ARPES studies of magnetic phases in parents of iron-based superconductors

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A surprise in 2008 : iron based superconductors

J|A|C|S COMMUNICATIONS

Published on Web 02/23/2008

Iron-Based Layered Superconductor $La[O_{1-x}F_x]FeAs$ ($x = 0.05-0.12$) with $T_c = 26$ K

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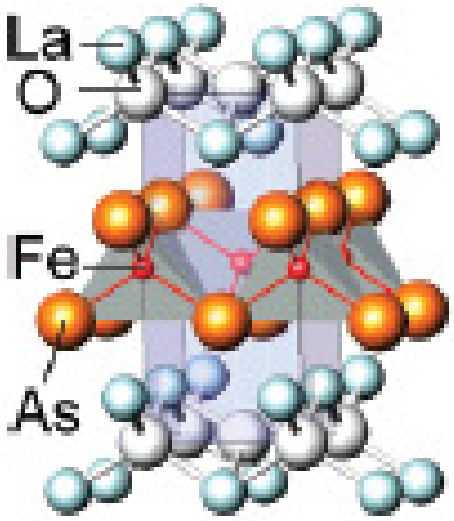


=> 55K in $Sm(O_{1-x}F_x)FeAs$

Ren et al., Chinese Phys. Letters April 2008

- Electron-phonon coupling is expected and calculated to be weak (λ=0,2) !

  L. Boeri et al., PRL 2008

- Unconventional superconductivity ? Magnetic pairing ??

- Similar to cuprates ?

Outline

- What can we learn about magnetism by studying the electronic structure ?

- How can we learn about the electronic structure ?

  => Angle Resolved PhotoElectron Spectroscopy (ARPES)

- Itinerant or localized magnetism in iron pnictides ?

  Almost all magnetic phases are metallic, but they are correlated and cannot be described by a simple spin density wave picture.

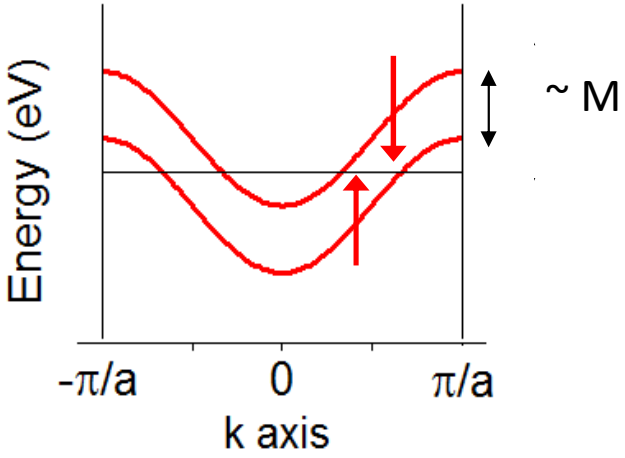
  => $BaFe_2As_2$ (T_N=140K) : the AF ordering corresponds to good FS nesting

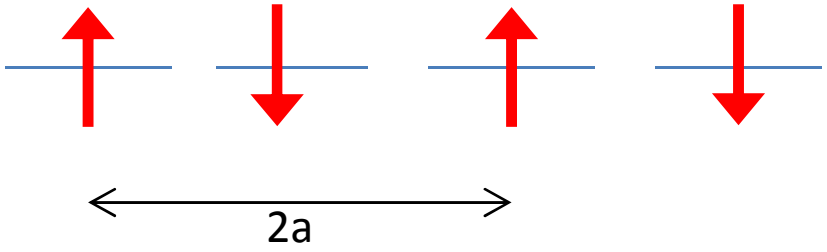
  => FeTe (T_N=76K) : the AF ordering does not correspond to FS nesting

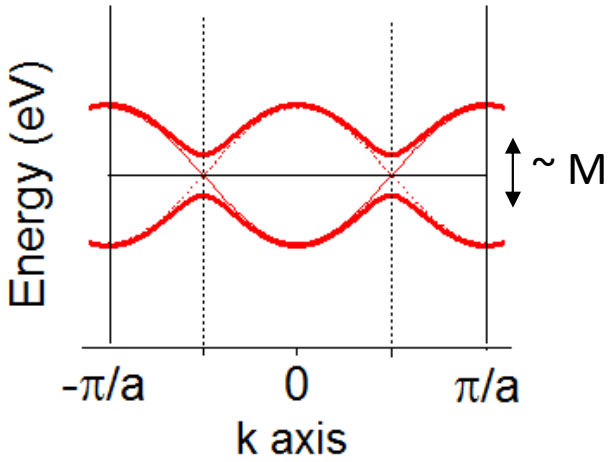
  => $CaCo_2As_2$ (T_N=72K) : ferromagnetic ordering in the planes

  => see poster by J. Mansart

What can we learn about magnetism by studying the electronic structure ?

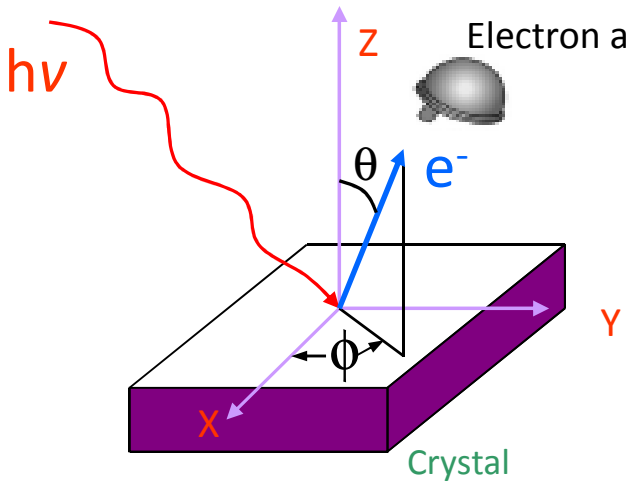






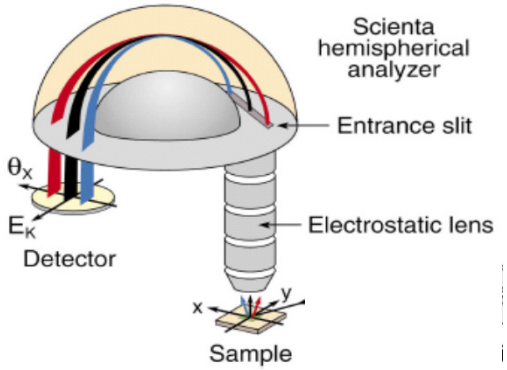
How can we learn about the electronic structure ?

