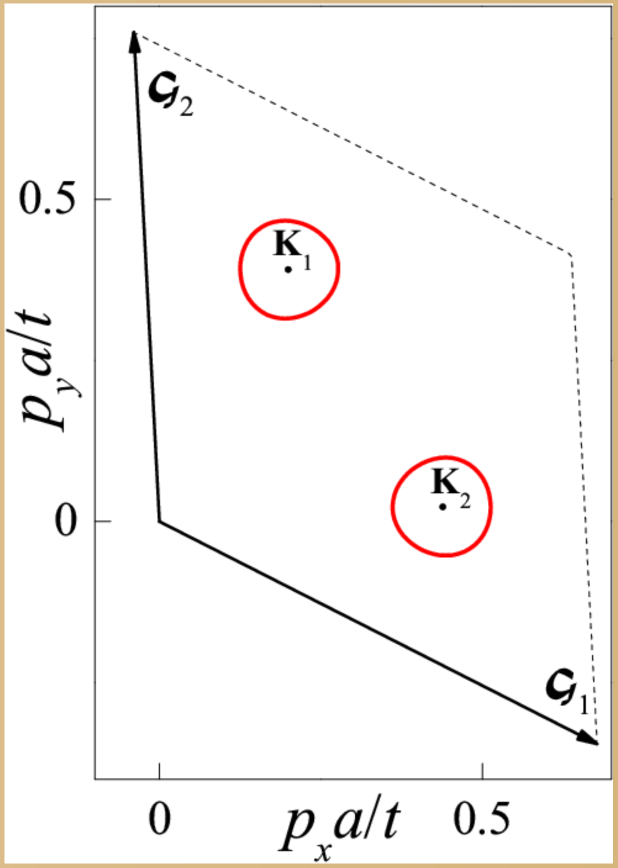

Fermi level

Fermi surfaces near $\mathbf{K}_1$ and $\mathbf{K}_2$ points are doubly degenerate

