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SAPIENZA UNIVERSITÀ DI ROMA

Interplay between orbital degrees of freedom and spin fluctuations in the nematic phase of iron-based superconductors

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14 July 2016

Collaborations

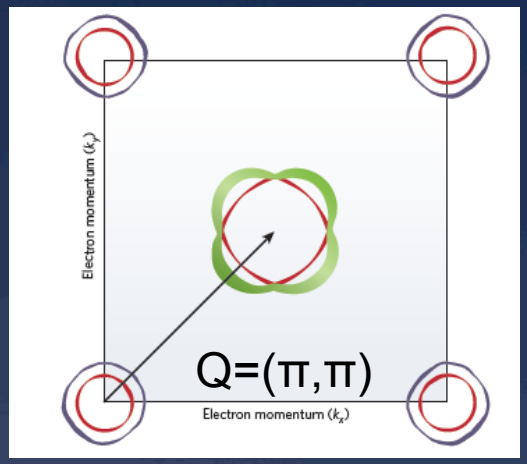
* Theory:
  * Emmanuele Cappelluti (Rome)
  * Laura Fanfarillo (SISSA Trieste)
  * Belen Valenzula (CSIC Madrid)

* Experiments:
  * Veronique Brouet (CNRS Orsay Paris)

What is new in pnictides?

* Multiband systems

(already seen in MgB2, graphene, etc.)



* Proximity/coexistence with an AF phase, possible relevance of spin-fluctuations mediated interactions

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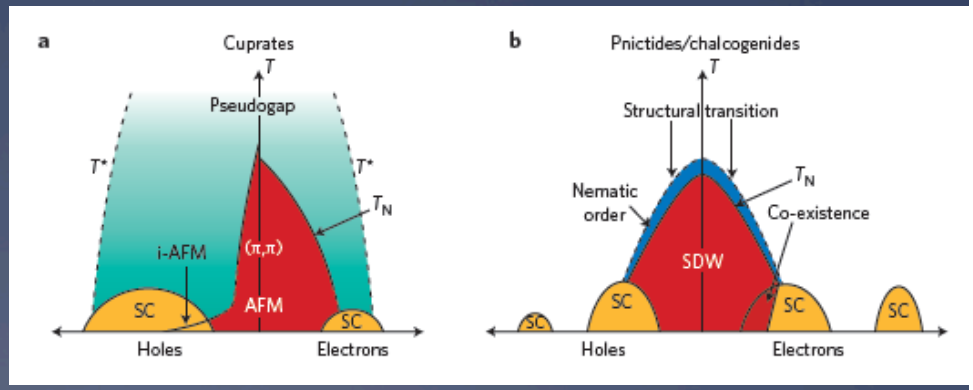
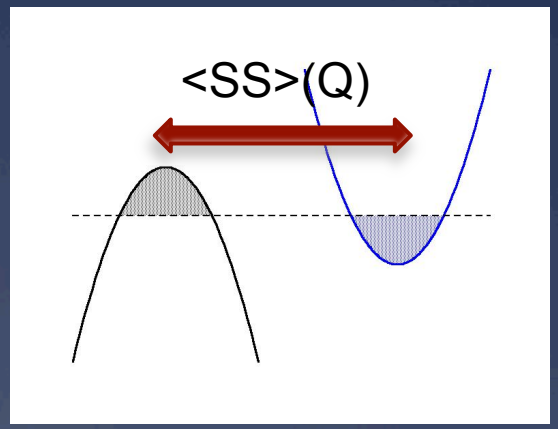


What is new in pnictides?

* Multiband systems

(already seen in MgB2, graphene, etc.) → Coexistence of **hole** and **electron** bands



* Proximity/coexistence with an AF phase, possible relevance of spin-fluctuations mediated interactions

(already seen in heavy fermions, cuprates, etc.) → Interband interaction

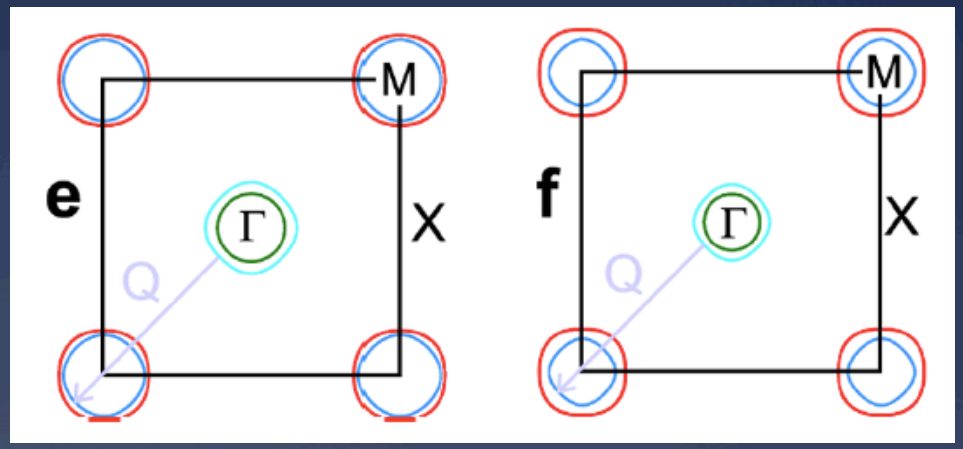
More
(interacting
electron-hole bands)
is different!

Fermi-surface shrinking

- De Haas Van Alphen experiments measure the Fermi surface areas for various bands

A. Coldea et al., Phys. Rev. Lett. **101**, 216402 (2008)

unshifted LDA shifted LDA



- Shrinking of all the FS with respect to DFT
- Total number of particles is still conserved

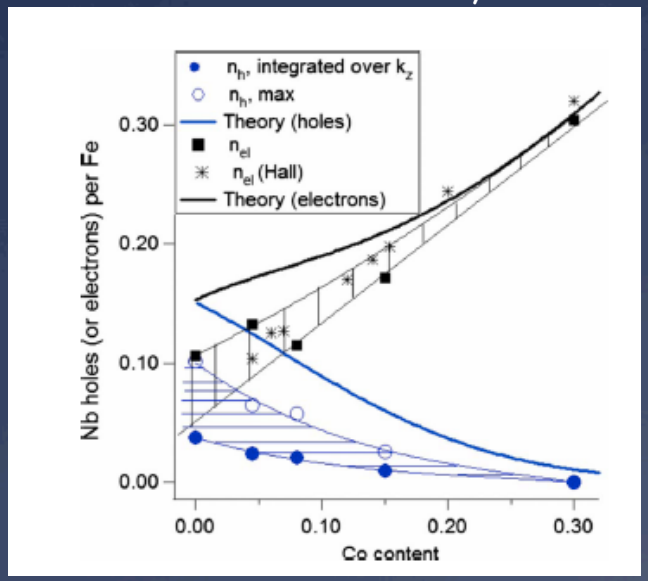
$n=n_e+(2-n_h)$

n_e-n_h is conserved, not n_e+n_h

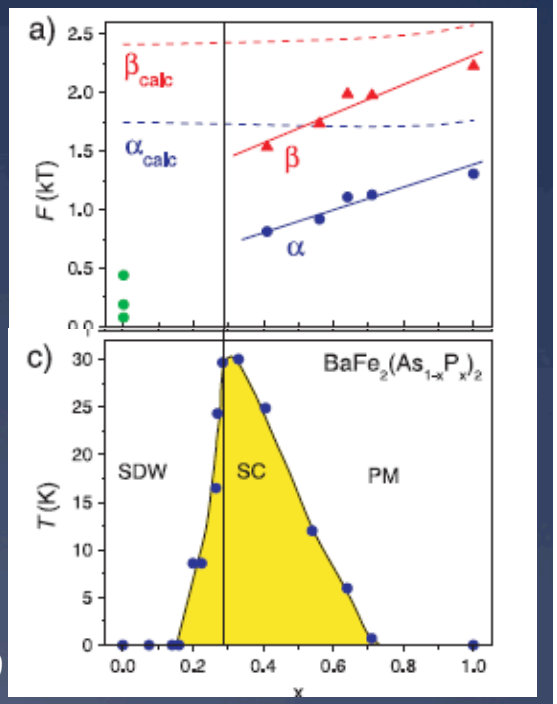
Fermi-surface shrinking

* Both dHvA and ARPES show a **systematic** shrinking of the Fermi surface that can hardly be understood as a systematic inaccuracy of DFT

V. Brouet et al. PRB 2009, PRL2013



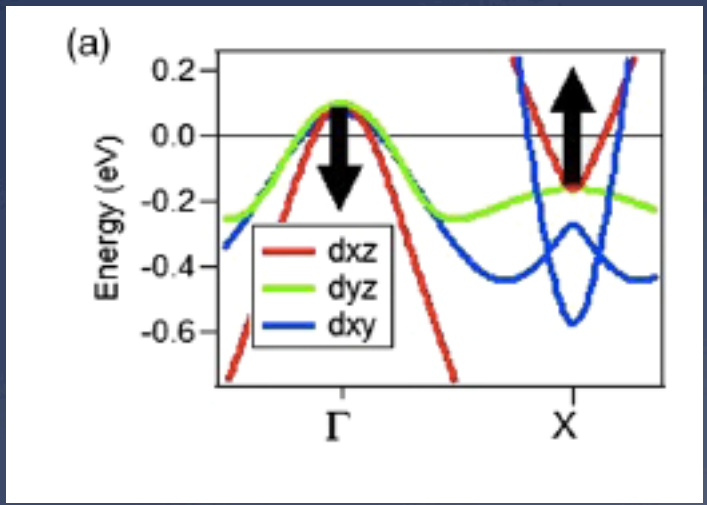
H. Shishido et al. PRL 2010

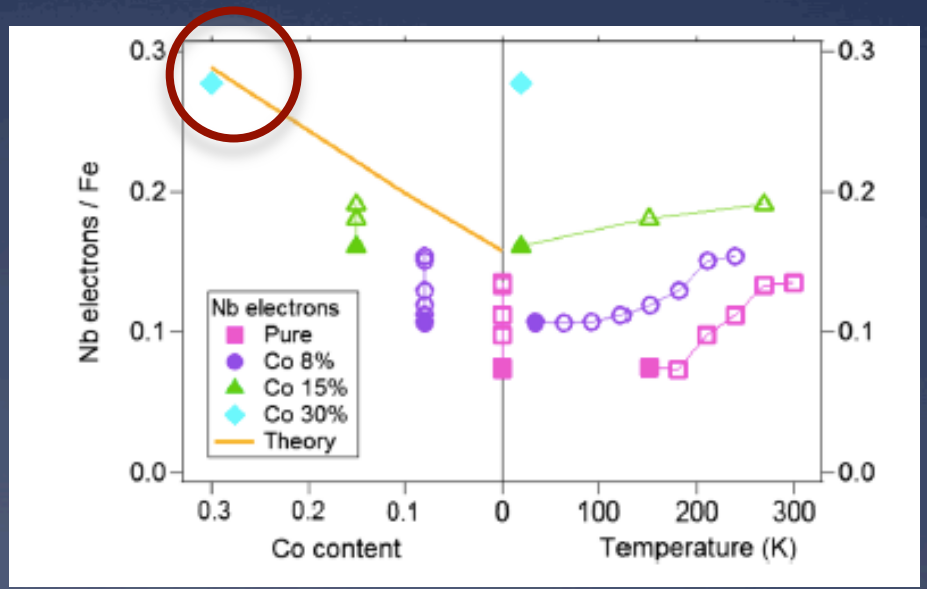


Fermi-surface shrinking

* The effect is stronger at lower doping and lower temperatures. In e-doped 122 it disappears when hole pockets are completely filled