ARPES : Angle Resolved PhotoElectron Spectroscopy

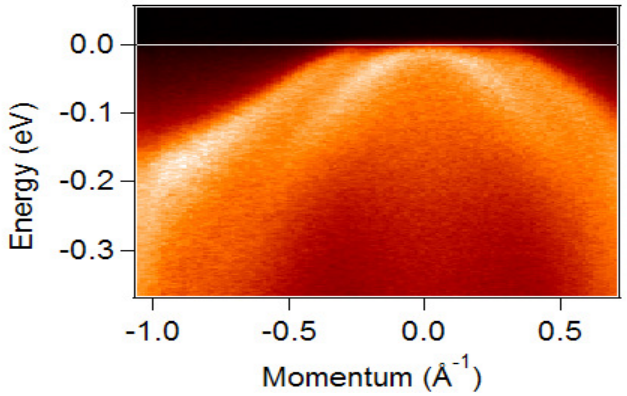


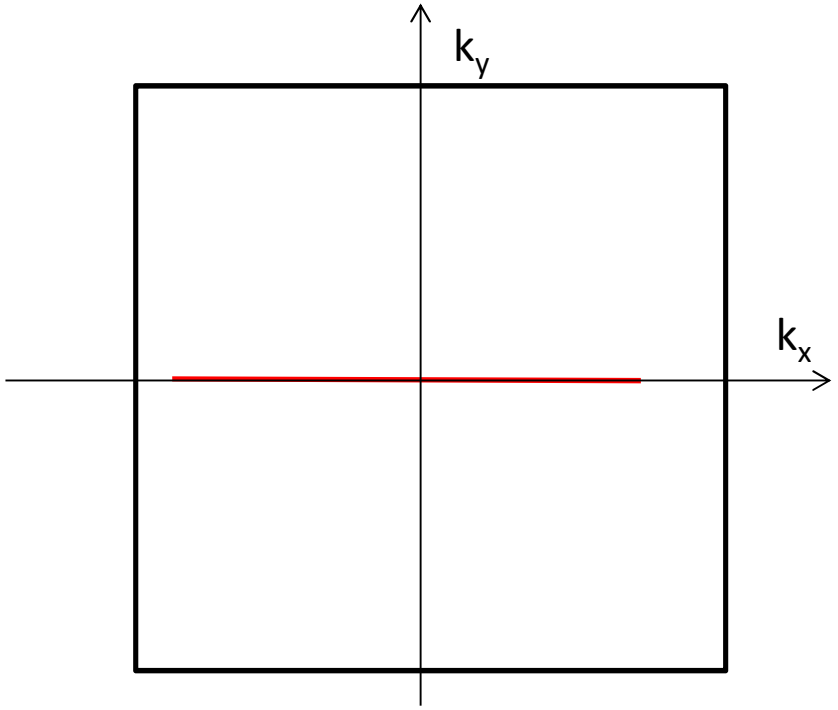
$$E_{kin} = h\nu - W - |E_B|$$

$$\hbar \mathbf{k}_{\parallel} = \sqrt{2mE_{kin}} \sin\theta$$



Hole pockets





How can we learn about the electronic structure ?

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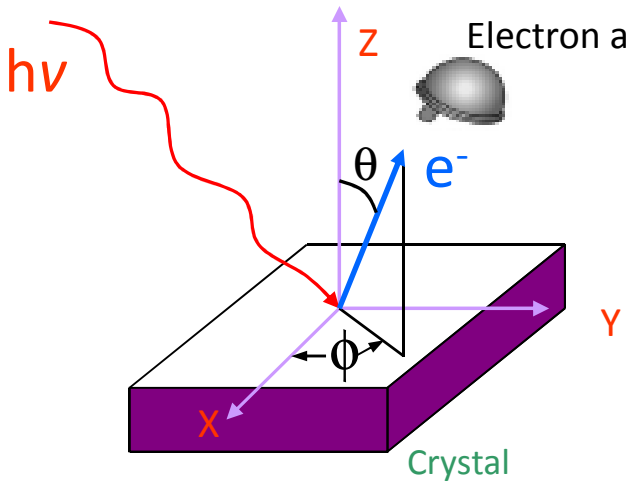

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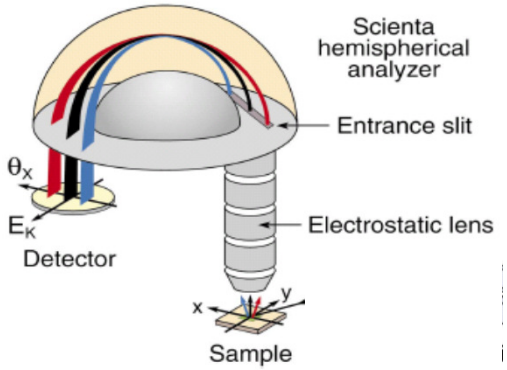
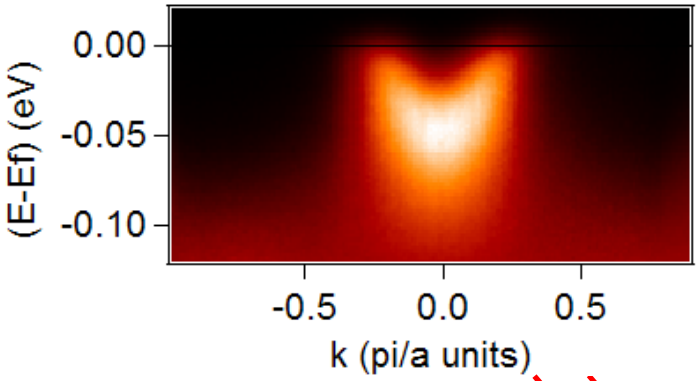
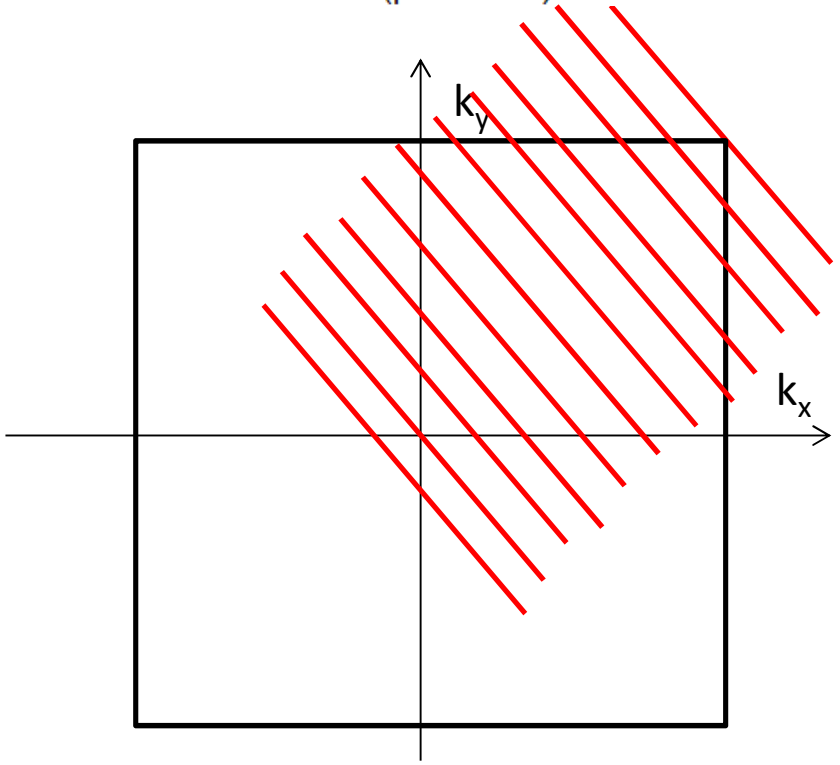
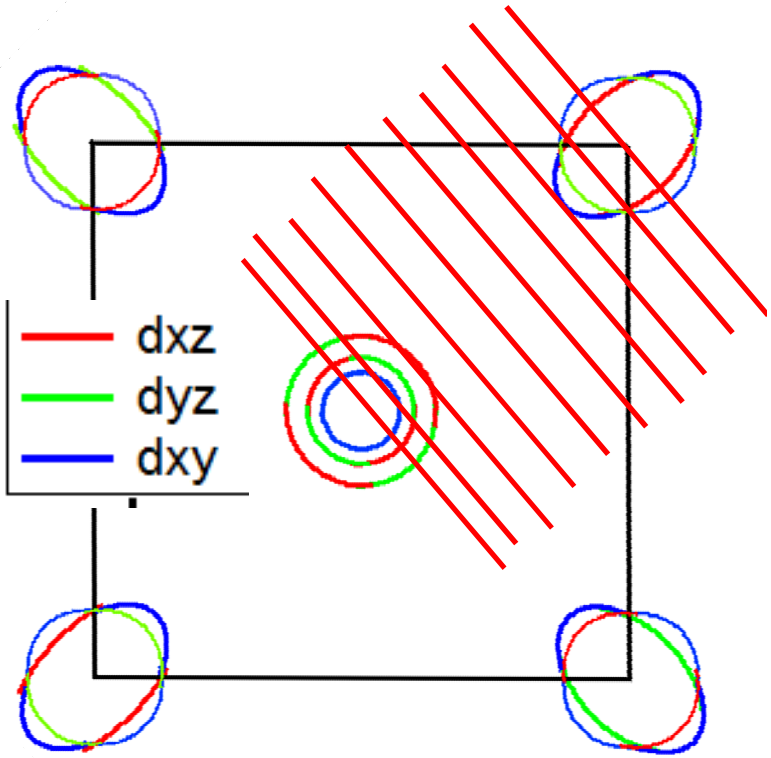


