Spin-orbit coupling in Fe-based superconductors

Maxim M. Korshunov

L.V. Kirensky Institute of Physics, Krasnoyarsk, Russia

[ES&ES-May-2013]

In collaboration with

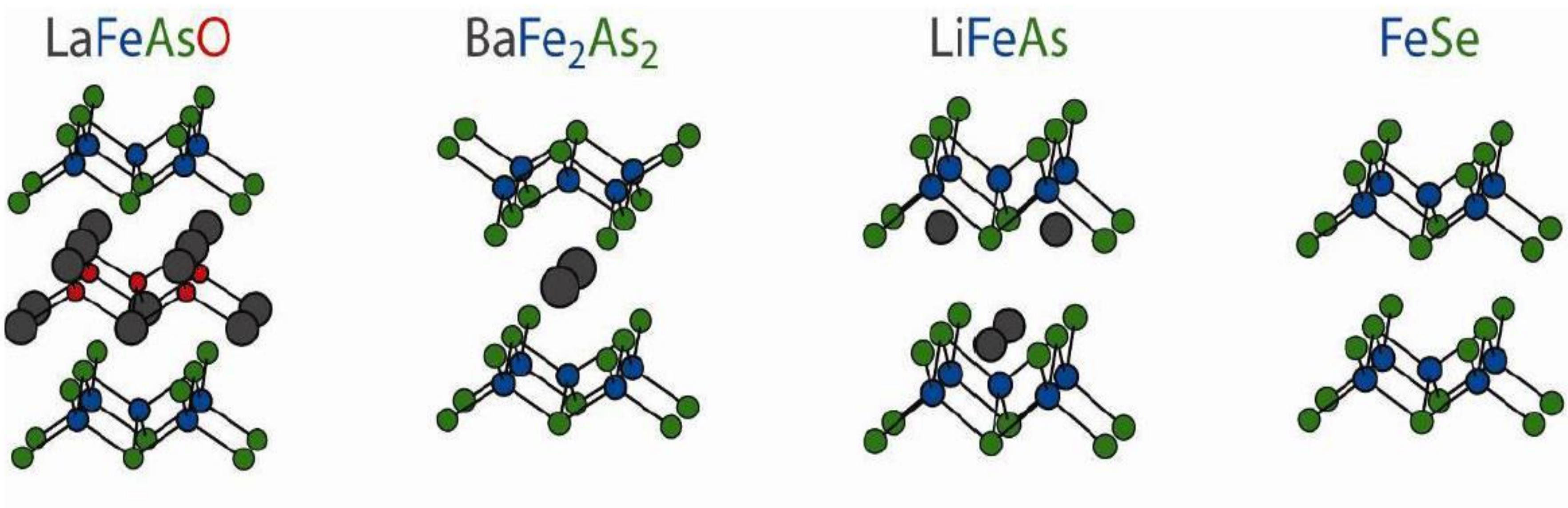
- Yuliya Togushova (Siberian Federal University)
- Ilya Eremin (Bochum University)
- Peter Hirschfeld, Andreas Kreisel, and Yan Wang (University of Florida)

Outline

- **Introduction:** structure, Fermi surface, etc.
- **Spin-resonance as evidence for the $s_{\pm}$ gap symmetry**
- **Experimental evidences for spin-space anisotropy**
  - Inelastic neutron scattering
  - NMR
- **Spin-orbit coupling**
  - Band structure renormalization
  - Fermi surface changes
  - Spin-resonance splitting
- **Conclusions**

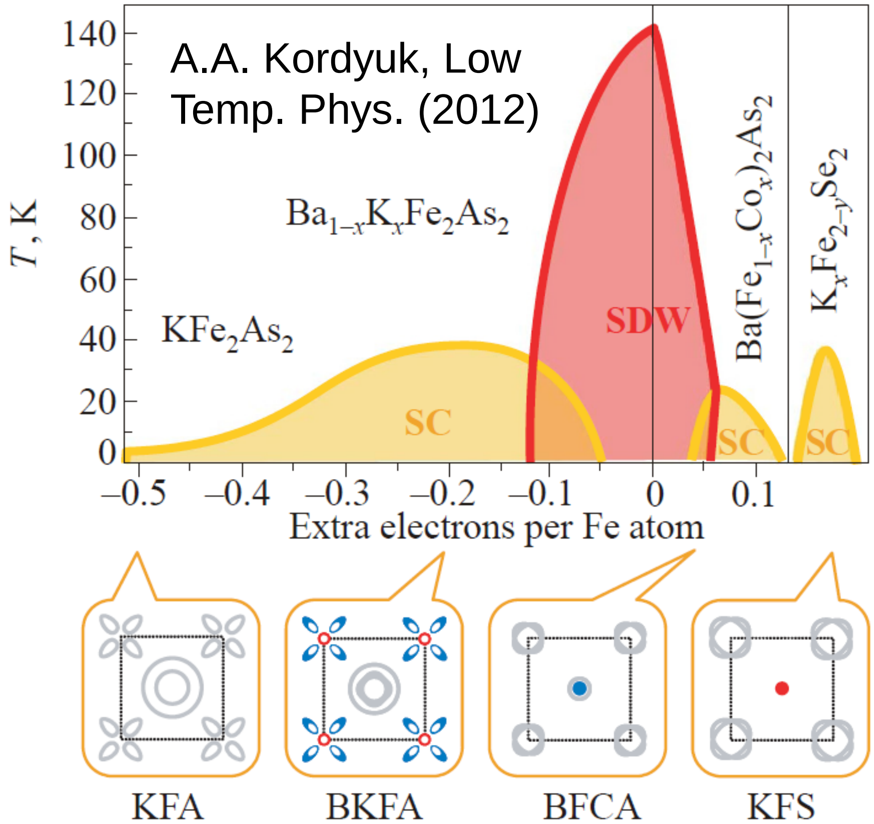
1111 vs. 122 vs. 111 vs. 11 materials

Big family of pnictides and chalcogenides

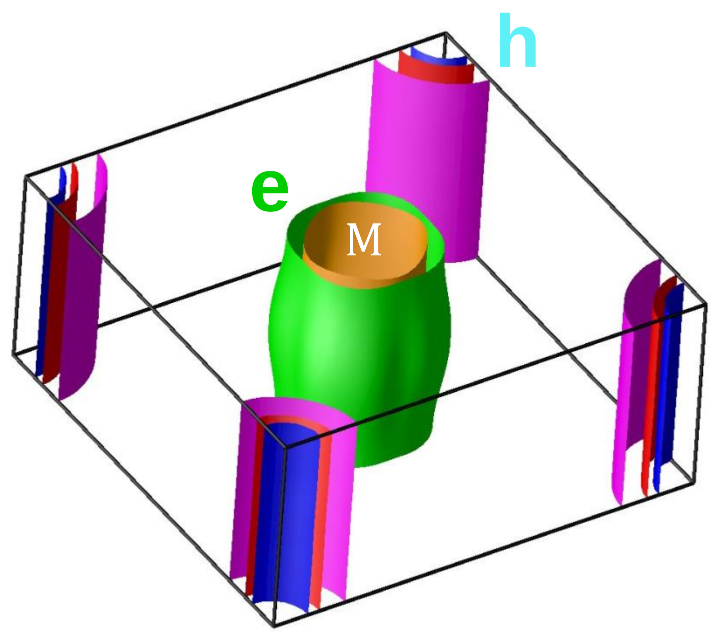


T_c=26K (55K for **Sm**, Chen et al., Nature 2008; Ren Chin. Phys. Lett. 2008)	T_c=38K Rotter et al., PRL 2008, Ni et al. PRB 2008	T_c=18K Wang et al., arXiv:0806.4688	T_c=8K Hsu et al., arXiv:0807.2369

Itinerant picture: LDA electronic structure (LaFeAsO)



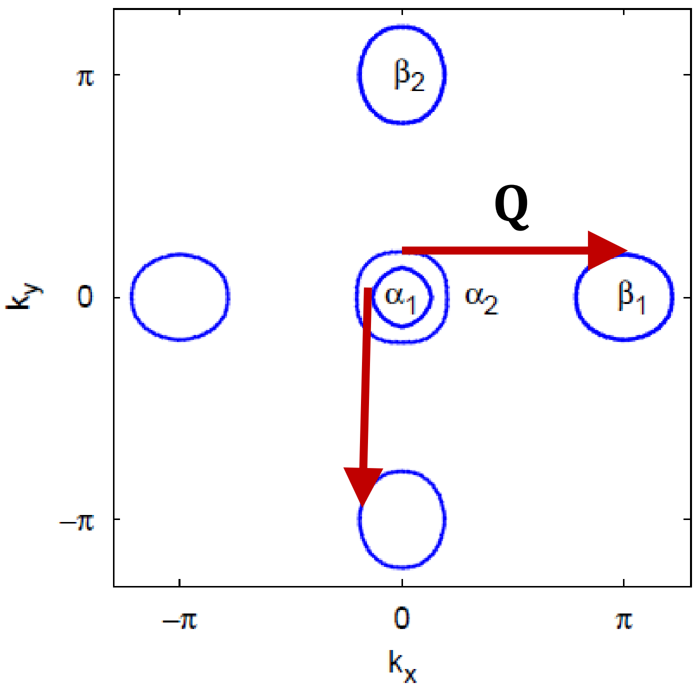
Weak CEF splitting: all 5 orbitals ($d_{x^2-y^2}$, $d_{3z^2-r^2}$, d_{xy}, d_{xz}+d_{yz}) are near the Fermi level



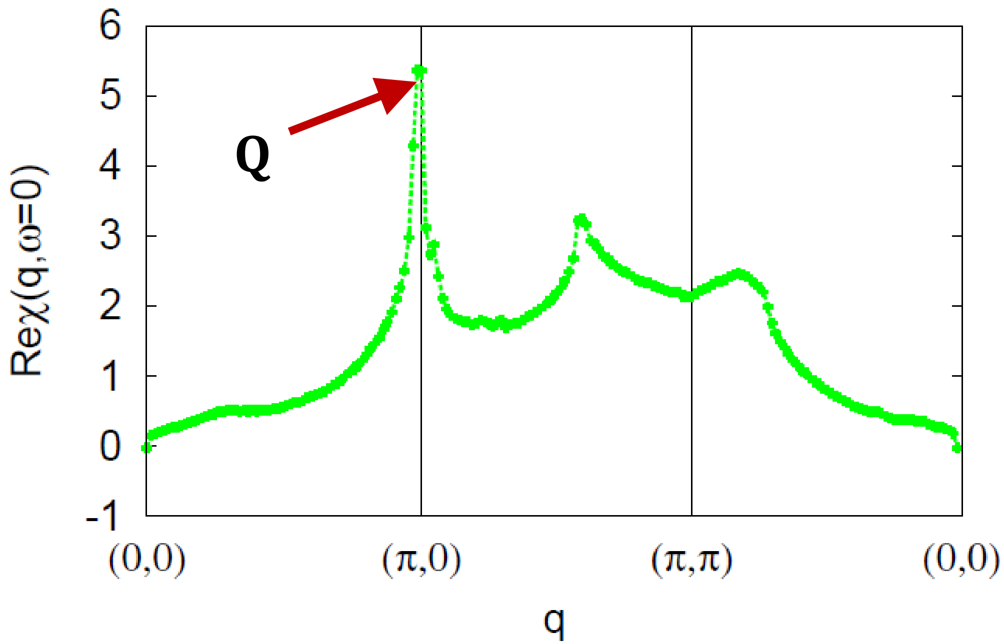
1. Both electron and hole pockets do exist (quantum oscillations, ARPES)
2. There is a Fermi surface even at zero doping (ARPES)

S. Lebegue, PRB 75, 035110 (2007); D.J. Singh and M.-H. Du, PRL 100, 237003 (2008); I.I. Mazin et al., PRL 101, 057003 (2008)

Spin susceptibility $\chi(q, \omega = 0)$



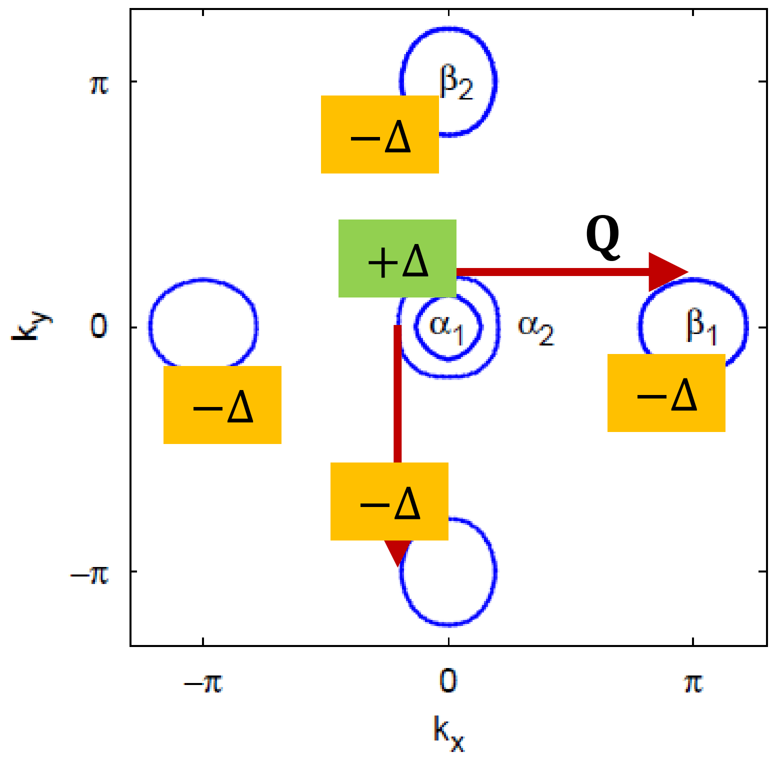
Spin fluctuations – repulsive interaction at $\mathbf{Q} = (\mathbf{0}, \boldsymbol{\pi})$ (in the unfolded BZ)



Local parameters (eV):
U=1.2, J=0.3, U'=0.6, J' =J

I.I. Mazin et al. (2008), Dong et al. (2008), MMK and I. Eremin (2008), Kuroki et al. (2008), …

Pnictides: nesting wave vector and the gap symmetry



$$\Delta_k(\mathrm{T}) = -\sum_{k'} \frac{V(k-k')}{2E_{k'}} \Delta_{k'}(T) \tanh\left(\frac{E_{k'}}{2k_B T}\right)$$

$V(q = Q) > 0$ (repulsive interaction) – Δ have to change sign!