Ba(Fe1-xCox)2As2
V. Brouet et al., PRL 110, 167002 2013





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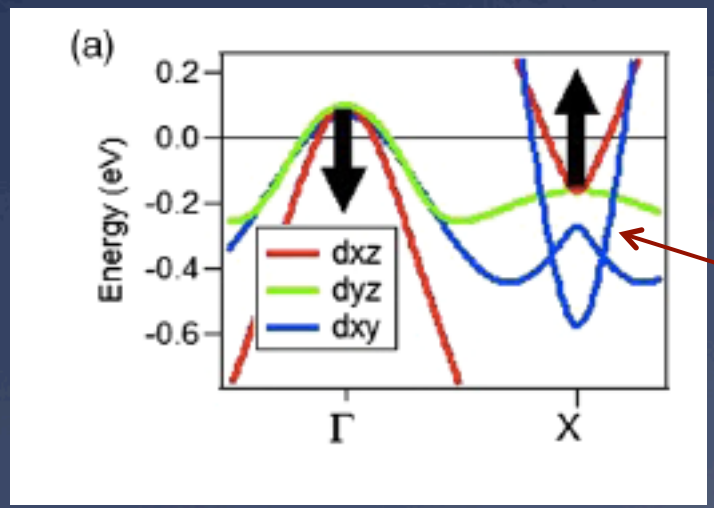


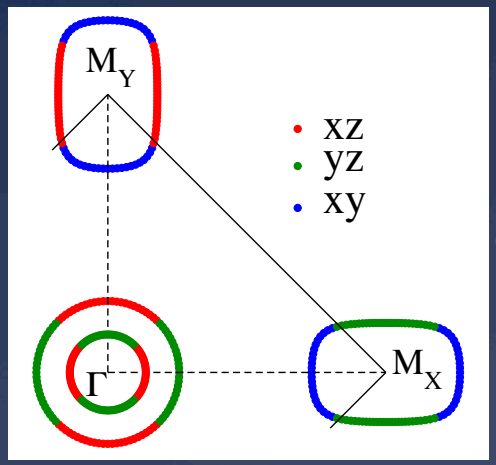
However, not all ***orbital*** components are affected in the same way

xy band is NOT shifted

Orbital effects on the FS shrinking

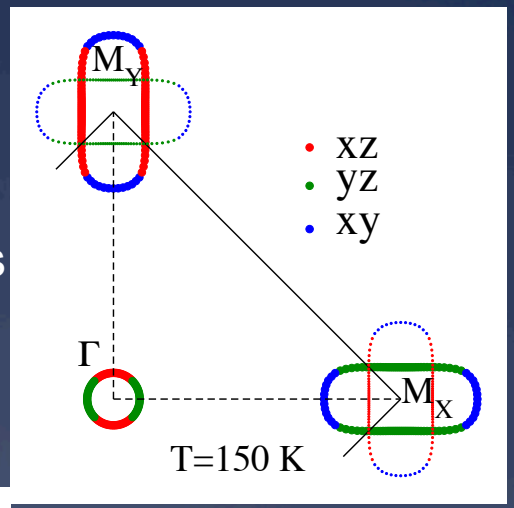
* Already evident in 122, best seen in FeSe

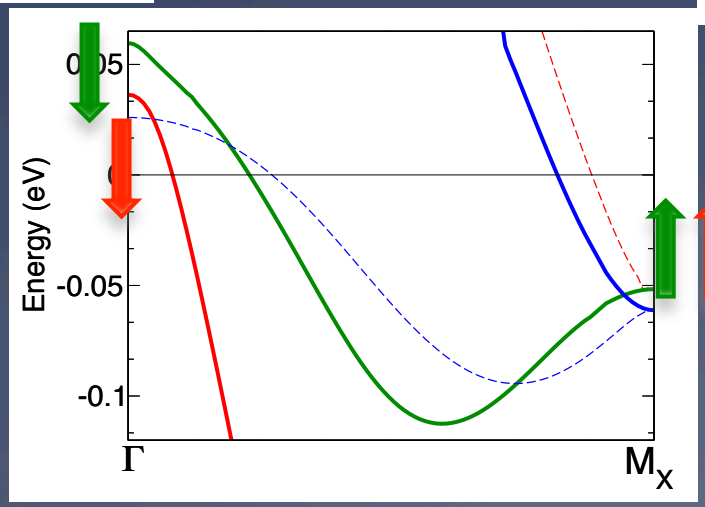
LDA



Only xz,yz shifted, leading to more elliptical electron pockets

Experiments





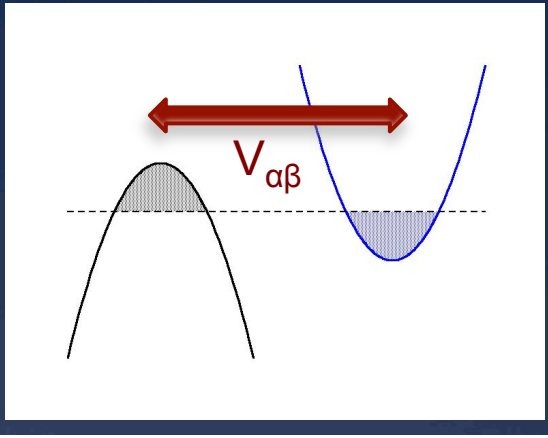
L. Fanfarillo, L.B. et al. arXiv:1605.02482

The FS shrinking is a common feature of all iron-based superconductors

Let us try to understand it first
within the "band" language
No orbital degrees of freedom for the moment

Eliashberg approach

* hole+electron (parabolic) bands
* Multiband interaction mediated by a bosonic mode with characteristic energy ω_0 and coupling λ=VN



$$\Sigma_\alpha(i\omega_n) = -T\sum_{m,\beta} V_{\alpha,\beta} D(\omega_n - \omega_m) G_\beta(i\omega_m)$$

$$D(\omega_l) = \int d\Omega \frac{2\Omega B(\Omega)}{(\Omega^2 + \omega_l^2)} \qquad B(\Omega) = \frac{1}{\pi}\frac{\Omega\omega_0}{\omega_0^2 + \Omega^2}$$

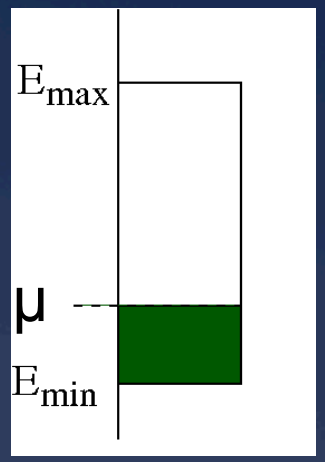
* Imaginary part of the self-energy: broadening of the energy levels
* Real part of the self-energy: mass renormalization and band shift (FS shrinking)

(1) The standard Eliashberg theory for the one-band case

* Infinite bandwidth: mass renormalization λ=NV

$$\Sigma'(\omega) = -\lambda\omega, \qquad \lambda = NV$$

$$G^{-1}(\omega,k) = \omega(1+\lambda) - \varepsilon_k + \mu$$



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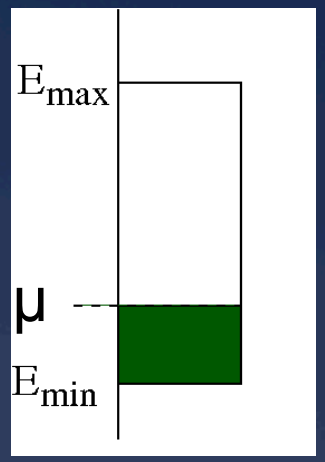

* Finite bandwidth: ω=0 self-energy is finite

$$\Sigma'(\omega) = \chi - \lambda\omega$$

$$G^{-1}(\omega,k) = \omega(1+\lambda) - \varepsilon_k + \mu - \chi = \omega(1+\lambda) - \varepsilon_k + \tilde{\mu}$$

$$\chi \approx -\omega_0 \frac{VN}{2} \ln\left|\frac{E_{\max} - \mu}{E_{\min} - \mu}\right|$$

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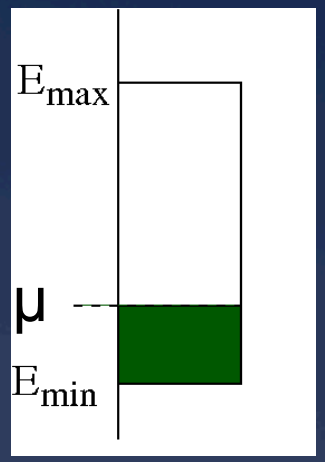

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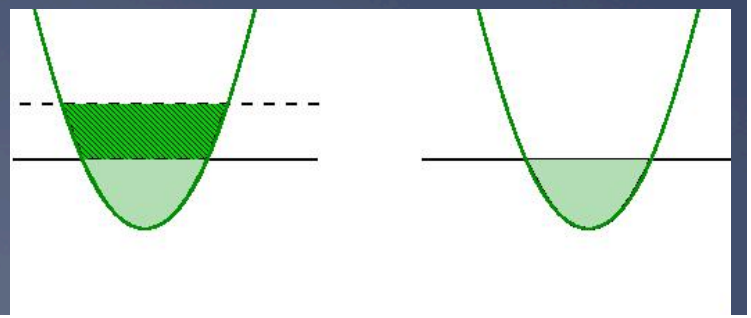
- However, this effect is immaterial because it is re-adsorbed in a chemical-potential shift, to guarantee particle-number conservation