Electron pocket

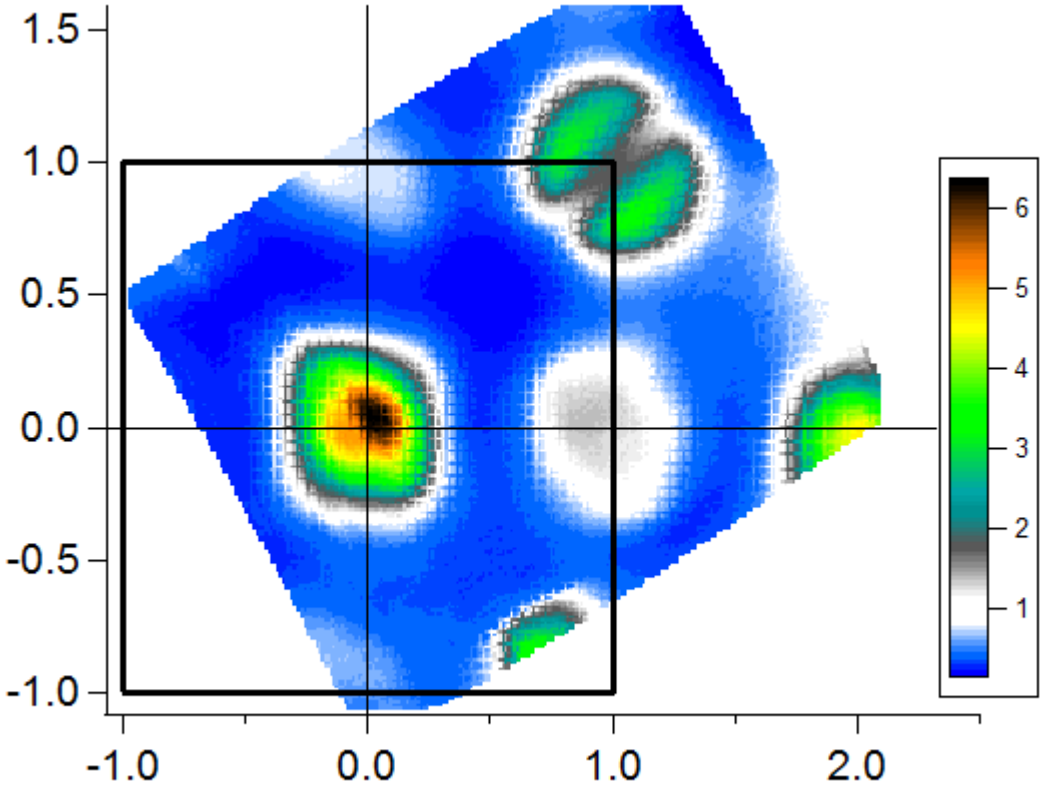




How can we learn about the electronic structure ?

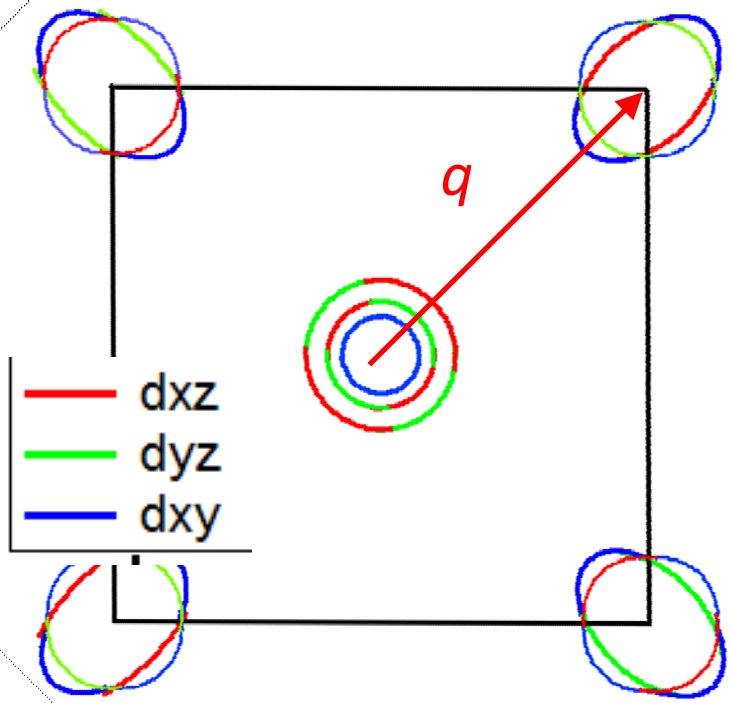


Fermi Surface

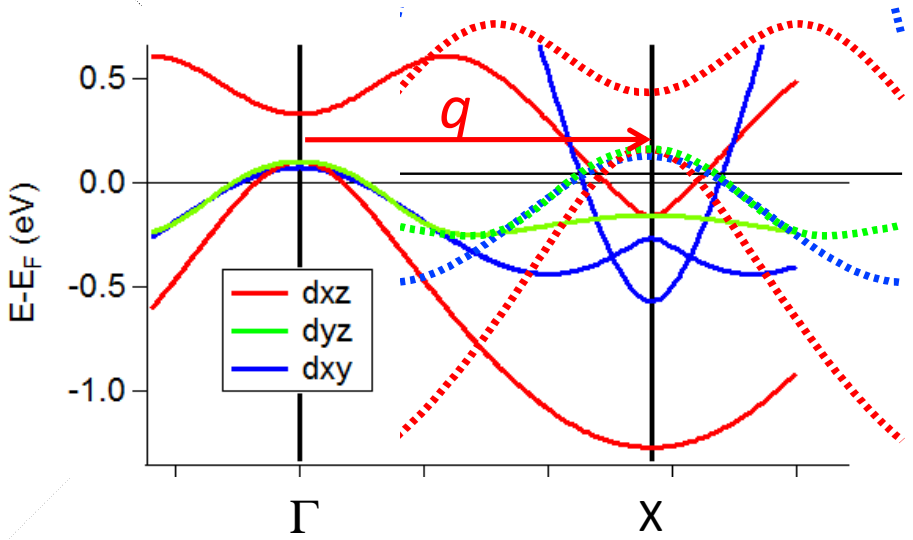


The Fermi Surface is made out of small hole and electron pockets made out of at least three different orbitals.

How can we learn about the electronic structure ?



Band structure along diagonal

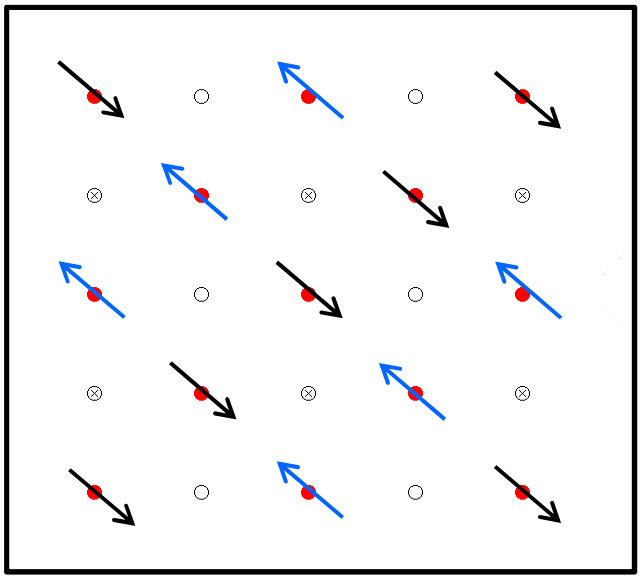


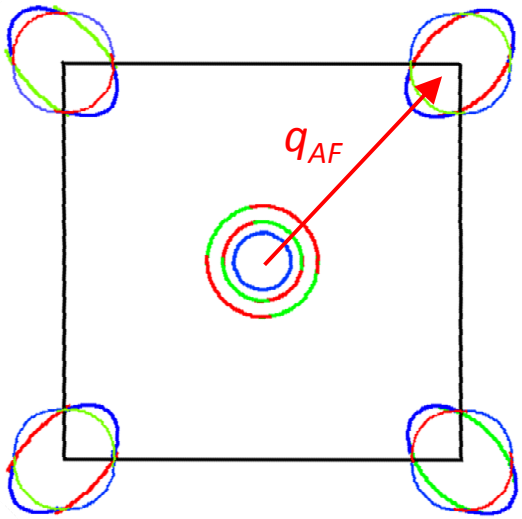
=> Good nesting between hole and electron pockets for q=(π, π)

6e$^-$/Fe

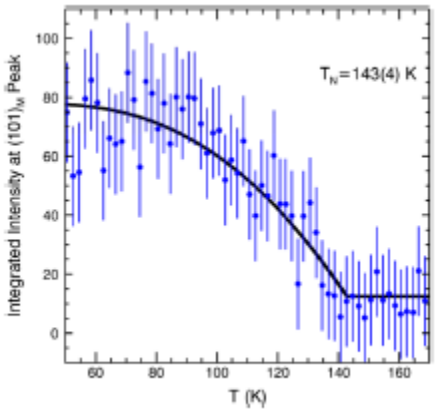
The Fermi Surface is made out of small hole and electron pockets made out of at least three different orbitals.

