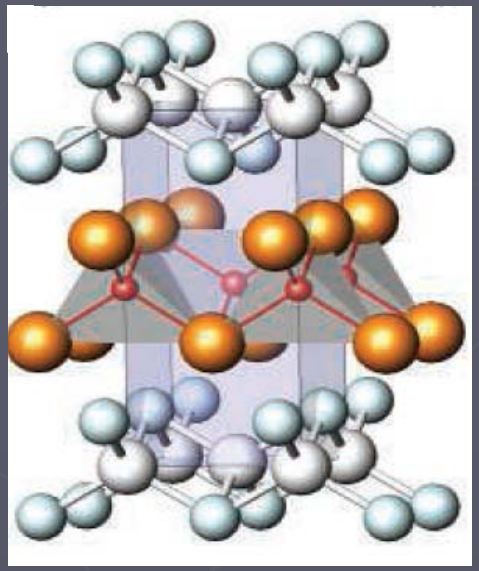
Fe-based SC

Koenigstein School
April 2014



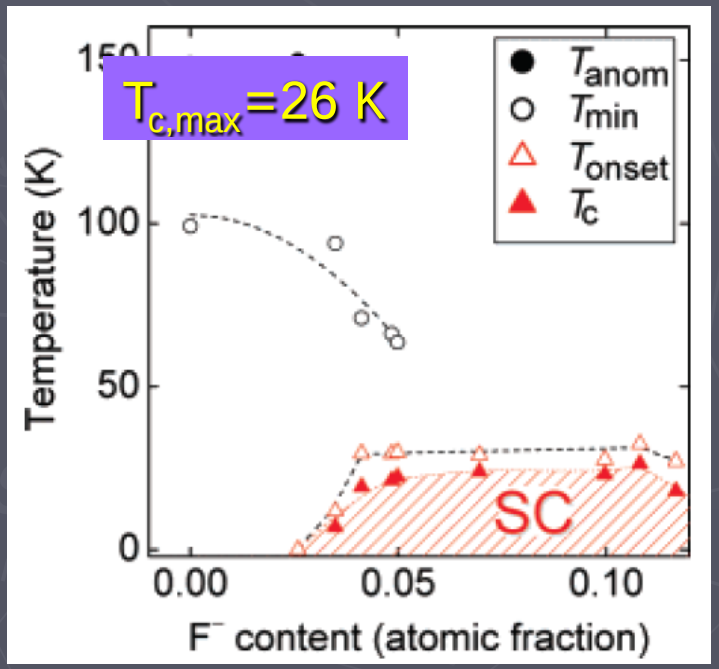
- review of normal state
- review of sc state
- standard model
- new materials & directions

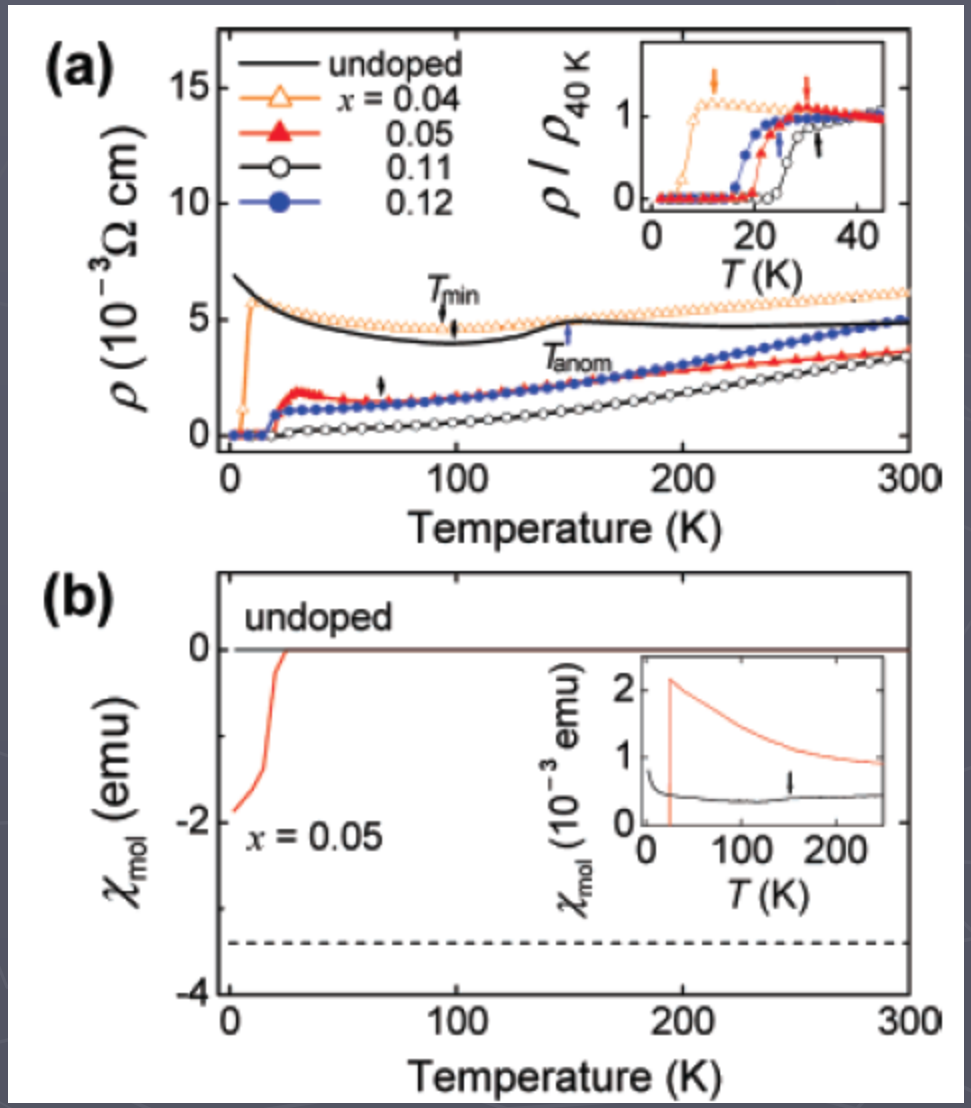
Reviews: P.J. Hirschfeld et al, Rep. Prog. Phys. 74, 124508 (2011);
G.R. Stewart RMP 2012; Dagotto and Dai, Nat. Phys. 2012; A. Chubukov, Ann. Rev. 2012

Discovery of $LaO_{1-x}F_xFeAs$

Kamihara et al JACS 2008

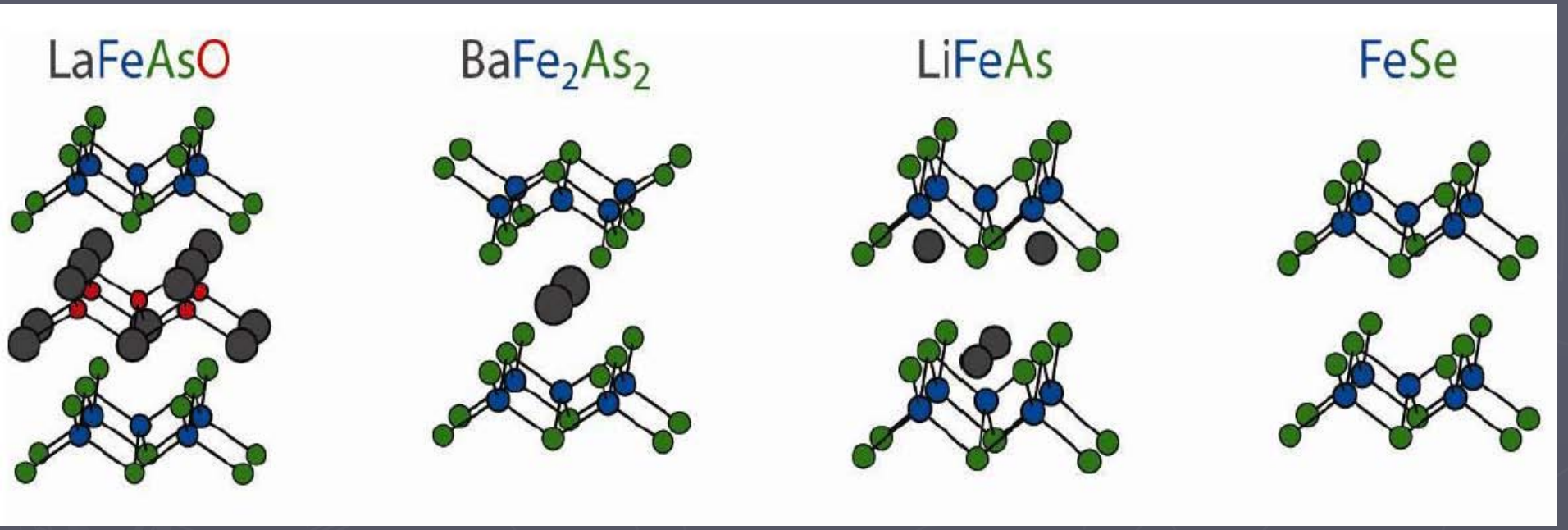
H. Hosono





Iron-based superconductors

Recent reviews: G.R. Stewart RMP 2012, Paglione & Greene Nat Phys 2010; Johnston Adv. Phys. 2010



T_c=28K
(55K for Sm)

- Kamihara et al JACS (2008)
- Ren et al Chin. Phys. Lett. (2008)

T_c=38K

- Rotter et al. arXiv: PRL (2008)
- Ni et al Phys. Rev. B 2008 (single xtals)

T_c=18K

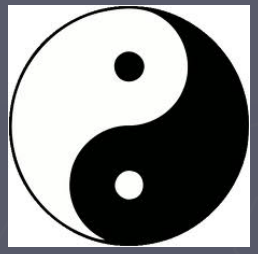
Wang et al
Sol. St. Comm. 2008

T_c=8K

Hsu et al
PNAS 2008

No arsenic ☺!

Comparison with cuprates



Strong vs. weak coupling?

Single vs. multibands?

2D vs. 3D?

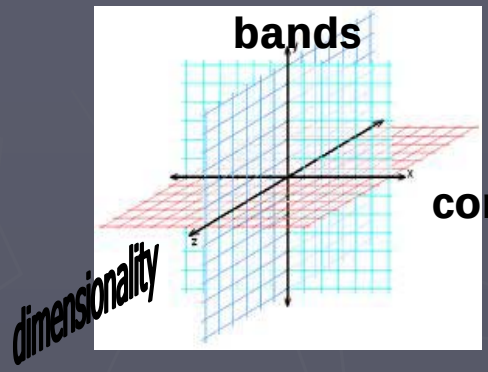


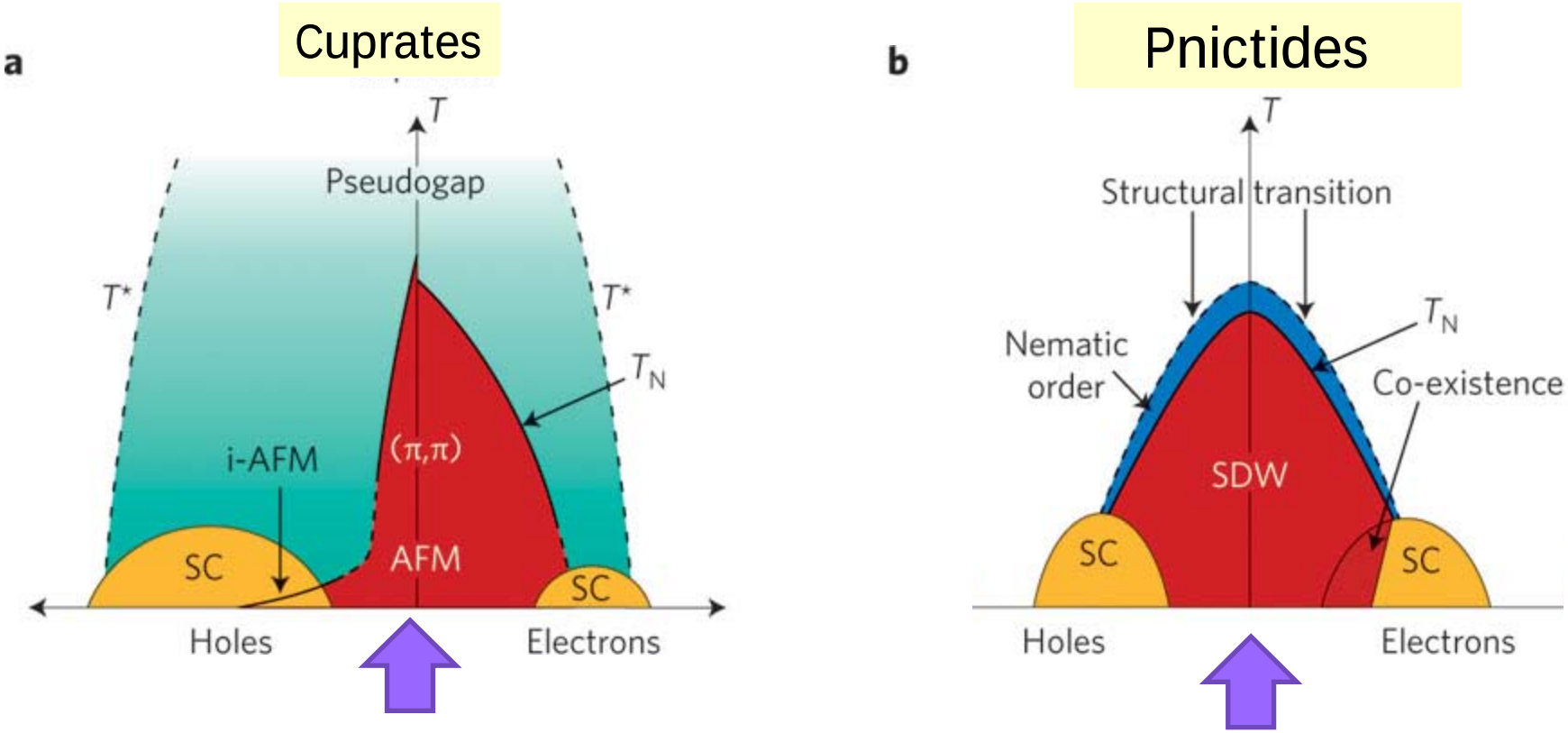
Table 1 | Properties of different classes of superconductor

Property	Conventional superconductors	Copper oxides	MgB_2	Iron-based superconductors
T_c (maximum)	<30 K	134 K	39 K	56 K
Correlation effects	None (nearly-free electrons)	Strong local electronic interaction	None (nearly-free electrons)	Long-range (non-local) magnetic correlations
Relationship to magnetism	No magnetism	Parent compounds are magnetic insulators	No magnetism	Parent compounds are magnetic metals
Order parameter	One band, same-sign *s* wave	One band, sign-changing *d* wave	Two band, same-sign *s* wave	Two band, presumably sign-changing *s* wave
Pairing interaction	Electron–phonon	Probably magnetic (no consensus)	Electron–phonon	Presumably magnetic
Dimensionality	Three dimensional	Two dimensional	Three dimensional	Variable

I. Mazin, Nature 2010

Can we learn what the essential ingredients for high-T_c are from the comparison?

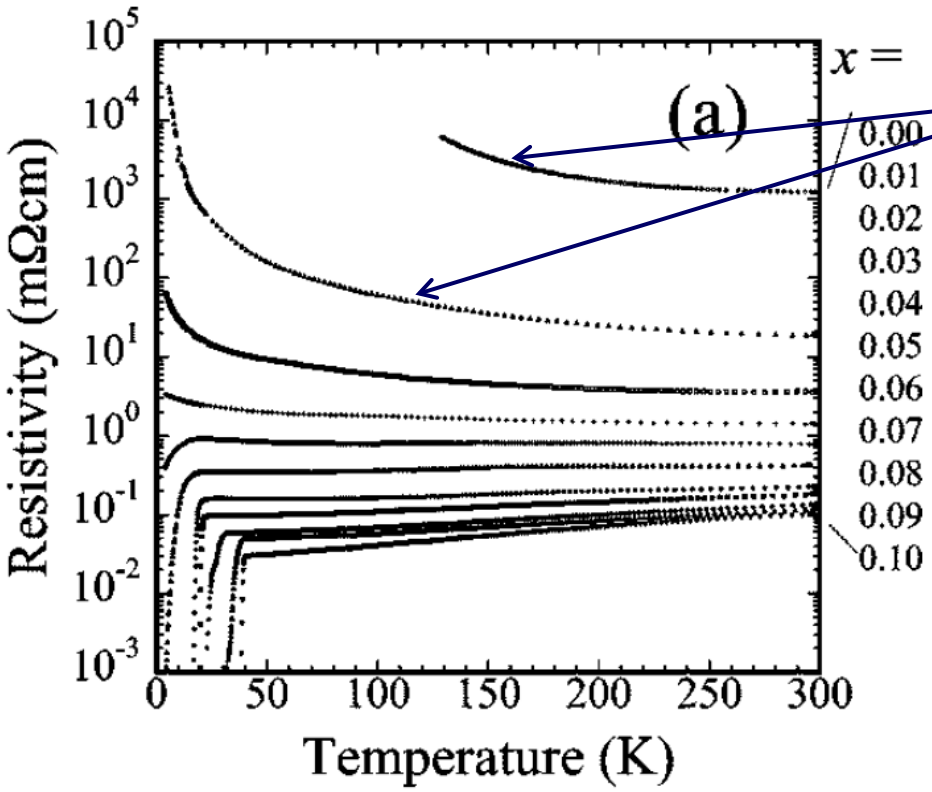
Phase diagrams of Cu-based and Fe-based superconductors are similar