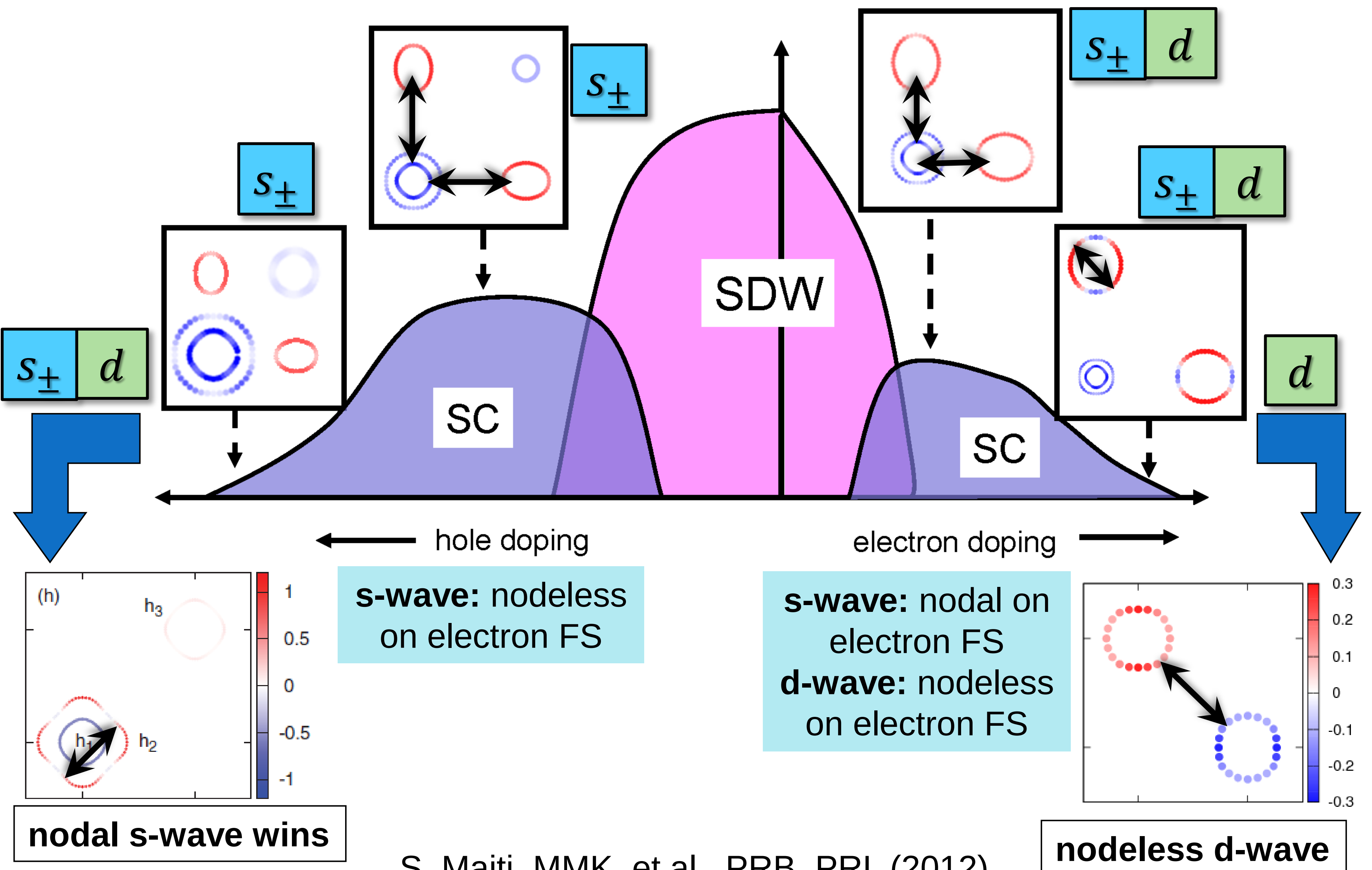
$$\Delta_1 = \Delta_2 e^{-i\pi}$$

Interband scattering with the SDW wave vector **Q**=(π,0) enhance intraband Cooper-pairing: extended s-wave ($s_{\pm}$)

I.I. Mazin et al., PRL 101, 057003 (2008)

This symmetry most naturally comes out of the spin-fluctuation pairing theories

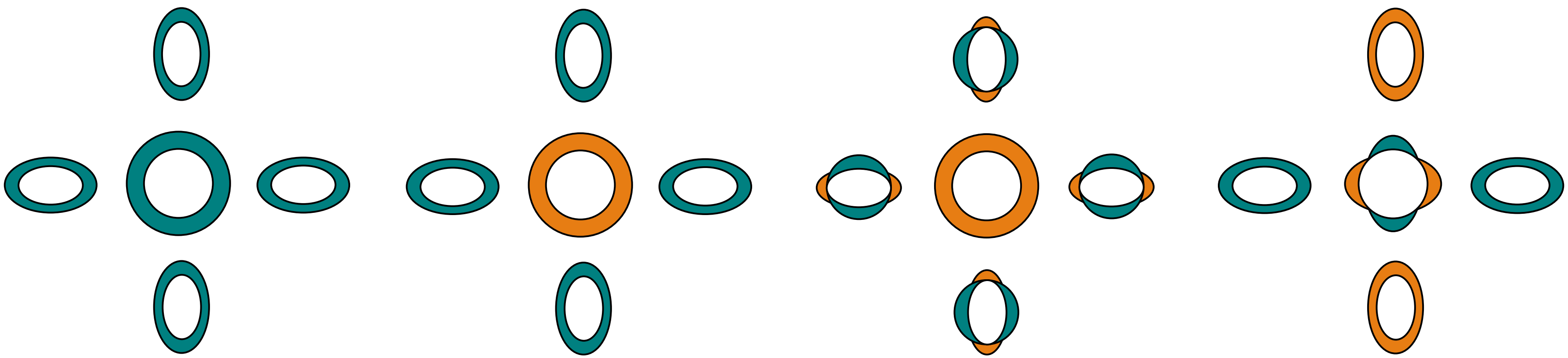
Spin-fluctuations pairing expectations in FeBS



S. Maiti, MMK, et al., PRB, PRL (2012)

Symmetry proposals for FeBS

s_{++} | $s_{\pm}$ | nodal $s_{\pm}$ | d



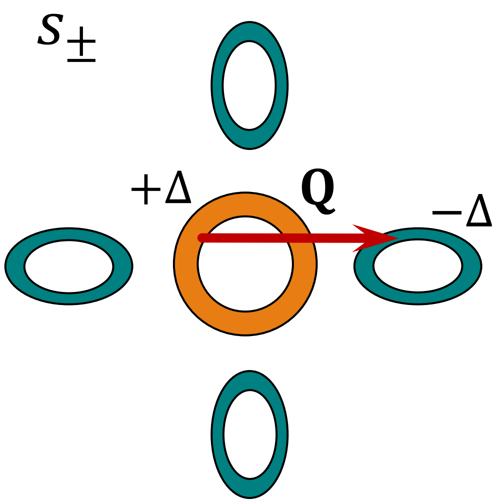
Orbital fluctuations, Phonons | Spin fluctuations | “Realistic” Spin fluctuations | Mott-Hubbard-type theories

Family	Full gap	Highly anisotropic	Strong nodal
1111	$PrFeAsO_{1-y}$[52K] [290]	LaFeAs(O, F)[26K] [212]	LaFePO[6K] [201, 202, 291]
	SmFeAs(O, F)[55K] [211]	NdFeAs(O, F) [212]	
122	(Ba, K)Fe_2As_2[40K] [144, 234, 240, 292]	Ba(Fe, Co)$_2As_2$[OD] [236, 239]*	KFe_2As_2[4K] [209, 304]
	Ba(Fe, Co)$_2As_2$[OP, 23K] [236, 206]	Ba(Fe, Ni)$_2As_2$ [293]*	$BaFe_2$(As, P)$_2$[OP, 31K] [203, 147]
		Ba(Fe, Co)$_2As_2$[UD] [239]*	(Ba, K)Fe_2As_2[UD] [240]
111	LiFeAs[18K] [294, 256]		LiFeP[6K] [295]
11		Fe(Se, Te)[27K] [229, 244]	

Note: Symbol * indicates possible evidence for ‘*c*-axis nodes’.

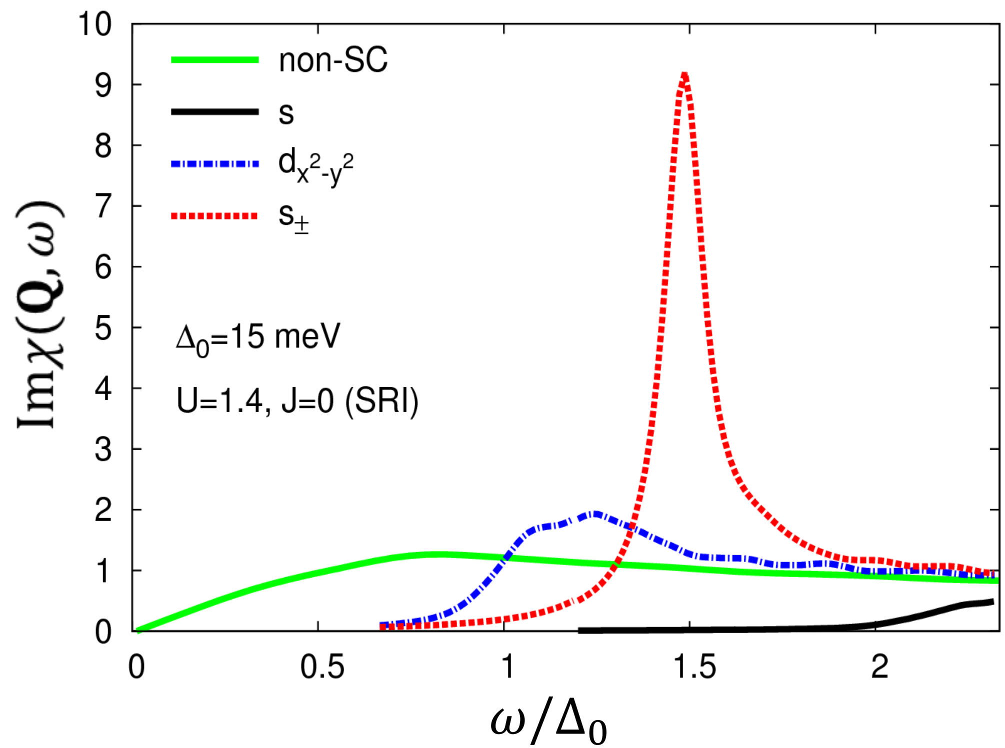
P.J. Hirschfeld, MMK, and I.I. Mazin, Rep. Prog. Phys. 74, 124508 (2011)

Resonance peak in INS: hallmark of $s_\pm$ symmetry



For $s_\pm$ symmetry $\Delta_{\mathbf{k}}^{\alpha} = -\Delta_{\mathbf{k+Q}}^{\beta}$

Coherence factors in **Imχ:** $\left(1 - \frac{\Delta_{\mathbf{k}}\Delta_{\mathbf{k+Q}}}{|\Delta_{\mathbf{k}}||\Delta_{\mathbf{k+Q}}|}\right) \neq 0$