$BaFe_2As_2$: magnetic order at (π, π)





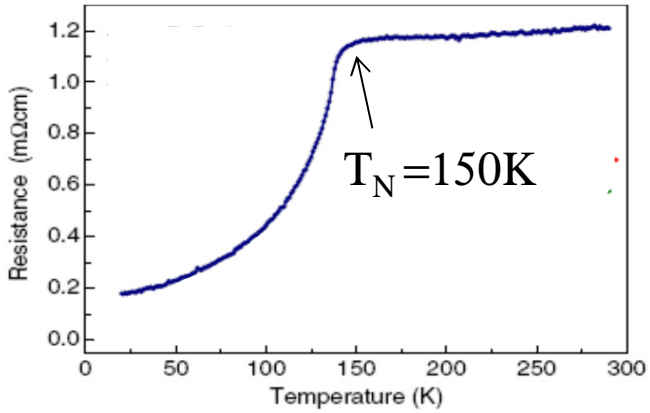
Neutrons



$Q_{AF} = (\pi,\pi)$
$M = 0,87\ \mu_B$

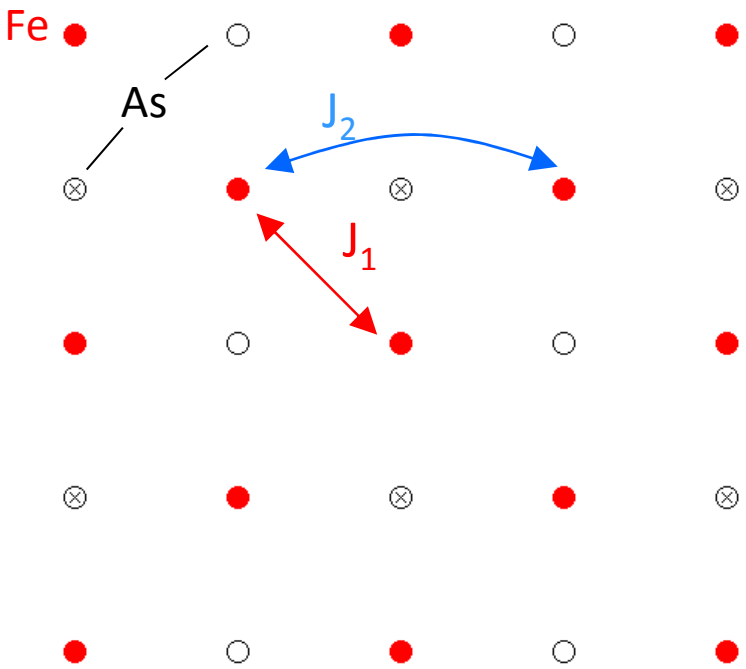
Huang et al., PRL 2008

Resistivity



Localized magnetism point of view

Magnetic ordering patterns can also be understood from localized picture



- *Frustrated* AF interactions :

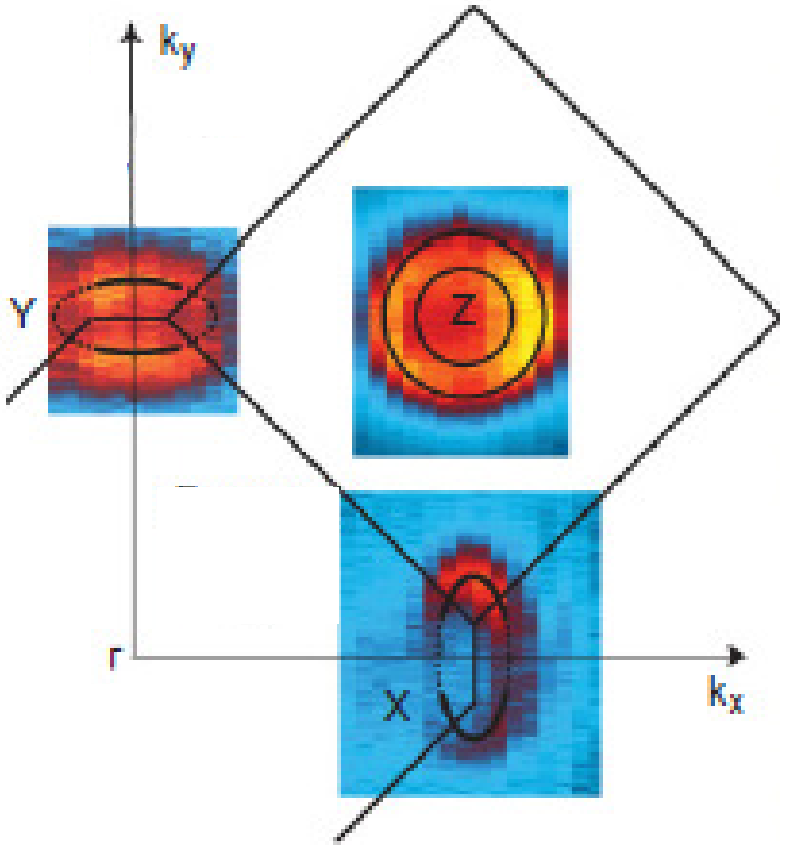
  => Checkerboard for $J_1 > 2J_2$

  => Stripe for $J_2 > J_1/2$

  Yildirim, PRL2008

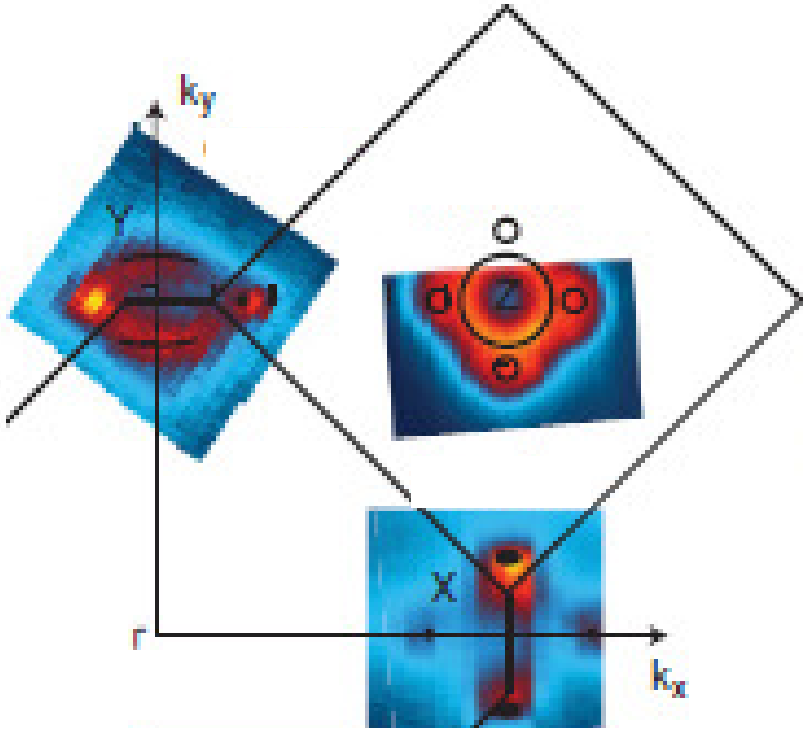
Fermi Surface in $BaFe_2As_2$ across T_{mag}