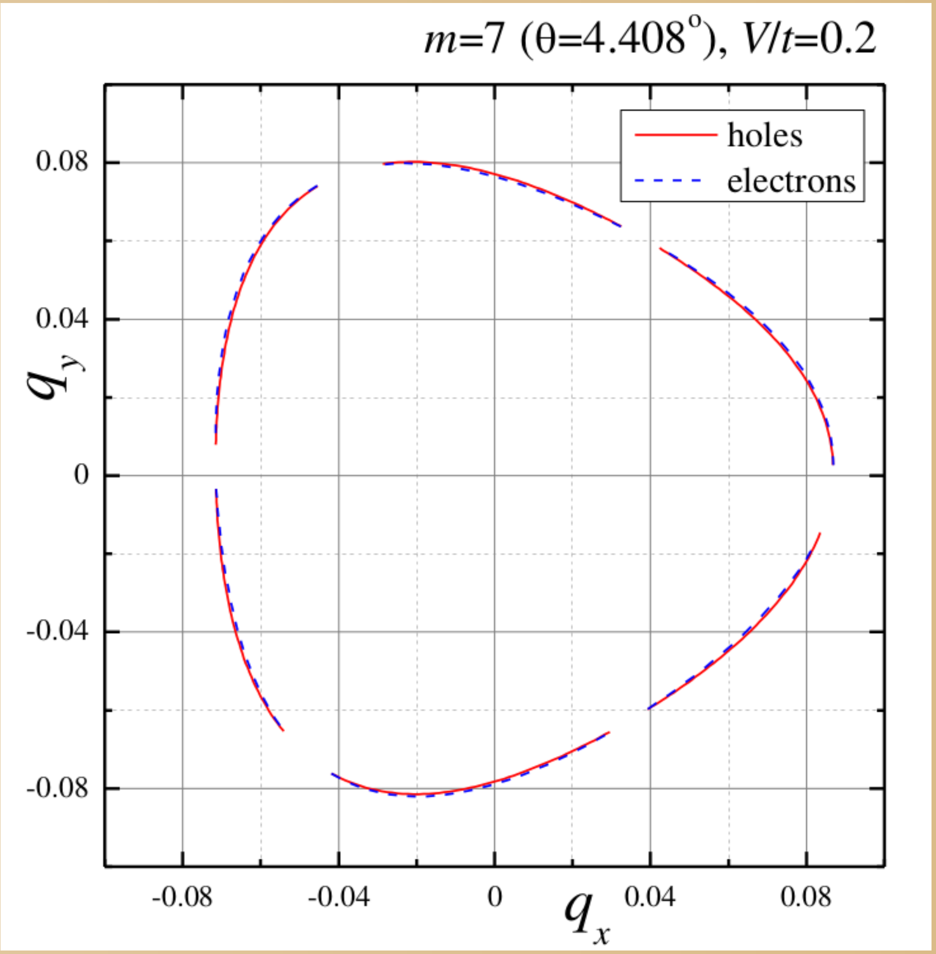


# Fermi surface (Fermi curve) with nesting

Fermi surfaces near $\mathbf{K}_1$ and $\mathbf{K}_2$ points are doubly degenerate (perfect nesting between hole- and electron-like bands). This leads to exciton band gap opening.