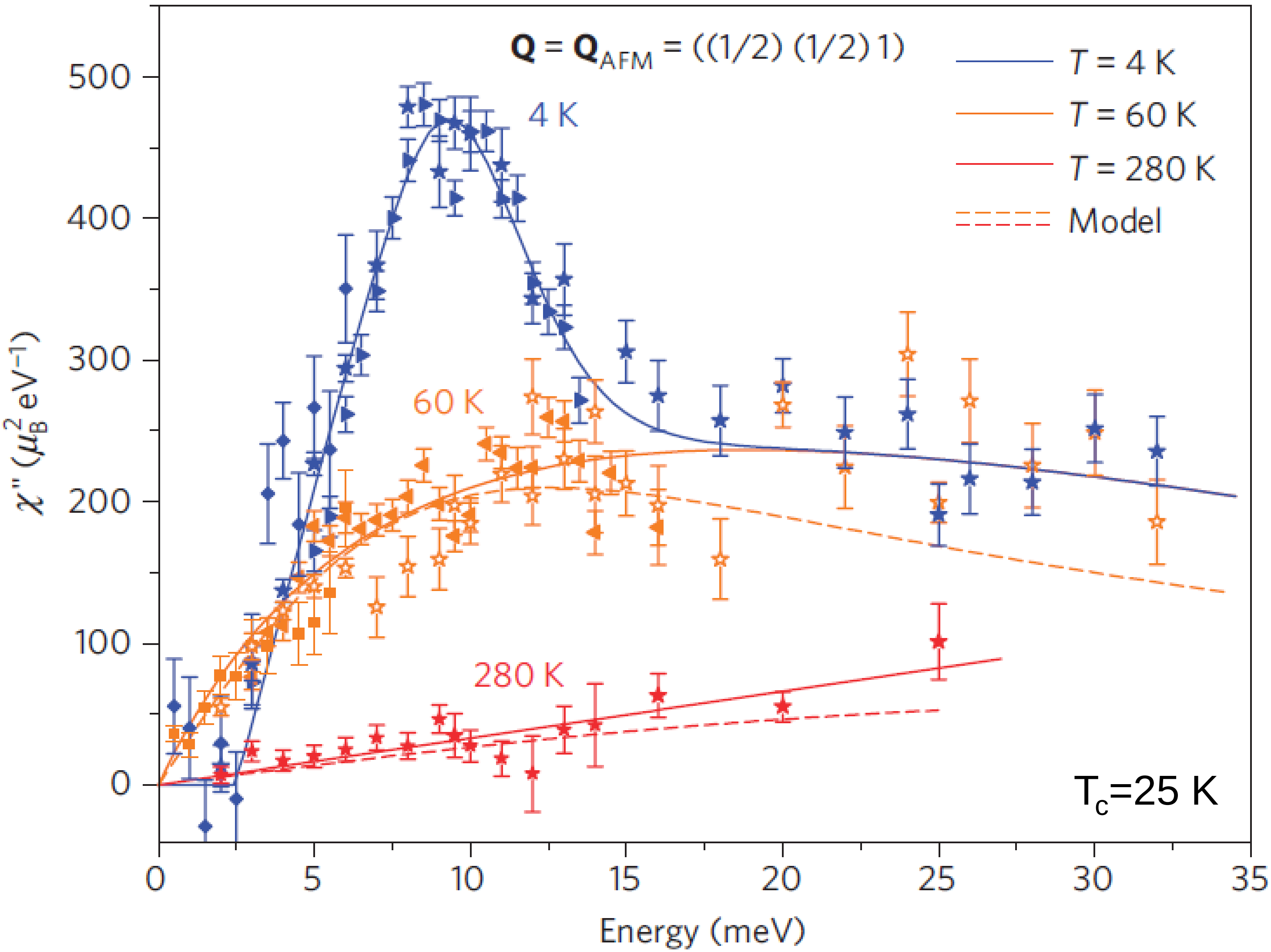


$s_\pm$ superconductivity →
resonance peak in INS,
$\boldsymbol{\omega_R \leq 2\Delta}$

***Observed experimentally*:**
A.D. Christianson et al., Nature 456, 930 (2008); M.D. Lumsden et al., PRL 102, 107005 (2009)

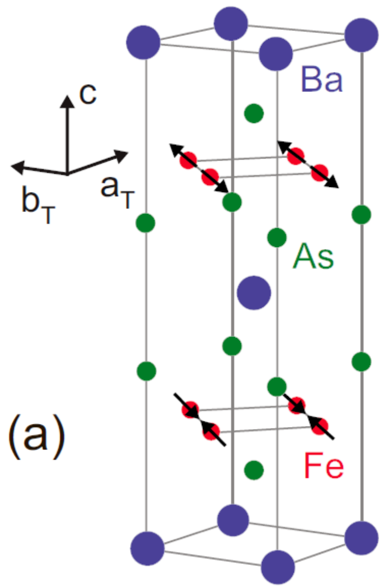
MMK and I. Eremin, PRB 78, 140509(R) (2008)
T.A. Maier and D.J. Scalapino, PRB 78, 020514(R) (2008)

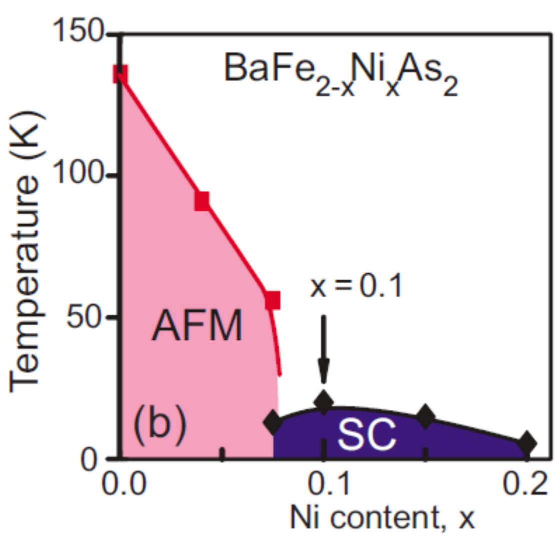
Example of inelastic neutron scattering data on $BaFe_{1.85}Co_{0.15}As_2$



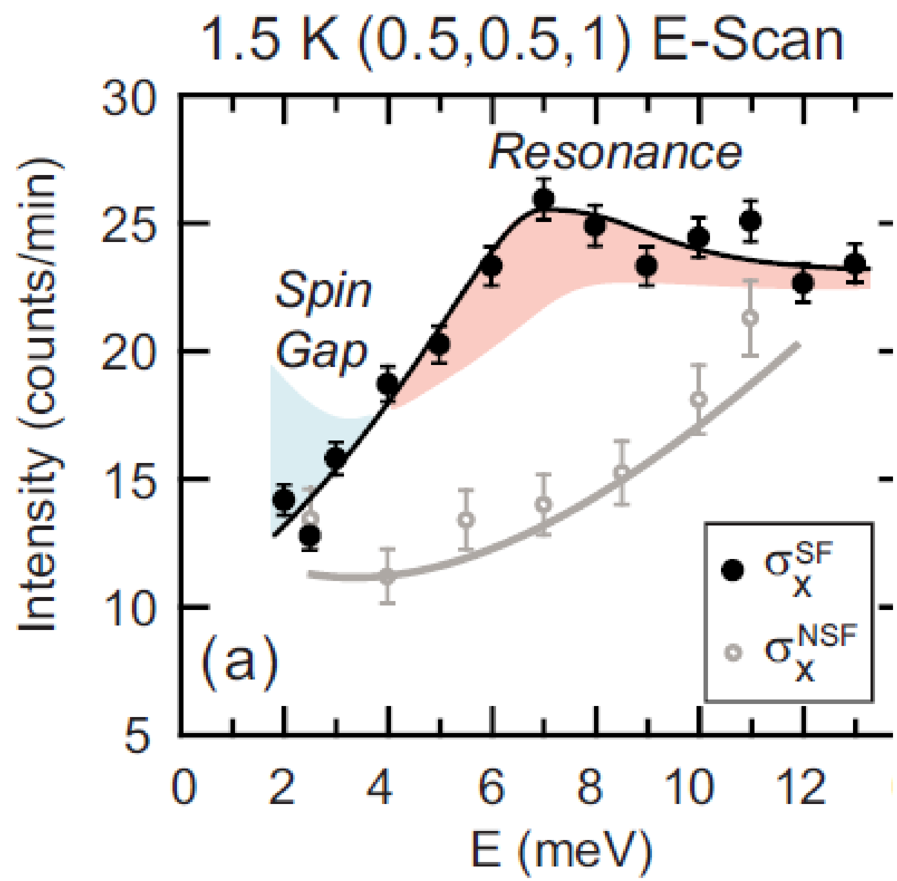
D.S. Inosov et al., Nature Physics 6, 178 (2010)

Polarized neutron scattering on $BaFe_{2-x}Ni_xAs_2$



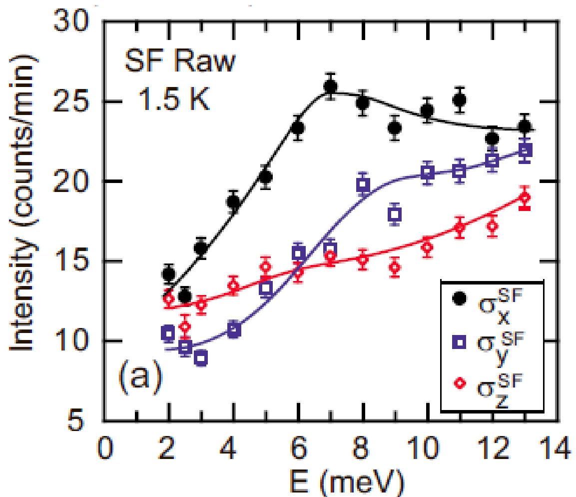


Spin-resonance at 7 meV



O.J. Lipscombe et al., PRB 82, 064515 (2010)

Polarized neutron scattering: spin-resonance anisotropy

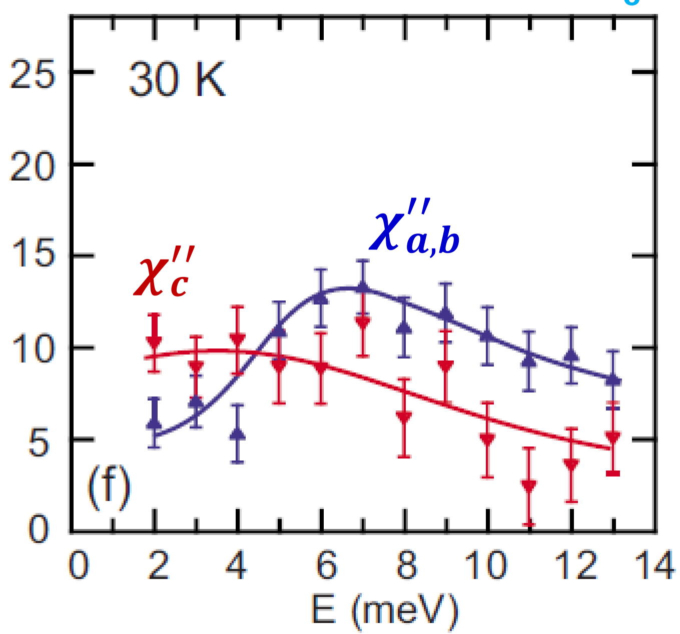


$$\langle S^x S^x \rangle = \langle S^y S^y \rangle = \langle S^z S^z \rangle$$

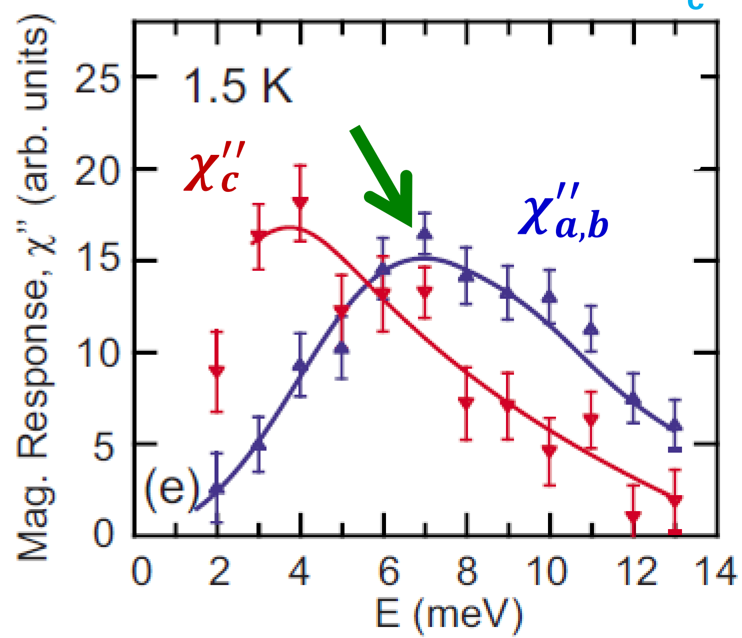
$$\chi_{+-} = \chi_{xx} + \chi_{yy} = 2\chi_{zz}$$

$\chi''_{a,b} \neq \chi''_c$: Spin-rotational invariance is broken!