Fermi Surface at 150K



Fermi Surface at 20K

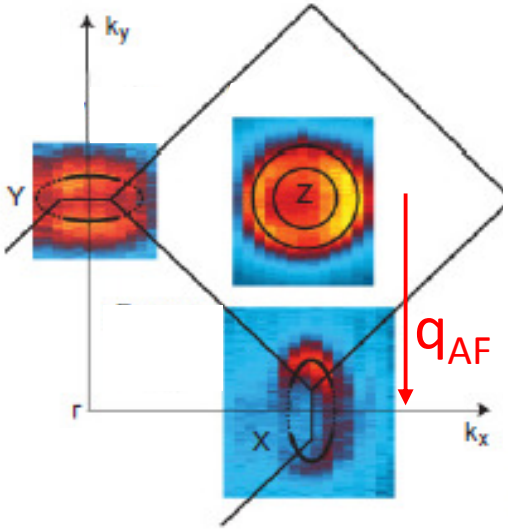
« droplets » *[de Jong, EPL10]*

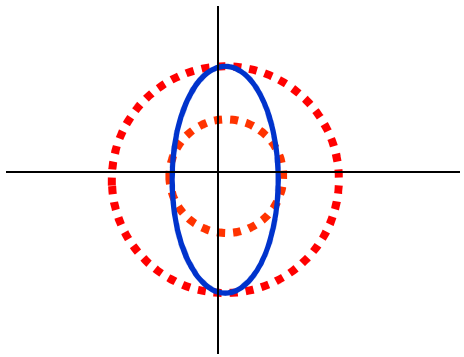


M.F. Jensen, V. Brouet et al, PRB 2011

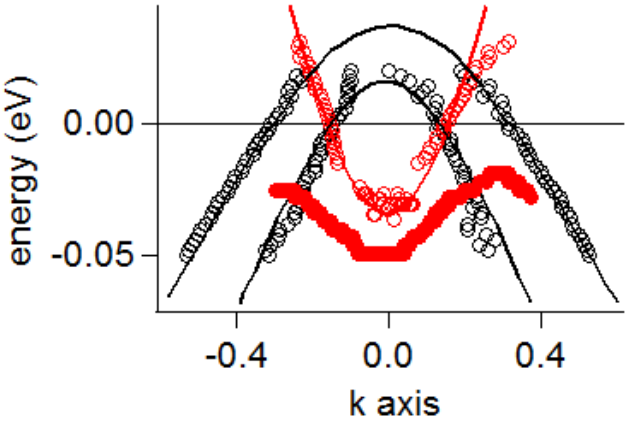
Nesting of hole and electron pockets in $BaFe_2As_2$