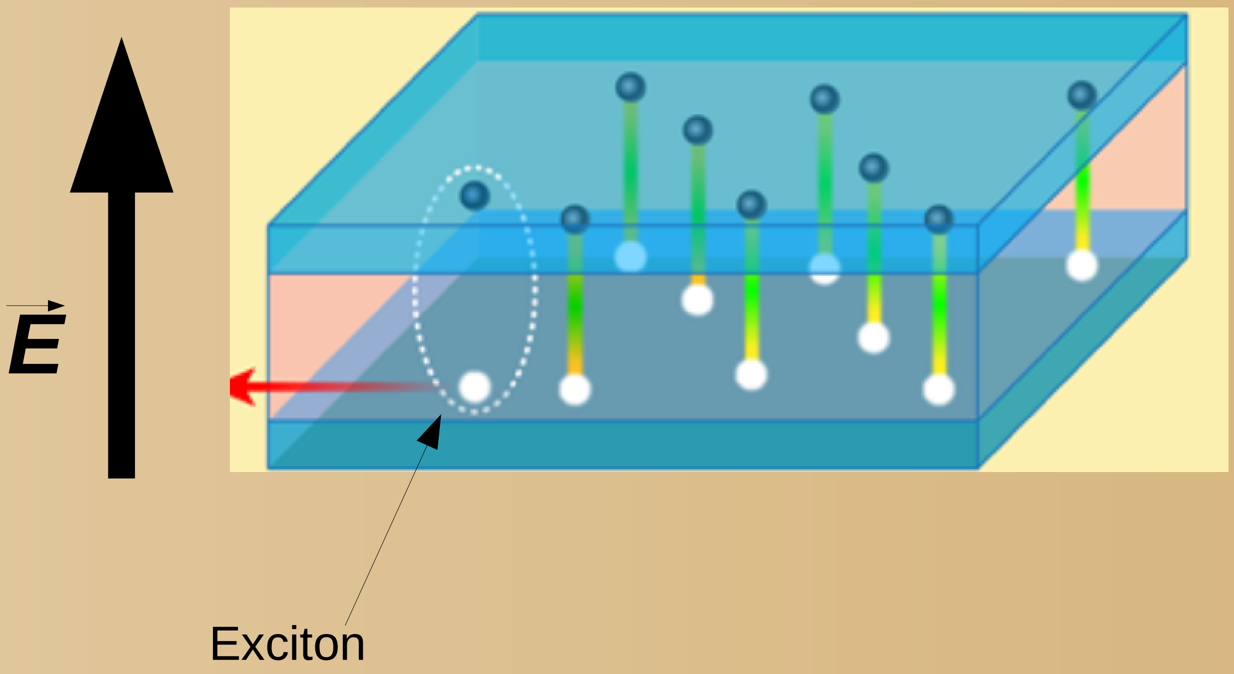
# Quality of nesting



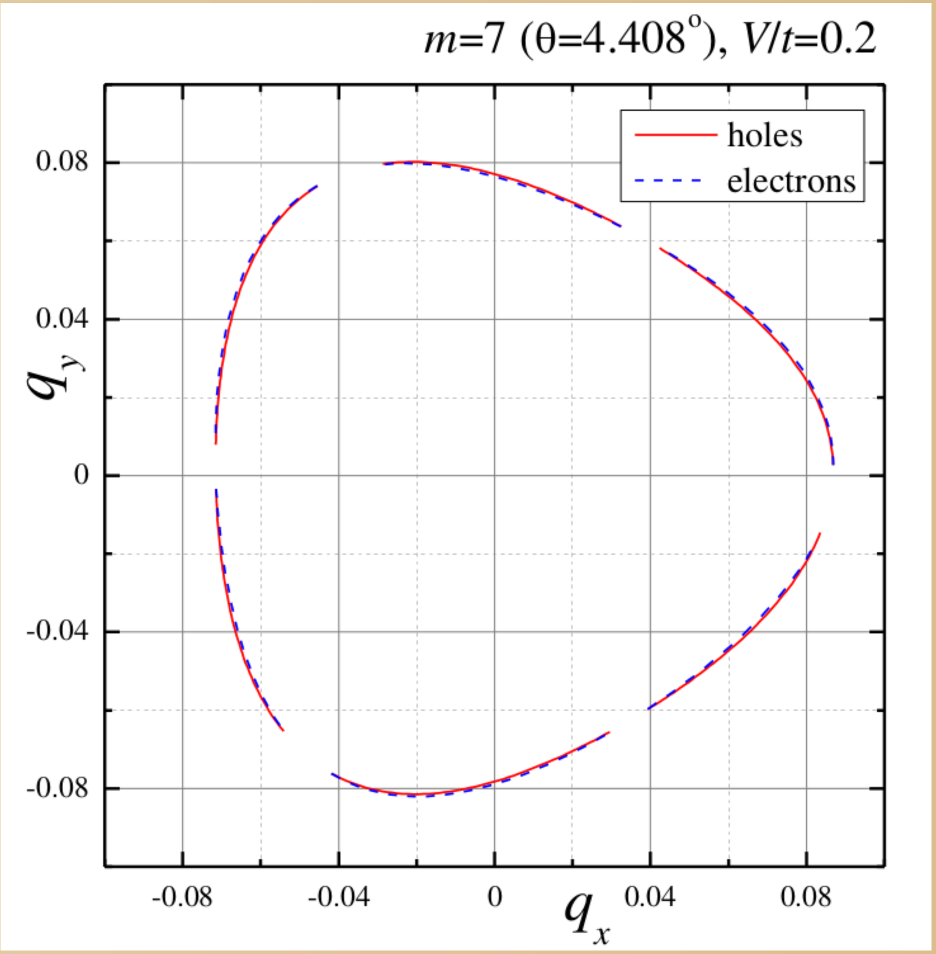

Electron Fermi surface and hole Fermi surface are almost identical

# Ordered state

Electron in one layer + hole in another + e-e repulsion = exciton



# Ordered state:
# why nesting is important?




For any electron with low energy and momentum ***p*** there is a hole with low energy and momentum ***p***

# Some technical remarks

Model hamiltonian: $H = H_0 + H_{\rm int}$

Tight-binding part:

$$\hat{H}_0 = \sum_{\substack{i\mathbf{n}j\mathbf{m}\\ ss'\sigma}} t(\mathbf{r}_{\mathbf{n}}^{is};\mathbf{r}_{\mathbf{m}}^{js'})\hat{d}^{\dagger}_{\mathbf{n}is\sigma}\hat{d}_{\mathbf{m}js'\sigma} + \frac{V_b}{2}\sum_{\mathbf{n}}(\hat{n}_{\mathbf{n}1} - \hat{n}_{\mathbf{n}2})$$

Interaction part (*U* is screened Coulomb interaction):