T>T$_c$

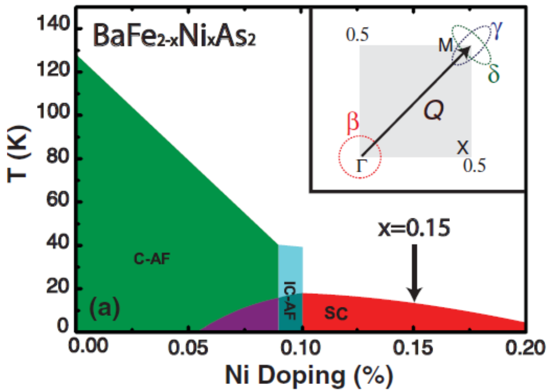


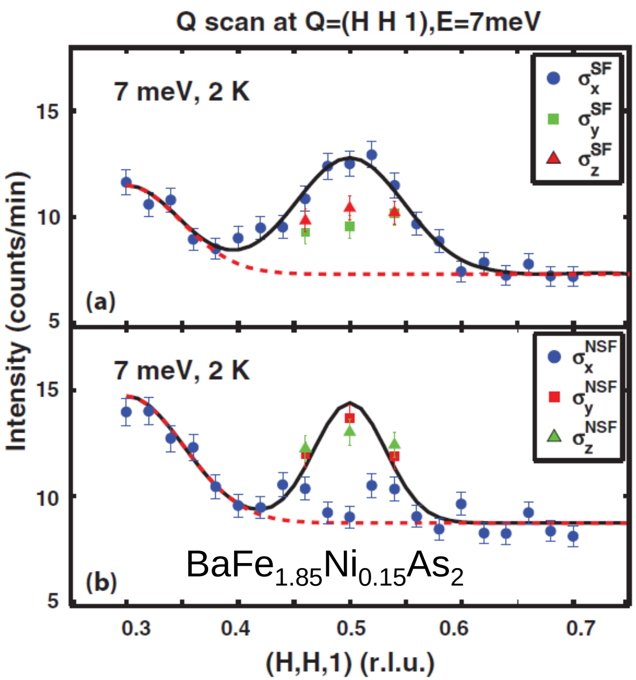
T<T$_c$



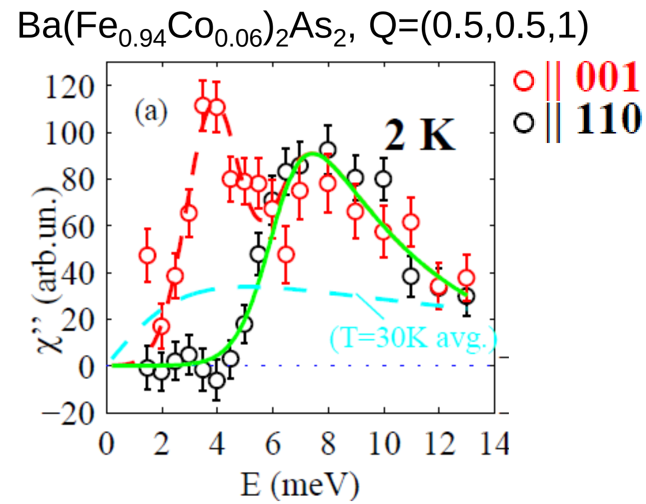
O.J. Lipscombe et al., PRB 82, 064515 (2010)

Spin-resonance anisotropy: other studies

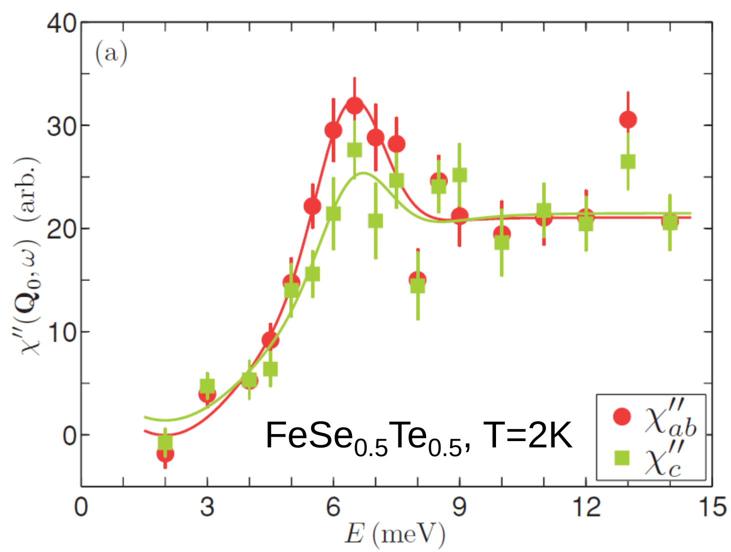




M. Liu et al., PRB 85, 214516 (2012)



P. Steffens et al., arXiv:1210.6386v1



P. Babkevich et al., PRB 83, 180506(R) (2011)

NMR above T_c: $1/T_1$ anisotropy in $Ba_{1-x}K_xFe_2As_2$

x=0.32, T_c =38.5 K and x=0.28, T_c =31.5 K

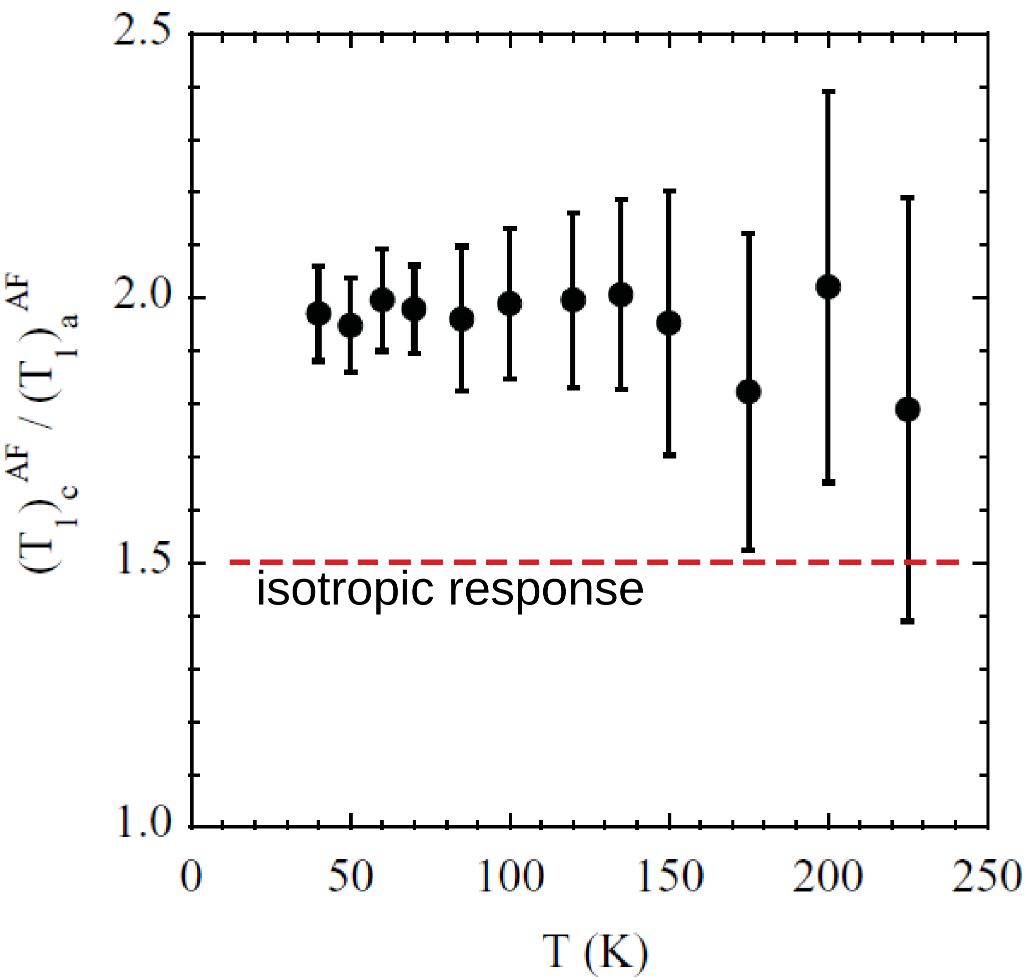
^{75}As-NMR

$$R = \frac{(1/T_1)_a}{(1/T_1)_c} = \frac{\chi''_a + \chi''_b}{2\chi''_c} + \frac{1}{2}$$

$$R^{\text{iso}} = 1.5$$

$$\frac{1}{2}\chi_{+-} > \chi_{zz}$$

by about 50%



K. Matano et al., EPL 87, 27012 (2009)
Z. Li et al., PRB 83, 140506(R) (2011)

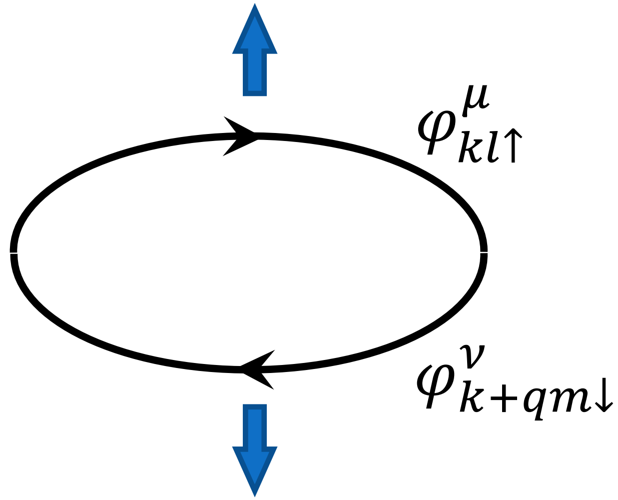
What can cause violation of spin-rotational invariance?

Spin-orbit coupling:

$$H_{SO} = \lambda \sum_f \boldsymbol{L}_f \cdot \boldsymbol{S}_f$$

Spin-orbit coupling affects the spin susceptibility

$\chi_{+-} \propto$

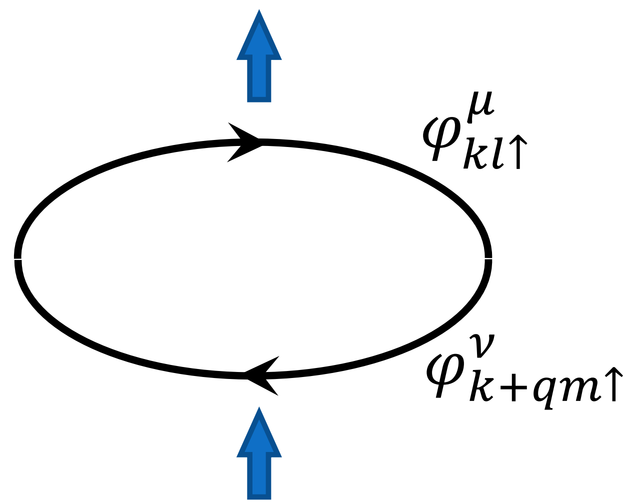


Matrix elements (orbitals l – bands μ):

$$d_{kl\sigma} = \sum_{\mu} \varphi^{\mu}_{kl\sigma}\, b_{k\mu\sigma}$$

$$\hat{H}_{SO} = \frac{\lambda}{2}\begin{pmatrix} \widehat{L_z S_z} & \widehat{L_- S_+} \\ \widehat{L_+ S_-} & -\widehat{L_z S_z} \end{pmatrix}$$