Fermi Surface at 150K

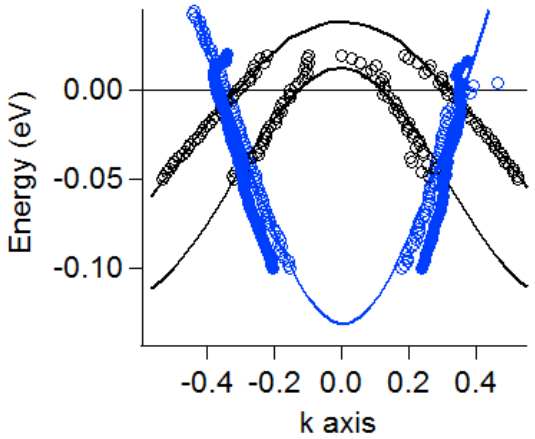




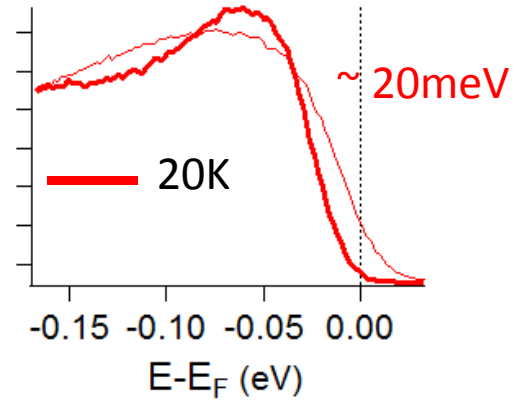
Minor ellipse axis

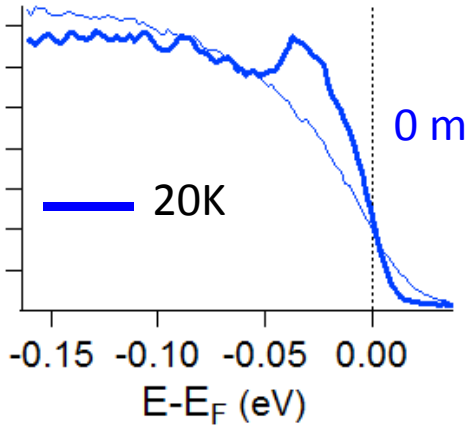


Major ellipse axis



Gap from ARPES spectra

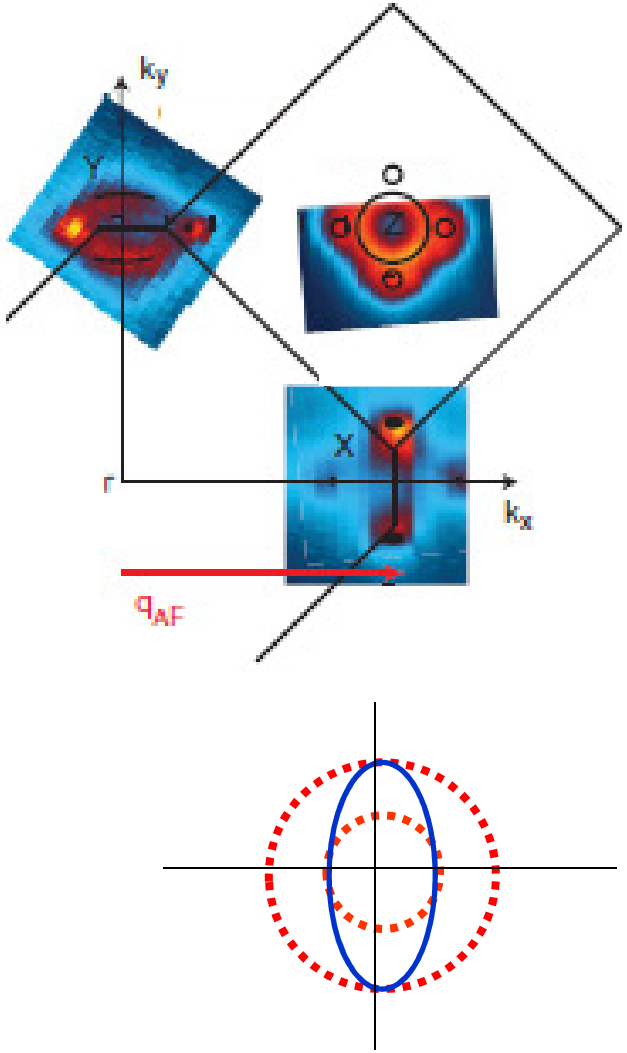




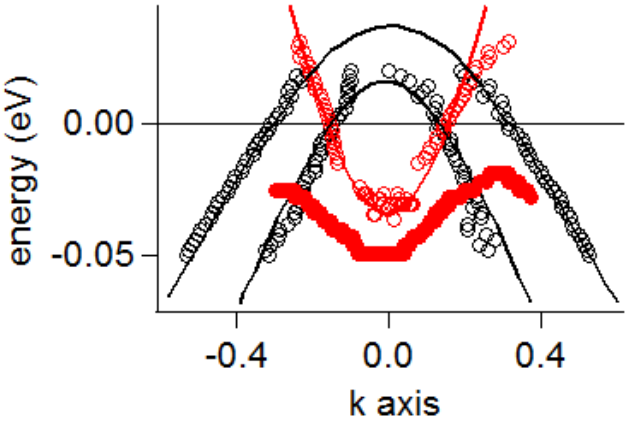
M.F. Jensen, V. Brouet et al, PRB 2011

Nesting of hole and electron pockets in $BaFe_2As_2$

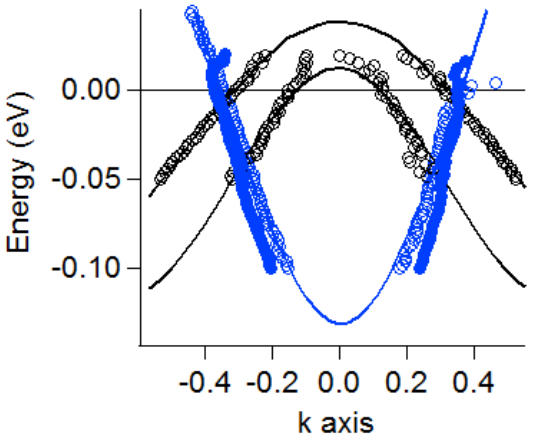
Fermi Surface at 20K



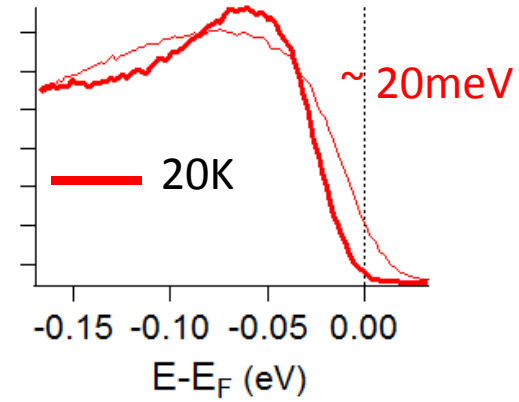
Minor ellipse axis

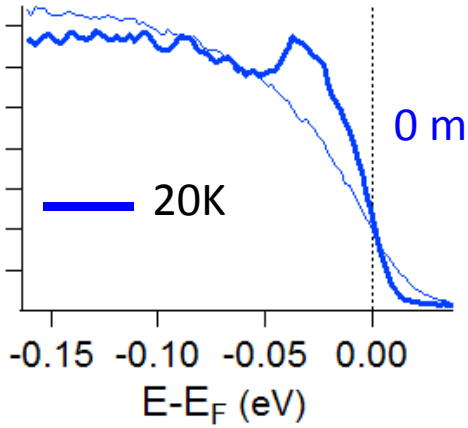


Major ellipse axis



Gap from ARPES spectra

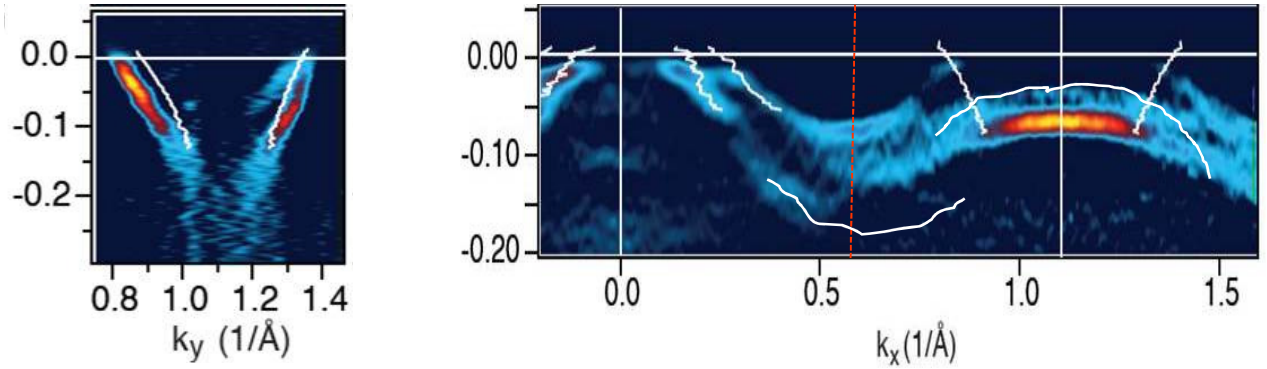




M.F. Jensen, V. Brouet et al, PRB 2011

Reconstruction beyond nesting

Band move with respect to PM state

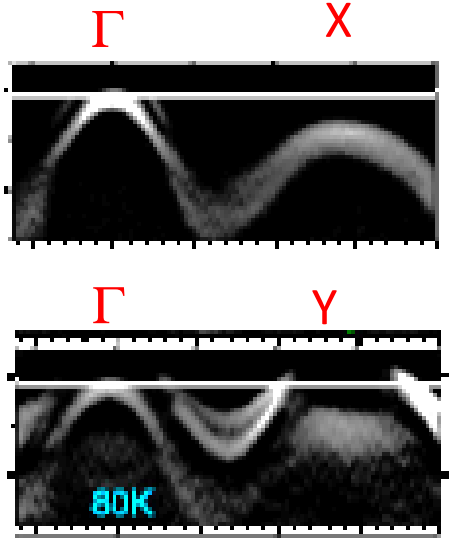


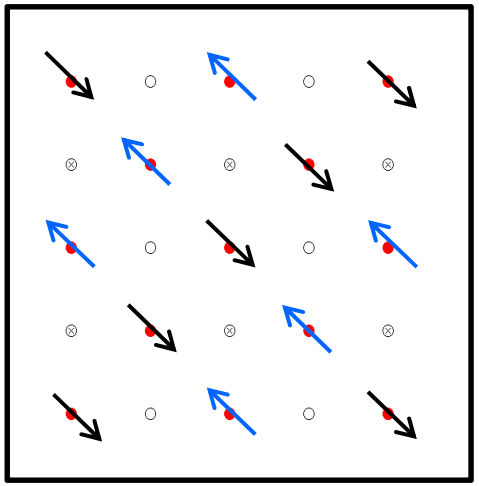
=> Gaps and shifts of bands have a similar order of magnitude (20-30meV). They stabilize equally the AFM state.

See M.D. Johannes and I.I. Mazin, PRB 2009

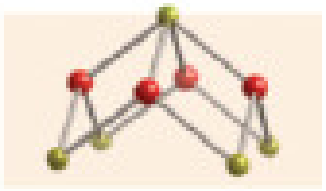
Orbital ordering between d_{xz} and d_{yz}

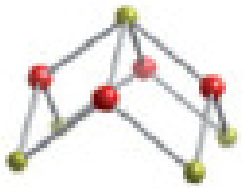
Detwinned experiment
Yi, Shen et al., PNAS 2011