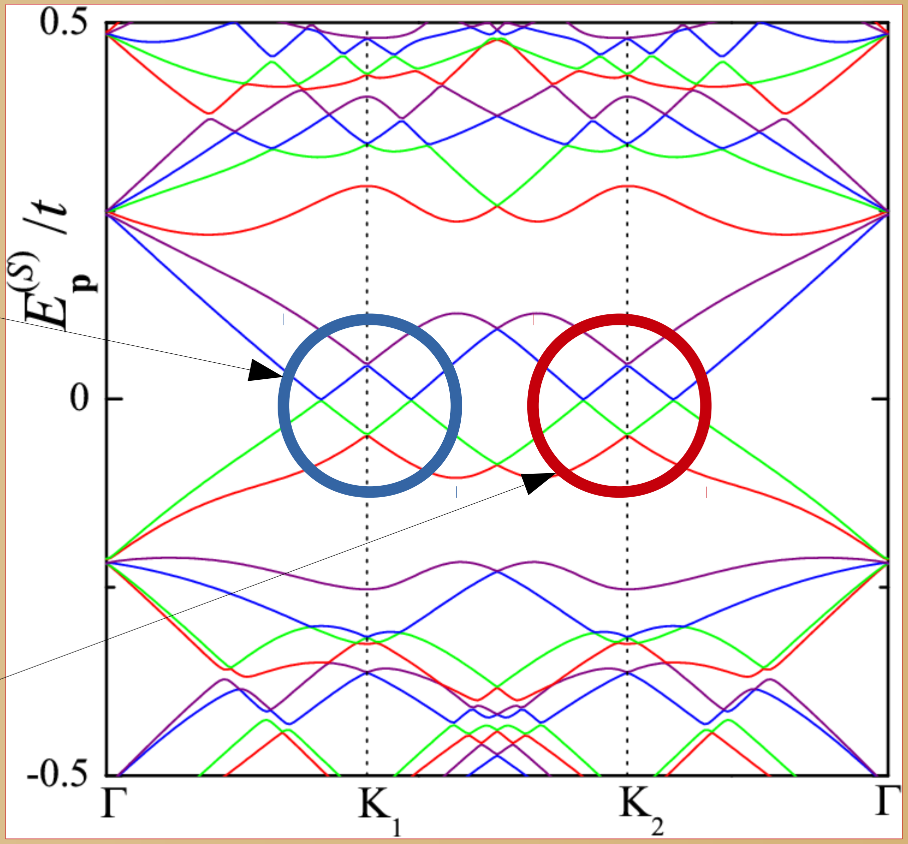
$$\hat{H}_{\rm int} = \frac{1}{2}\sum_{\substack{i\mathbf{n}j\mathbf{m}\\ ss'\sigma\sigma'}} \hat{d}^{\dagger}_{\mathbf{n}is\sigma}\hat{d}_{\mathbf{n}is\sigma}U_{ij}(\mathbf{r}_{\mathbf{n}}^{is} - \mathbf{r}_{\mathbf{m}}^{js'})\hat{d}^{\dagger}_{\mathbf{m}js'\sigma'}\hat{d}_{\mathbf{m}js'\sigma'}$$