Parent compounds are insulators

Parent compounds are metals

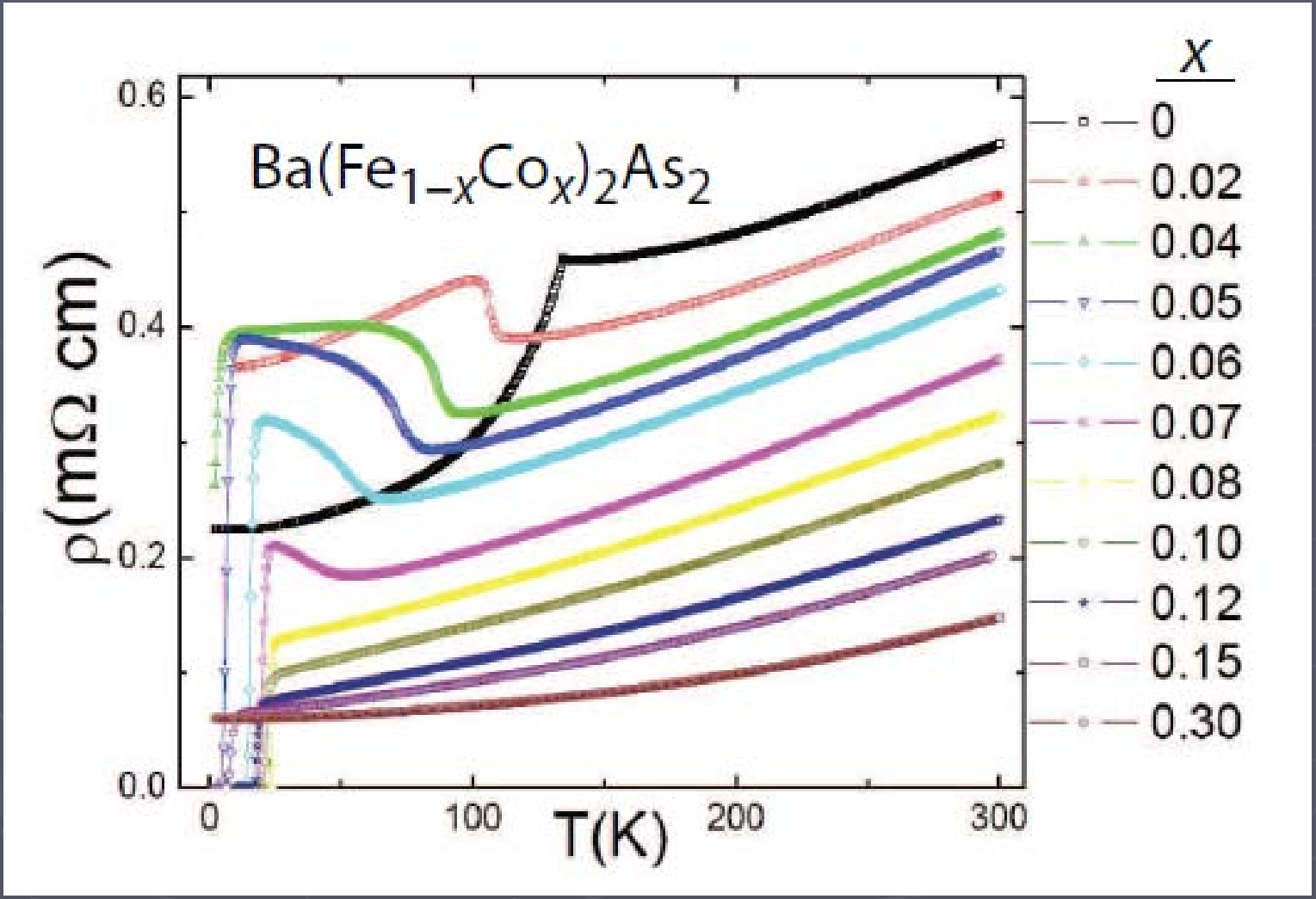
Insulating behavior of parent compounds of the cuprates



parent compounds

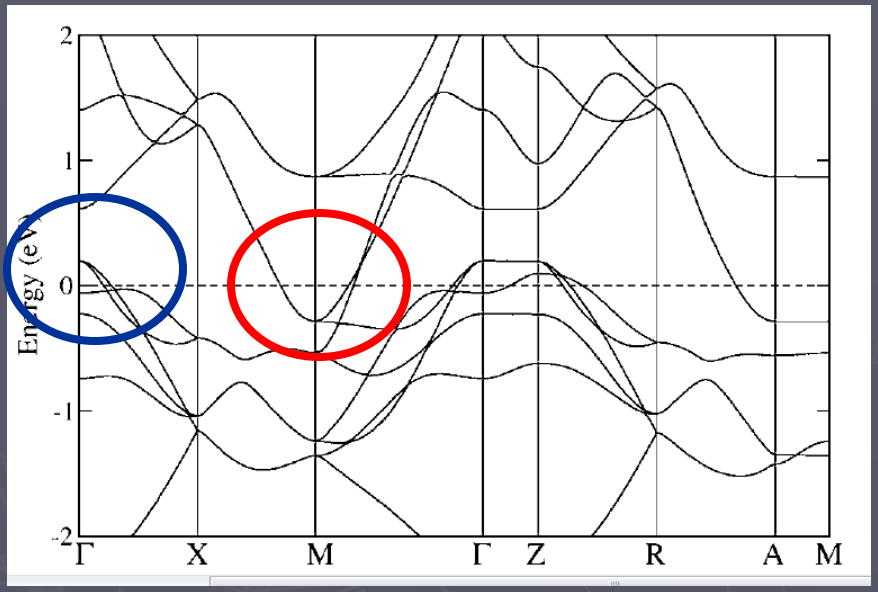
Metallic behavior of parent compounds of Fe pnictides

Fang et al 2009

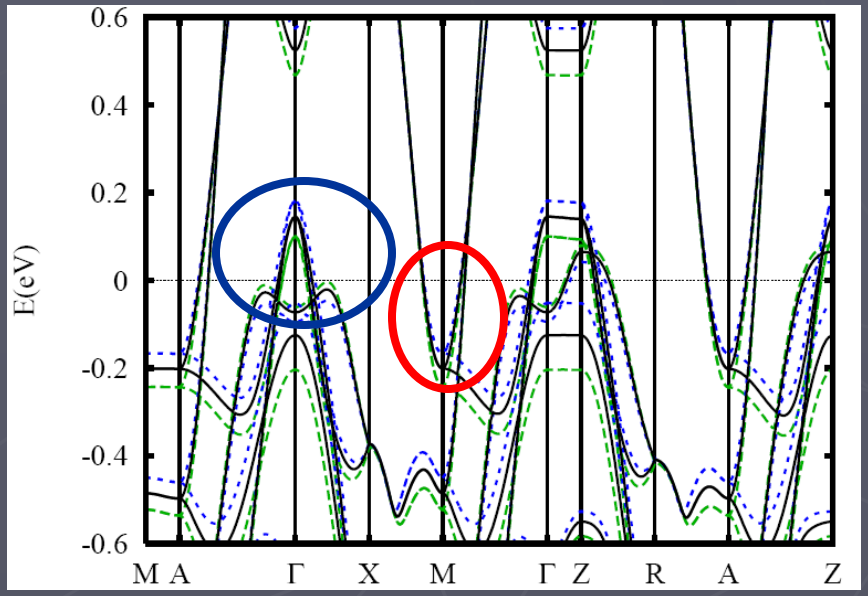


Electronic structure calculations

LOFP Lebegue 2007 (T_c=6K)

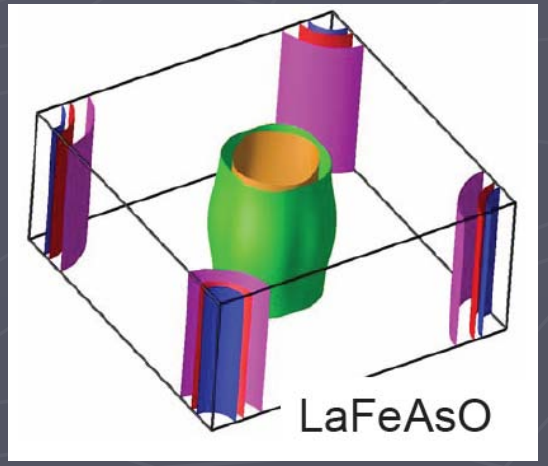


LOFA Singh & Du 2008 (T_c=26K)



Band structures for 2 materials nearly identical!
Hole pocket near Γ, electron pocket near M

Kotliar et al, Cao et al: correlations can be significant



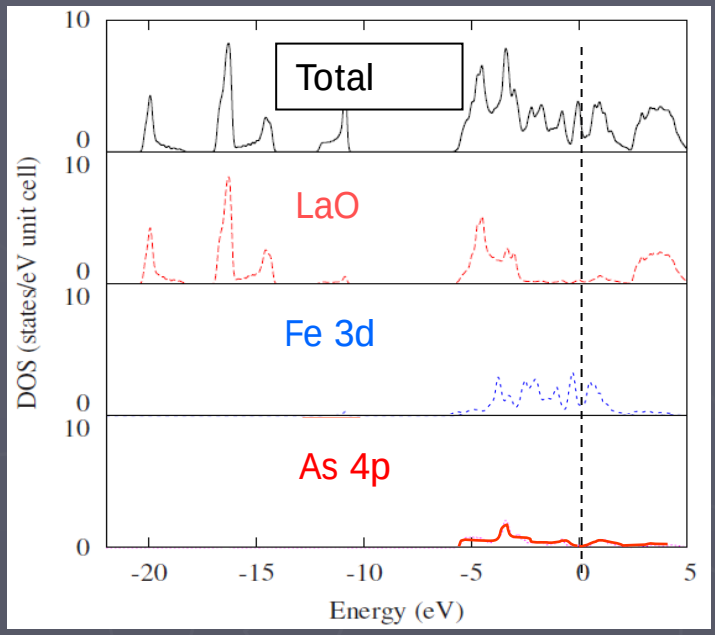
2D!

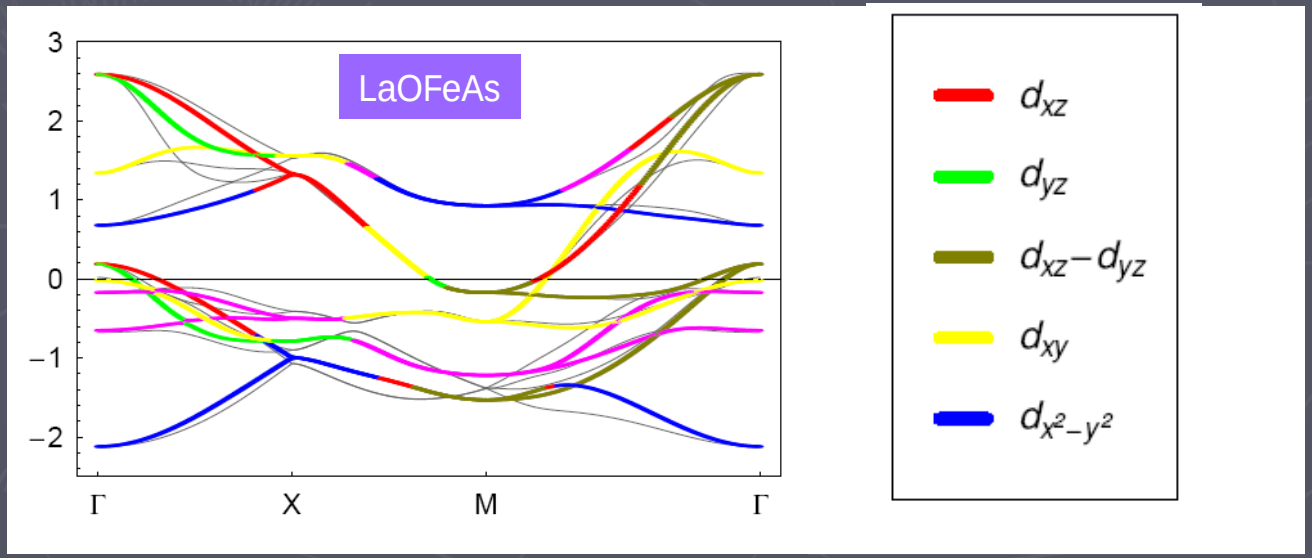
Multiorbital physics

DOS near Fermi due almost entirely to 5 Fe d-states

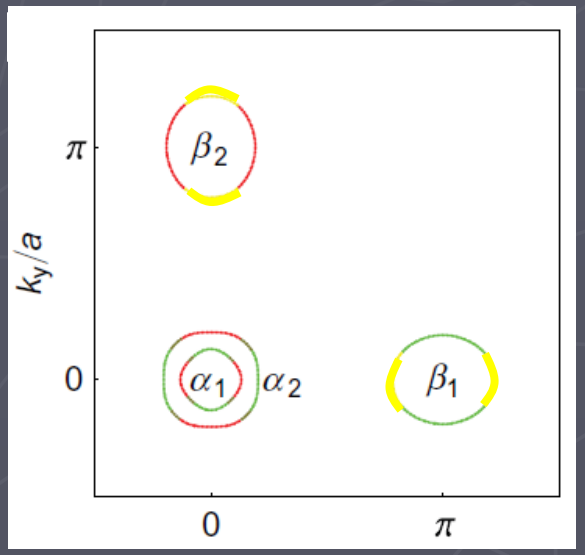
Complications: calculations will be harder

Novelty: surprising new aspects of multiorbital/ multiband physics





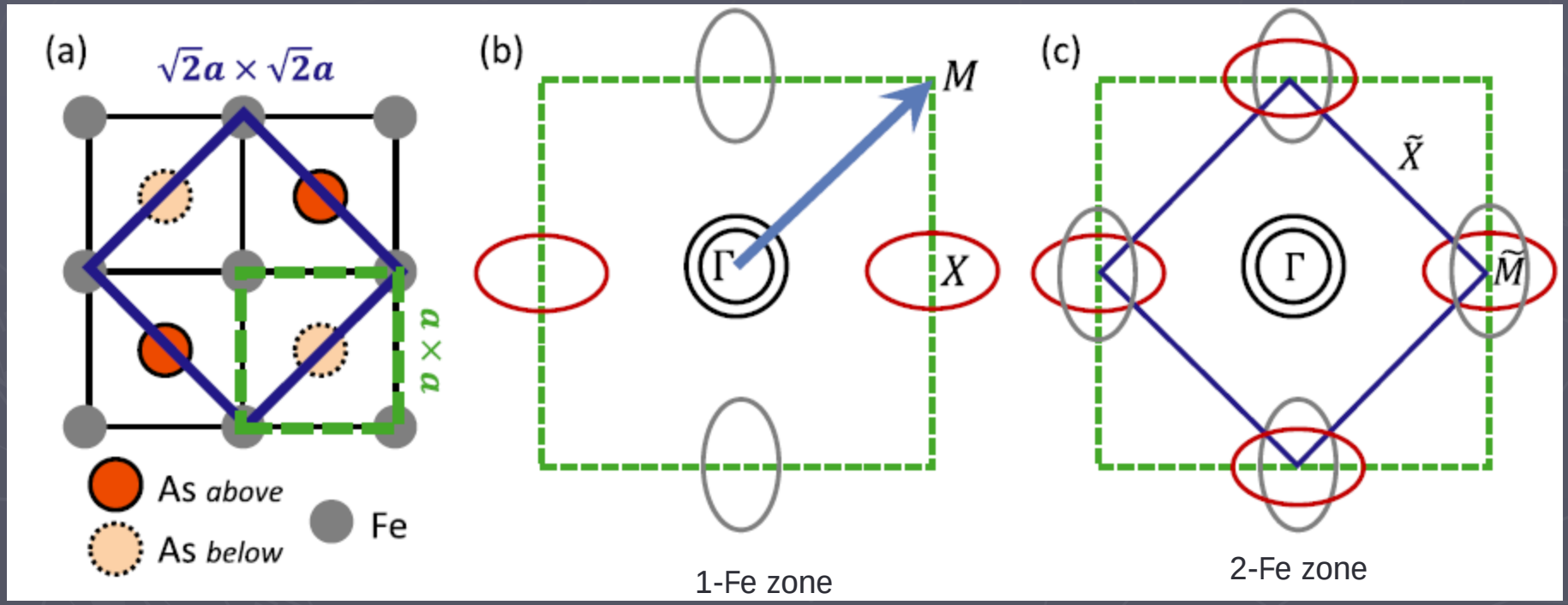
Band structure



Fermi surface

(Some) theorists find folded BZ already too complex

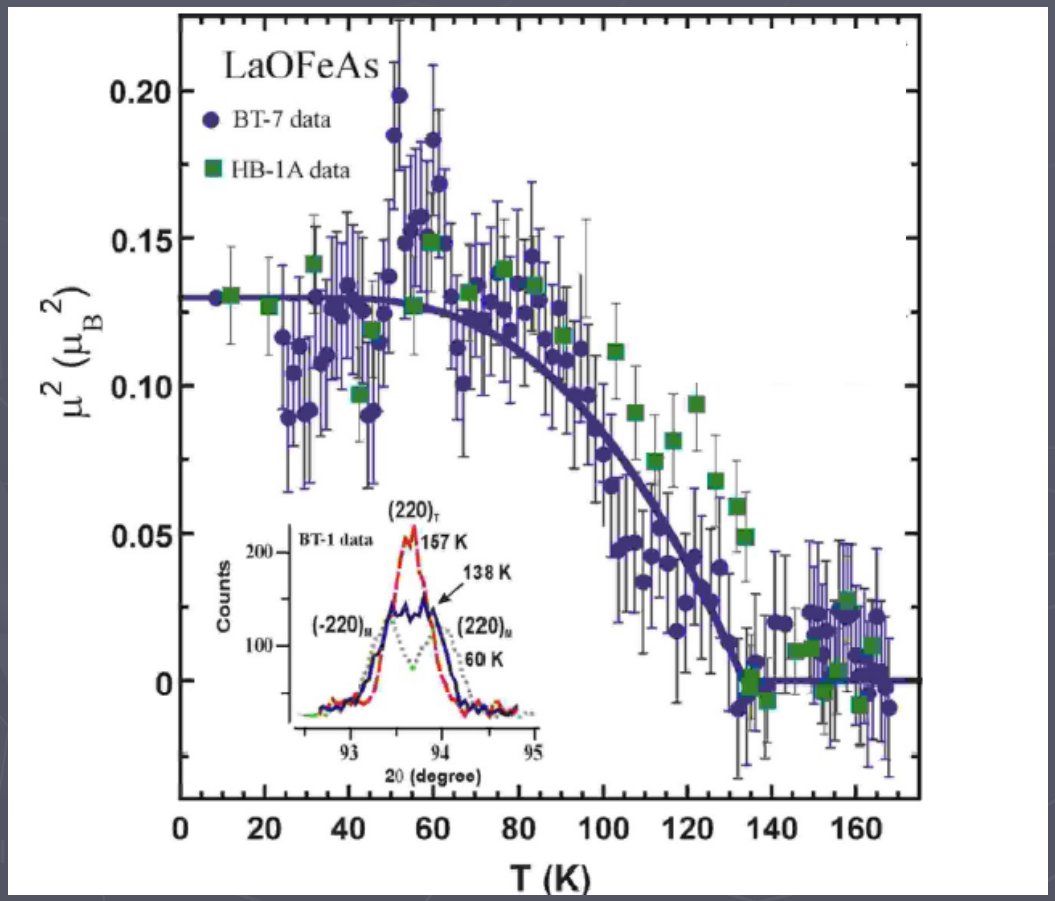
Unfolded BZ Folded BZ

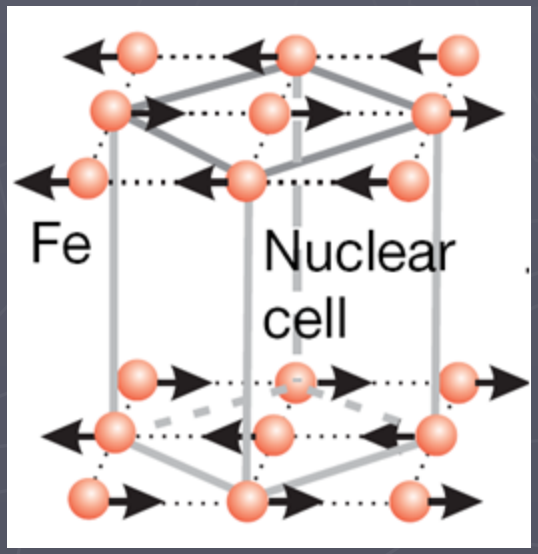


2D cross-sections

Magnetic order in most (not all) parent compounds

de la Cruz et al Nature 453, 899 (2008)





Stripe like order w q=(π,0)

Ordered magnetism in FeSC

Material	T_S (K)	T_N(Fe) (K)	μ_{Fe} (μ_B)	q_{Fe}	Spin direction	T_N(R) (K)	μ_R (μ_B)	q_R	Spin direction
LaOFeAs	155	137	0.36	101	likely *a*	-			
CeOFeAs	158	140	0.8	100	*a*	4.0	0.94	101	*a,b,c*
PrOFeAs	153	127	0.48	100	*a*	14	0.84	100	*c*
NdOFeAs	150	141	0.25	101	likely *a*	1.96	1.55	100	*a,c*
$CaFe_2As_2$	173	173	0.80	101	*a*	-			
$SrFe_2As_2$	220	220	0.94	101	*a*	-			
$BaFe_2As_2$	142	143	0.87	101	*a*	-			
$Fe_{1.068}Te$	67	67	2.25	100	*b*	-			

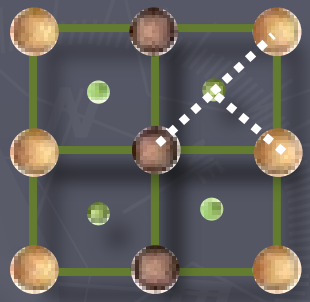
"double stripe" q=(π/2,π/2)

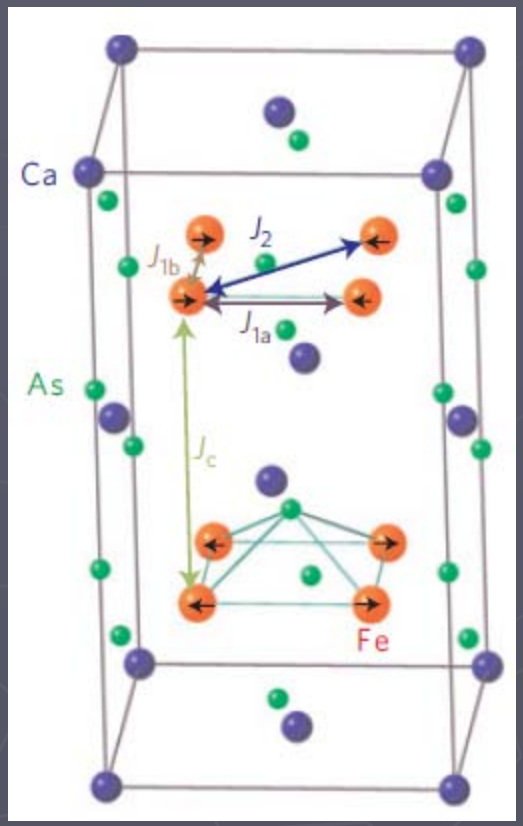
Lynn, Dai 2009

Weak coupling/strong coupling picture of magnetism?