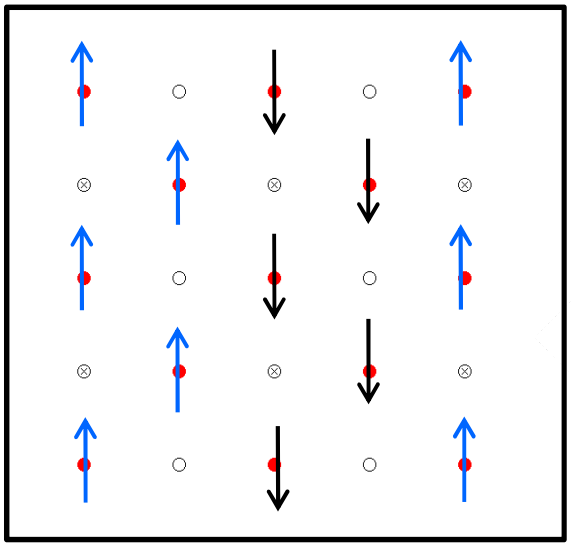


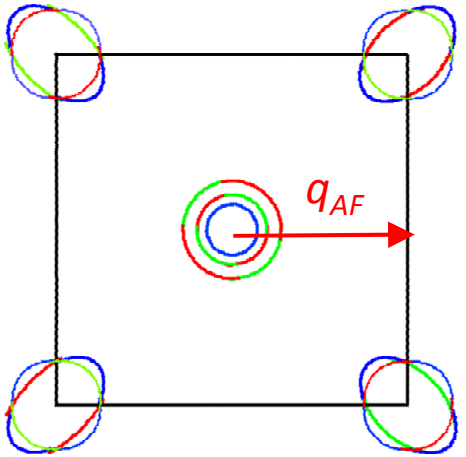
Magnetic order in FeTe



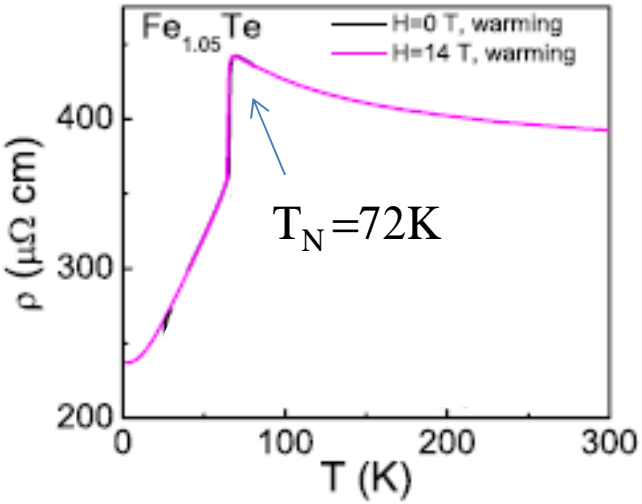


FeTe





Resistivity



Chen, PRB 2009

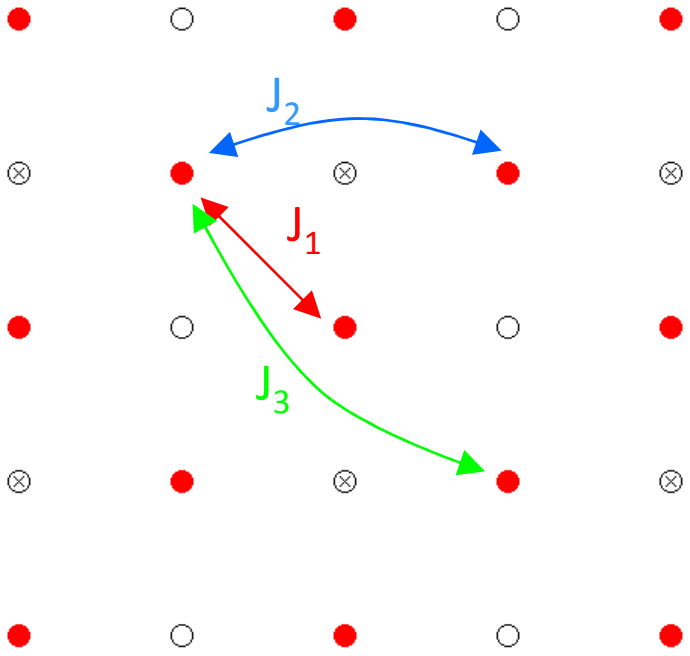
Much larger magnetic moment

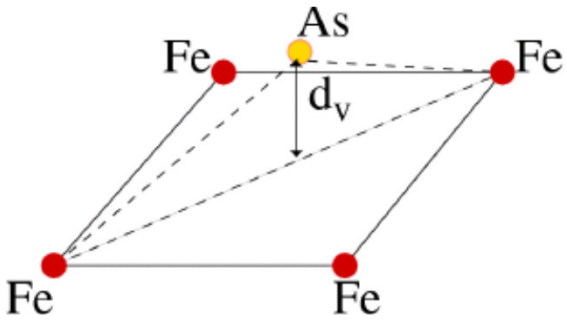
=> M=2,1μ_B

Bao, PRL 2009

Localized magnetism point of view

Magnetic ordering patterns can also be understood from localized picture





- *Frustrated* AF interactions :