(2) Multiband case

* In a multiband system particle-number conservation follows from a balance between electron and hole bands, so energy shifts are visible

$$\chi_\alpha \approx -\omega_0 \sum_\beta \frac{V_{\alpha,\beta} N_\beta}{2} \ln \left| \frac{E_{\max,\beta} - \mu}{E_{\min,\beta} - \mu} \right|$$

e band: $E_{max} - \mu > \mu - E_{min}$ ➡ $\chi < 0$

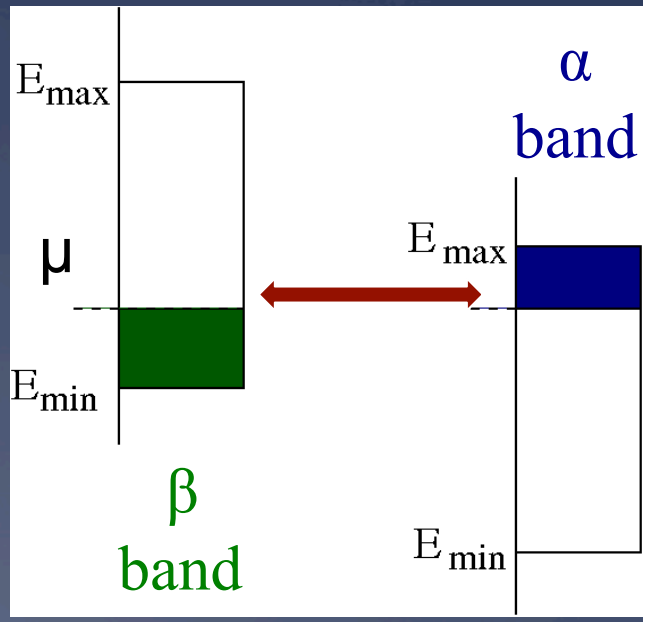
h band: $E_{max} - \mu < \mu - E_{min}$ ➡ $\chi > 0$

$$k_F^2 = 4\pi N [E_{\max} + \chi(0)]$$

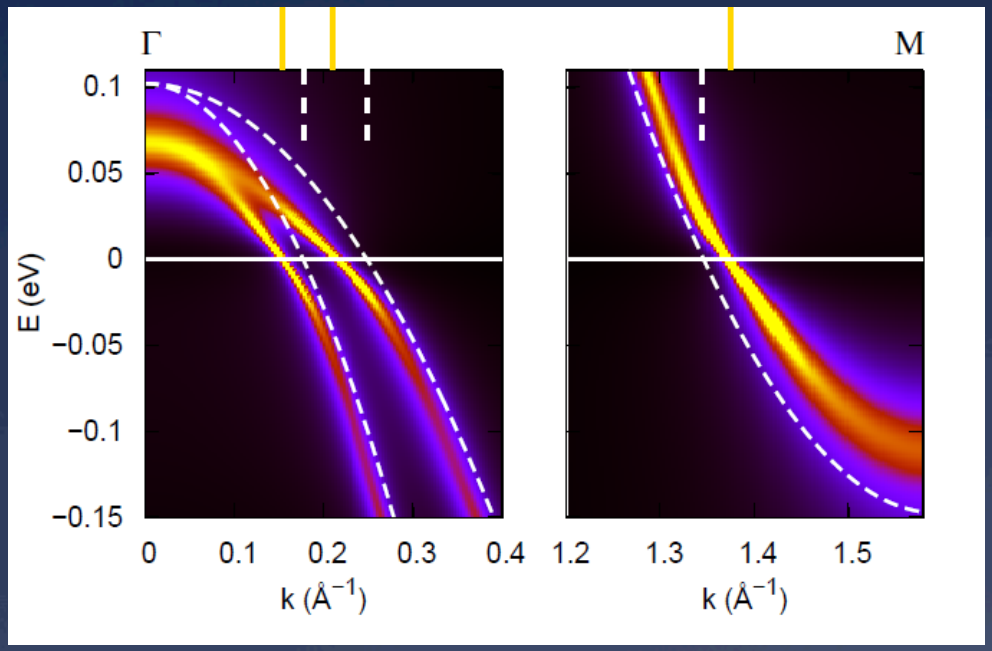
← Hole band

Intraband interactions:
$\chi > 0$, **expansion** of the FS

Interband interactions:
$\chi < 0$, **shrinking** of the FS



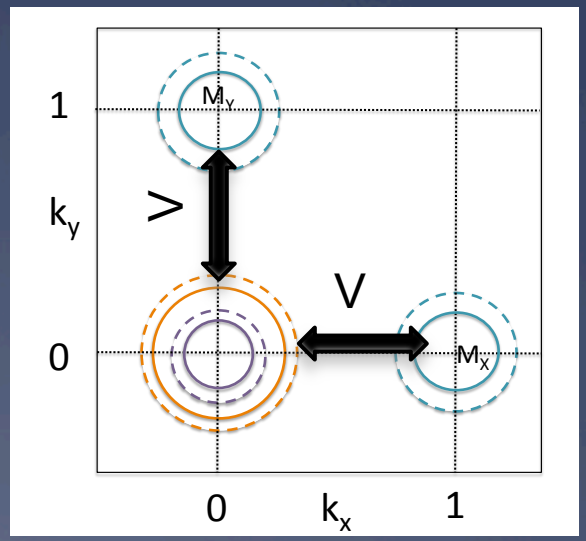
Fermi-surface shrinking = interband interactions



- Parabolic bands, no orbital character, including an overall high-energy renormalization
- Only interband coupling
- Uniform shrinking of all the bands

L.Ortenzi, E.Cappelluti, L.B., L.Pietronero, Phys Rev Lett 103, 046404 (2009)

$$\Sigma_h(i\omega_n) = -TV\sum_m D(\omega_n - \omega_m)G_e(i\omega_m)$$



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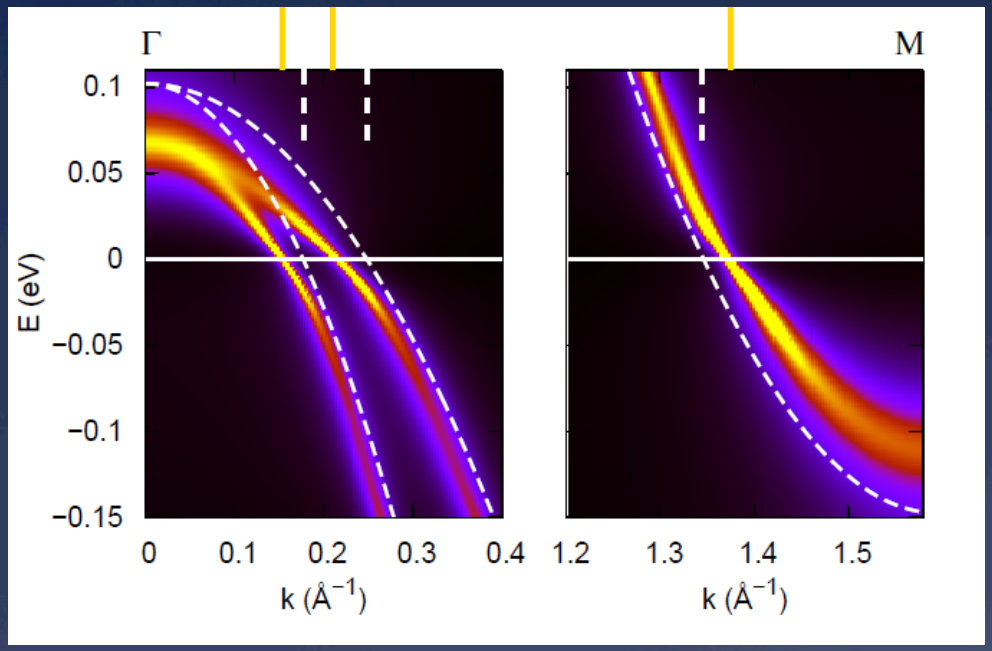

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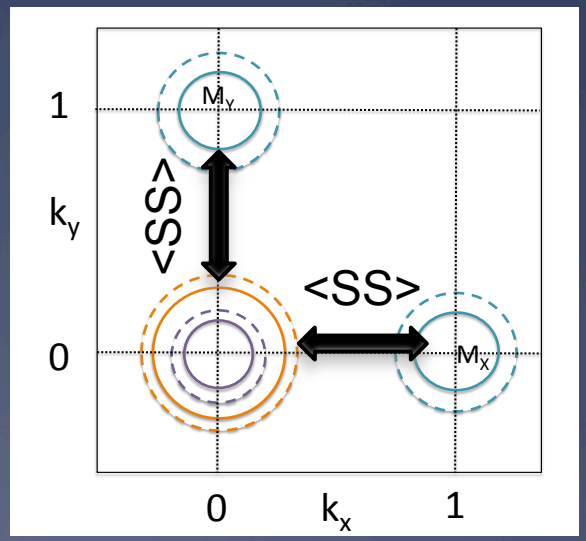
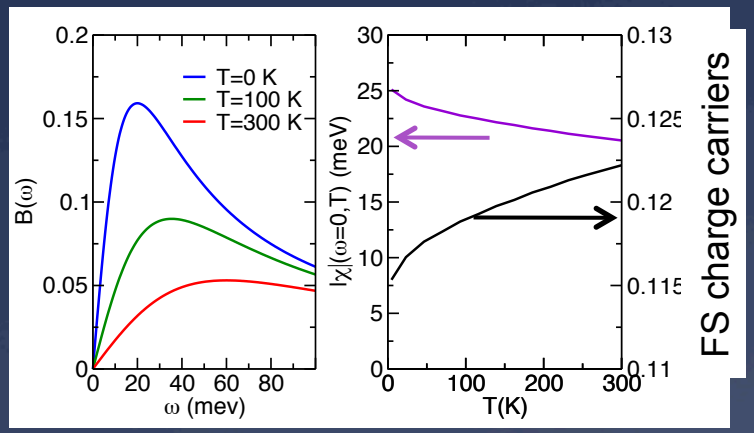
The most-likely candidate for interband interactions are **spin fluctuations**

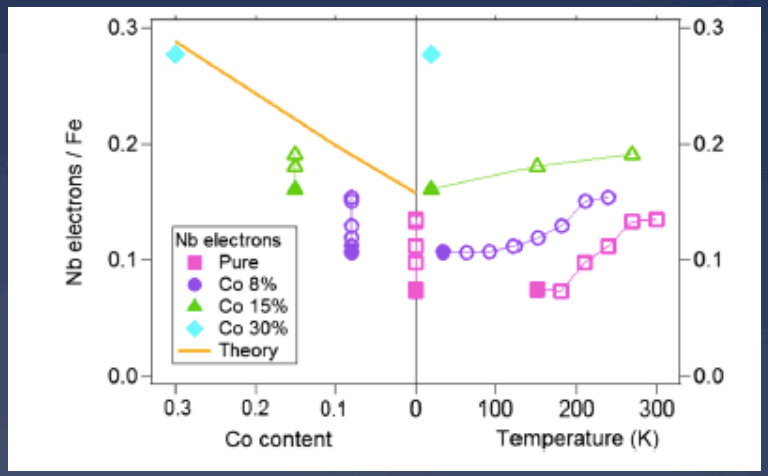


Temperature dependence

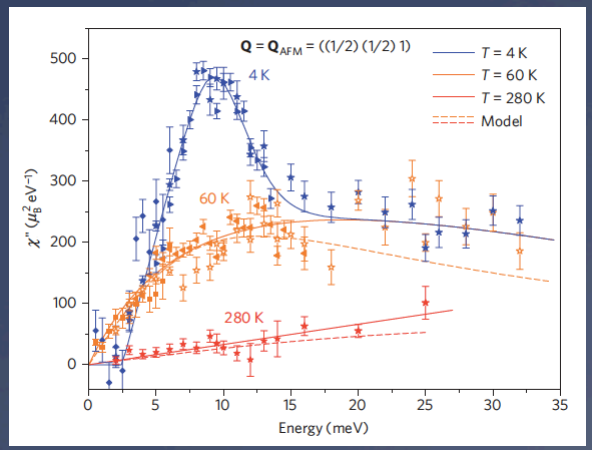
* By using the T dependence of the spin spectrum measured by neutrons we can reproduce the T-dependent FS shrinking