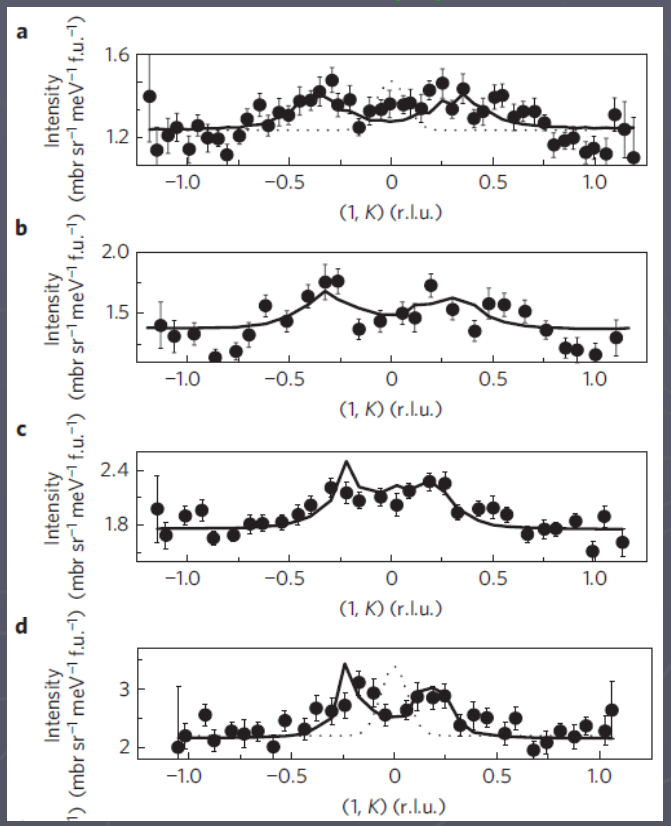
Early theories proposing strong coupling: Yildrim 08; Fang et al 08, Cvectovic & Tesanovic 08, Abrahams & Si 08, Manousakis et al 08

Stripe order stabilized for large J_2



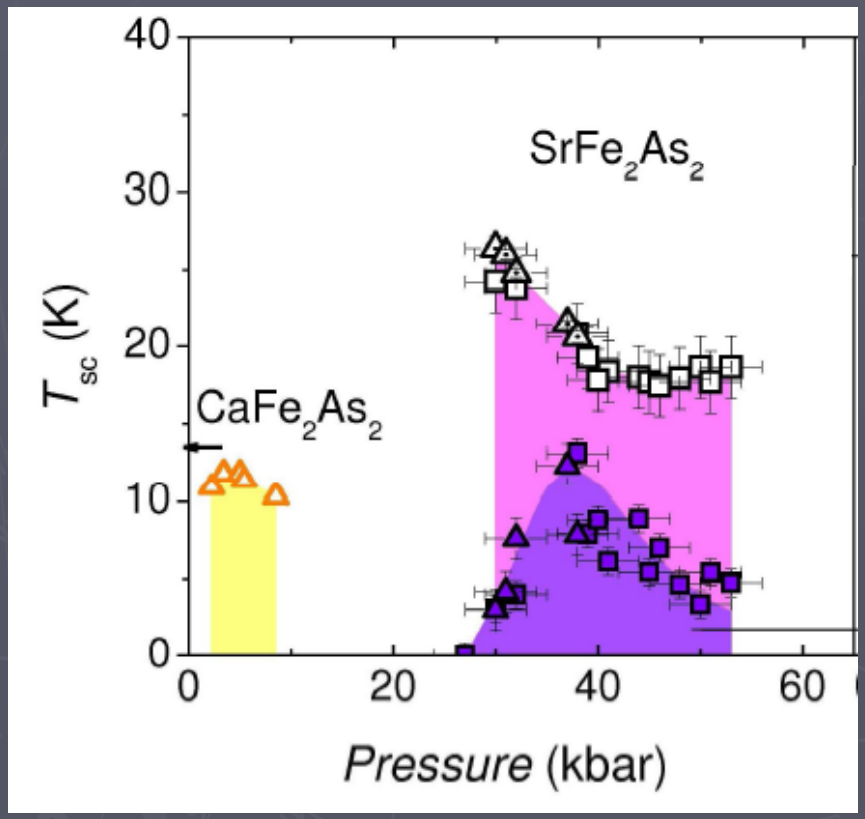


Zhao et al. Natphys 09

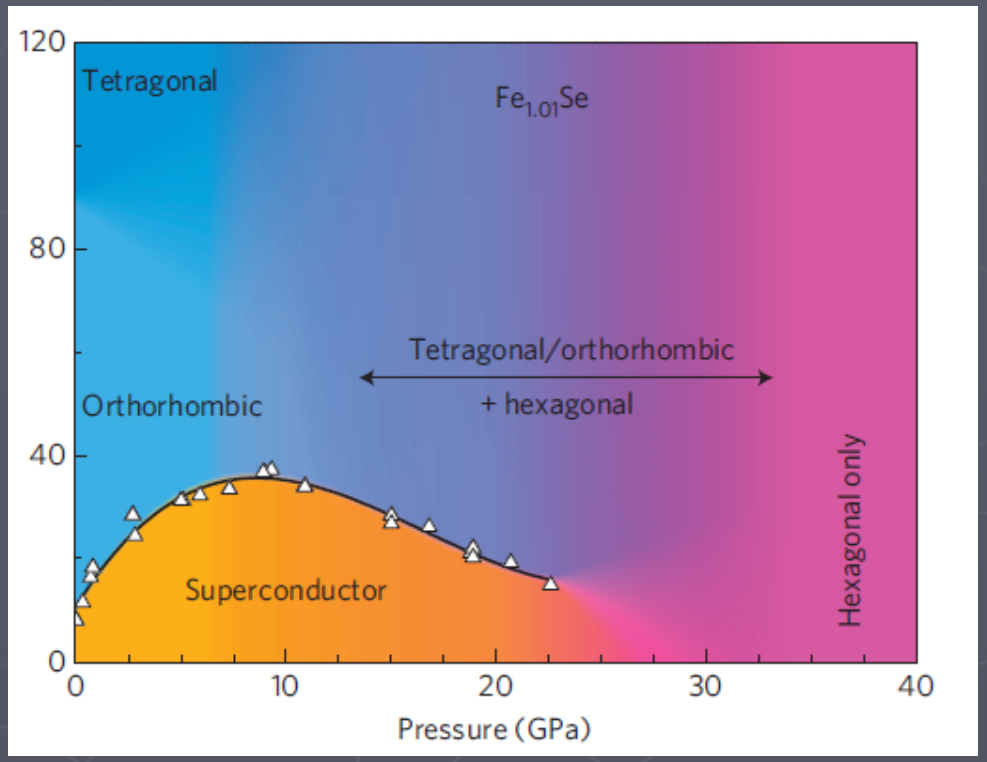


Zhao et al. Natphys 09 spin excitations fit Heisenberg without need for Stoner continuum, but a-b anisotropy hard to understand.
Diallo et al PRL 09: poor fit at higher E, spin waves are damped by p-h excitations; good fit from 1st principles susceptibility

Also: “doping” with pressure

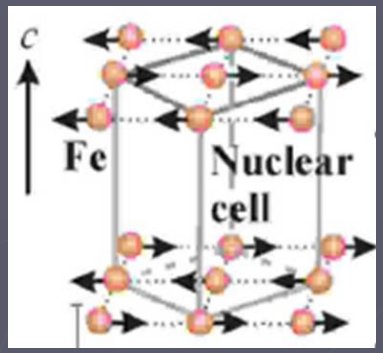


Alireza *et al.* (2008)



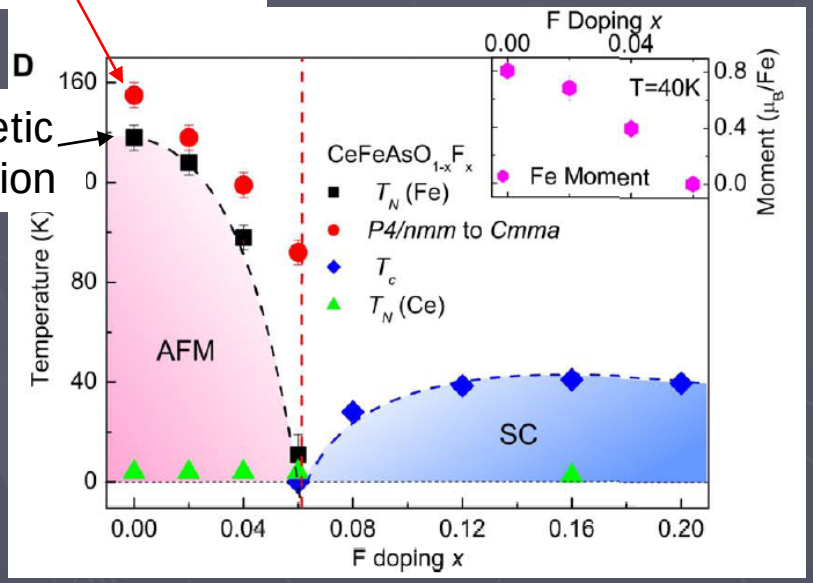
Medvedev *et al.* (2009)

- Magnetic order tied to structural phase transition
- possible coexistence with superconductivity?

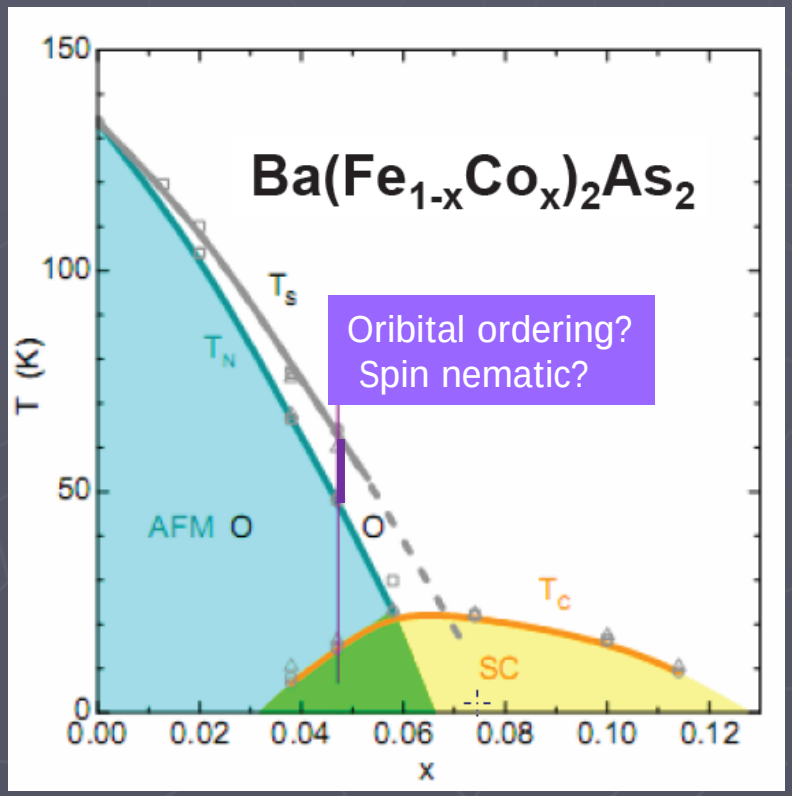


structural transition

magnetic transition



Zhao et al 2008



D.K. Pratt et al 09

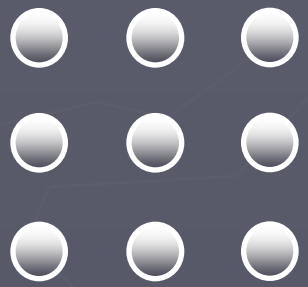
Best guess at present: 1111—NO; 122--YES

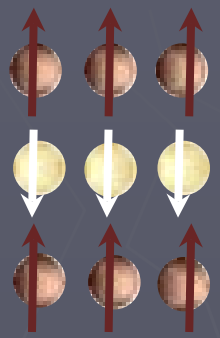
Two phase transitions

I) Structural Transition

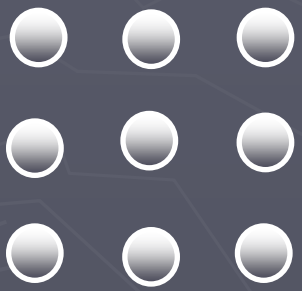
II) Magnetic Transition

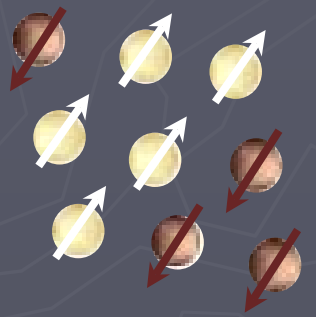
122/1111





FeTe





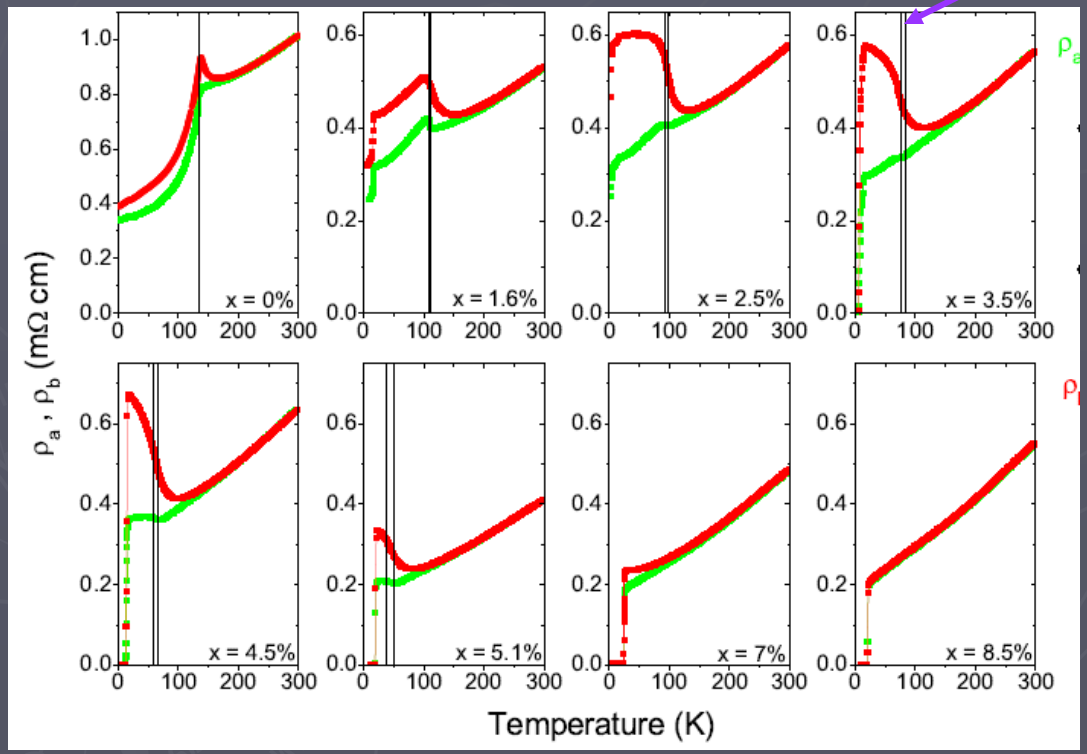
DFT correctly reproduces (or even predicts) correct magnetic and structural ground states, but requires magnetism as a prior condition for distortion

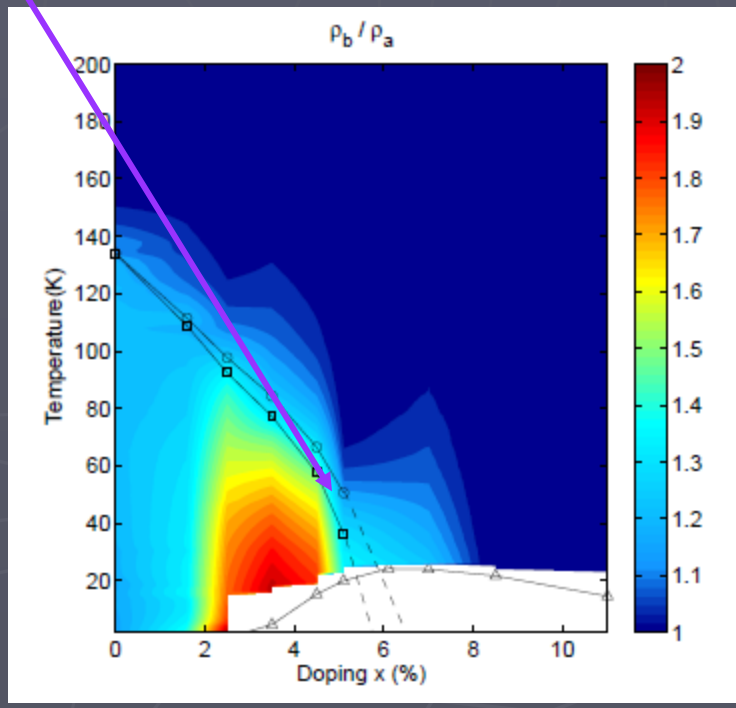
Courtesy of M. Johannes & I. Mazin

Transition driven by orbital ordering?

Theory: Xu et al, Kruger et al, Fang et al 08

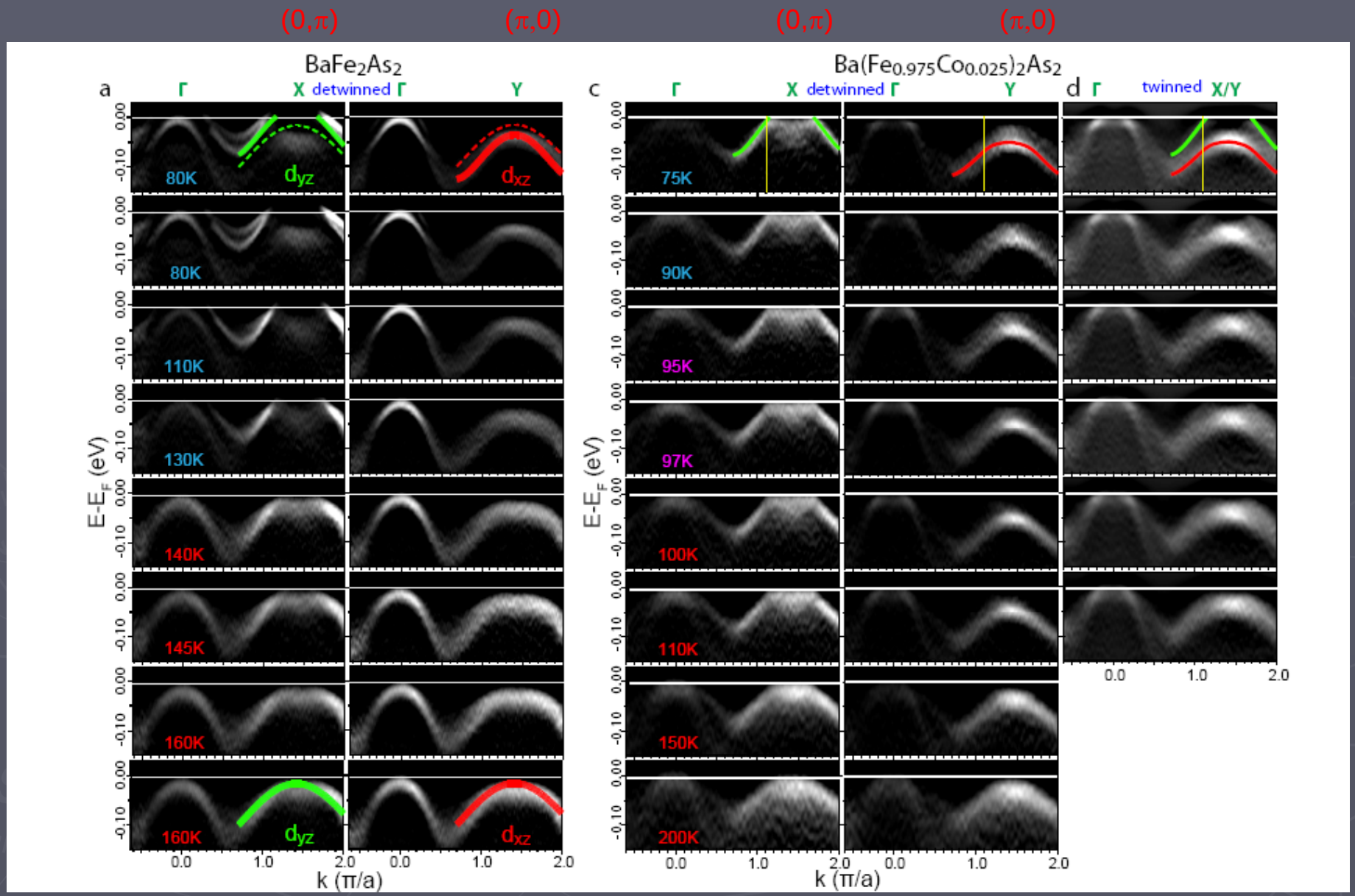
Experiments on untwinned samples: “nematic” susceptibility above T_s?