# Some more technical remarks

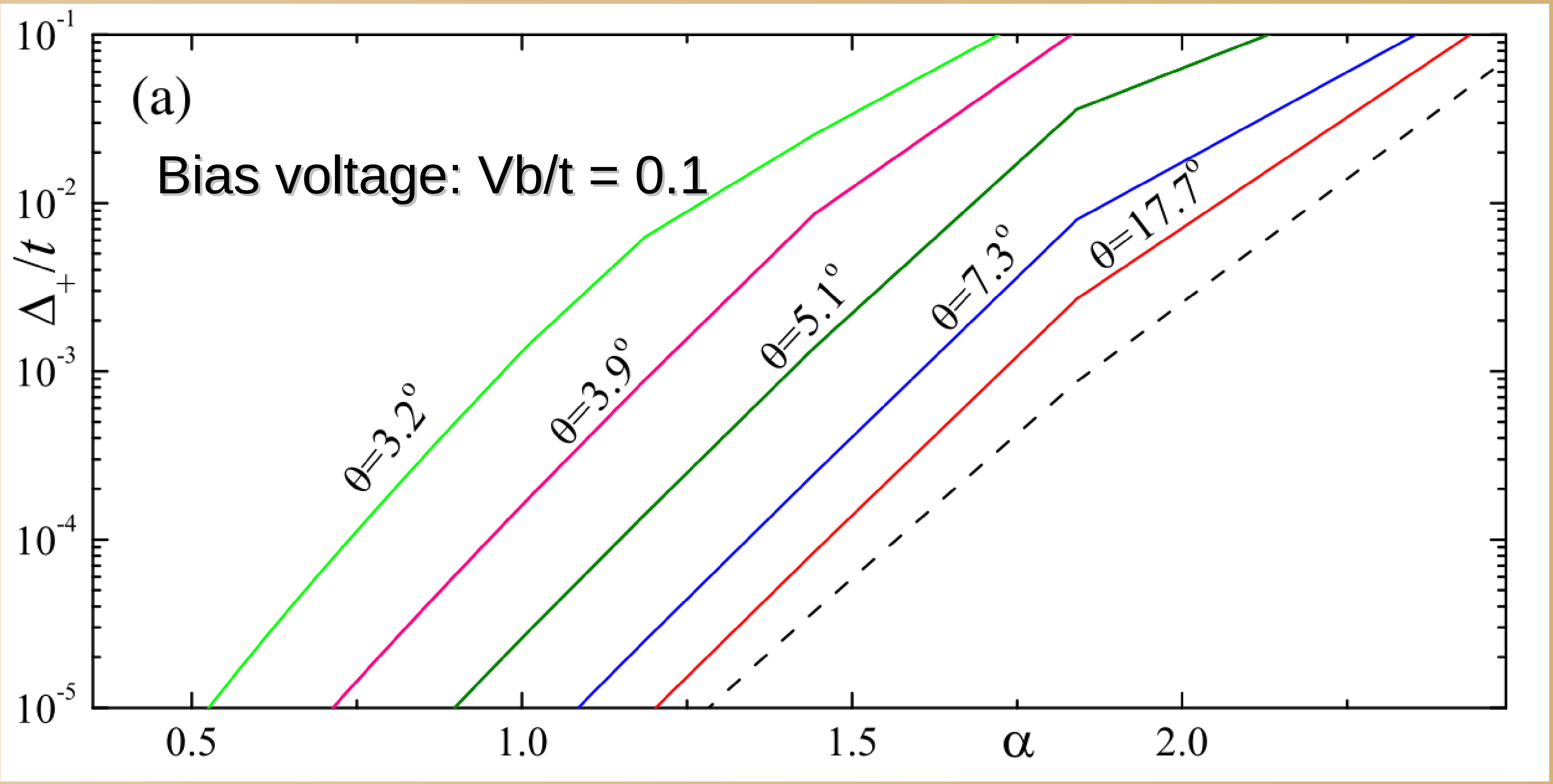
Order parameter  is of SDW type
two such order parameters (one per Dirac point)