L.B. and E. Cappelutti, PRB 83, 104516 (2011)





V. Brouet et al., PRL 110, 167002 2013

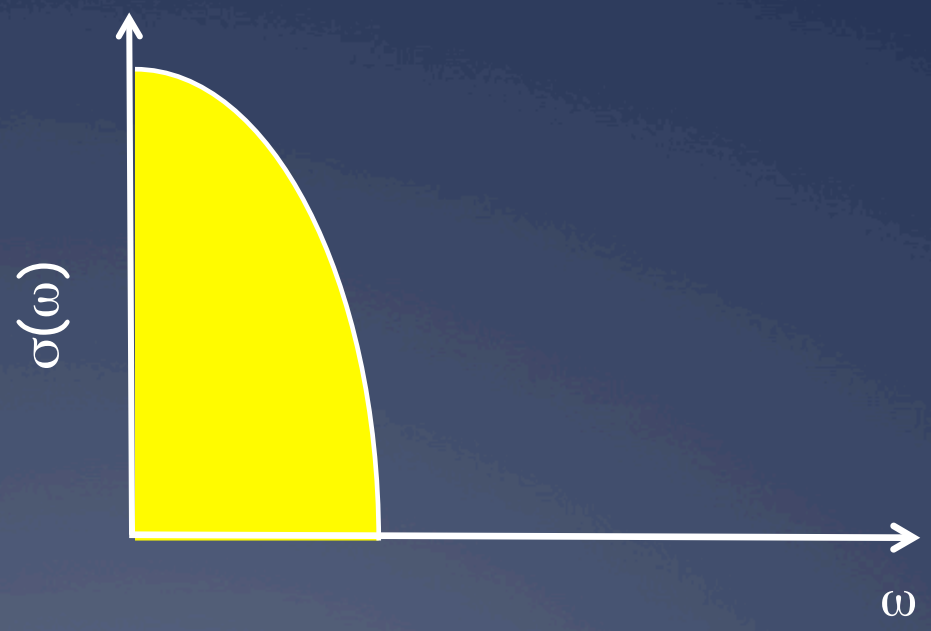


Inosov et al, Nat.. Phys. 2010

The FS shrinking is stronger at low T
This has also profound implications for the optical sum rule

Optical sum rule

$$W = \int_0^\infty d\omega \mathrm{Re}\sigma_{xx}(\omega) = \frac{\pi e^2 n}{m}$$

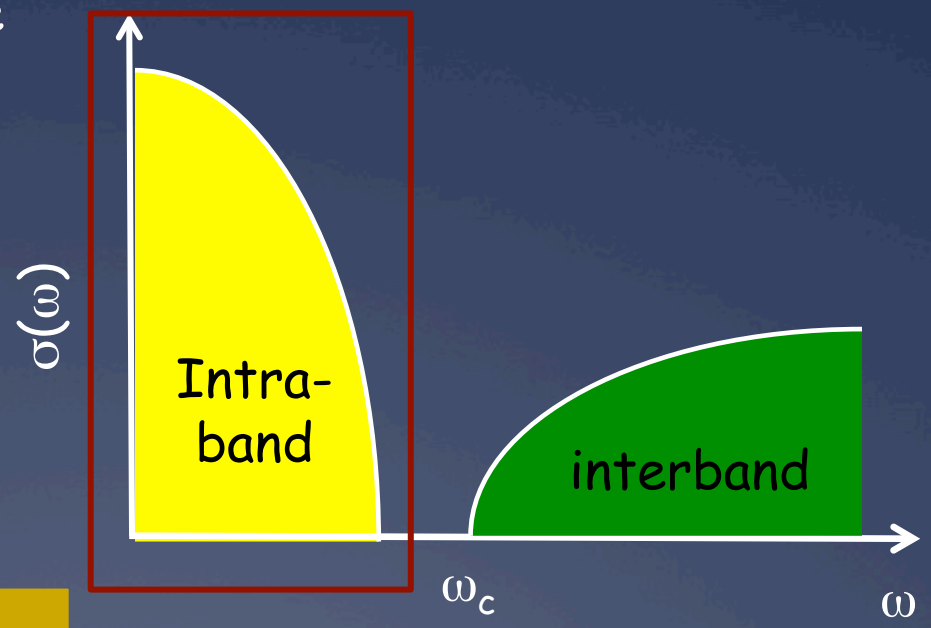


Optical sum rule

$$W = \int_0^{\omega_c} d\omega \mathrm{Re}\sigma_{xx}(\omega) = \frac{\pi e^2}{2N} \sum_{\mathbf{k},\sigma} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_x^2} n_{\mathbf{k},\sigma}$$

* W(T) *decreases* as T^2/D in the normal state (Sommerfeld) (D=bandwidth)

$$W(T)=W(0)-BT^2$$



Interacting systems: correlations affect the T dependence

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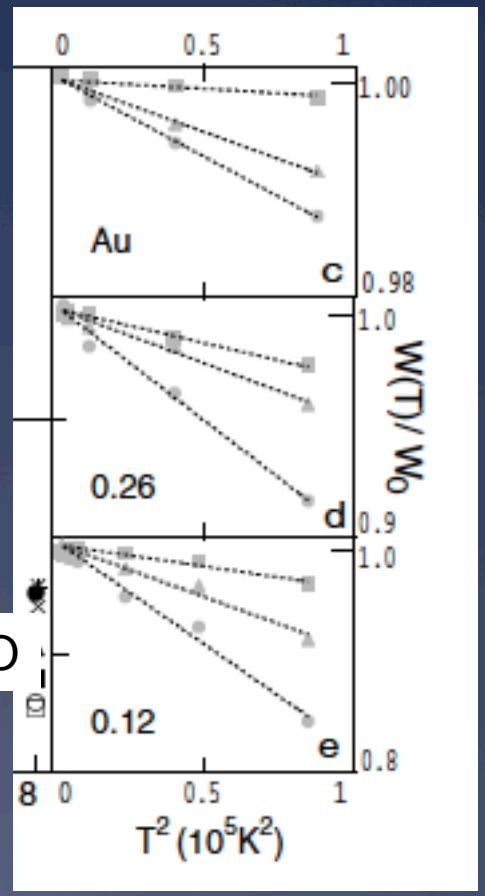


LSCO

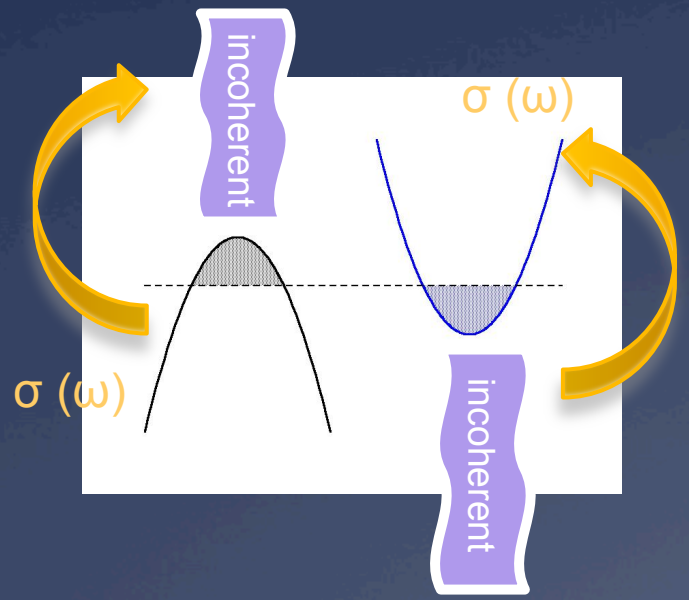
Interacting systems: correlations affect the T dependence

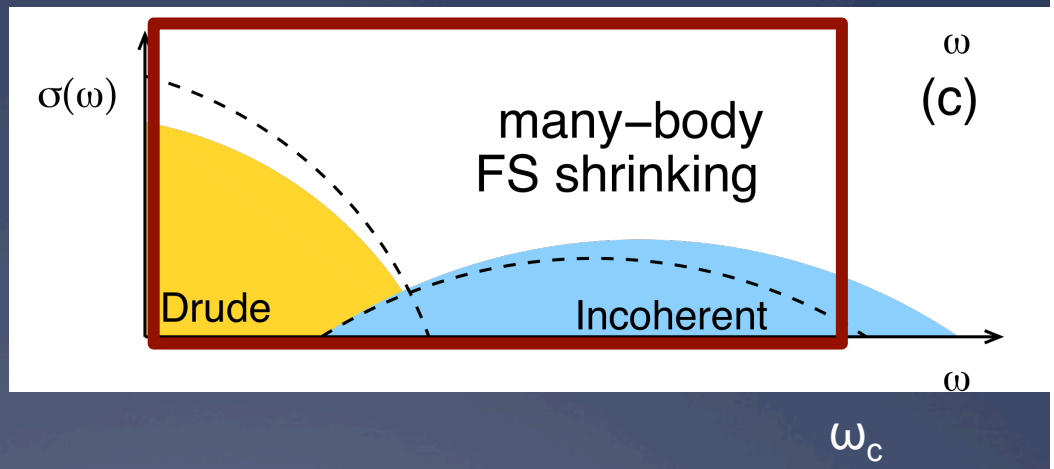
M.Ortolani et al. PRL 05

FS shrinking and optical sum rule

The interband interaction leads to a finite DOS in the otherwise unoccupied part of the spectrum

The incoherent spectral weight is transferred up to energies much larger than the typical threshold ω_c for interband transitions



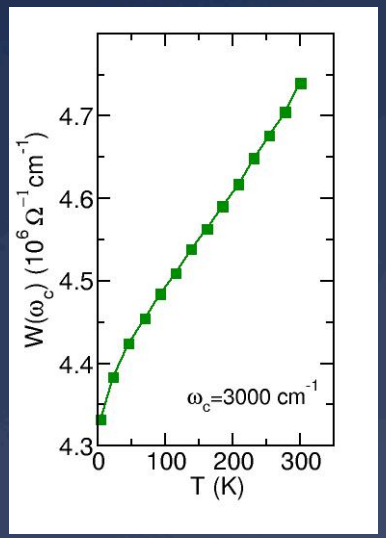


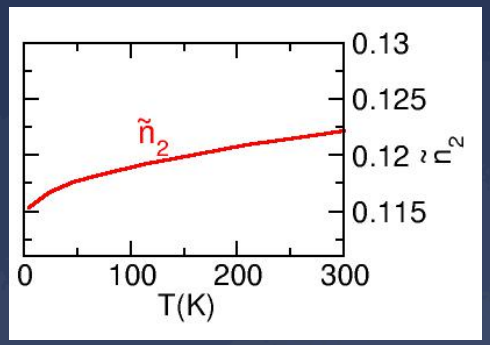
The optical spectral weight up to ω_c, $W(\omega_c)$ scale with the T dependent FS area