Implications for superconductivity?

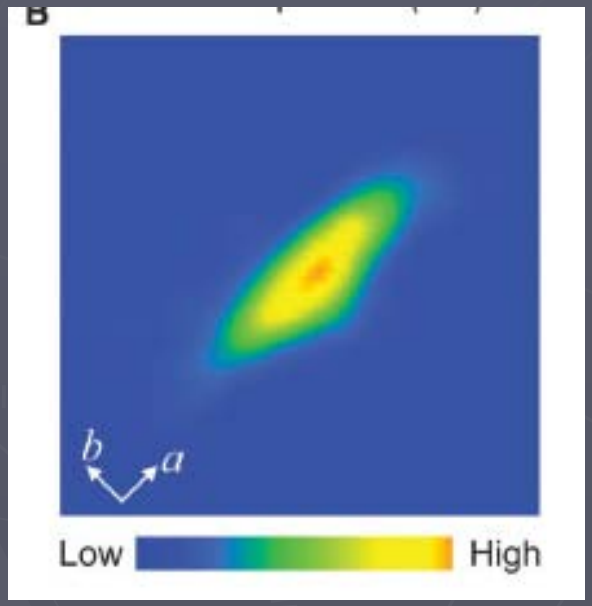
ARPES: orbital ordering



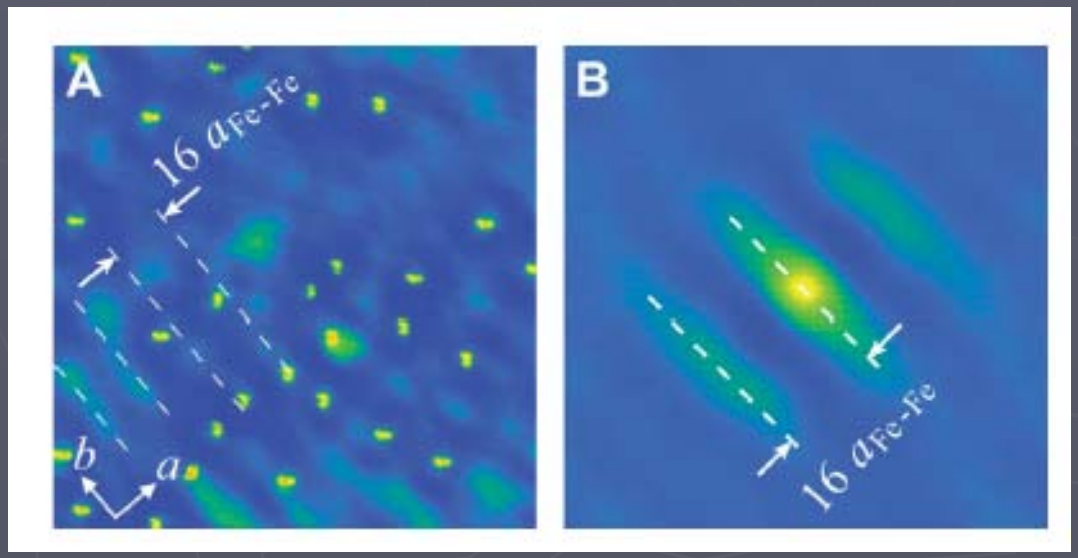
Yi et al PNAS 2011

Nematic behavior also in superconducting state!

STM on FeSe, Song et al., Science 2011



Vortex



Impurity states

Strongly 1D defect structures in (barely orthorhombic system)!

Three different types of order which break x/y symmetry

- stripe spin order (neutrons)
- structural order $a_x \neq a_y$ (X-ray diffraction)
- orbital order - dxz and dyz orbitals occupied differently (ARPES)

which one is the driving force?

?

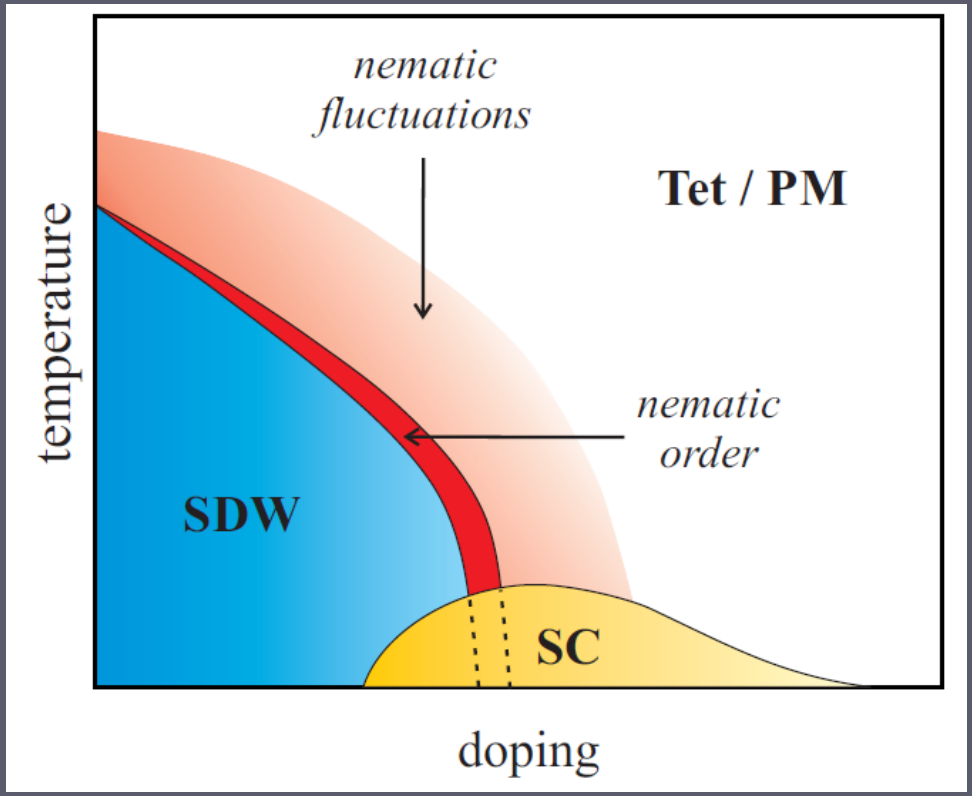
Courtesy of A. Chubukov

Magnetic origin for nematicity?

J1-J2 model:

Chandra et al (1990)

Si et al (2008)
Fang et al (2008)
Xu et al (2008)



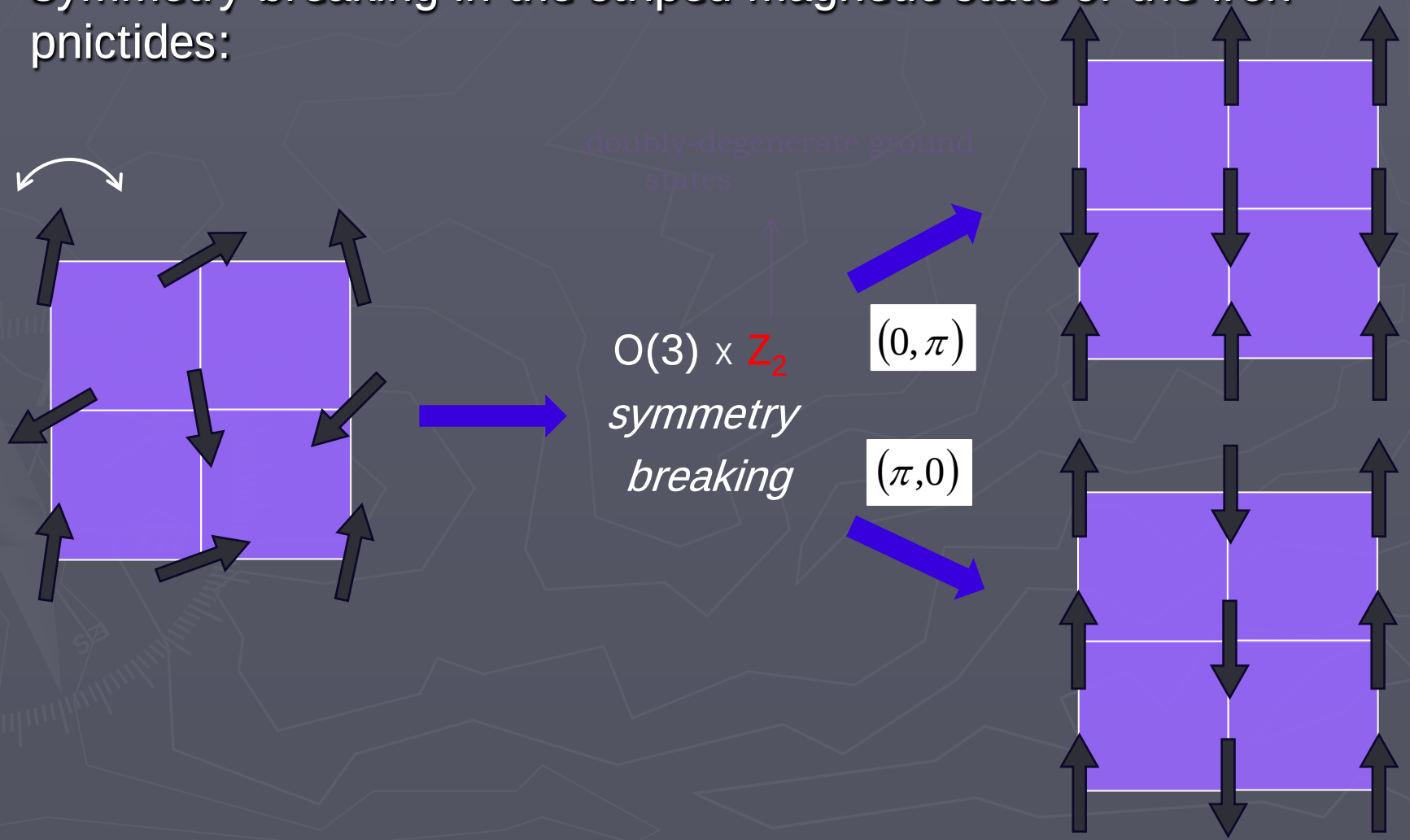
Itinerant version:

Fernandes, Schmalian, Eremin, Chubukov...

- Nematic order is a natural consequence of the magnetism of the pnictides (no need to introduce extra degrees of freedom)
- Nematic degrees of freedom affect the macroscopic properties across much of the phase diagram

Magnetic origin for nematicity?

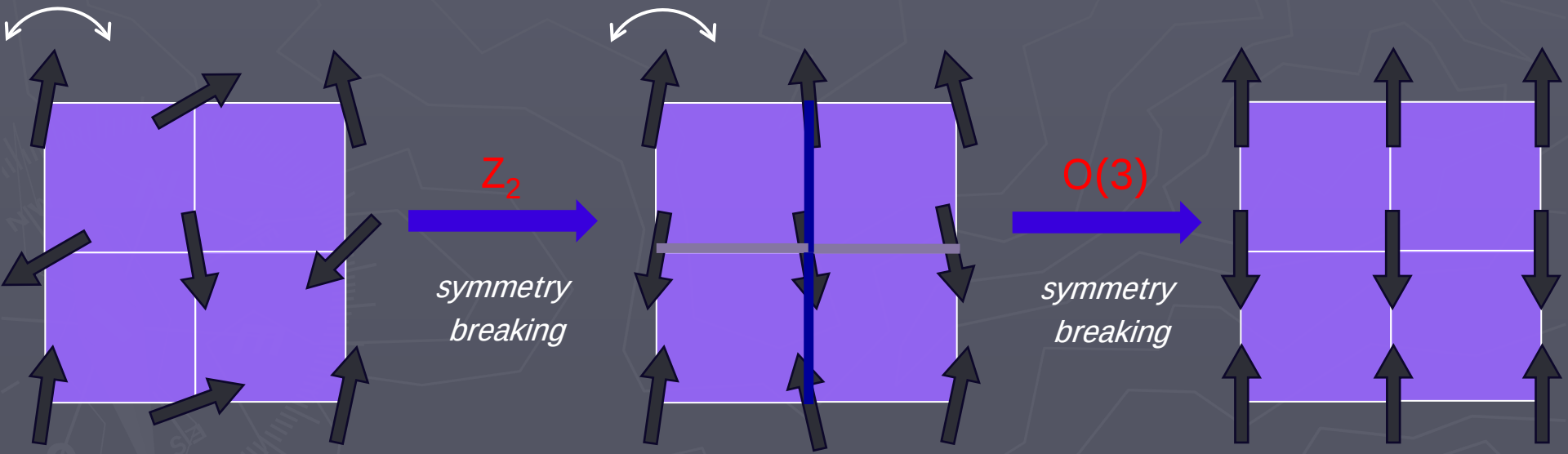
- Symmetry breaking in the striped magnetic state of the iron pnictides:



Magnetic origin for nematicity?

- A state that breaks Z_2 symmetry but remains paramagnetic

spontaneous tetragonal symmetry breaking



disordered state

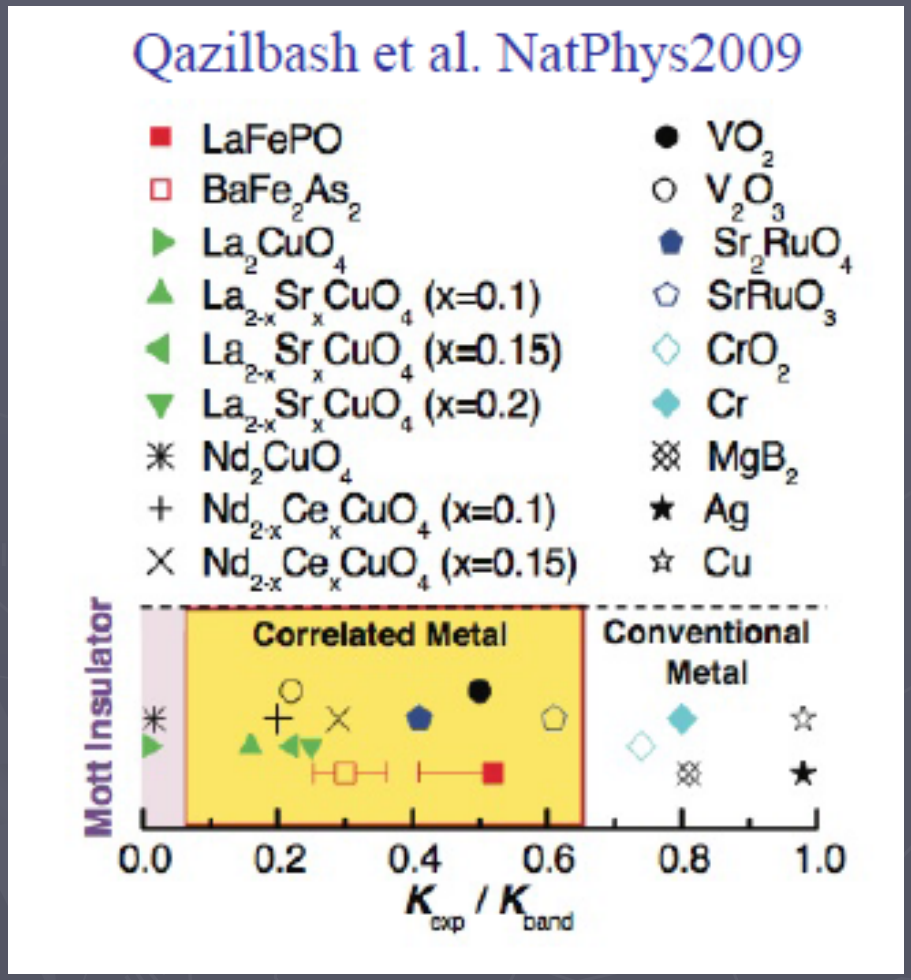
nematic state

$$\langle M_1^2 \rangle \neq \langle M_2^2 \rangle$$
$$\langle M_1 \rangle = \langle M_2 \rangle = 0$$

magnetic state

$$\langle M_1 \rangle \neq 0$$

Correlation strengths across materials



Specific heat (mJ/ mol K^2)	
LaFePO	7
$Ba(Co_xFe_{1-x})_2As_2$	15-20
$Ba_{1-x}K_xFe_2As_2$	50
$FeSe_{0.88}$	9.2
KFe_2As_2	69-102
$K_{0.8}Fe_{1.6}Se_2$	6

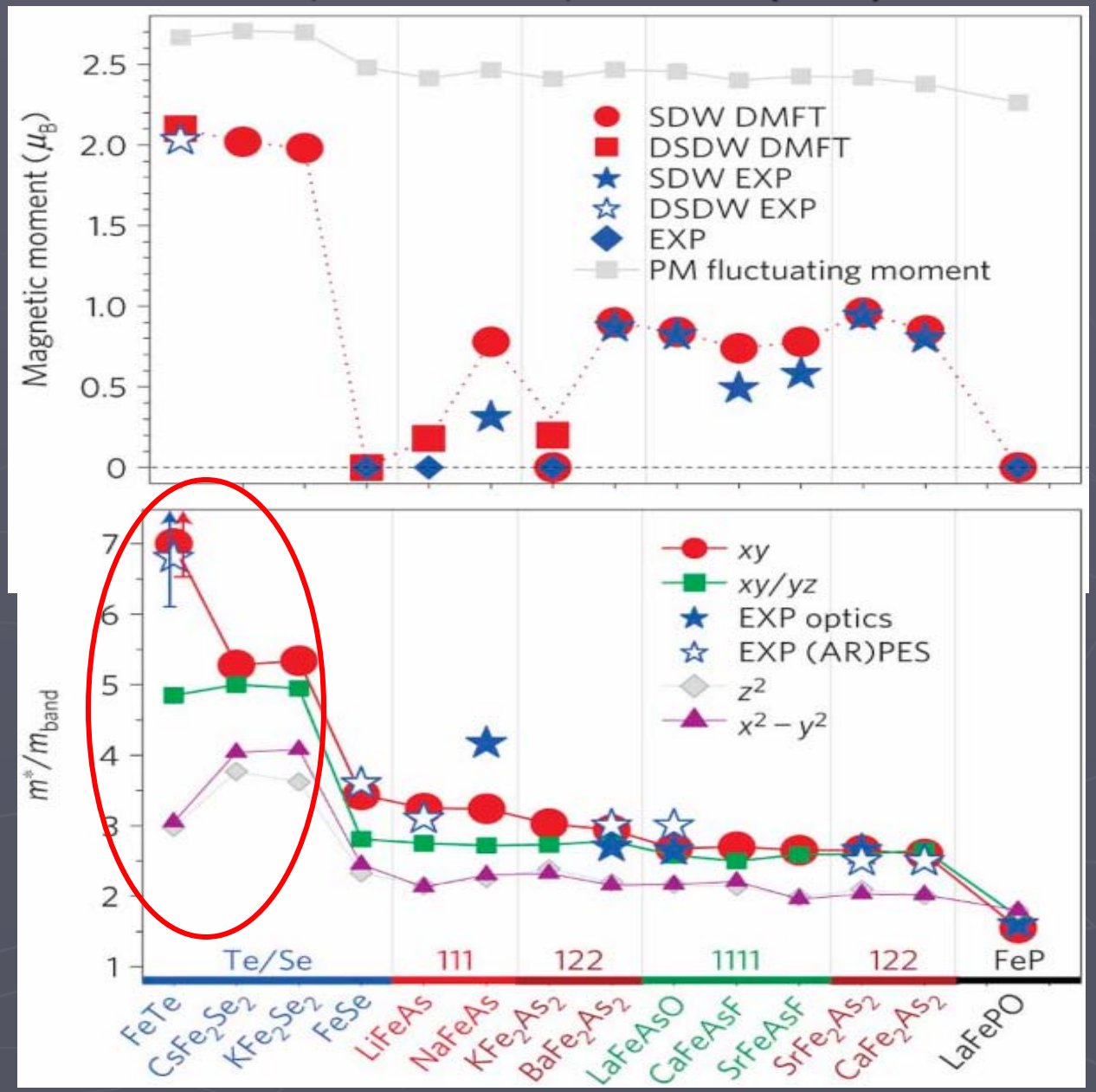
Review: Stewart, RMP (2011)