  => Checkerboard for $J_1 > 2J_2$

  => Stripe for $J_2 > J_1/2$

  Yildirim, PRL2008

- At high d_v

  J_1 and J_2 decrease

  J_3 increase

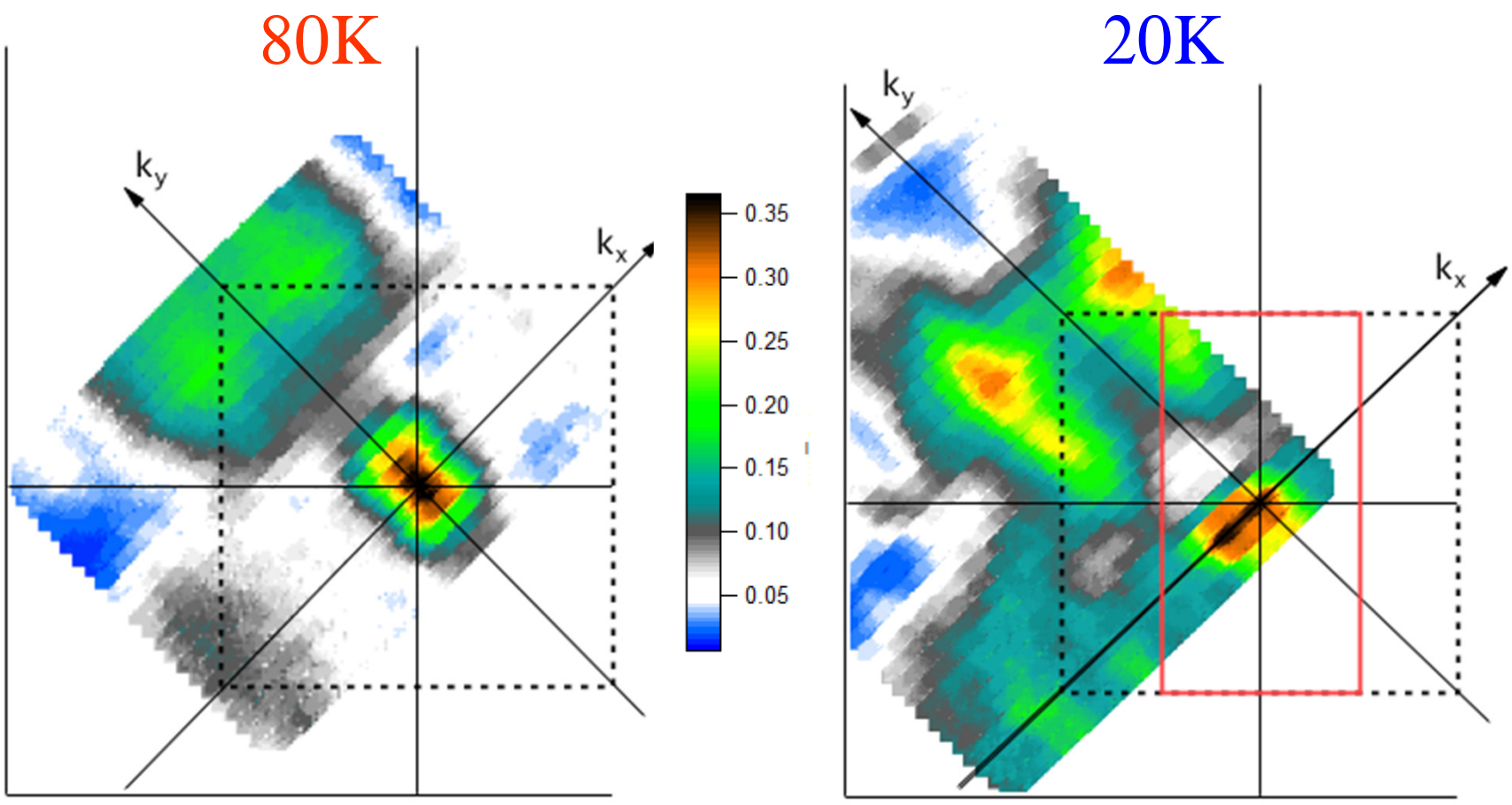
  => Double stripe for $J_3 > J_2/2$

  Ma et al.,PRL2009

  Moon and Choi, PRL2010

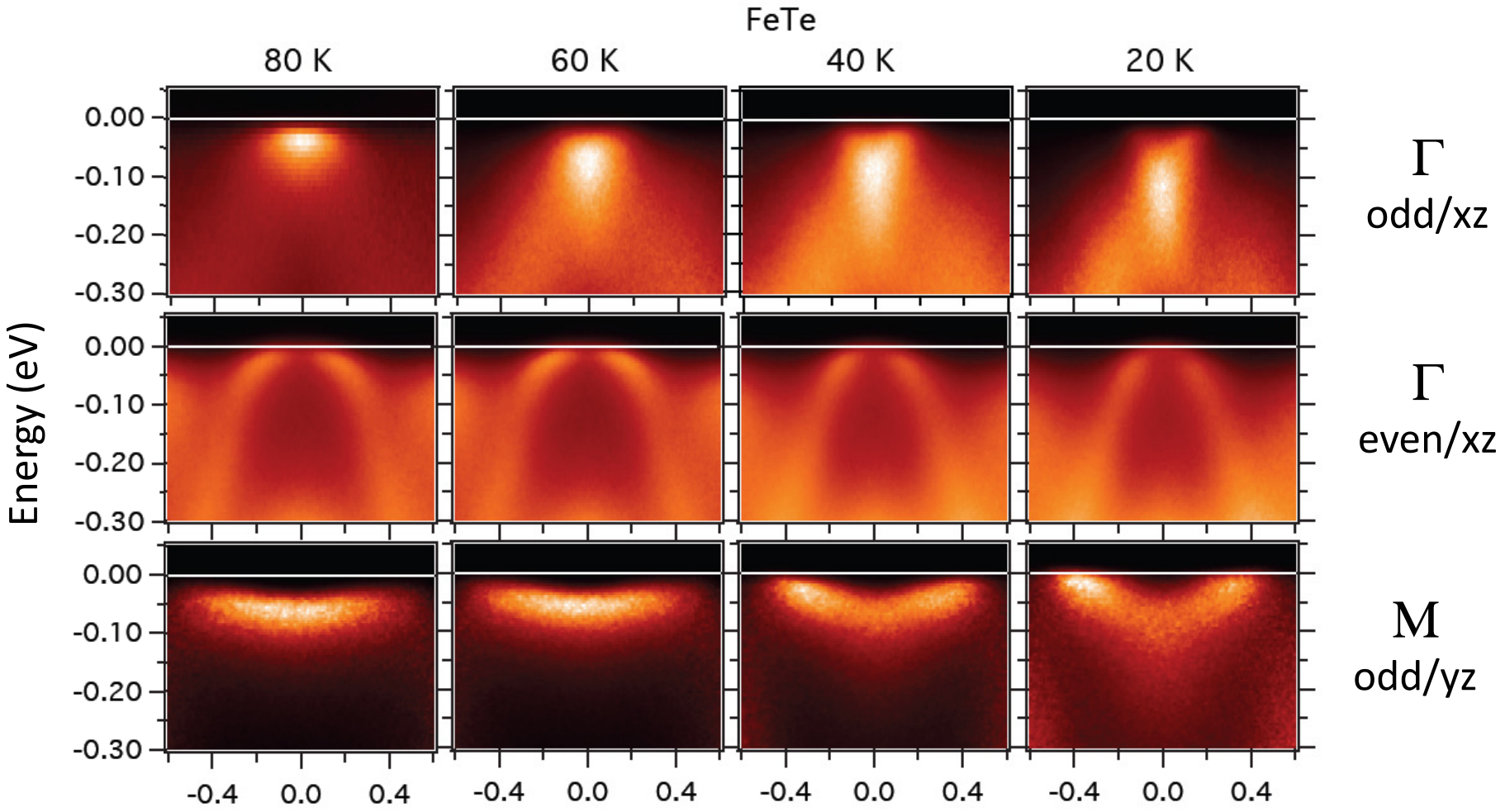
Fermi Surface through the magnetic transition

See also : Zhang et al., PRB 2012
Liu et al., PRL 2013



Different evolution compared to $BaFe_2As_2$: no « droplets »

Evolution of the different bands

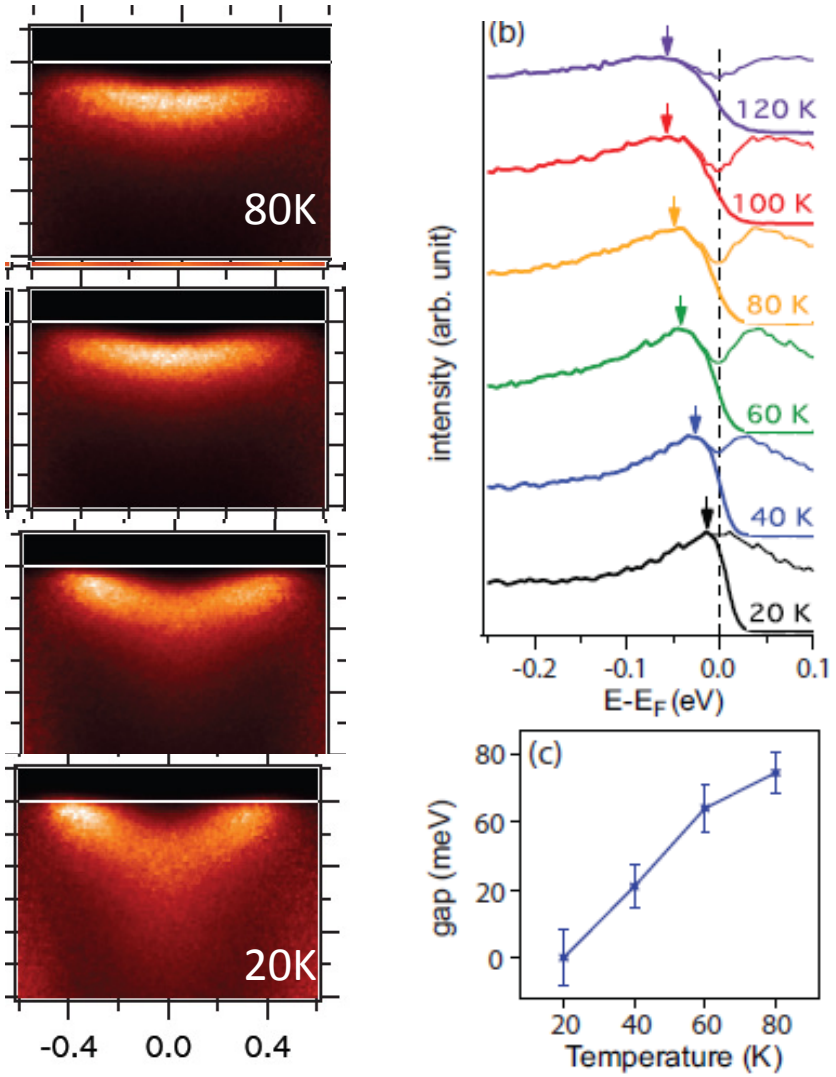


⇒ No folded band, no gap opening

⇒ Shift of some bands and changes in lineshapes

P.H. Lin et al., to appear in Phys. Rev. Letters

« Pseudogap » on the electron pocket

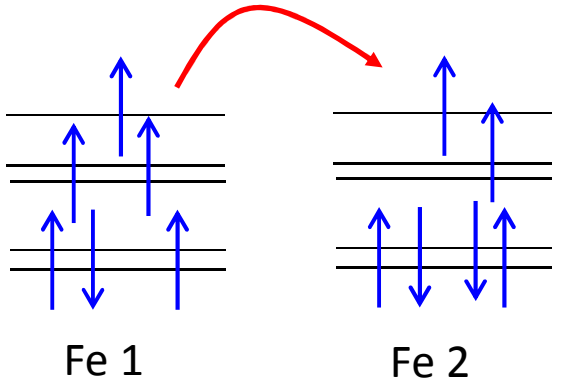


P.H. Lin et al., to appear in Phys. Rev. Letters

- The pseudogap explains very well the « bad metallic behavior » in the PM state.

- It shows that magnetic fluctuations are detrimental to metallicity

« Hund's metals » : new type of correlations due to the interplay between local moment and itinerancy



K. Haule and G Kotliar, New J. of Phys. 2009
L. deMedici, Mravlje, Georges, PRL 2011

Conclusions

=> Very different reconstruction of the electronic structure are observed with ARPES, where nesting does not play the leading role.

=> The formation of magnetic moment is mostly a local effect, but the magnetic structure optimizes conducting channel.

=> New types of correlations emerge form this particular magnetic background.