FS shrinking and optical sum rule

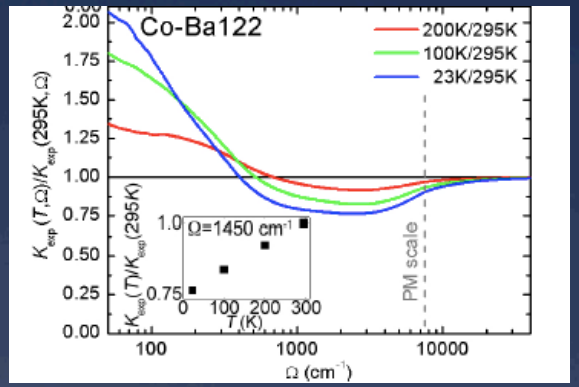
Anomalous ***increase*** of the the optical sum rule with T

L.B. and E. Cappelutti, PRB 83, 104516 (2011)



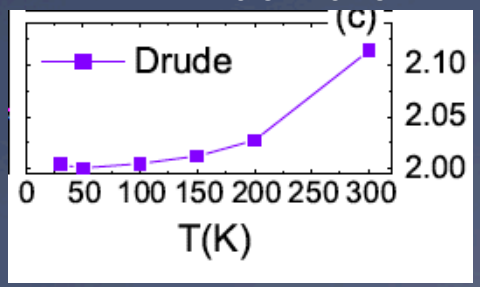


W(ω_c)~FS shrinking

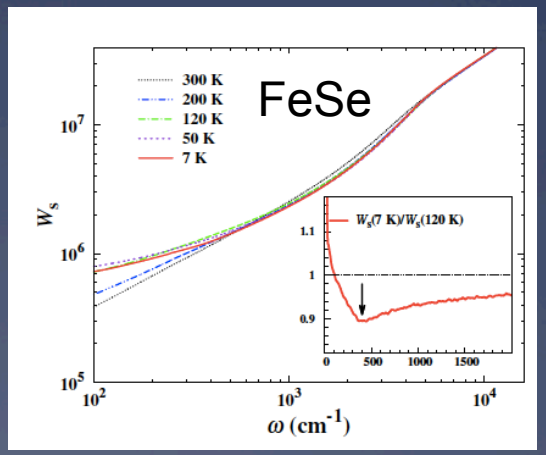


A.A.Schafgans et al. PRL 108, 147002

$EuFe_2(As_{0.82}P_{0.18})_2$



D. Wu et al. PRB 83, 100503 (11)

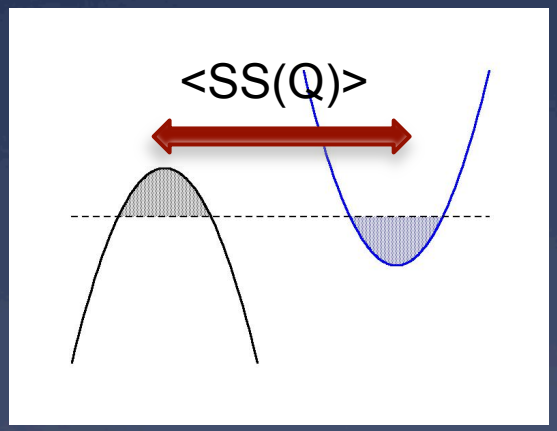


H. Wang, arXiv:1606.02198

Take-home message I

* FS shrinking in iron-based systems is a non-trivial effect due to the multiband character and to the interband interactions

Strong particle-hole asymmetry (almost full/empty bands)



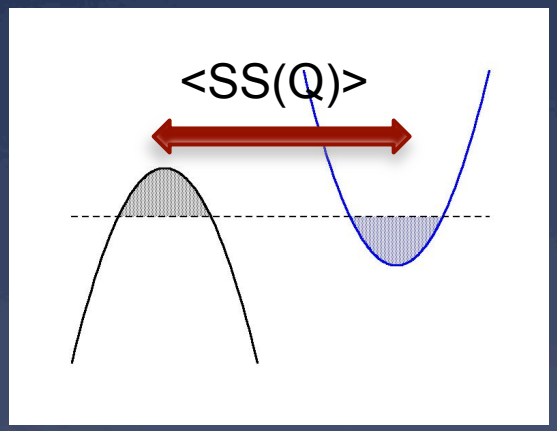
Hole&Electron pockets connected by interband interactions

Interband=spin fluctuations

Doping/T dependence FS shrinking= strength of spin fluctuations

We still miss the orbital degrees of freedom
Let us go back from the band basis to the orbital basis

Strong particle-hole asymmetry (almost full/empty bands)



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Interband=spin fluctuations

Doping/T dependence FS shrinking= strength of spin fluctuations

Low-energy orbital model

* Approximate description of the bands with three orbital components xz,yz and xy

$$\hat{H}_0^l = h_0^l \tau_0 + \vec{h}^l \cdot \vec{\tau}^l = \begin{pmatrix} h_0^l(\mathbf{k}) + h_3^l(\mathbf{k}) & h_1^l(\mathbf{k}) - i h_2^l(\mathbf{k}) \\ h_1^l(\mathbf{k}) + i h_2^l(\mathbf{k}) & h_0(\mathbf{k}) - h_3^l(\mathbf{k}) \end{pmatrix}$$

* Only yz, xz at Γ, only yz/xz, xy at X/Y

$$\hat{H}_0^\Gamma = \begin{pmatrix} \varepsilon_\Gamma - a_\Gamma k^2 + b_\Gamma (k_x^2 - k_y^2) & -2 b_\Gamma k_x k_y \\ -2 b_\Gamma k_x k_y & \varepsilon_\Gamma - a_\Gamma k^2 - b_\Gamma (k_x^2 - k_y^2) \end{pmatrix}$$

$$\Psi^\Gamma = (c^{yz}, c^{xz})$$

$$E^{\Gamma,\pm} = \varepsilon_\Gamma - (a_\Gamma \pm b_\Gamma) k^2$$

See V. Cvektovic and O. Vafek, PRB 88, 134510 (2013)

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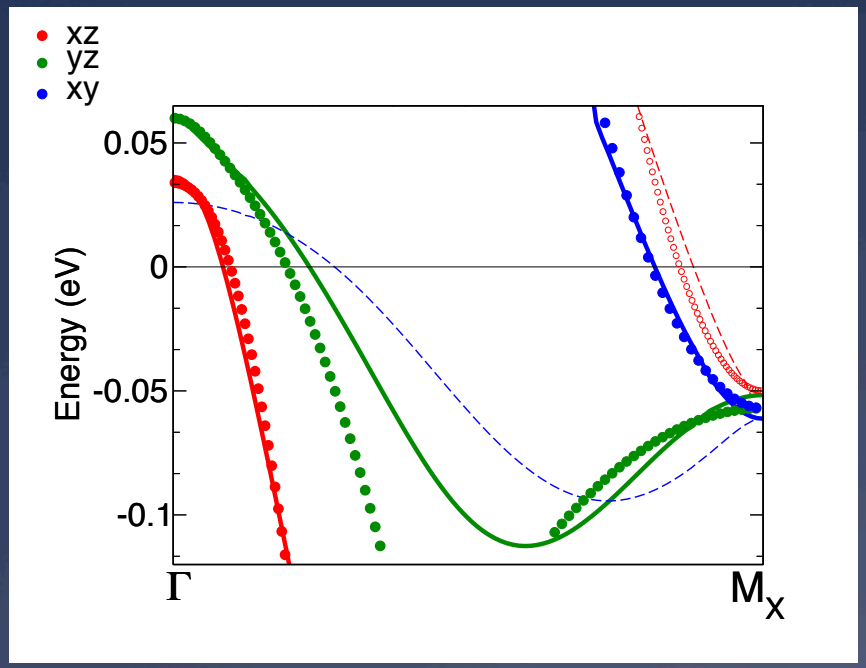
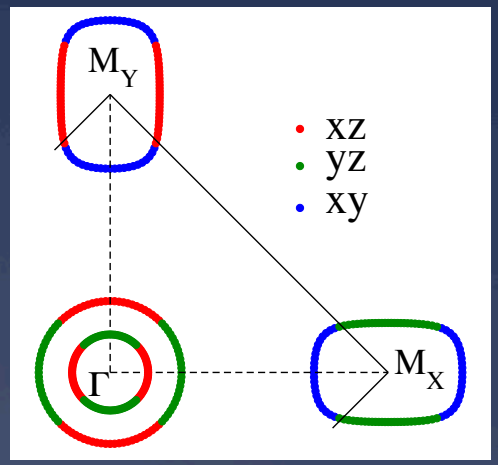
* Approximate description of the bands with three orbital components xz,yz and xy





* Mass renormalization and SOC fitted to the experiments

Low-energy orbital model

* Approximate description of the bands with three orbital components

* Self-energy effect must be computed in the orbital basis

$$\hat{G}^{-1} = \hat{G}_0^{-1} - \hat{\Sigma}$$

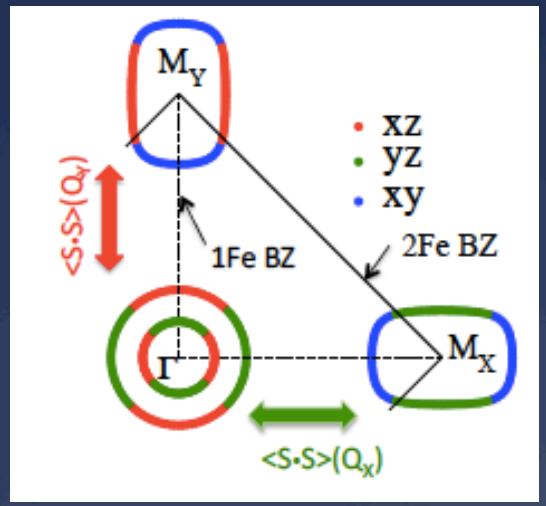
* Also the microscopic spin-spin interaction carries information on the orbital degrees of freedom

$$H_{int} = -1/2 \sum_{\mathbf{q}\,'} U_{\eta\eta'} \mathbf{S}^{\eta}_{\mathbf{q}} \cdot \mathbf{S}^{\eta'}_{-\mathbf{q}},$$

$$\mathbf{S}^{\eta}_{\mathbf{q}} = \sum_{\mathbf{k}ss'} (c^{\eta\dagger}_{\mathbf{k}s} \sigma_{ss'} c^{\eta}_{\mathbf{k}+\mathbf{q}s'})$$

Orbital character and spin fluctuations

* The SF along X or Y select different orbitals



$$\langle \mathbf{S}\cdot\mathbf{S}\rangle(\mathbf{Q}_X) \Rightarrow \langle \mathbf{S}^{yz}_{\mathbf{Q}_X}\cdot\mathbf{S}^{yz}_{\mathbf{Q}_X}\rangle$$
$$\langle \mathbf{S}\cdot\mathbf{S}\rangle(\mathbf{Q}_Y) \Rightarrow \langle \mathbf{S}^{xz}_{\mathbf{Q}_Y}\cdot\mathbf{S}^{xz}_{\mathbf{Q}_Y}\rangle$$