Results from LDA+DMFT

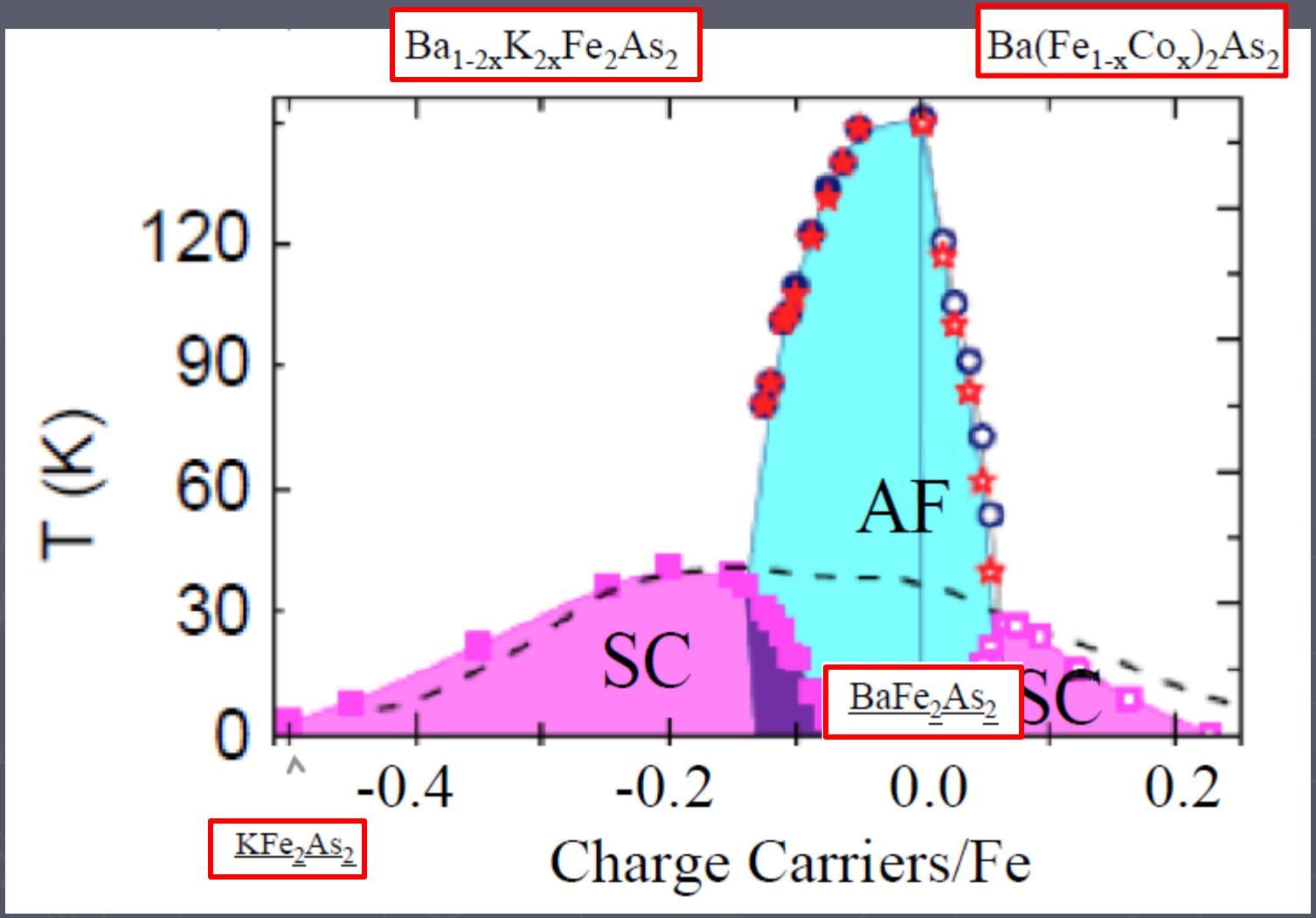
Z. P. Yin, K. Haule, & G. Kotliar, Nat. Mat. 10, 932–935 (2011)

Fix interactions U,J, vary material

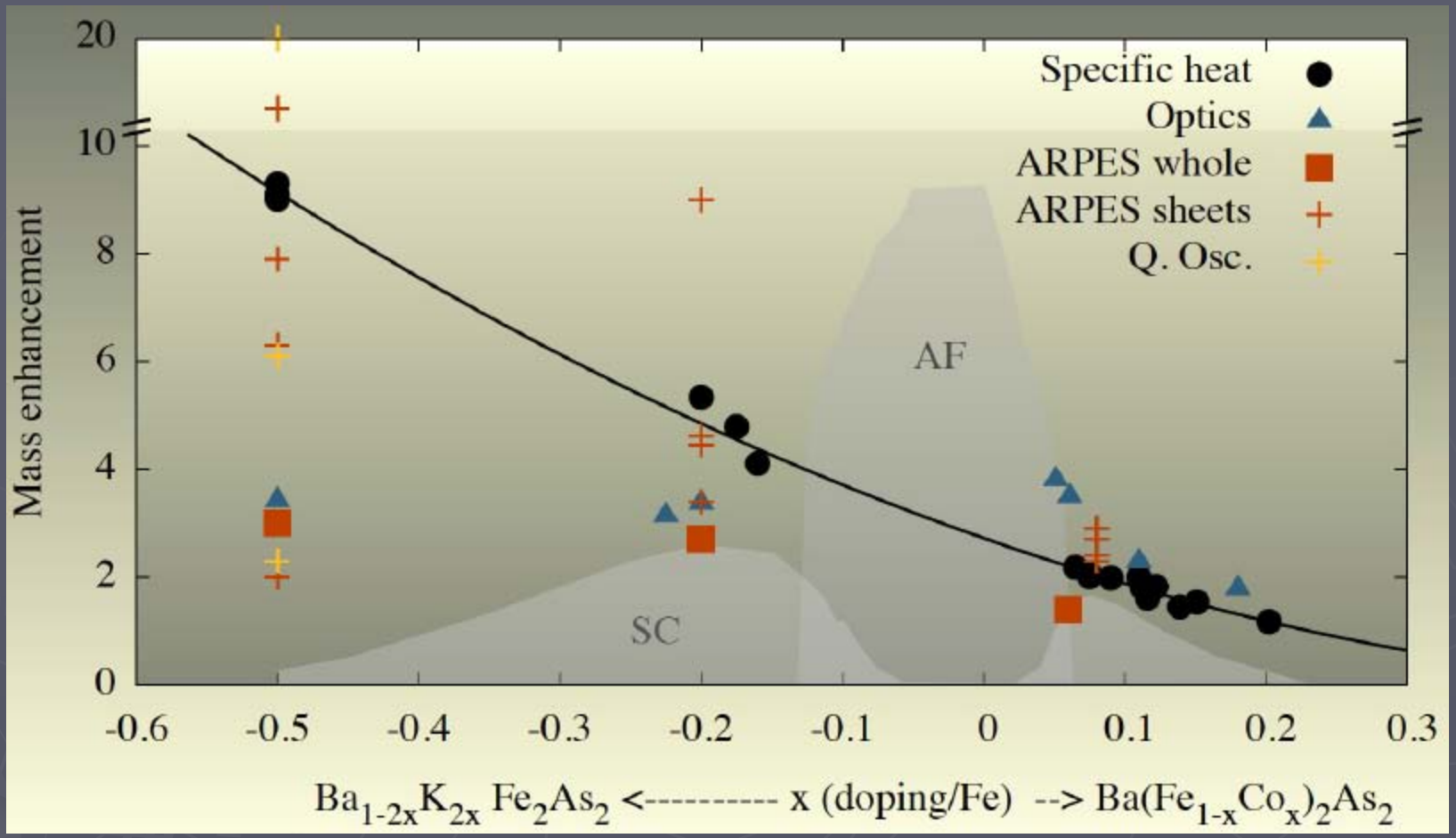
Not all orbitals are equally correlated!



Can we understand evolution of correlations across 122 phase diagram?



Some empirical measures of correlations



References in: L. de Medici et al, ArXiv:1212.3966 (all data in high-T tetragonal phase)

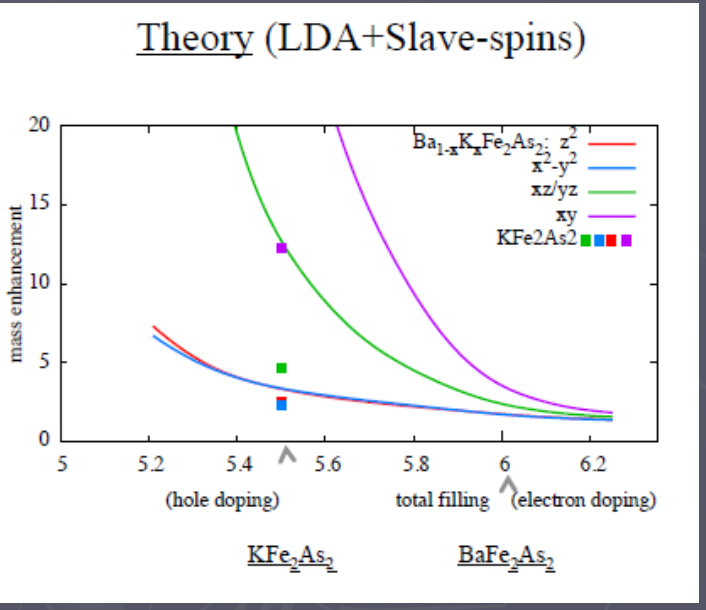
Sommerfeld coefficient $\gamma \sim N^*(E_F) = \sum_\alpha (m^*/m_b)_\alpha N_b^\alpha(E_F)$

Optics: Drude contribution $D^* = \sum (m_b/m^*)_\alpha D_b^\alpha$

$\Rightarrow$ *selective* orbital mass enhancement

Multiorbital Mott physics: J acts as orbital decoupler:

- suppresses inter-orbital correlations
- differentiate orbitals with respect to distance from Mott transition



de Medici et al, ArXiv:1212.3966

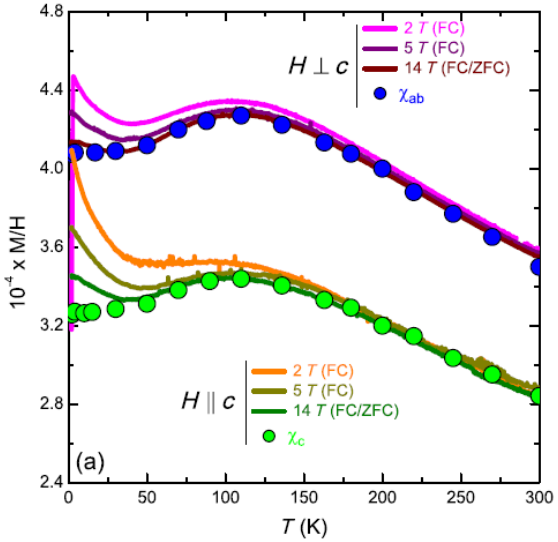
PRL 111, 027002 (2013) PHYSICAL REVIEW LETTERS week ending 12 JULY 2013

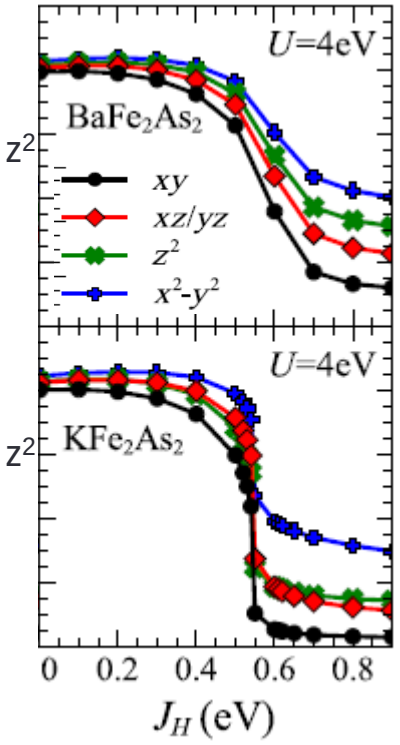
Evidence of Strong Correlations and Coherence-Incoherence Crossover in the Iron Pnictide Superconductor KFe_2As_2

F. Hardy,[1,*] A. E. Böhmer,[1] D. Aoki,[2,3] P. Burger,[1] T. Wolf,[1] P. Schweiss,[1] R. Heid,[1] P. Adelmann,[1] Y. X. Yao,[4] G. Kotliar,[5] J. Schmalian,[6] and C. Meingast[1]

[1]*Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany*
[2]*INAC/SPSMS, CEA Grenoble, 38054 Grenoble, France*
[3]*IMR, Tohoku University, Oarai, Ibaraki 311-1313, Japan*
[4]*Ames Laboratory US-DOE, Ames, Iowa 50011, USA*
[5]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*
[6]*Karlsruher Institut für Technologie, Institut für Theorie der Kondensierten Materie, 76128 Karlsruhe, Germany*

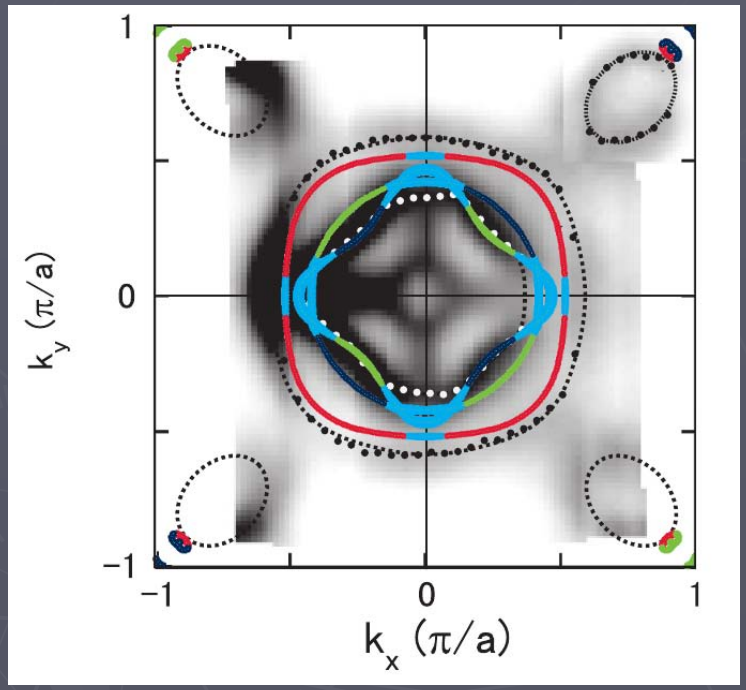
(Received 15 January 2013; published 9 July 2013)

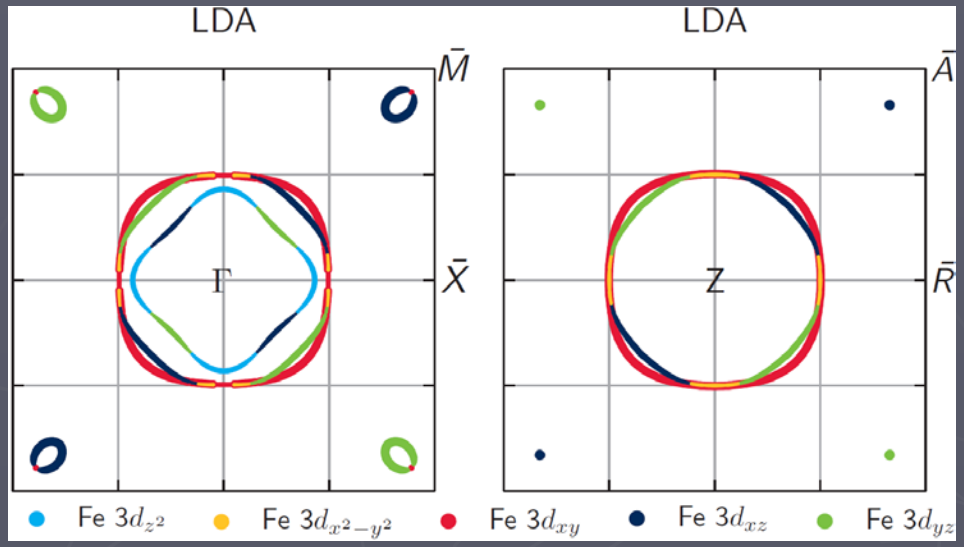


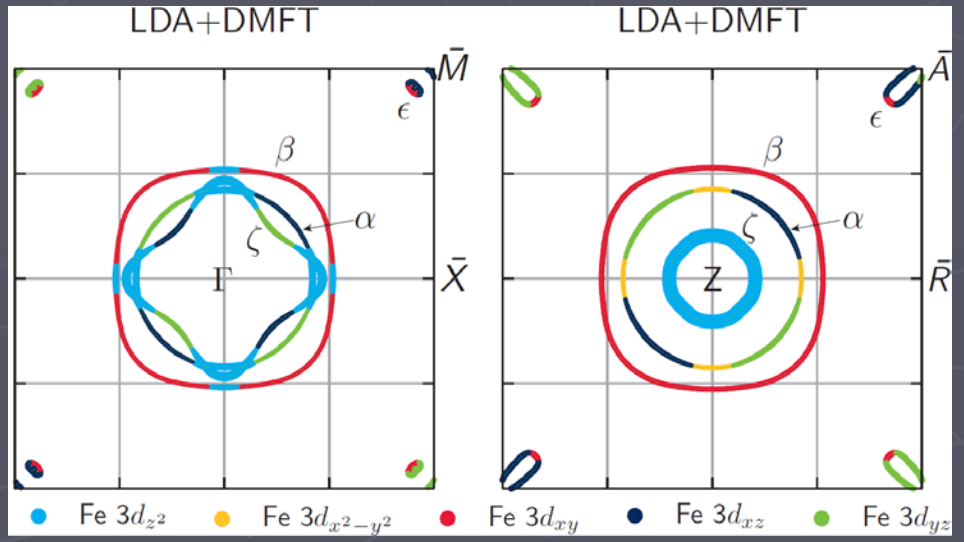


Correlations have strong effect on LDA+DMFT Fermi surface of KFe2As2 (unlike BaFe2As2)