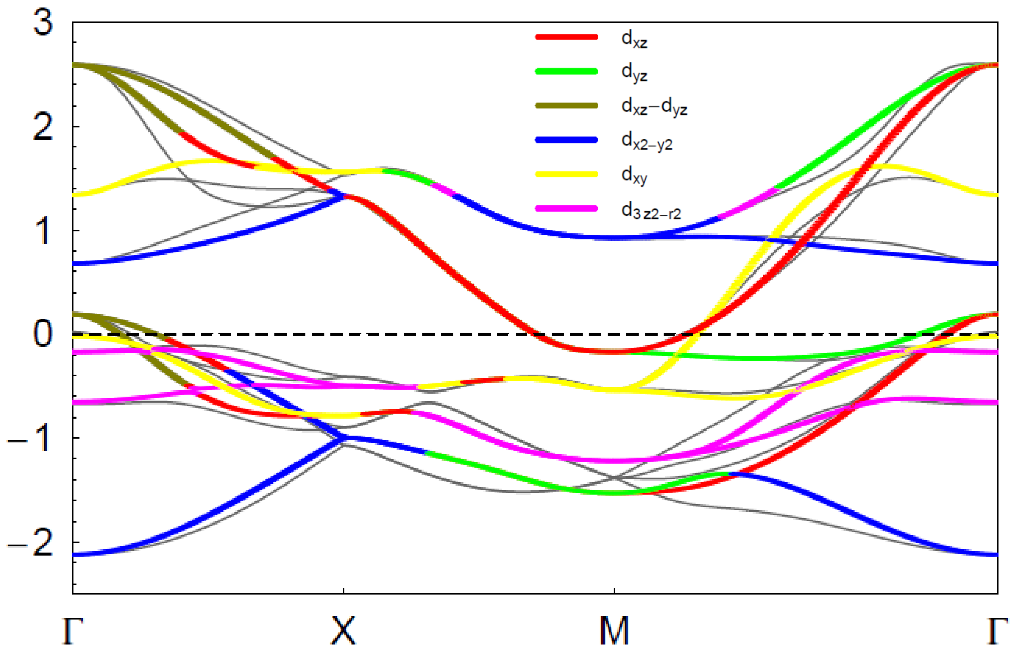
$\chi_{zz} \propto$

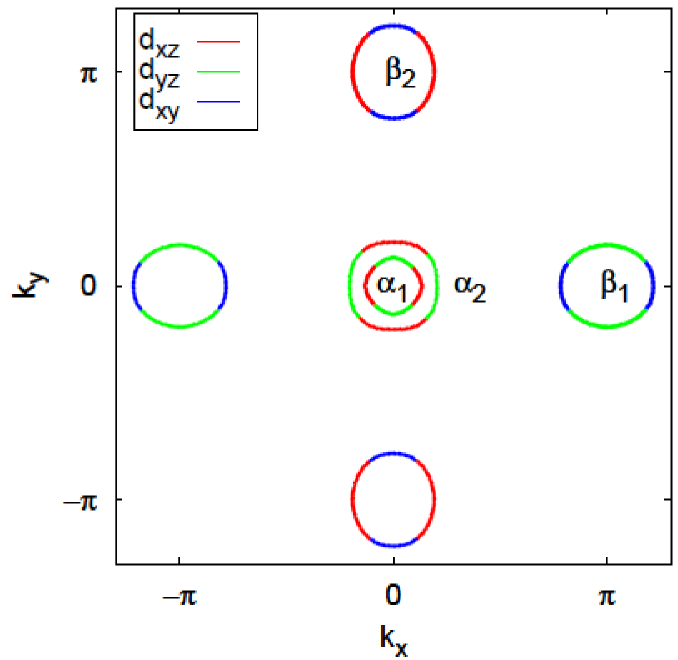


Hamiltonian and interactions

$H = H_0 + H_{int}$

H_0 =5-orbital tight-binding model





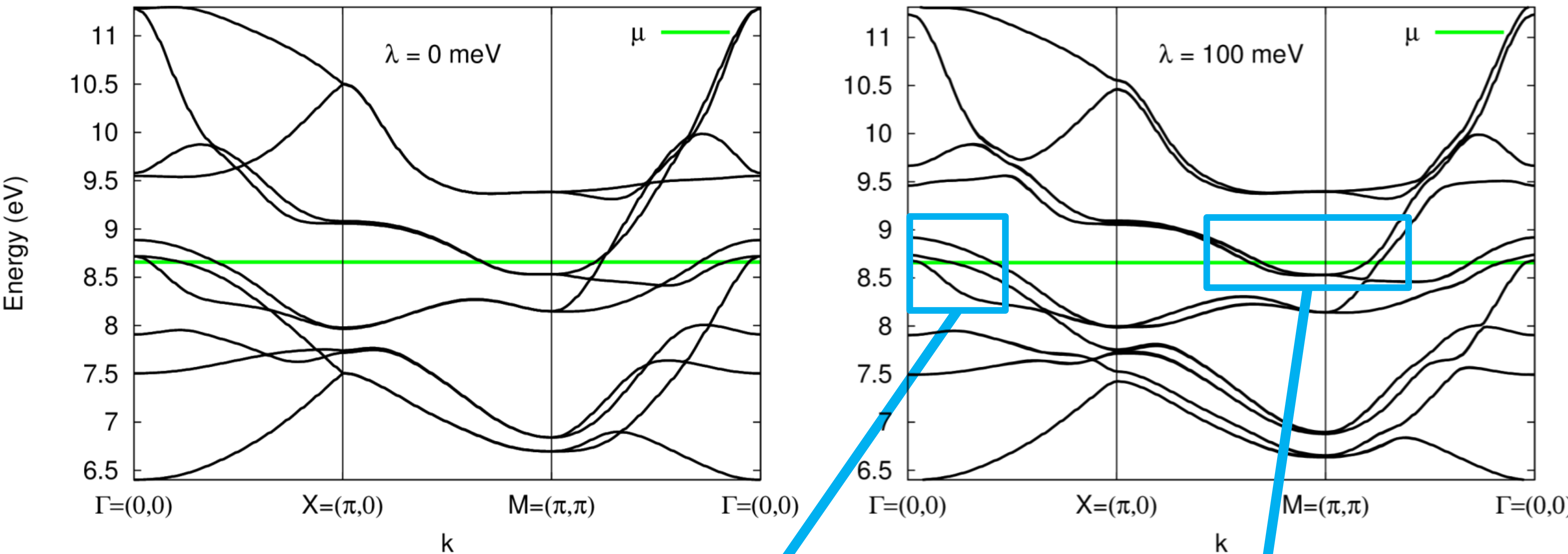
Matrix elements (orbitals l – bands μ): $d_{kl\sigma} = \sum_\mu \varphi^\mu_{kl\sigma}\, b_{k\mu\sigma}$

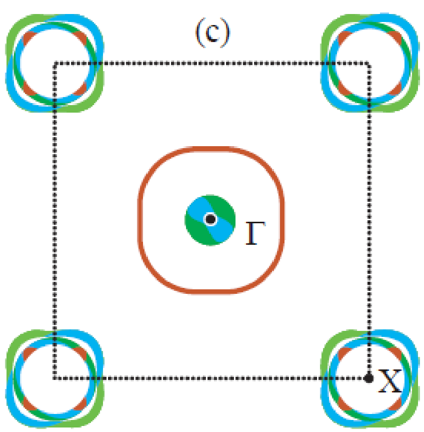
Most general 2-body Hamiltonian with intrasite interactions only

$$H_{int} = U\sum_{i,m} n_{im\uparrow}n_{im\downarrow} + J\sum_{i,m<n}\sum_{\sigma,\sigma'} d^\dagger_{in\sigma}d^\dagger_{im\sigma'}\, d_{in\sigma'}d_{im\sigma} + U'\sum_{i,m<n} n_{in}n_{im} + J'\sum_{i,m\neq n} d^\dagger_{in\uparrow}d^\dagger_{in\downarrow}\, d_{im\downarrow}d_{im\uparrow}$$

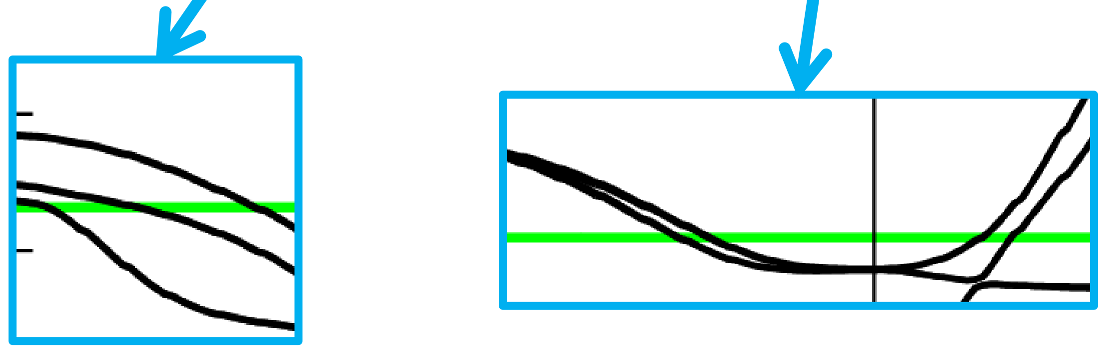
S. Graser, T.A. Maier, P.J. Hirschfeld, and D.J. Scalapino, NJP 11, 025016 (2009)

Band structure changes due to the SO coupling: 10-orbital model for LiFeAs



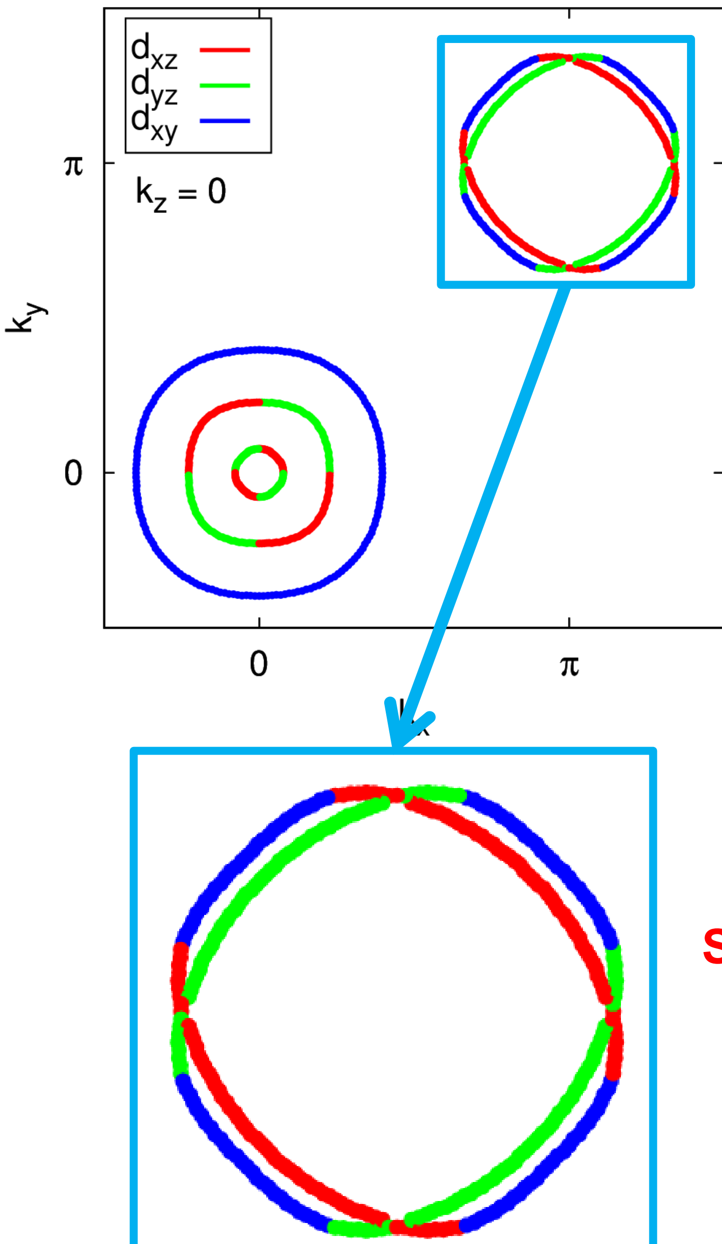


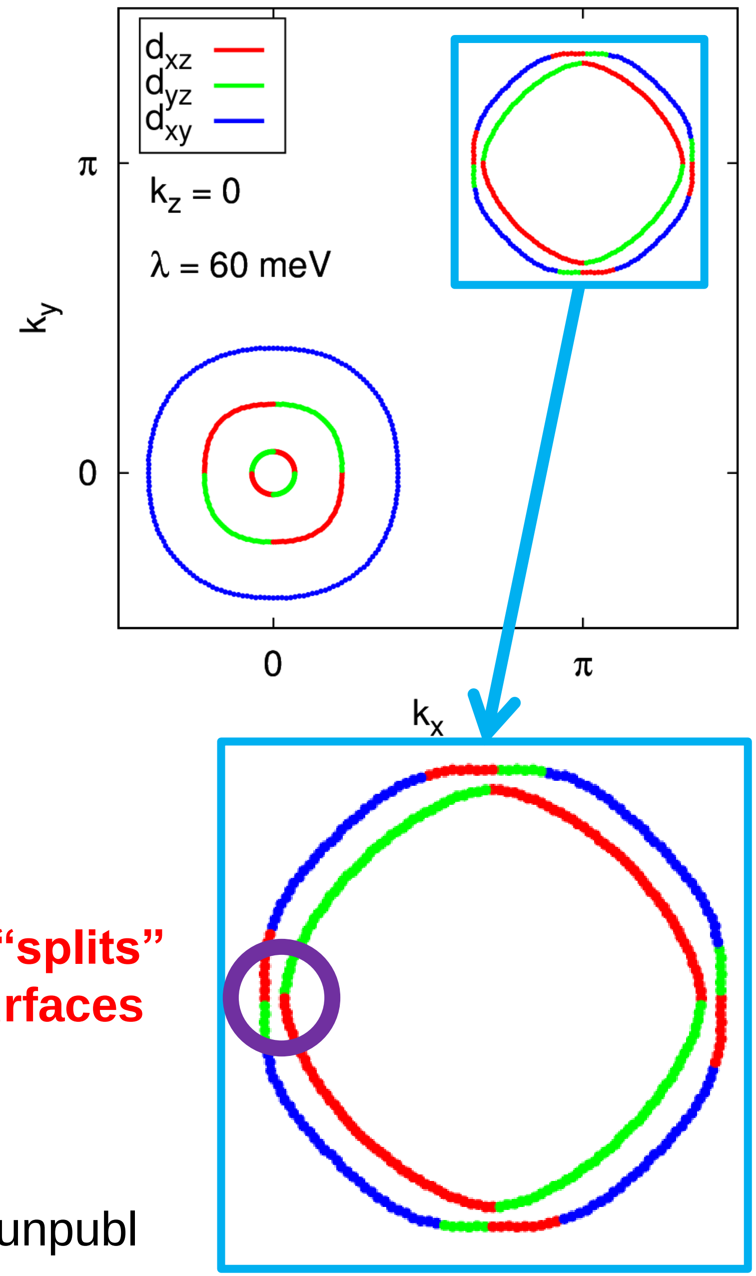
From A.A. Kordyuk review, Low Temp. Phys. (2012)