See L. Fanfarillo, A.Cortijo and B. Valenzuela, PRB 91, 214515 (15)

Orbital character and spin fluctuations

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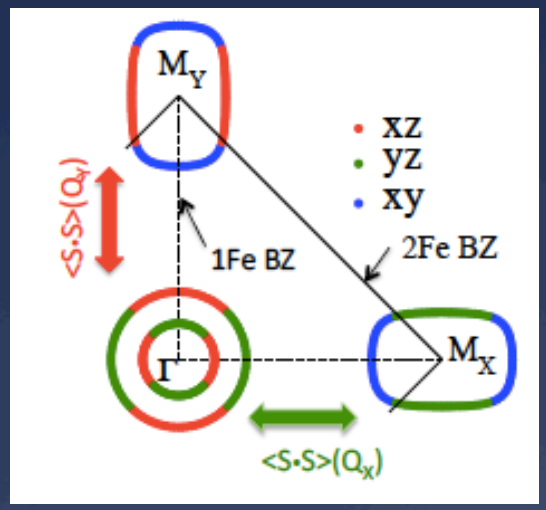

$$\langle \mathbf{S}\cdot\mathbf{S}\rangle(\mathbf{Q}_X) \Rightarrow \langle \mathbf{S}^{yz}_{\mathbf{Q}_X}\cdot\mathbf{S}^{yz}_{\mathbf{Q}_X}\rangle$$
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See L. Fanfarillo, A.Cortijo and B. Valenzuela, PRB 91, 214515 (15)

Orbital-selective FS shrinking

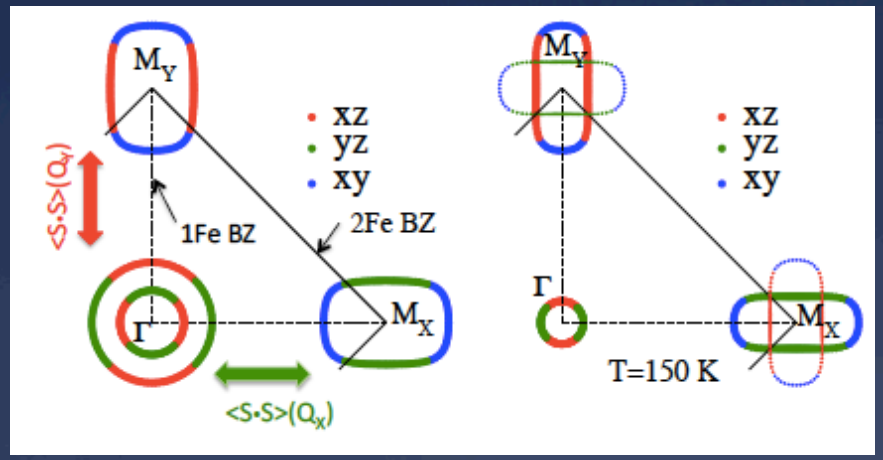
* The self-energy corrections probe SF in different directions, while the sign is still dictated by the particle-hole asymmetry of the band+interband interaction

$$\hat{\Sigma}^{\Gamma} = \begin{pmatrix} \Sigma^{\Gamma}_{yz} & 0 \\ 0 & \Sigma^{\Gamma}_{xz} \end{pmatrix} \qquad \hat{\Sigma}^{X} = \begin{pmatrix} \Sigma^{X}_{yz} & 0 \\ 0 & 0 \end{pmatrix} \qquad \hat{\Sigma}^{Y} = \begin{pmatrix} \Sigma^{Y}_{xz} & 0 \\ 0 & 0 \end{pmatrix}$$

$$\Psi^{\Gamma} = \begin{pmatrix} c_{yz} \\ c_{xz} \end{pmatrix} \qquad \Psi^{X} = \begin{pmatrix} c_{yz} \\ c_{xy} \end{pmatrix} \qquad \Psi^{Y} = \begin{pmatrix} c_{xz} \\ c_{xy} \end{pmatrix}$$

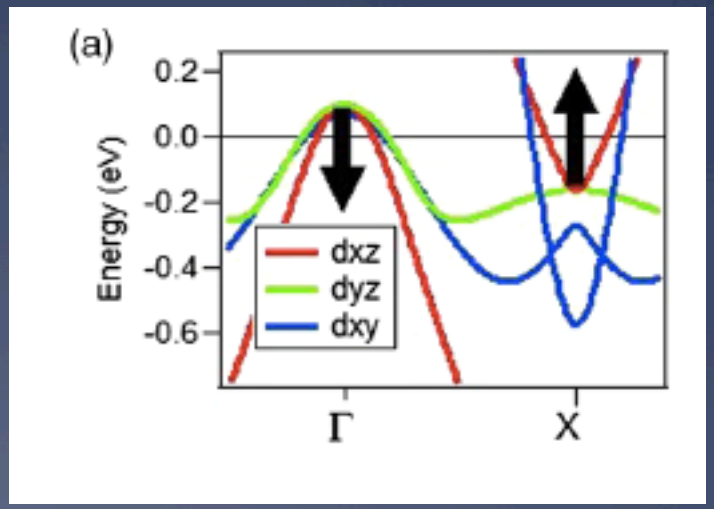
Orbital-selective FS shrinking

* No effect on the xy orbital at X/Y, enhanced ellepticity



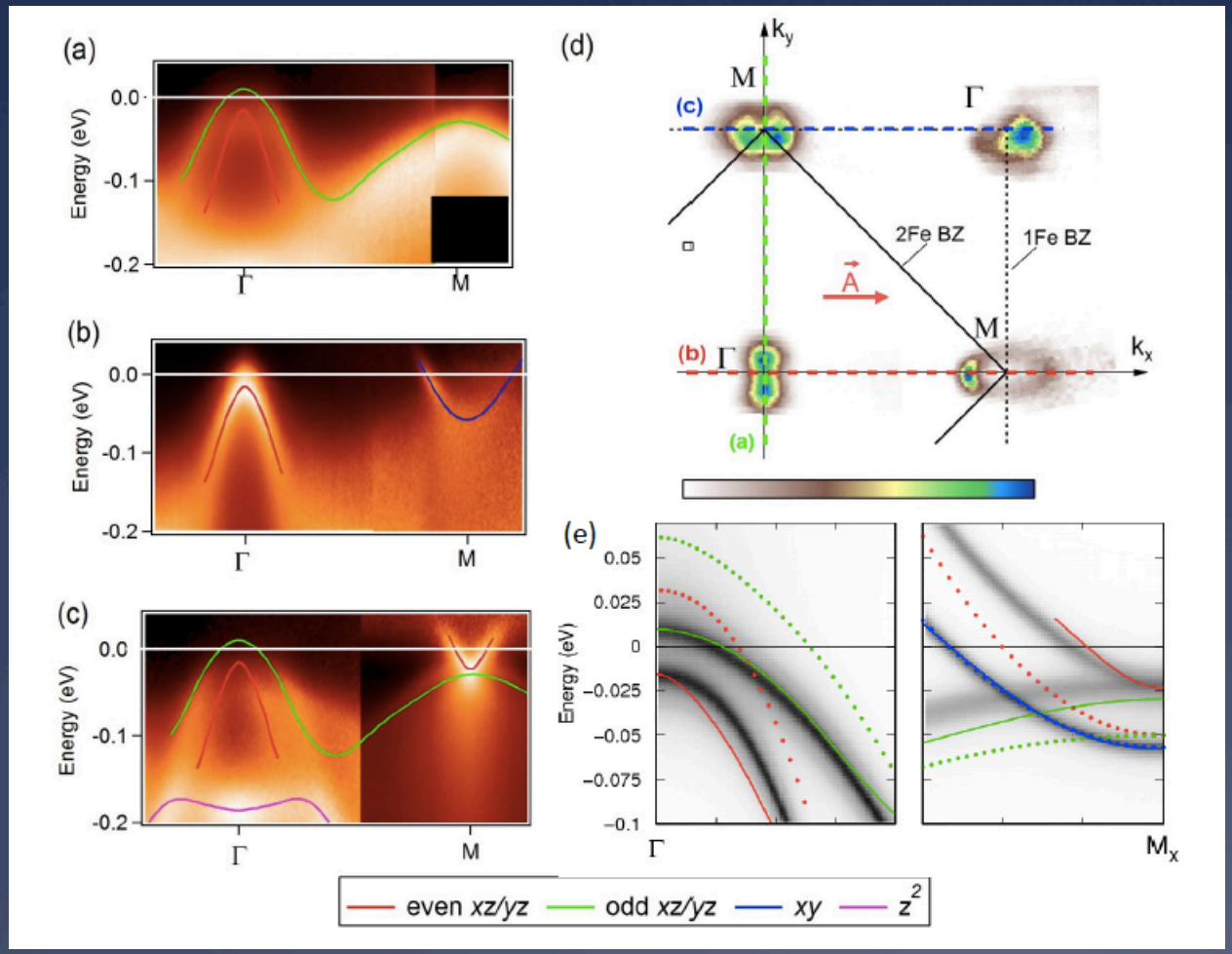
N.B.: in the usual paramgnetic states SF along X or Y are equal

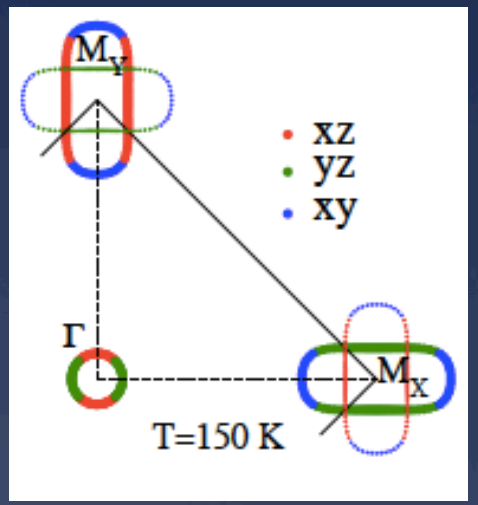
Ba(Fe1-xCox)2As2
V. Brouet et al., PRL 110, 167002 2013