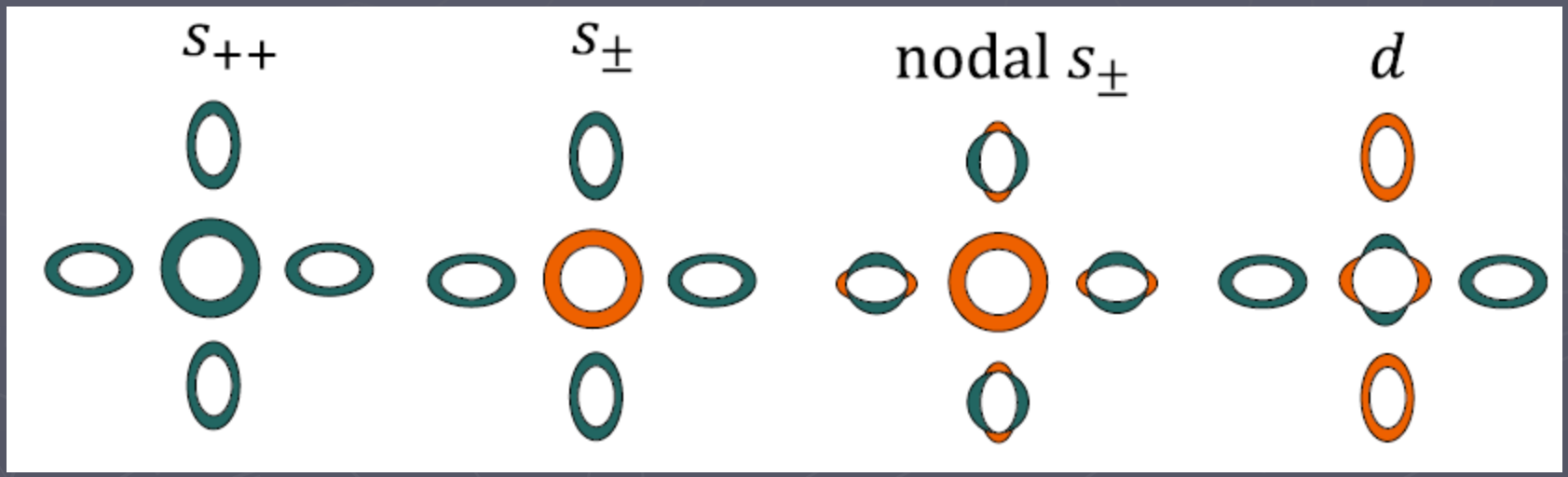
Backes et al (Frankfurt group)







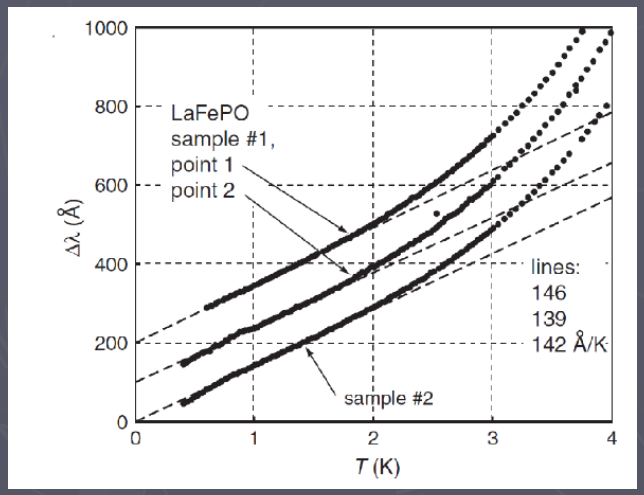
SC state: gap symmetry vs. structure



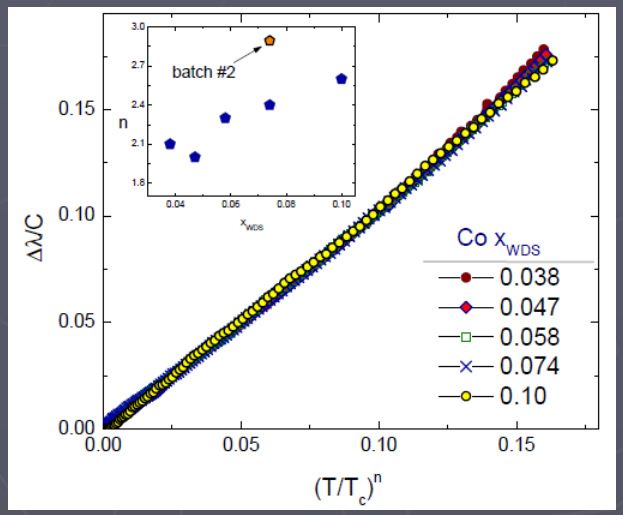
A_{1g} B_{1g}

SC state: experimental "lack of universality" e.g., penetration depth experiments

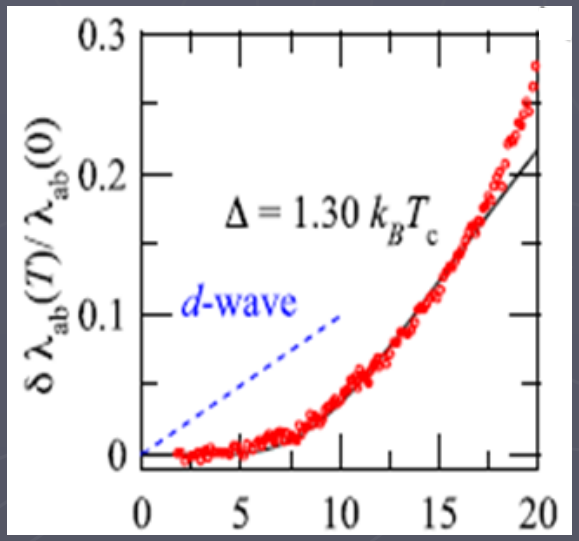
Hicks et al 2008
LaFePO T_c=6K



Prozorov, 2011
Co-doped Ba122 T_c=25K



Hashimoto et al 2009
K-doped Ba122 T_c=40K



$$\Delta\lambda \simeq \int d\omega \left(-\frac{\partial f}{\partial \omega}\right) N(\omega)$$

- dirty — *nodal SC*: $N(\omega) \simeq N_0 + a\omega^2$
- clean — *nodal SC*: $N(\omega) \simeq \omega$
- *gapped SC*

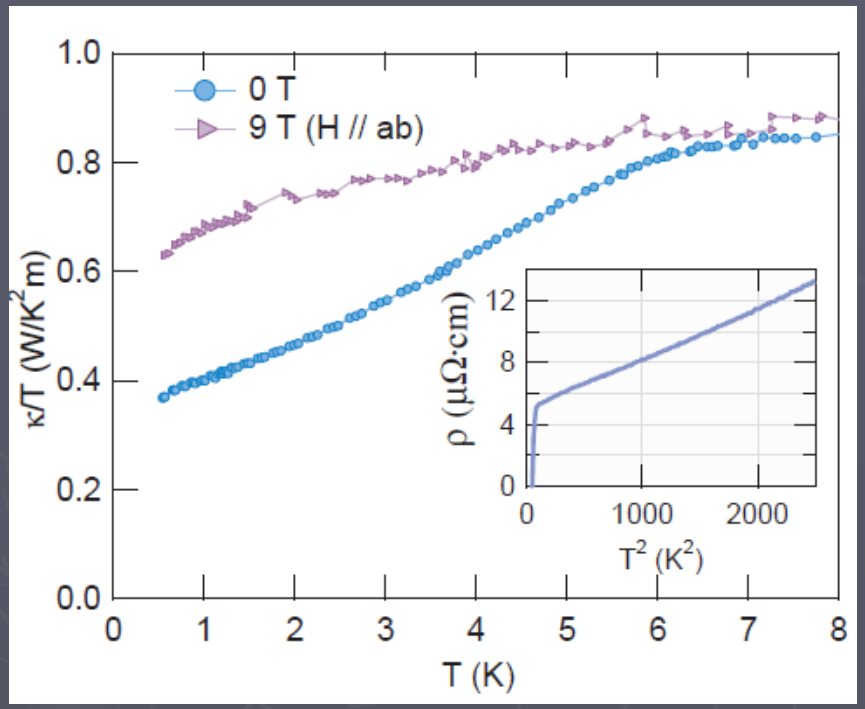
so $\Delta\lambda \simeq \begin{cases} T^2 & \text{dirty} \\ T & \text{clean} \end{cases}$

so $\Delta\lambda \; e^{-\Delta/T}$

Thermal conductivity (H=0)

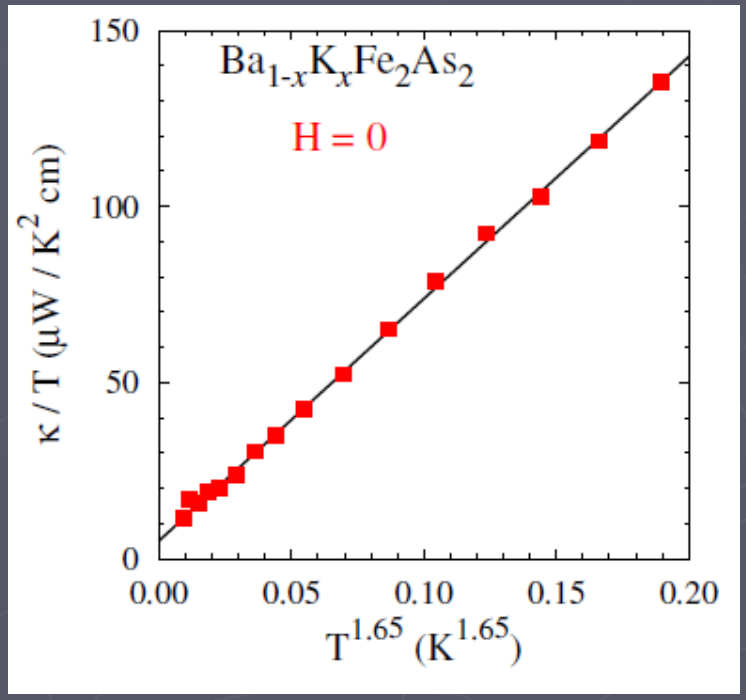
(bulk probe, lowest temperatures thus far)

LaFePO: Yamashita et al aXv:0906.0622



Big linear T term

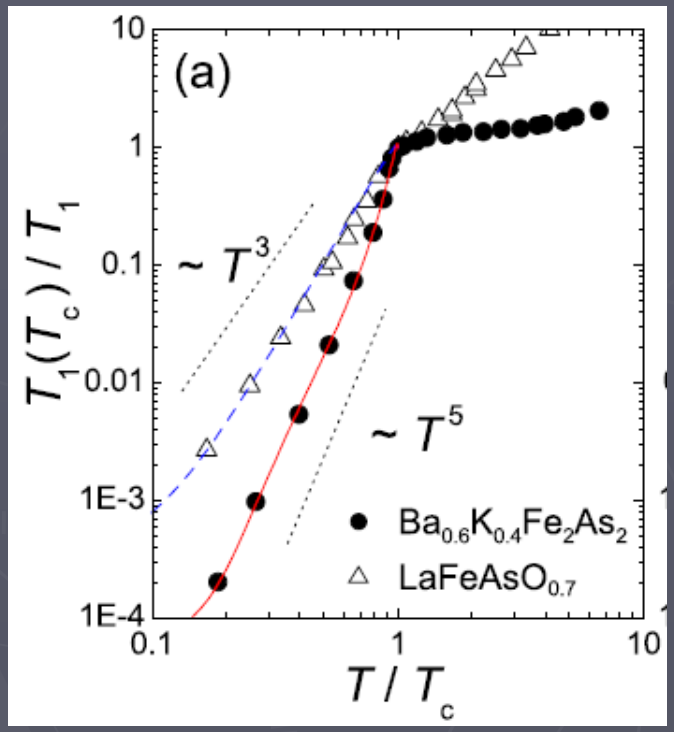
K-doped Ba-122: Luo et al aXv:0904.4049



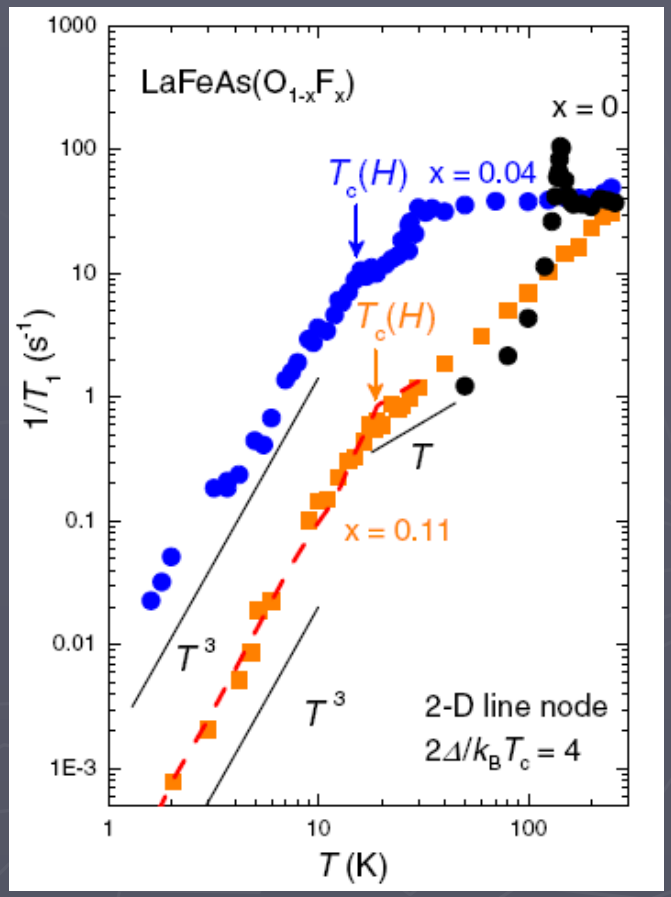
Tiny or zero linear T term

Recall in theory of nodal SC linear T term ⇒ residual qp excitations (metallic-like)
for d-wave superconductor this term is "universal" $\kappa/T \sim N_0 v_F^2/\Delta_0$

NMR spin-lattice relaxation



Yashima et al arXiv:0905.1896



Nakai et al. JPSJ (2008)

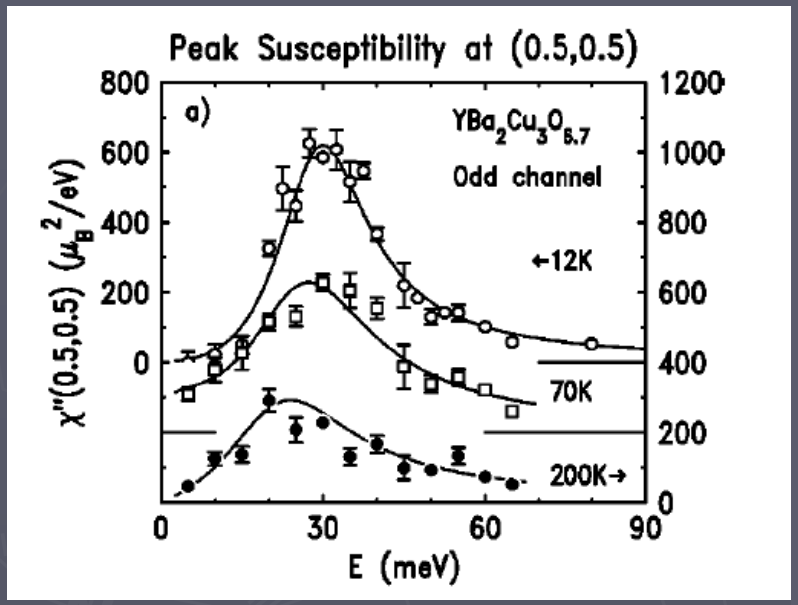
$$\frac{T_1^{-1}}{(T_1^{-1})_N} = 2\frac{T}{T_c}\int_0^\infty d\omega \left[\frac{-\partial f}{\partial \omega}\right]\left[\frac{N(\omega)}{N_0}\right]^2$$

$\longleftrightarrow$

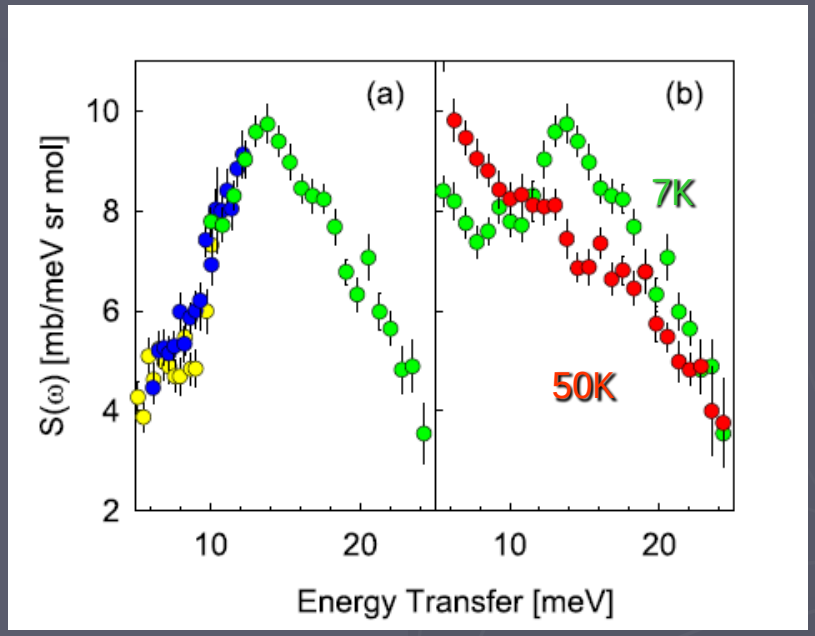
line nodes $\Rightarrow N(\omega) \sim \omega \Rightarrow T^3$!

Resonant mode in inelastic neutron scattering

Reminder: cuprates: Fong et al PRB 2000



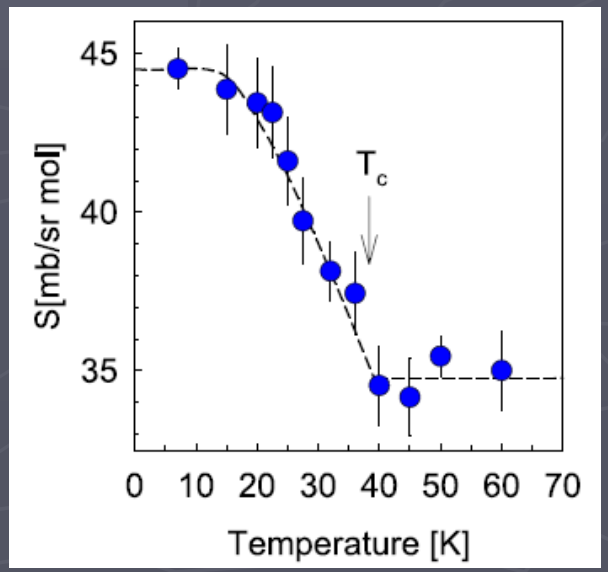
$Ba_{0.6}K_{0.4}Fe_2As_2$: Christianson et al Nature 2008



In Ba-122 resonance observed near Q=π,0 (1-Fe BZ)
Appears only in SC state (like opt. doped cuprates)

$$\text{Im}\,\chi \sim \sum_k \left[1 - \frac{\Delta_k \Delta_{k+q}}{E_k E_{k+q}}\right] \ldots$$

$\Delta_{k+Q} = -\Delta_k \Rightarrow$ sign change of order parameter



Multiband theory: Maier & Scalapino 2008, Korshunov & Eremin 2008, Maier et al 2009

questions

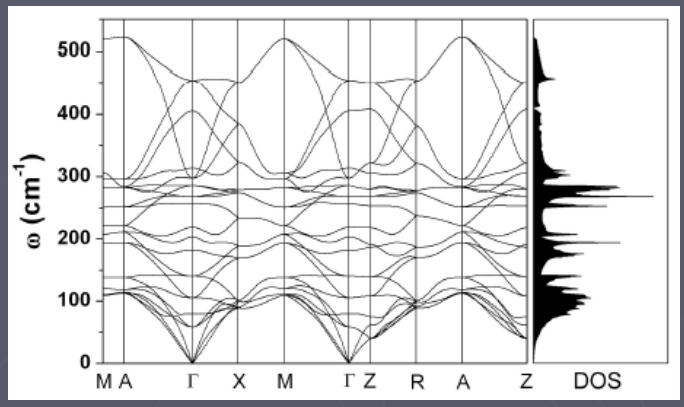
- What is the symmetry of SC order parameter?
- What controls whether Fe-based material is nodal or gapped superconductor?
- Why are these systems' superconducting states nonuniversal?

Pairing by spin fluctuations?

1) Electron-phonon interaction is weak:

We have calculated *ab initio* the electron-phonon spectral function, $\alpha^2F(\omega)$, and coupling, λ, for the stoichiometric compound [9]. Some moderate coupling exists, mostly to As modes, but the total λ appears to be ~ 0.2, with $\omega_{log} \sim 250$ K, which can in no way explain $T_c \gtrsim 26$ K.