SO coupling – splitting of many band crossings

Fermi surface topology changes due to the SO coupling

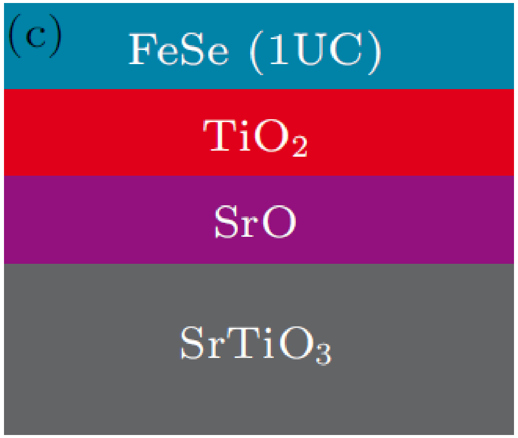




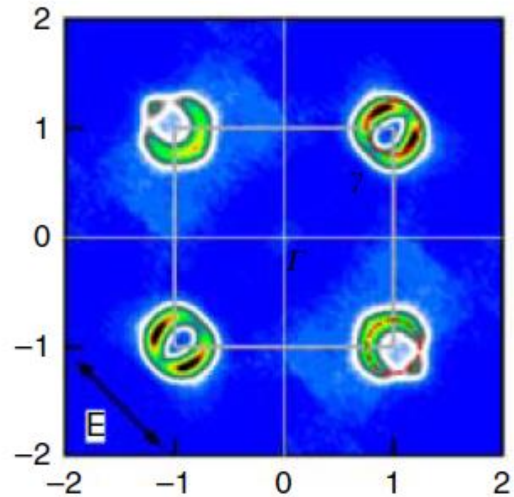
SO coupling "splits" the Fermi surfaces

MMK et al., unpubl

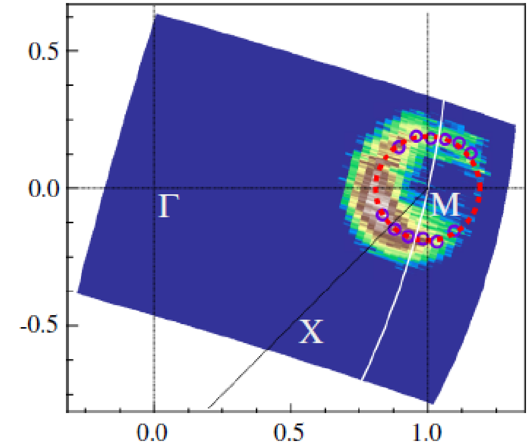
AFe_2Se_2 and FeSe monolayers



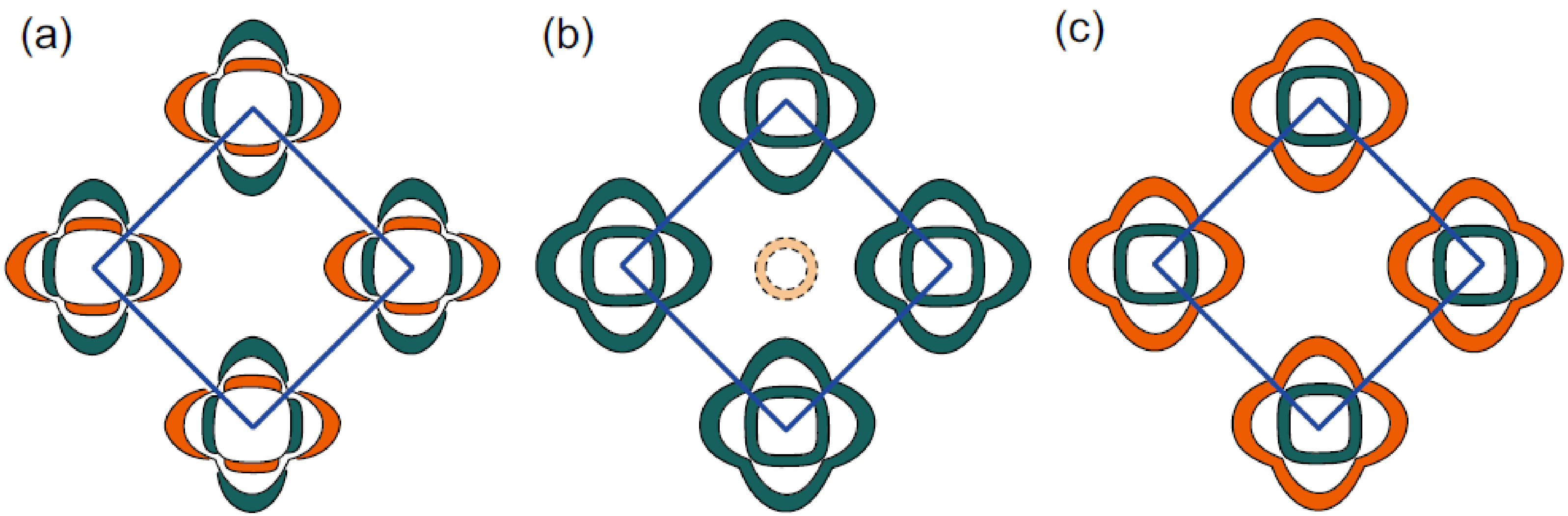
Wang et al, Chin. Phys. Lett. 29, 037402 (2012)



FeSe: Liu et al, Nat. Comm. 3, 931 (2012)



$K_{0.8}Fe_{1.7}Se_2$: Qian et al., PRL 106, 187001 (2011)

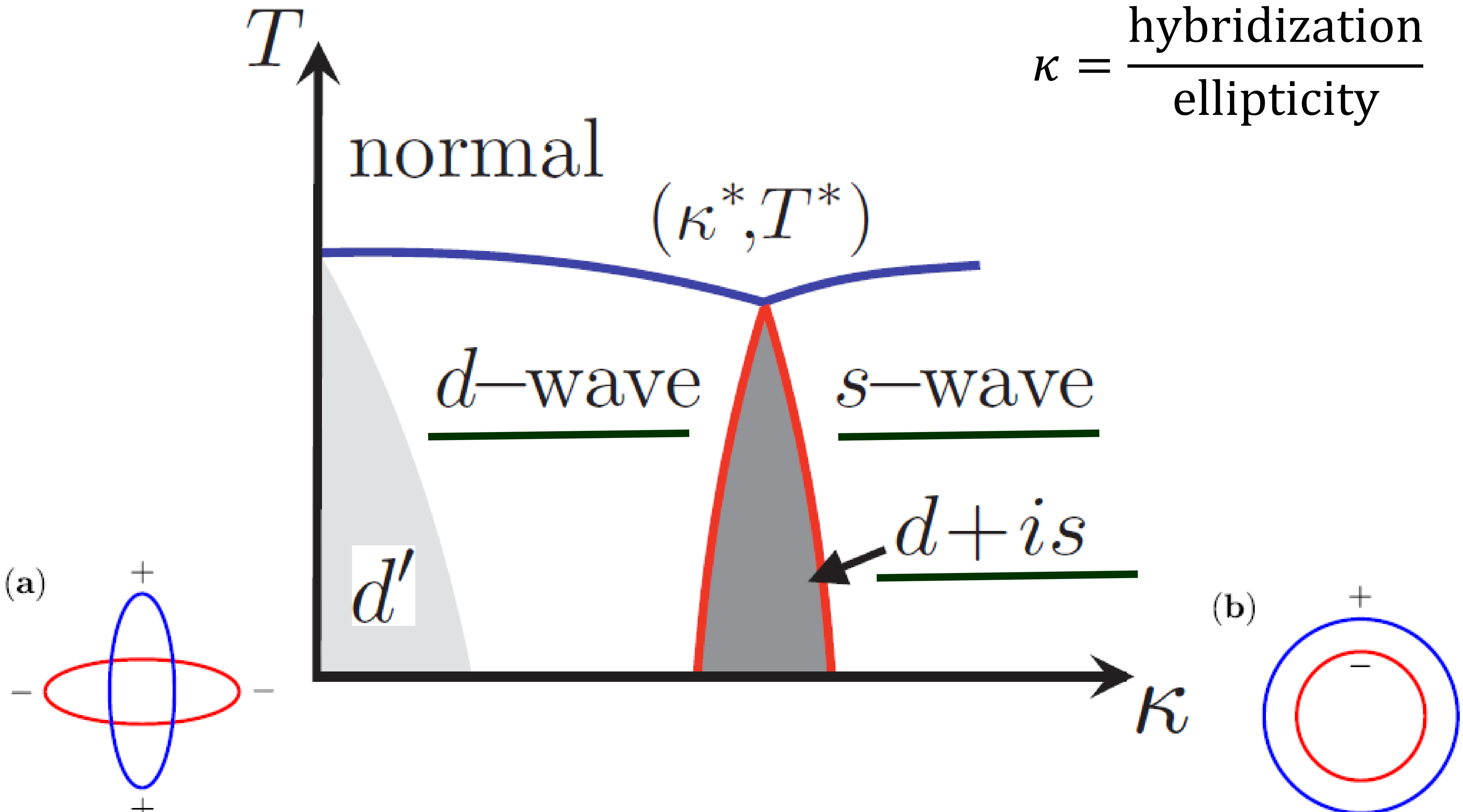


"quasi − nodeless" d "incipient" $s_{\pm}$ "bonding − antibonding" $s_{\pm}$

Role of hybridization and ellipticity (AFe_2Se_2)

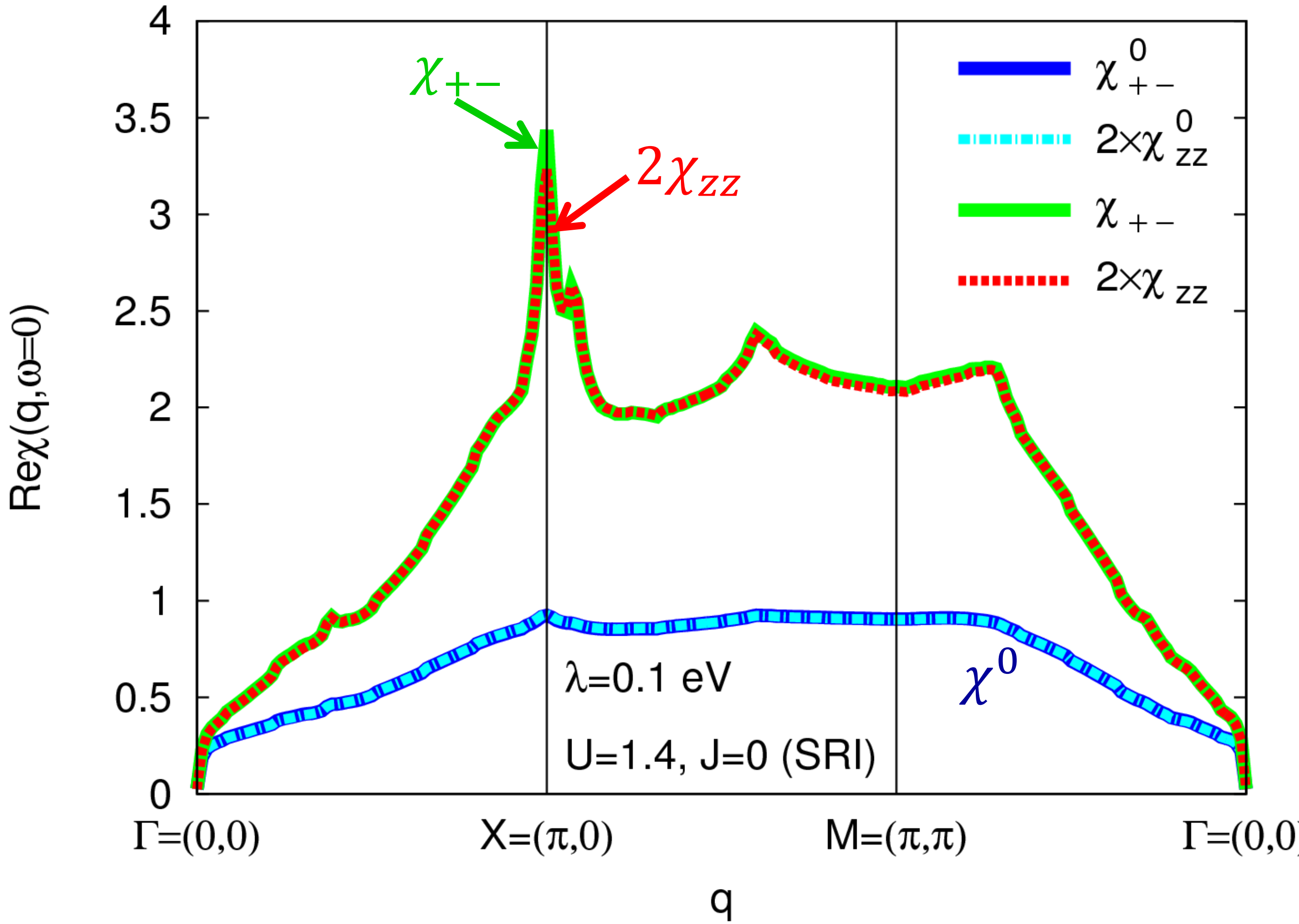
Two parameters: hybridization and the ellipticity of electron pockets