Orbital-selective FS shrinking

* No effect on the xy orbital at X/Y, enhanced ellepticity

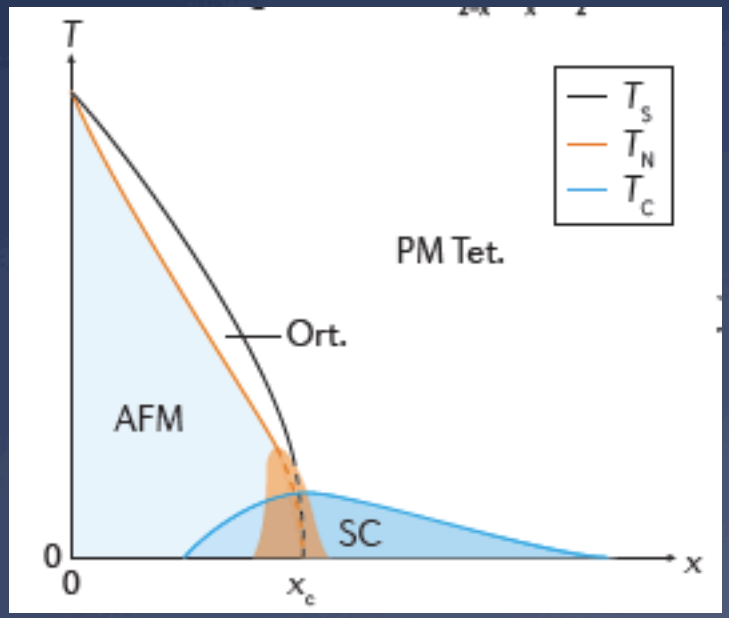


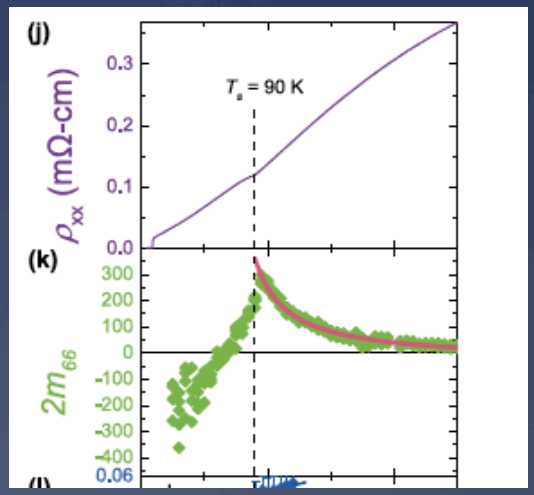


L. Fanfarillo, L.B. et al. arXiv:1605.02482

Nematicity

* Orthorhombic transition at Ts: electronic-properties anisotropy much larger than what expected from simple structural change



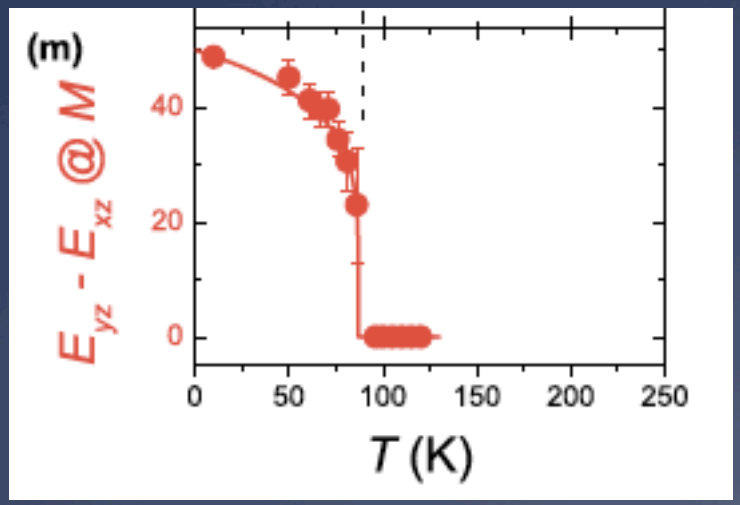


Elastoresistance tensor

Nematicity

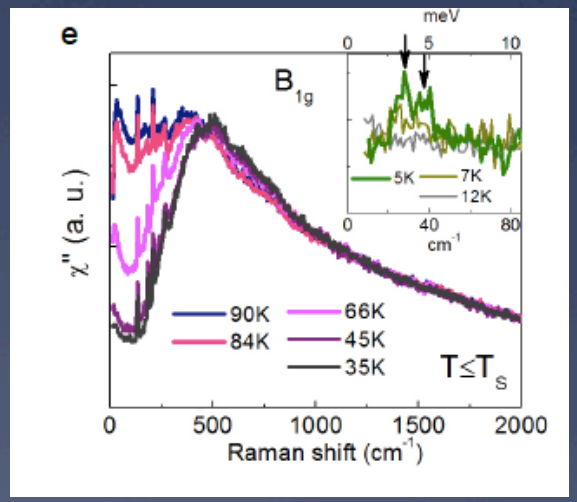
- Orthorhombic transition at Ts: electronic-properties anisotropy much larger than what expected from simple structural change
- "Hard": electronic structure (ARPES), orbital order
- "Soft": two-particle probes (Raman), spin fluctuations

Splitting of the xz/yz orbitals



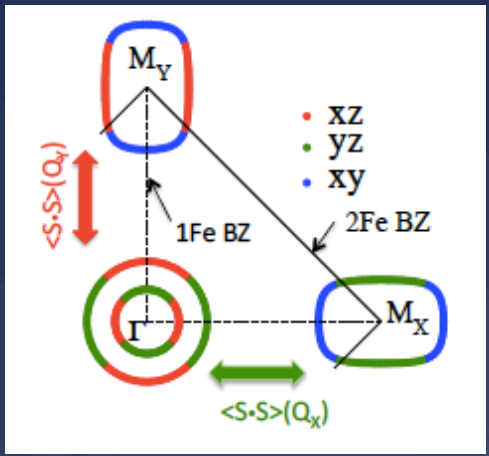
Watson et al. PRB 91, 155106 (15)

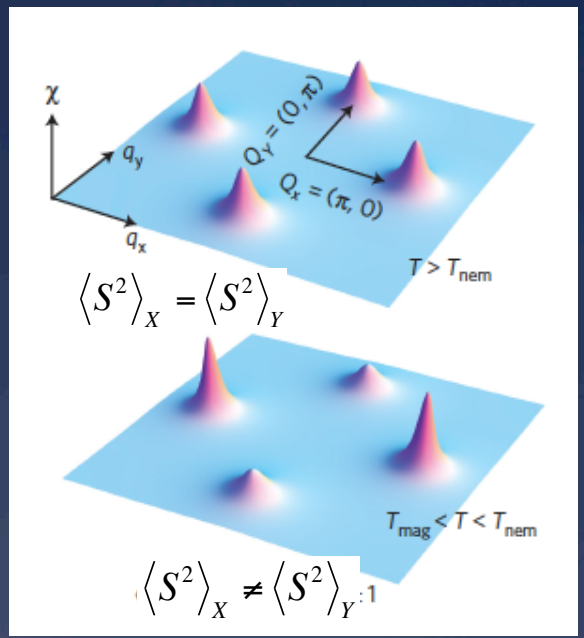
Enhanced B1g Raman response



P. Massat et al. arXiv:1603.01492

Nematicity

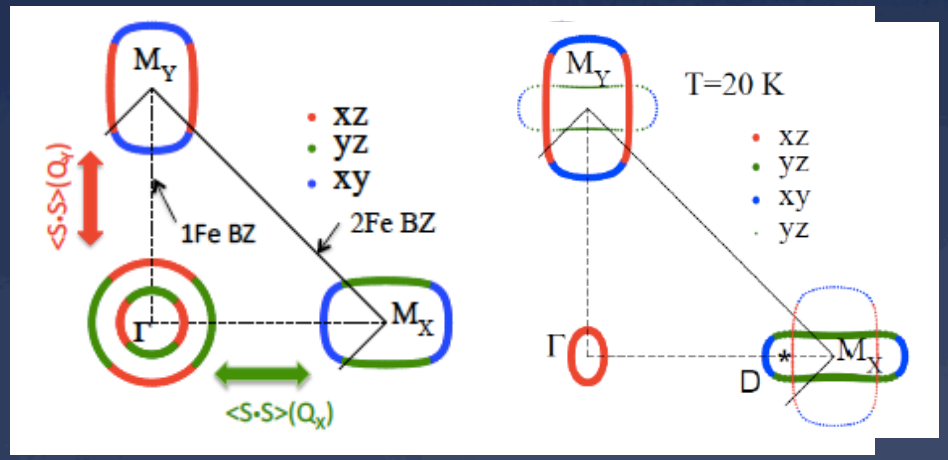




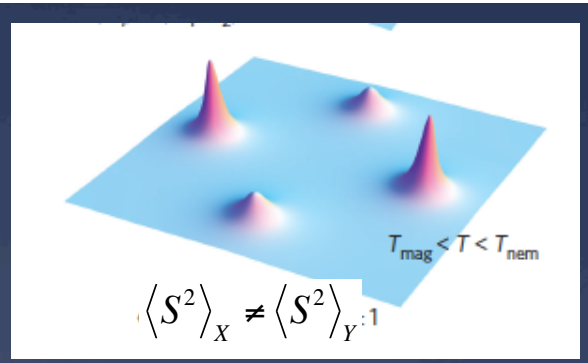
What happens when SF along X and Y become inequivalent?
"Soft" nematic transition

Fernandes et al. Nat. Phys'14

Nematicity



$$\Sigma^{\Gamma}_{yz}(\omega), \Sigma^{X}_{yz}(\omega) \Rightarrow \langle \mathbf{S}\cdot\mathbf{S}\rangle(\mathbf{Q}_X)$$
$$\Sigma^{\Gamma}_{xz}(\omega), \Sigma^{Y}_{xz}(\omega) \Rightarrow \langle \mathbf{S}\cdot\mathbf{S}\rangle(\mathbf{Q}_Y)$$



Inequivalent SF -> inequivalent orbital self-energy -> orbital ordering with different signs at Γ and X/Y

$$\hat{\Sigma}^{\Gamma} = \begin{pmatrix} \Sigma^{\Gamma}_{yz} & 0 \\ 0 & \Sigma^{\Gamma}_{xz} \end{pmatrix} \quad \hat{\Sigma}^{X} = \begin{pmatrix} \Sigma^{X}_{yz} & 0 \\ 0 & 0 \end{pmatrix} \quad \hat{\Sigma}^{Y} = \begin{pmatrix} \Sigma^{Y}_{xz} & 0 \\ 0 & 0 \end{pmatrix}$$

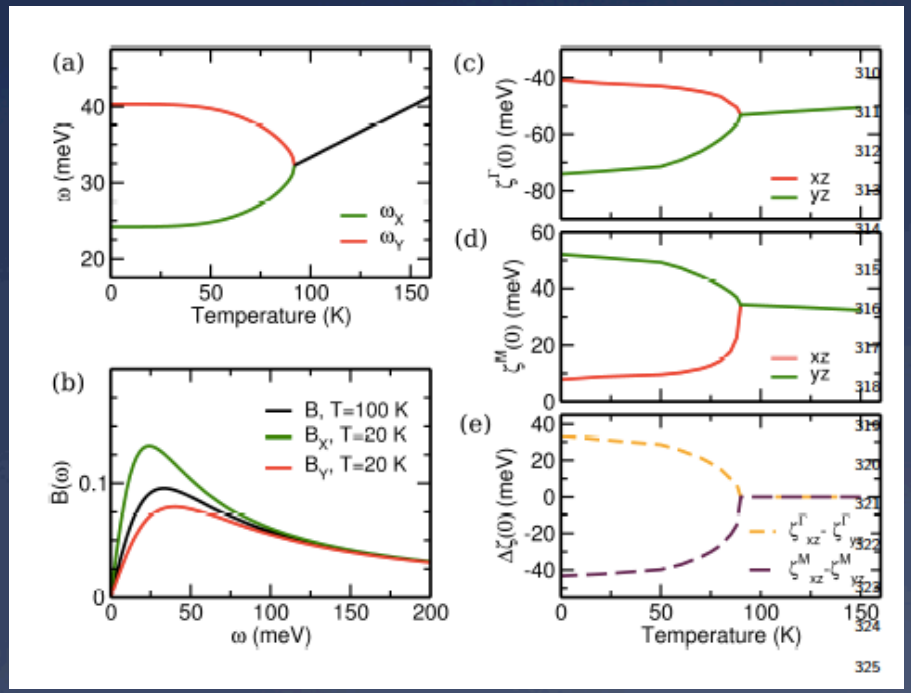
$$H_O = \Delta_b(T)\sum_k(\cos k_x - \cos k_y)[n_{xz}(k) + n_{yz}(k)] + \Delta_s(T)\sum_k[n_{xz}(k) - n_{yz}(k)] +$$