Mazin et al, PRL 2008, see also Mu et al CPL (2008), Boeri et al. PRL 2008

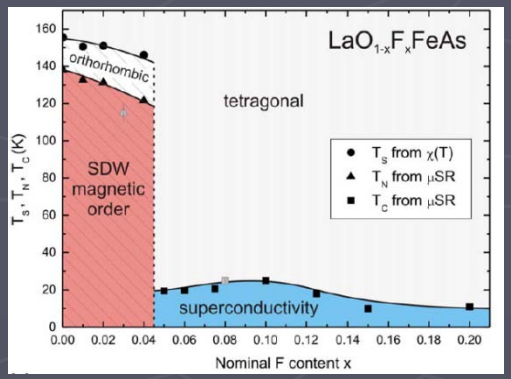


Singh & Du PRL 2008

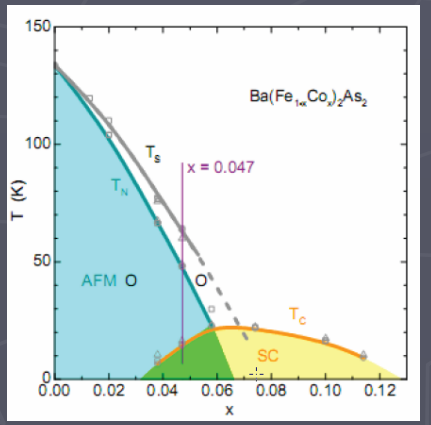
2) Magnetism is usually nearby:

1111-pnictides T_c =26-55K
LaFePO T_c=6K
KFe_2As_2 T_c=3.6K

nonmagnetic



Luetkens et al 08



Pratt et al 09

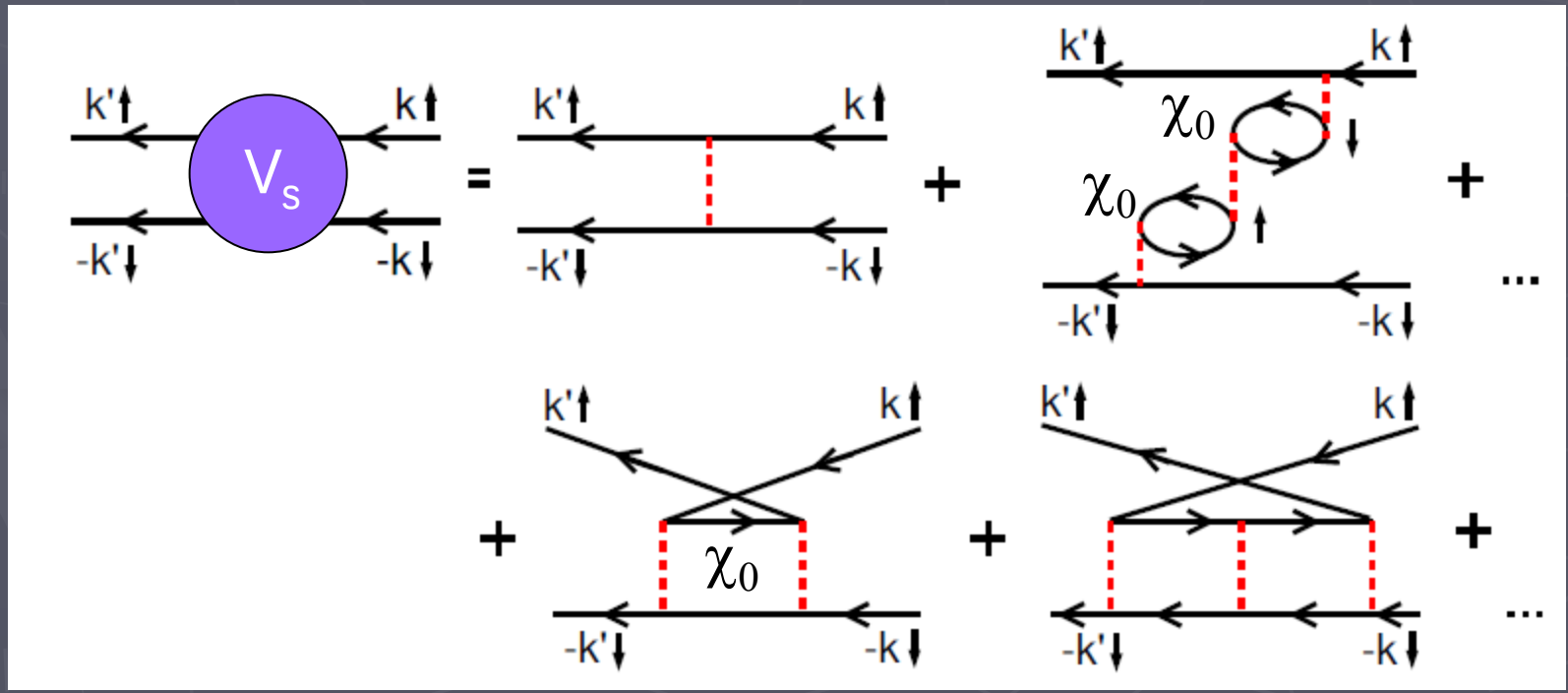
No magnetism ⇒ low T_c

Spin fluctuation theories of pairing

Effective interaction from spin fluctuations (Berk-Schrieffer 1966)

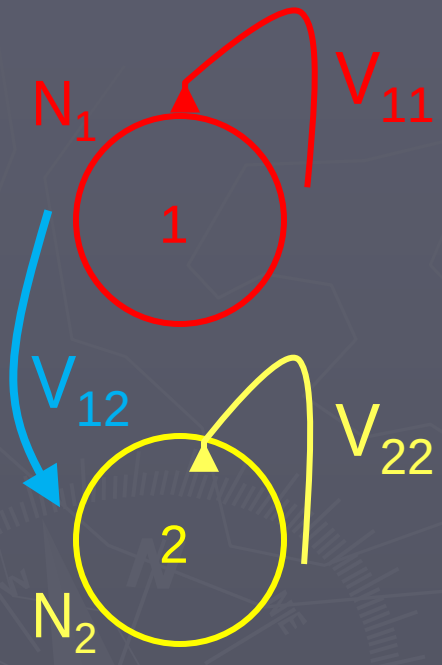
$$V_s(q,\omega) \cong \frac{3}{2}\frac{\bar{U}^2\chi_0(q,\omega)}{1-\bar{U}\chi_0(q,\omega)}$$

$$\chi_0(q,\omega) = \int \frac{d^3p}{(2\pi)^3}\frac{f(\varepsilon_{p+q})-f(\varepsilon_p)}{\omega-(\varepsilon_{p+q}-\varepsilon_p)+i\delta}$$



Multiband superconductivity

Suhl, Matthias and Walker PRL 1959



Assume gaps isotropic on each band:

$$\Delta_i = -\sum_j \Lambda_{ij}\Delta_j F(\Delta_j, T)$$

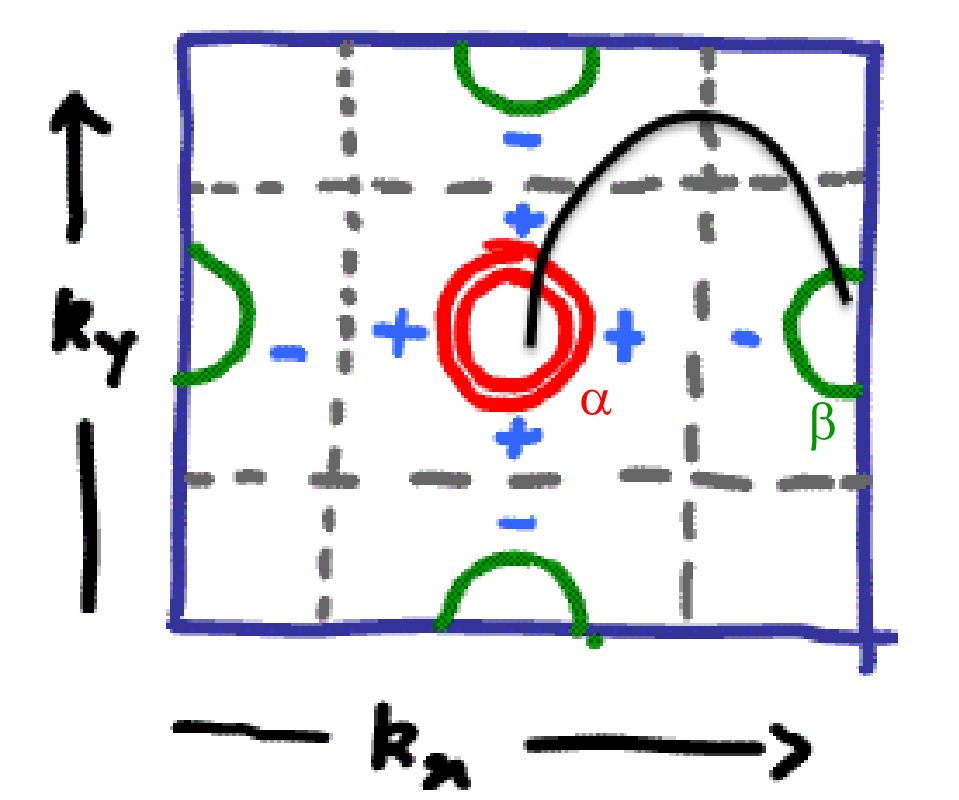
$$\Lambda_{ij} = V_{ij}N_j$$

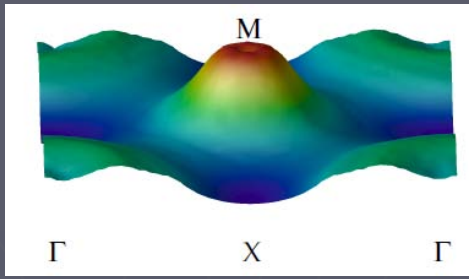
$$F = \int_{-\omega_D}^{\omega_D} d\xi \frac{1}{2\sqrt{\xi^2+\Delta^2}} \tanh\left(\frac{\sqrt{\xi^2+\Delta^2}}{2T}\right)$$

Equations may have solutions even when all elements of the interaction matrices are repulsive (>0).

The simplest example is an off-diagonal repulsion: $V_{11} = V_{12} = 0$, $V_{12} = V_{21} = -V < 0$. In this case the solution reads: $\lambda_{eff} = \sqrt{\Lambda_{12}\Lambda_{21}} = |V_{12}|\sqrt{N_1 N_2}$, $\Delta_1(T_c)/\Delta_2(T_c) = -\sqrt{N_2/N_1}$.

Similar argument from Mazin et al PRL 2008 for pnictides:
consider only α–β pair scattering





also:

Kuroki et al 2008
Seo et al. 2008
Chubukov et al 2008

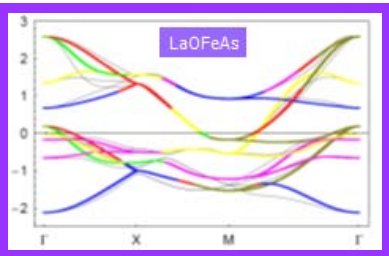
$$\Delta_p = -\sum_{p'} \frac{V(p-p')\Delta_{p'}}{2E_{p'}}$$

- nesting peaks interaction V_s at π,0 in 1-Fe zone.
- interaction is constant over sheet since they are small.
- therefore *isotropic* sign-changing $s_{+/-}$ state solves gap eqn

Spin fluctutation pairing theories in Fe-pnictides

$H = H_0 + H_{int}$

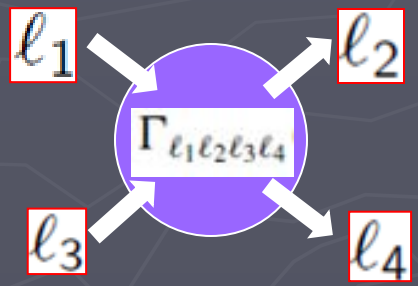
H_0=5-band tight-binding model



$$H = H_0 + \bar{U} \sum_{i,\ell} n_{i\ell\uparrow} n_{i\ell\downarrow} + \bar{U}' \sum_{i,\ell'<\ell} n_{i\ell} n_{i\ell'}$$

$$+\bar{J} \sum_{i,\ell'<\ell} \sum_{\sigma,\sigma'} c^{\dagger}_{i\ell\sigma} c^{\dagger}_{i\ell'\sigma'} c_{i\ell\sigma'} c_{i\ell'\sigma} + \bar{J}' \sum_{i,\ell'\neq\ell} c^{\dagger}_{i\ell\uparrow} c^{\dagger}_{i\ell\downarrow} c_{i\ell'\downarrow} c_{i\ell'\uparrow}$$

most general 2-body Hamiltonian
with intrasite interactions only!



Effective interaction between electrons in orbitals $\ell_1 \ell_2 \ell_3 \ell_4$

$$\Gamma_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}',\omega) = \left[\tfrac{3}{2}\bar{U}^s \chi_1^{\mathrm{RPA}}(\mathbf{k}-\mathbf{k}',\omega)\bar{U}^s + \tfrac{1}{2}\bar{U}^s - \tfrac{1}{2}\bar{U}^c \chi_0^{\mathrm{RPA}}(\mathbf{k}-\mathbf{k}',\omega)\bar{U}^c + \tfrac{1}{2}\bar{U}^c\right]_{\ell_3\ell_4\ell_1\ell_2}$$

Realistic theories: gaps display strong anisotropy/ nodes

$$\Gamma_{ij}(\mathbf{k},\mathbf{k}') = \mathrm{Re}\left[\sum_{\ell_1\ell_2\ell_3\ell_4} a_{\nu_i}^{\ell_2,*}(\mathbf{k}) a_{\nu_i}^{\ell_3,*}(-\mathbf{k}) \Gamma_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}',\omega=0) a_{\nu_j}^{\ell_1}(\mathbf{k}') a_{\nu_j}^{\ell_4}(-\mathbf{k}')\right]$$

band space interaction

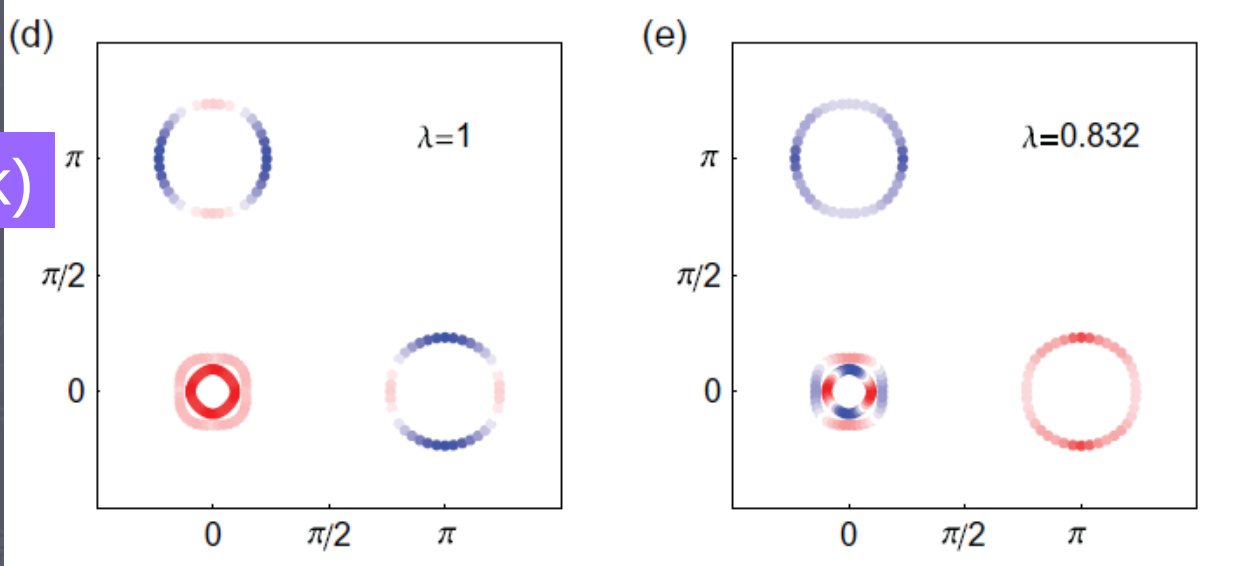
$$-\frac{1}{V_G}\sum_j \int_{\mathrm{FS}_j} dS'\, \Gamma_{ij}(\mathbf{k},\mathbf{k}') \frac{g_\alpha(\mathbf{k}')}{|v_{\mathrm{F}j}(\mathbf{k}')|} = \lambda_\alpha g_\alpha(\mathbf{k}),$$

gap eqn.

"anisotropic extended-s"-wave

close: $d_{x^2-y^2}$

$\Delta(k)$



(x=0.125 e-doped) U=1.54 J=0.3

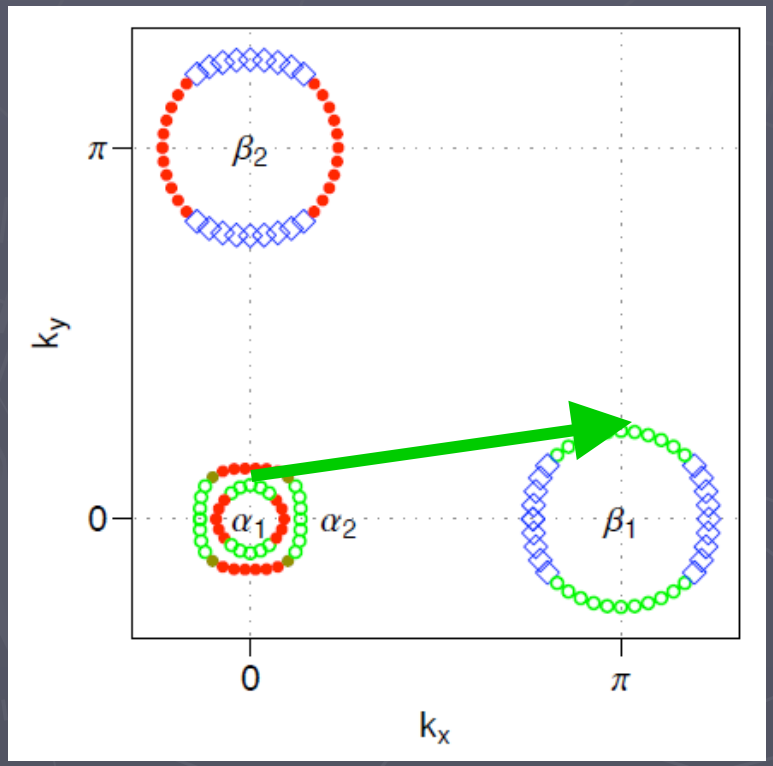
Two pairing channels nearly degenerate:

a) Can different FeAs materials have different symmetries?
b) Or, do all have s-wave *symmetry*, differing gap *structures* for different materials

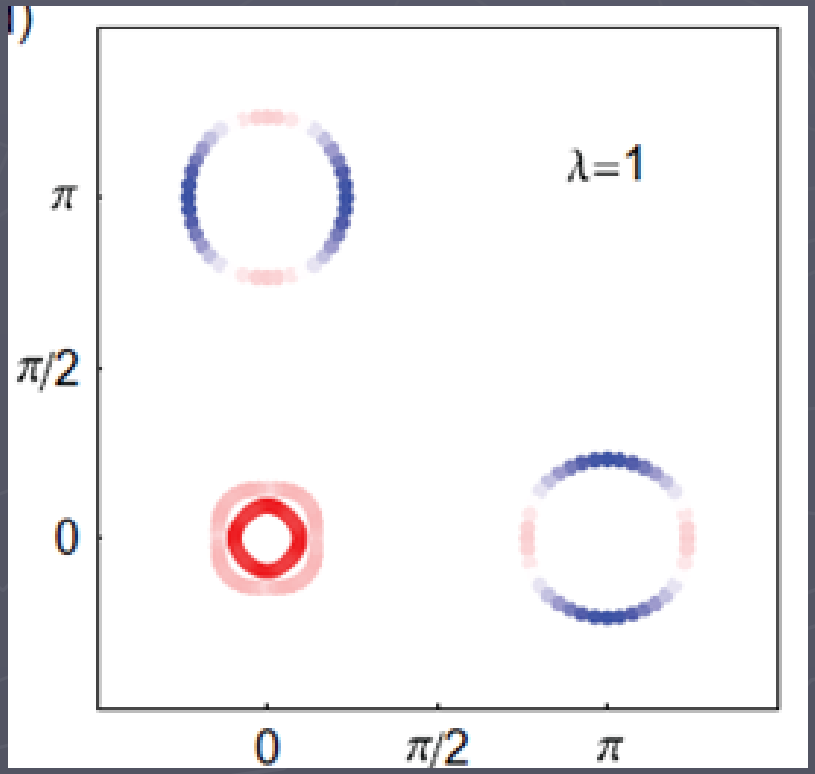
What is the origin of the gap anisotropy [Maier et al PRB 09]?