$$\kappa = \frac{\text{hybridization}}{\text{ellipticity}}$$



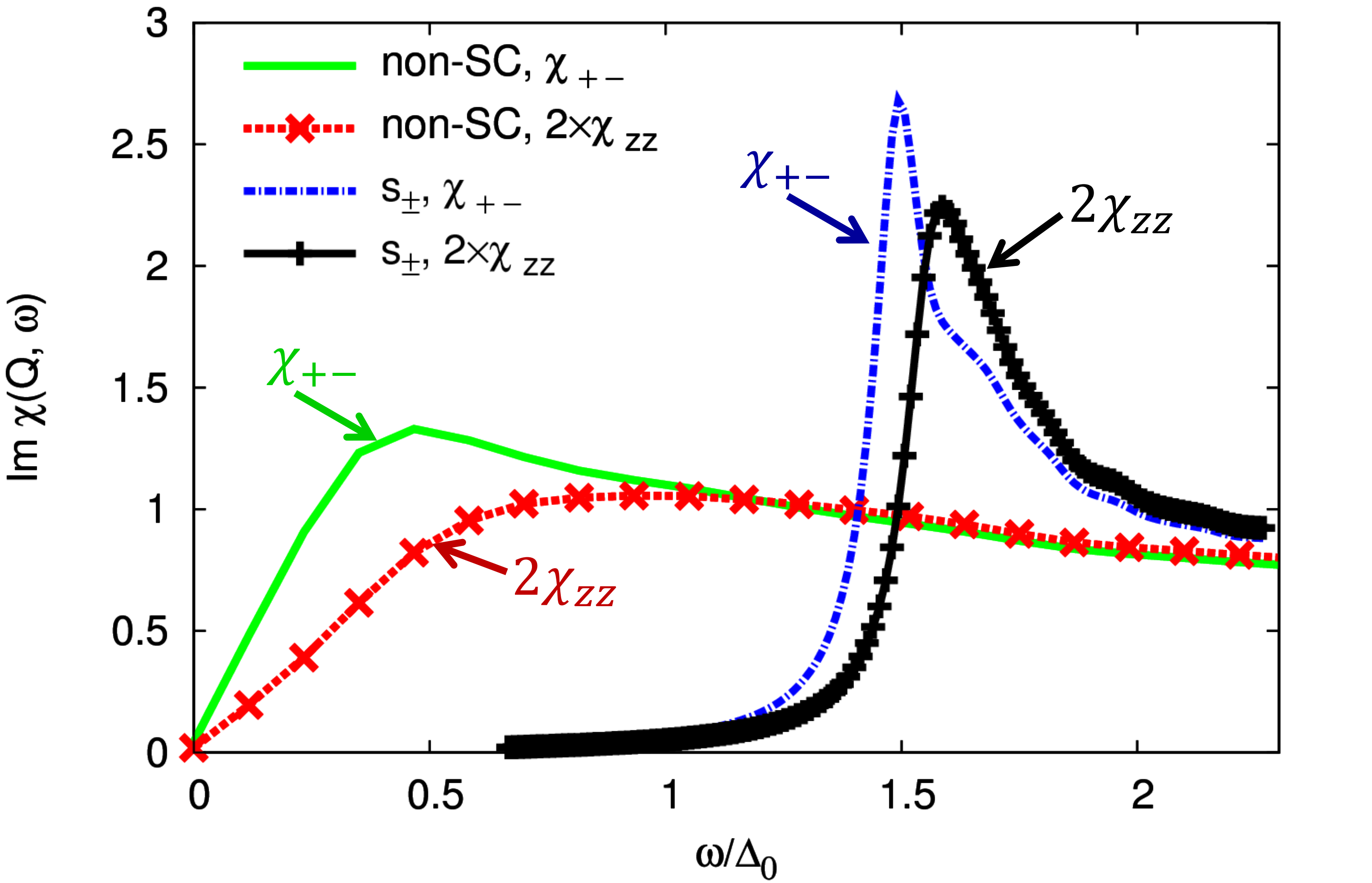
M. Khodas and A. Chubukov, PRL 108, 247003 (2012)

Spin susceptibility at $\omega = 0$ in the 5-orbital model with the SO



MMK et al., unpubl

Spin-resonance at $\boldsymbol{q} = \boldsymbol{Q}$ in the 5-orbital model with the SO



Spin-orbit coupling provides both asymmetry and frequency shift

$\lambda = 100$ meV, $U = 1.4, J = 0$ (SRI), $\Delta_0 = 15$ meV

MMK et al., unpubl

Conclusions

- **Spin-orbit (SO) coupling** provides momentum-dependent disparity between $+-$ and zz components of the spin susceptibility. This disparity is maximal at SDW wave vector and present in both normal and SC states.

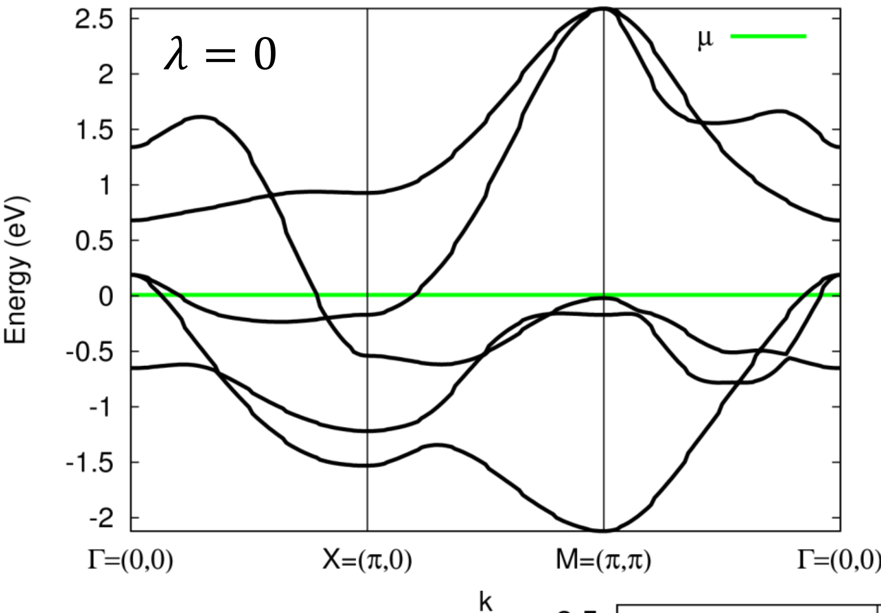
- **$+-$ wins over zz component in the normal state** that is consistent with the observation of in-plane orientations of spins in the magnetic SDW state.

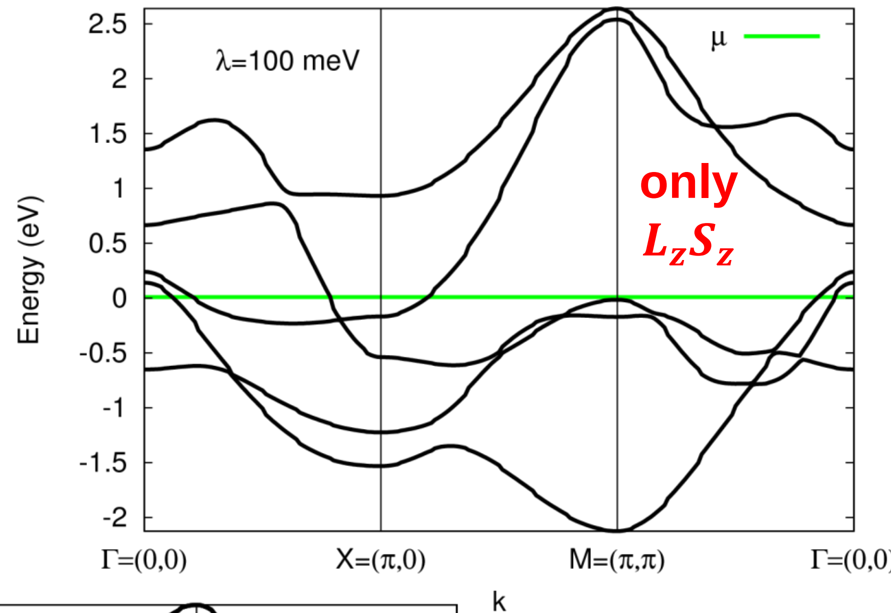
- **SO coupling gives qualitative understanding of the spin-space asymmetry** in neutron scattering and NMR data.

- **Spin-resonance for $s_{\pm}$ gap symmetry is partially suppressed in the out-of-plane (zz) component** as compared to the in-plane one.

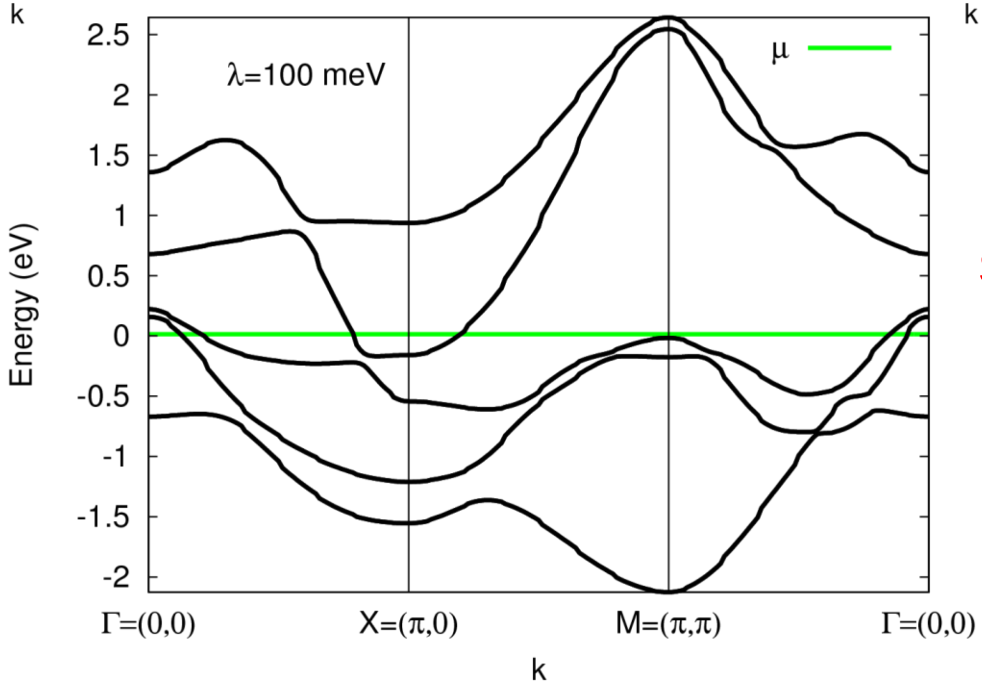
- **Band structure and Fermi surface are both affected by the SO coupling**.