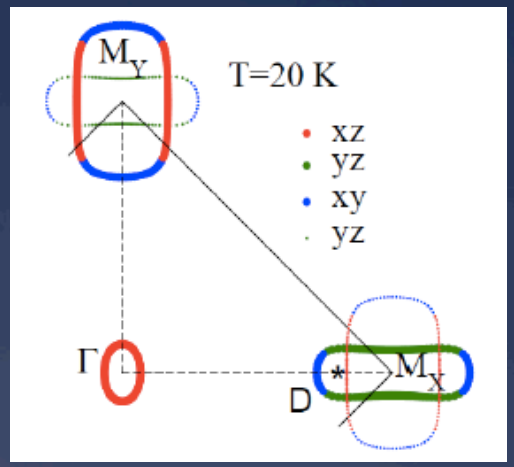
S. Mukherjee et al
PRL 115, 026402 (15);
PRB 92, 224515 (15)

Nematic FS shrinking

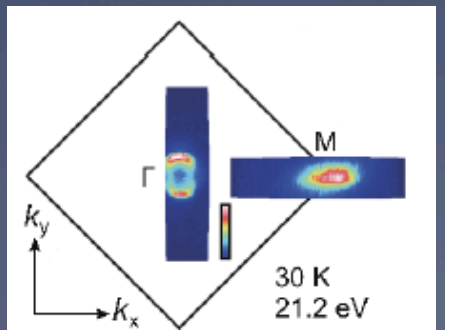
* T-dependent inequivalent spin fluctuations

L. Fanfarillo, L.B. et al. arXiv:1605.02482

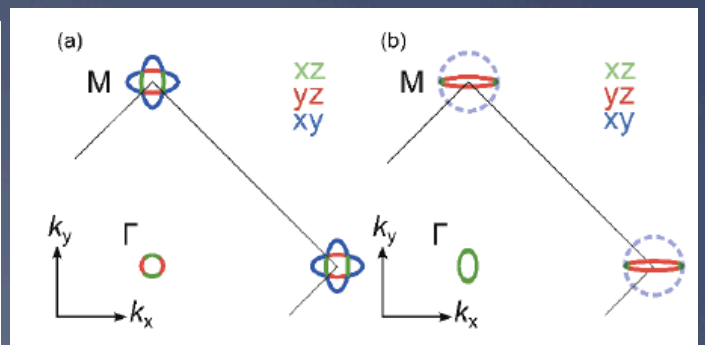




$$B_{X/Y}(\omega) = \frac{1}{\pi} \frac{\omega\omega_0}{(\omega_{sf}^{X/Y}(T))^2 + \Omega^2},$$



Y. Suzuki et al. PRB 92, 205117 (2015)



Nematic FS shrinking

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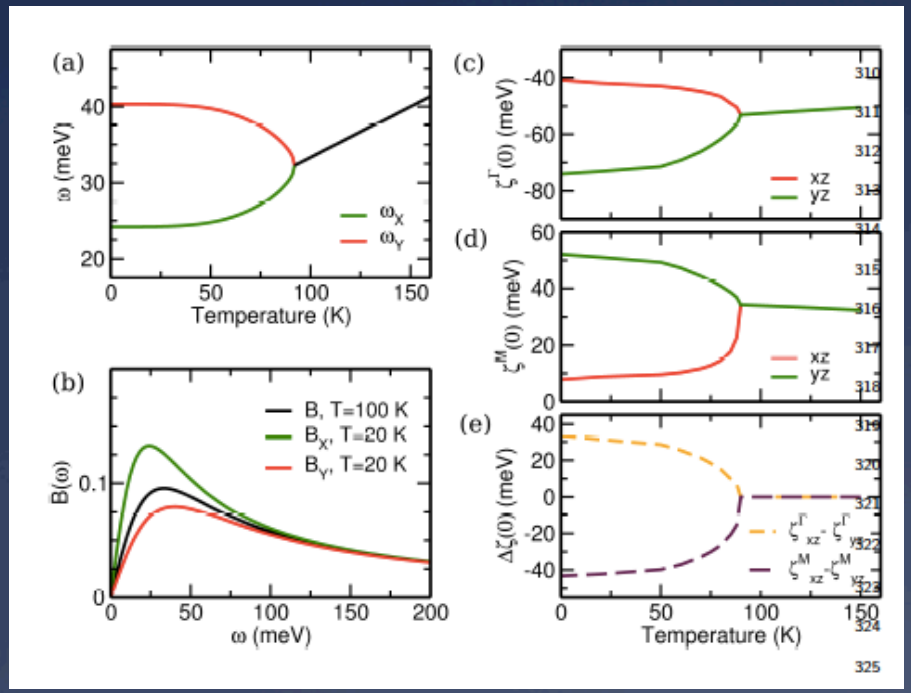

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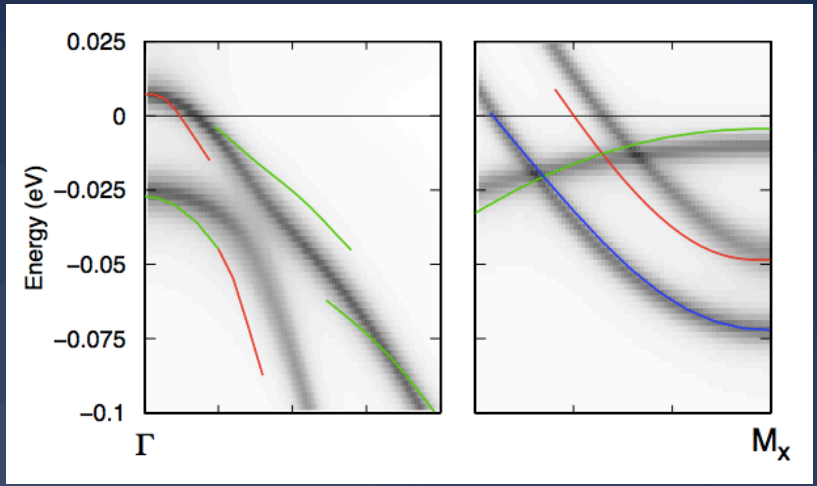
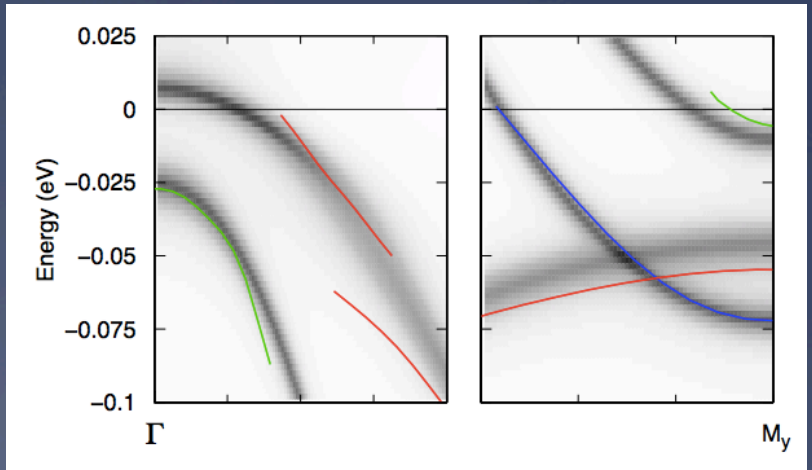
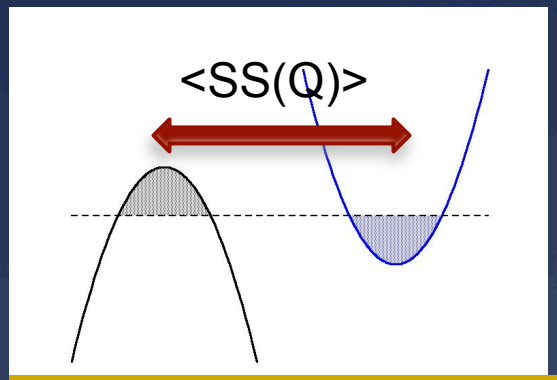


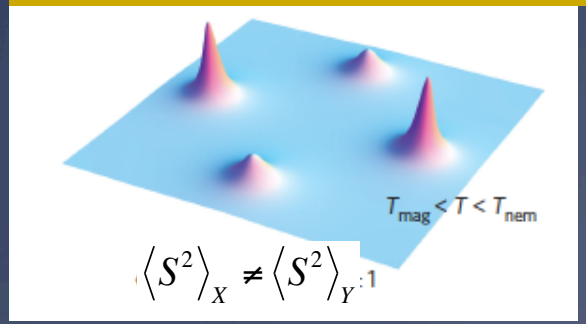


Take-home message (II)



FS shrinking

"soft" nematic mechanism



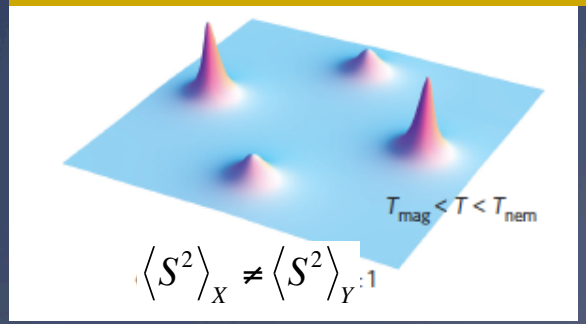
+ Orbital content = Orbital-selective FS shrinking

+ Orbital-selective FS shrinking = "hard" electronic nematicity

Take-home message (II)

Orbital order in the nematic phase is the "hard" side of the "soft" spin-fluctuation mechanism

"soft" nematic mechanism



+ Orbital-selective FS shrinking = "hard" electronic nematicity

More (interacting electron-hole bands) is different!

- Band shrinking an orbital ordering
- Optical sum rule
- Anomalous multiband Hall effect

L. Fanfarillo et al. PRL 109, 096402 (2012)

- Collective superconducting modes, Leggett mode and its signature in Raman

M. Marciani et al. PRB 88, 214508 (2013)
T. Cea and L.B. arXiv:1606.04874

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