One order parameter
lives here

Another order parameters
lives here

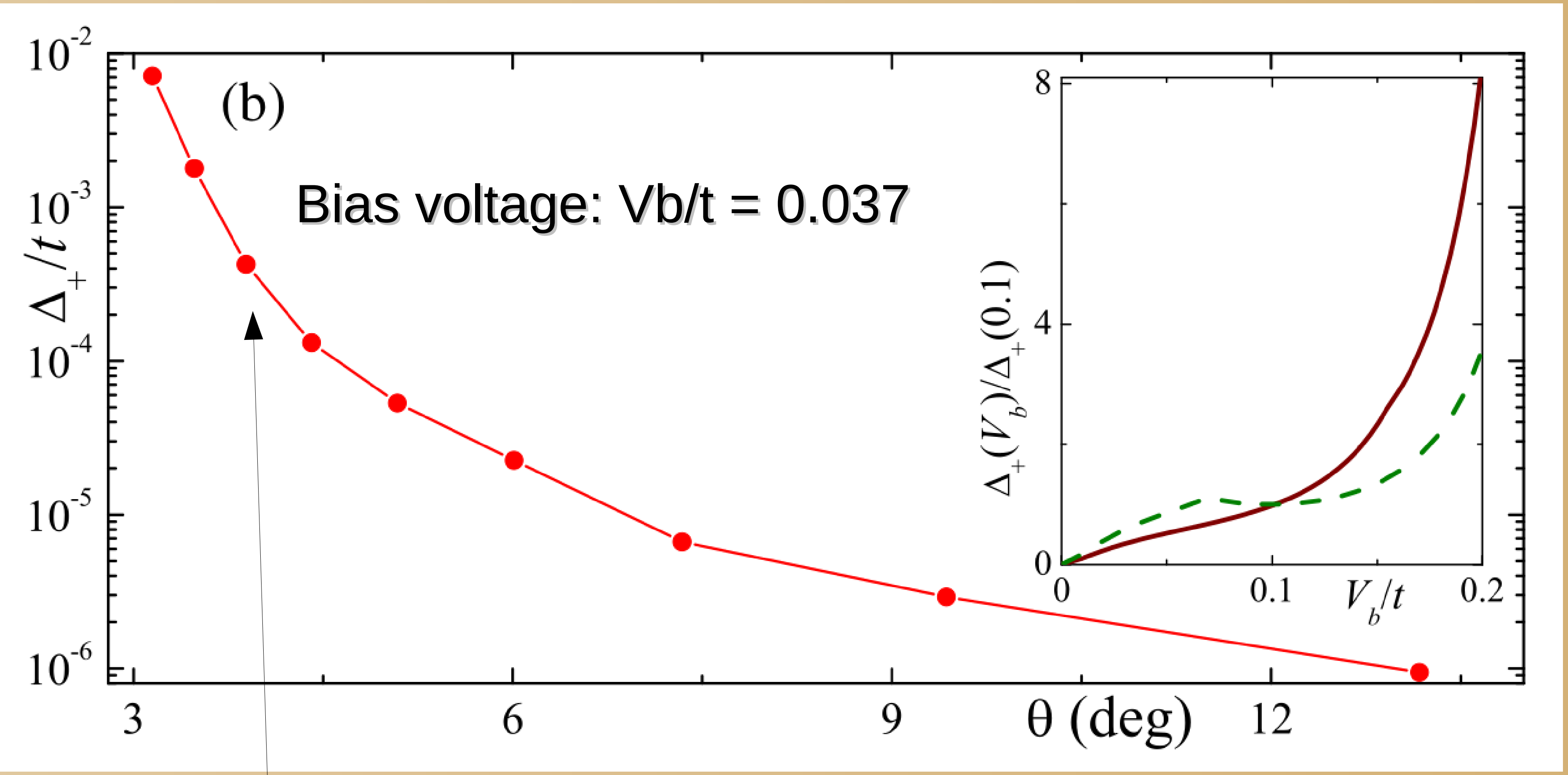


# Results



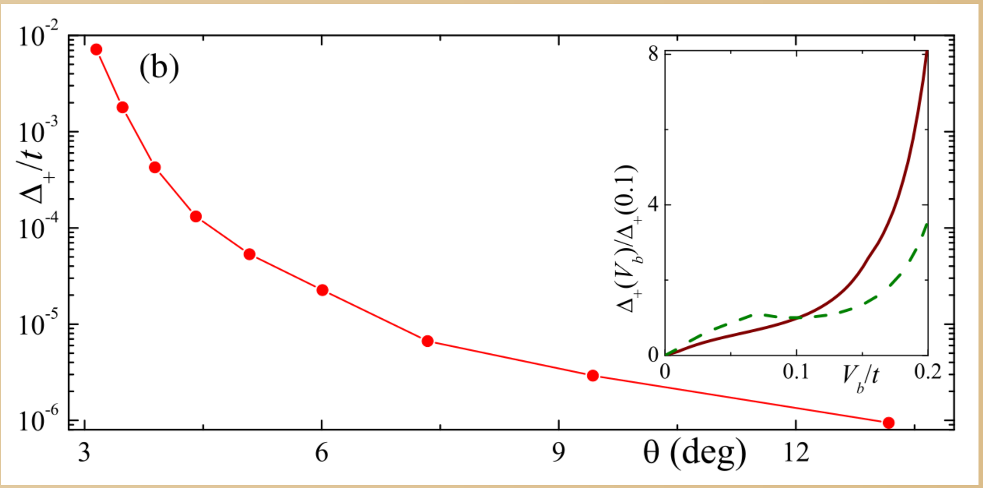
(a)
Bias voltage: Vb/t = 0.1
θ=3.2°
θ=3.9°
θ=5.1°
θ=7.3°
θ=17.7°
Δ+/t
α
10-1
10-2
10-3
10-4
10-5
0.5
1.0
1.5
2.0