Band structure changes with the finite SO coupling



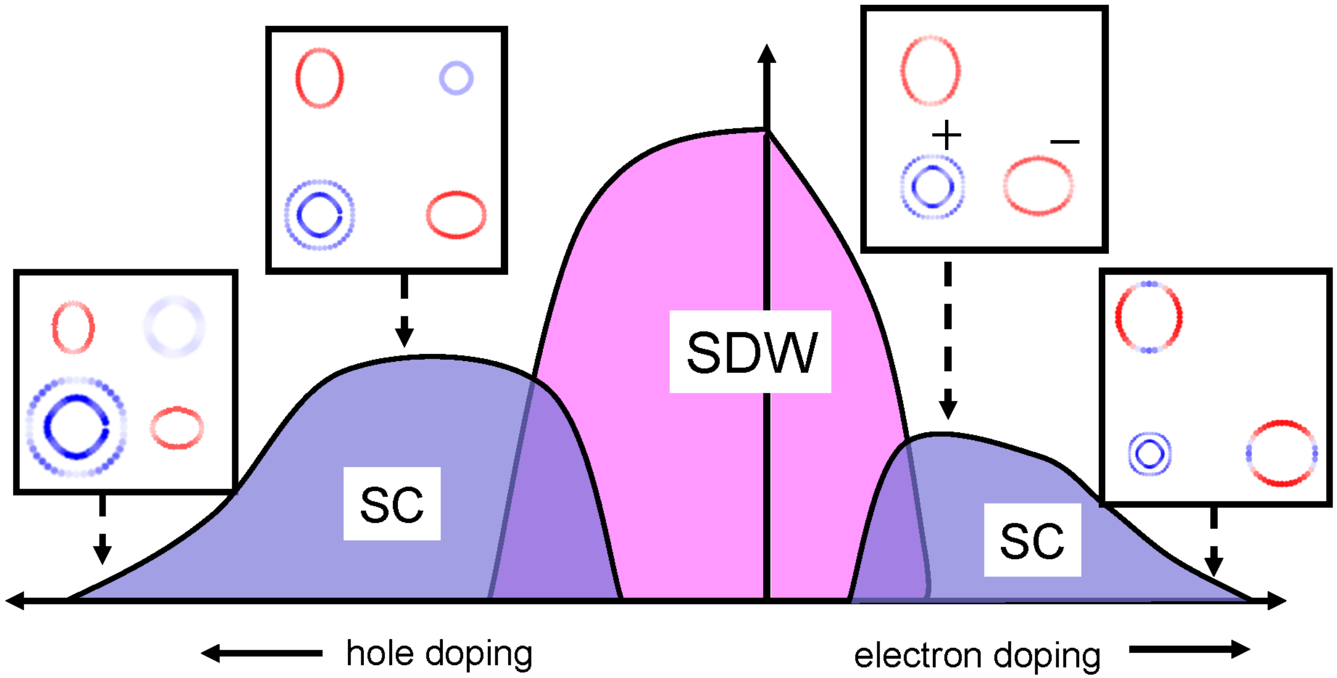


Full SO coupling

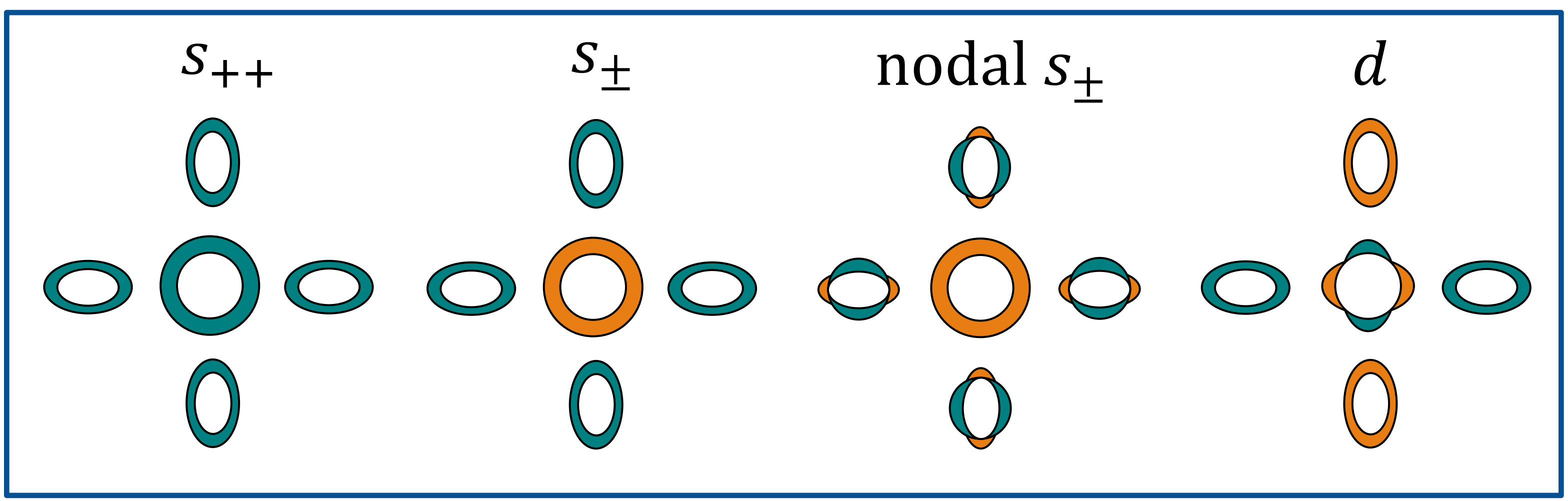


Splitting of many band crossings

2D spin-fluctuation pairing expectations in FeBS



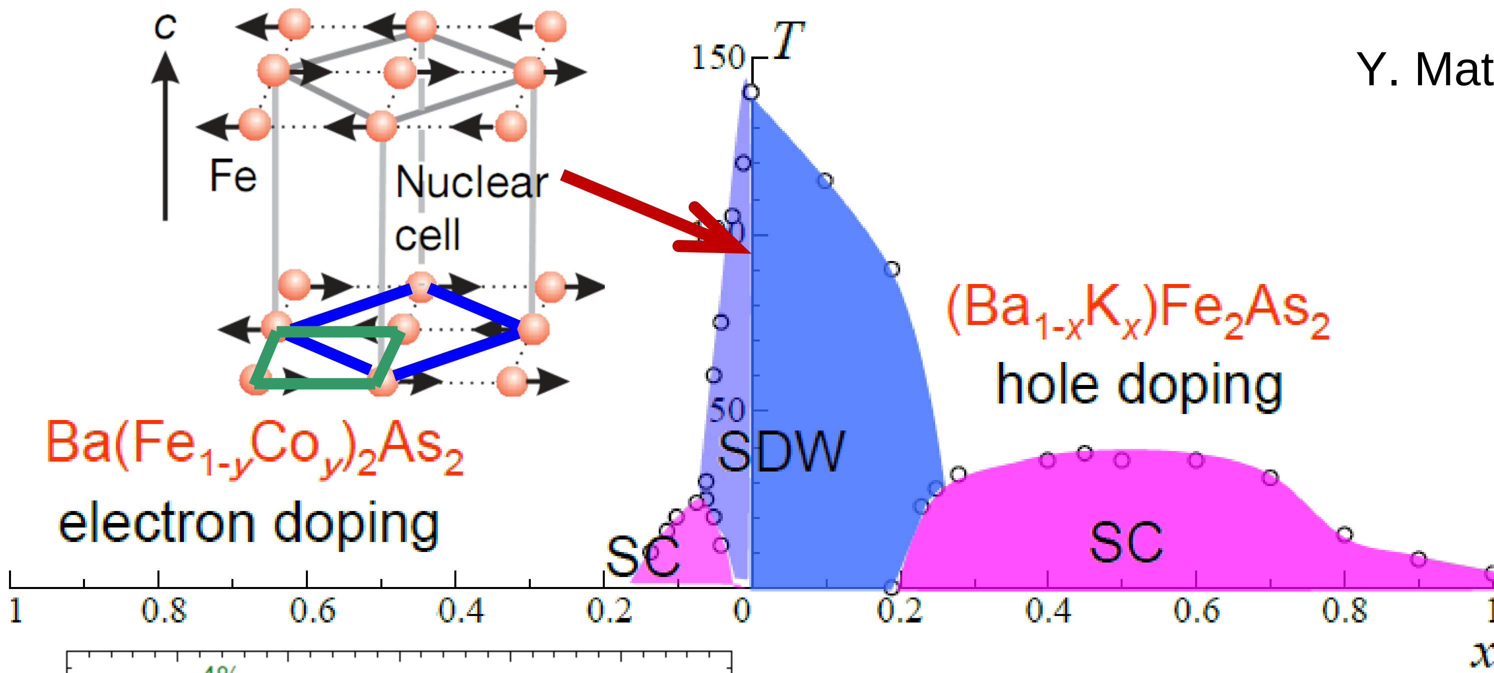
Other symmetry proposals for FeBS

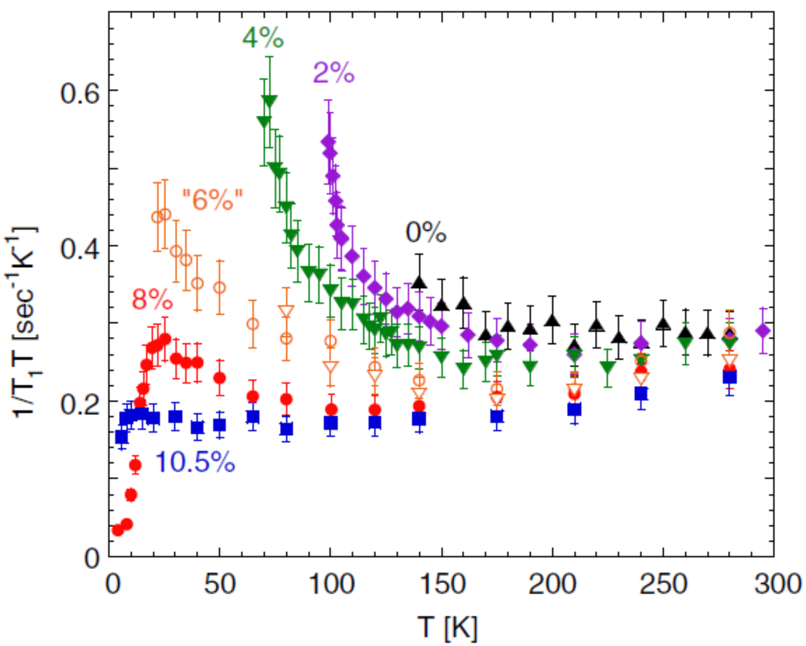


P.J. Hirschfeld, MMK, and I.I. Mazin, Rep. Prog. Phys. 74, 124508 (2011)

Phase diagram of Ba-122 system

Y. Matsuda



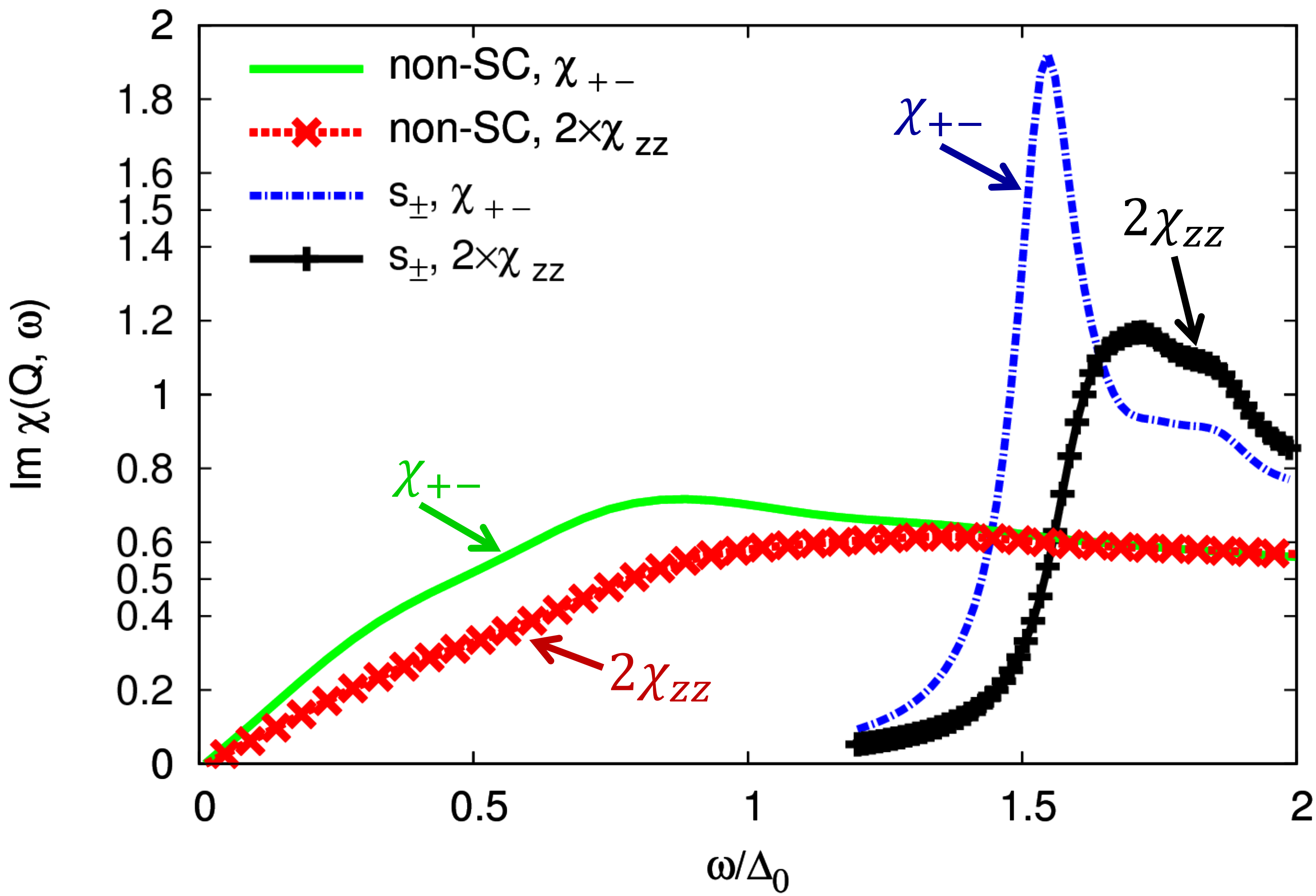


$Ba(Fe_{1-x}Co_x)_2As_2$

$1/T_1T$ from NMR

F. Ning et al., JPSJ 78, 013711 (2009)

Spin-resonance at $\boldsymbol{q} = \boldsymbol{Q}$ in the 5-orbital model: only L_zS_z-component of SO



Spin-resonance anisotropy if further enhanced

$\lambda = 100$ meV, $U = 1.4, J = 0$ (SRI), $\Delta_0 = 15$ meV