# Results

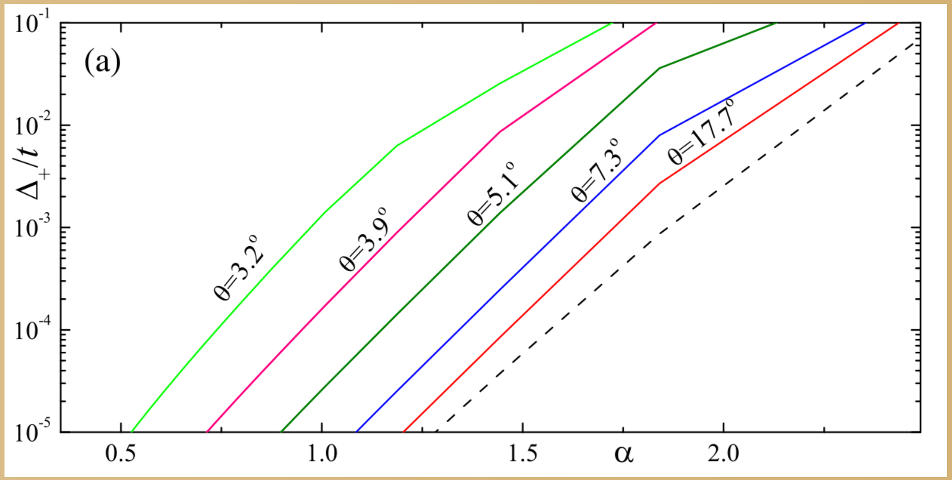



Effect of low Fermi velocity

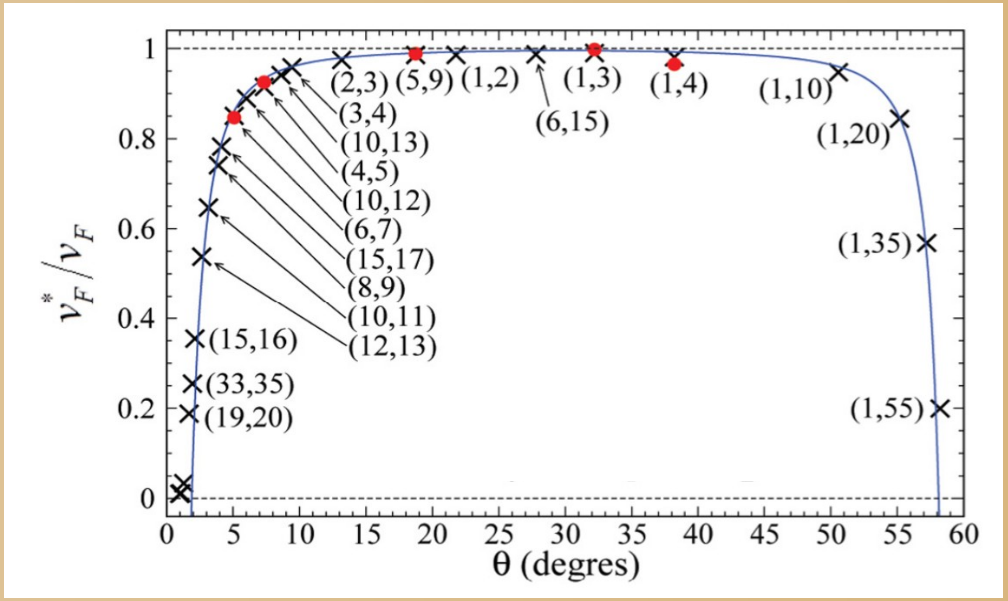
# Results



(b)
$\Delta_+/t$
θ (deg)
$\Delta_+(V_b)/\Delta_+(0.1)$
$V_b/t$

(a)
$\Delta_+/t$
α
θ=3.2°
θ=3.9°
θ=5.1°
θ=7.3°
θ=17.7°

$v_F^*/v_F$
θ (degres)
(2,3)
(5,9)
(1,2)
(1,3)
(1,4)
(6,15)
(1,10)
(1,20)
(1,35)
(1,55)
(3,4)
(10,13)
(4,5)
(10,12)
(6,7)
(15,17)
(8,9)
(10,11)
(12,13)
(15,16)
(33,35)
(19,20)

# Results: magnetism

Two SDW order parameters (one per Dirac point) => interference

# Conclusions

– Effect of the bias: nested Fermi surface

– Insulating gap + interference of 2 magnetic orders