1. **importance of orbital character on Fermi sheets**
2. scattering between β_1 and β_2 sheets
3. intraband Coulomb repulsion

See also: Chubukov et al 2009, Thomale et al 2009 (band picture), Thomale et al 2010, Kemper et al 2010



Fermi surface w/ orbital character

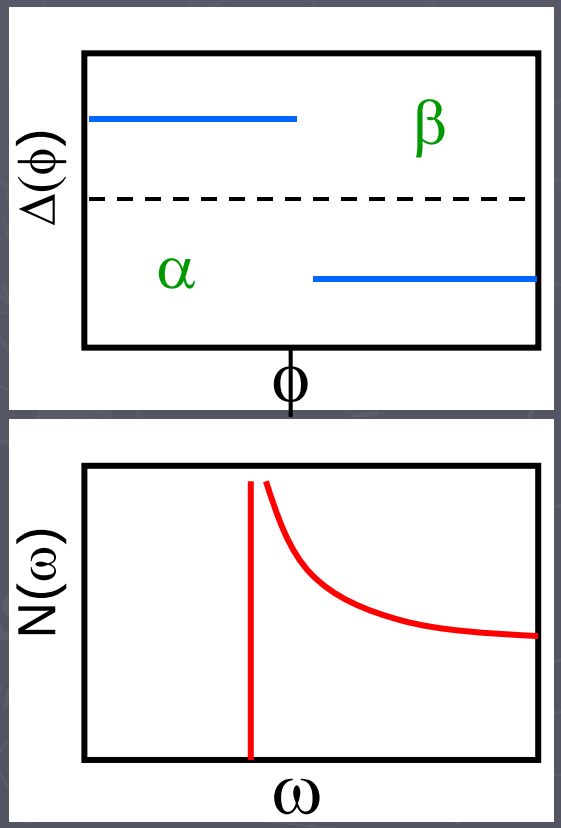


Gap

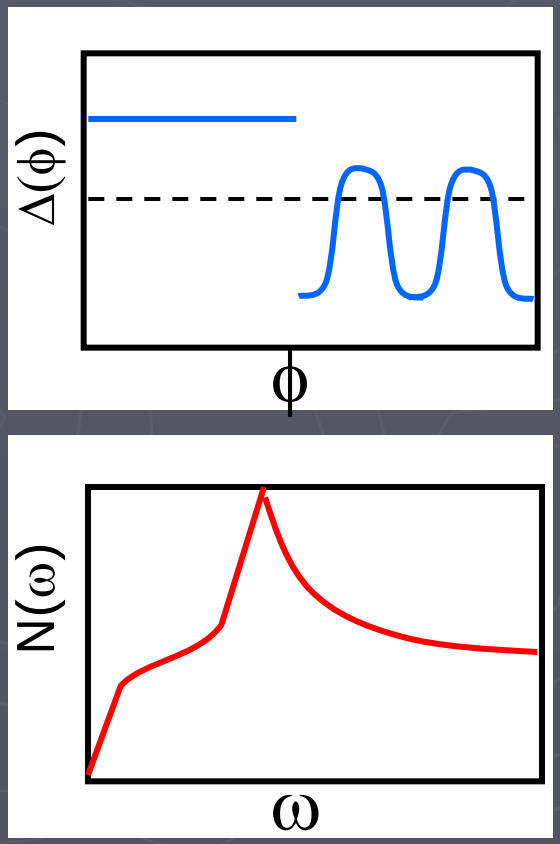
Nonuniversality in experiments: sensitivity to small changes in electronic structure, disorder

any nodes are *accidental* rather than symmetry-enforced in ext.-s states

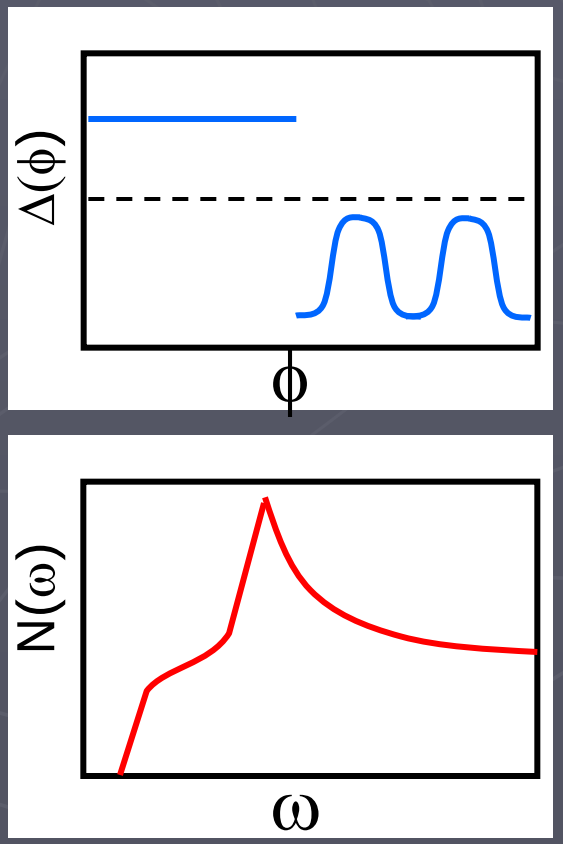
a) isotropic $s_{+/-}$



b) nodes

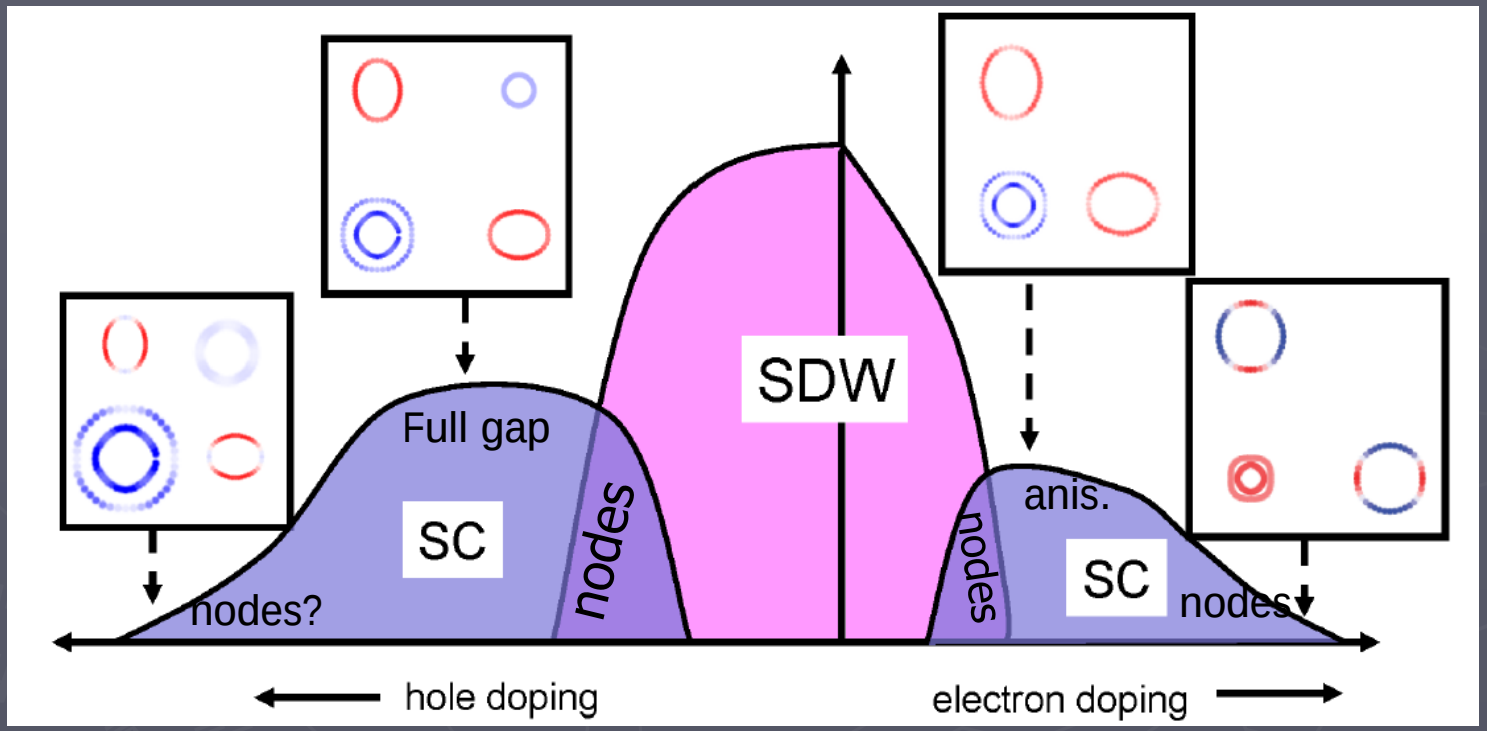


c) deep minima

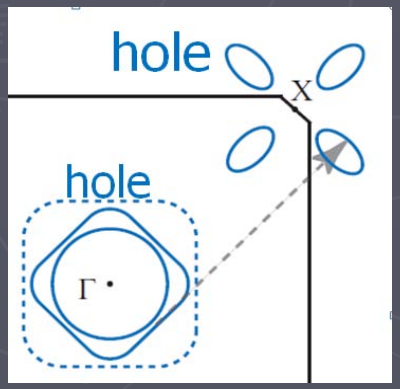


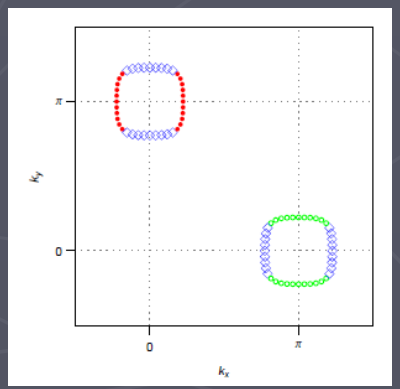
Big picture: evolution of gap with doping

PH, Korshunov and Mazin Rep. Prog. Phys. 2011



KFe_2As_2:
No electron pockets: d-wave?
Thomale et al

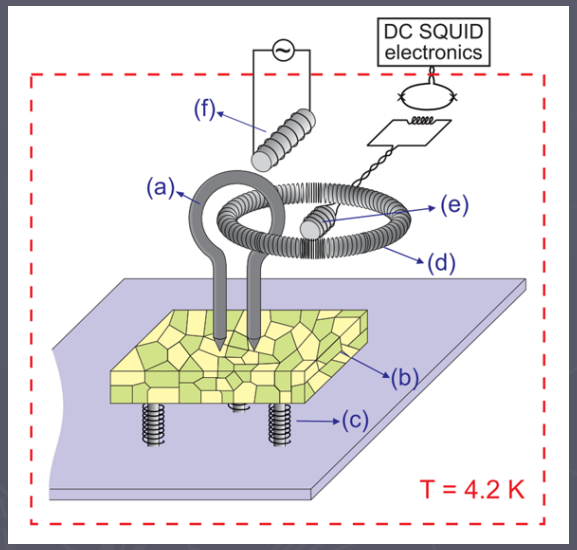




KFe_2Se_2:
No hole pockets: d-wave?
Wang et al
Graser et al
s-wave?
Mazin, Fang et al

s_{++} or s_{+-}? Few phase-sensitive expts.

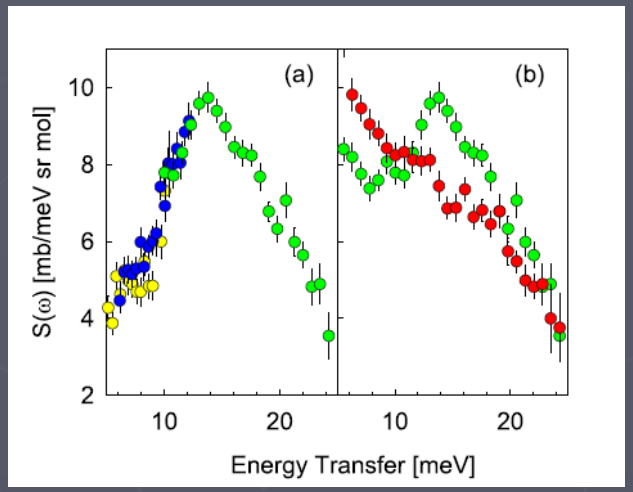
Chen et al, Nature 2010



$NdFeAsO_{0.88}F_{0.12}$

Half-integer fluxes detected (in a small fraction of loops)

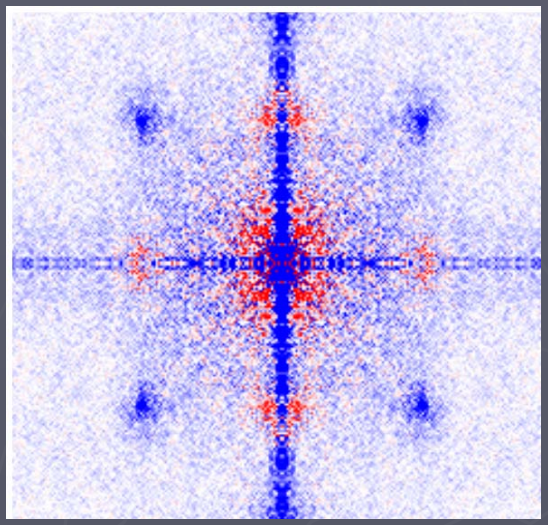
Christianson et al Nature 2008



$Ba_{0.6}K_{0.4}Fe_2As_2$

Enhanced susceptibility at Q below Tc ⇒ sign change of order parameter

Hanaguri et al Science 2010



Fe(Se,Te)

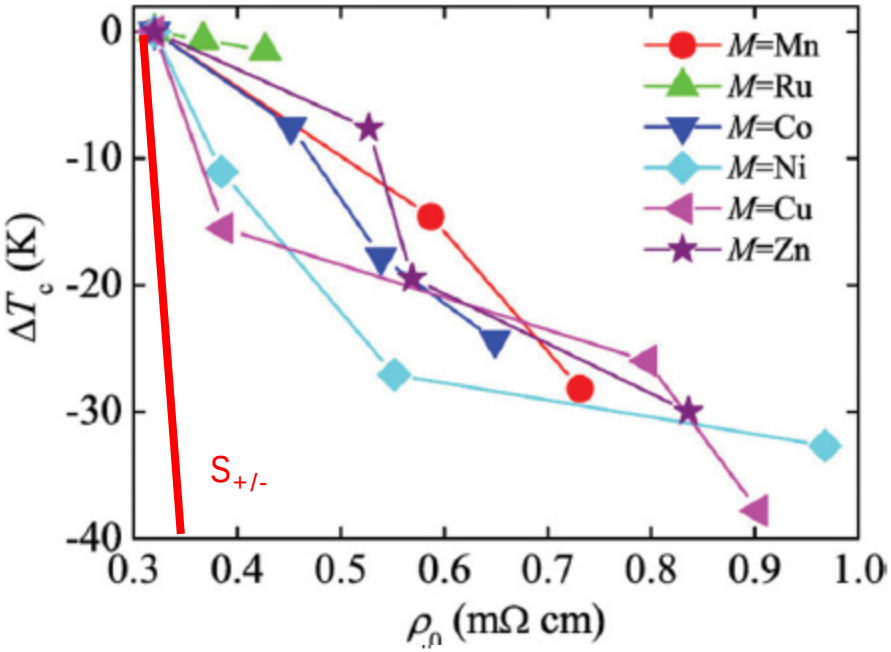
Field dependence of quasiparticle interference peaks depends on order parameter sign

Various critiques of all experiments, alternate scenarios: where is the

?

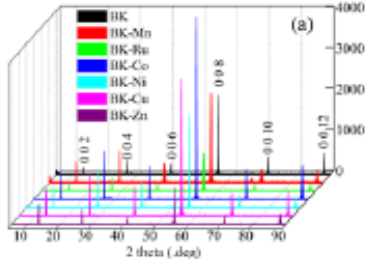
impurity effect in single crystal $(Ba,K)Fe_2As_2$

J.Li et al. PRB 85, 214509 (2012).



✓Vegard's law: good crystal

✓X-ray



other experiments:

1111 systems: Sato et al, JPSJ('08)
Ba122: Paglione et al, arXiv('12)
irradiation: Nakajima et al, PRB ('10)

Experiment:
T_c vanishes when
$\rho_{imp} > 500\mu\Omega cm$
$[l_{imp} \sim 3\,\text{Å}]$

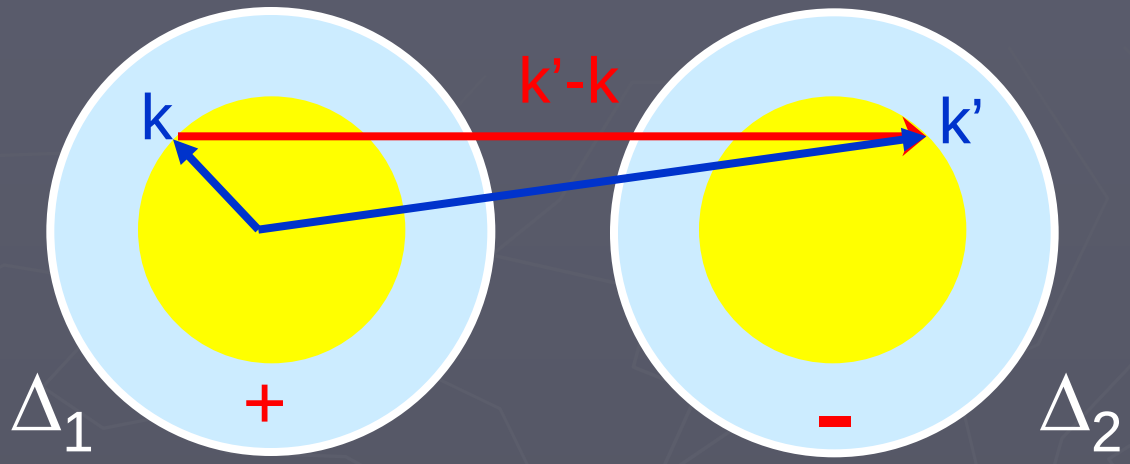
⇔

Theory:
S±wave state
disappears when
$\rho_{imp} = 20\sim40\mu\Omega cm$

local impurity
on Fe-sites

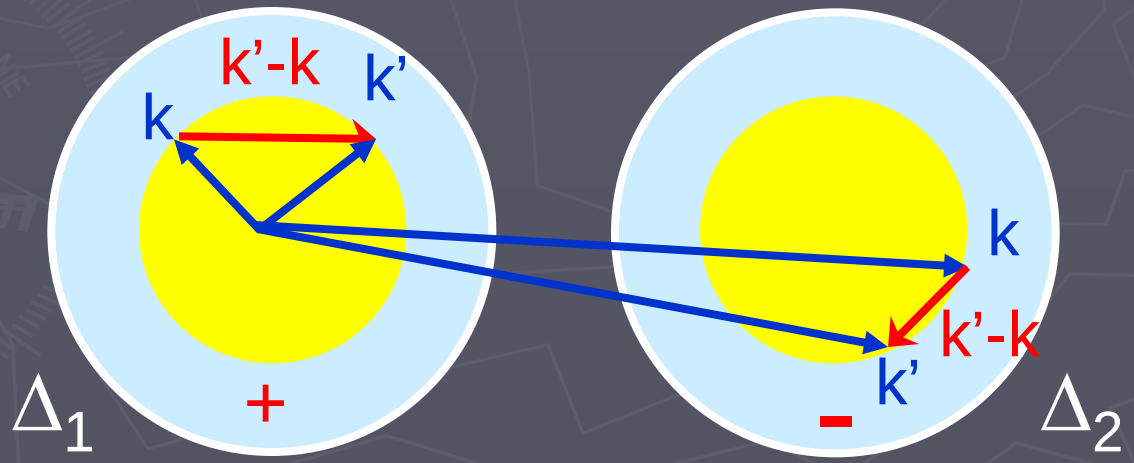
Inter- and intraband impurity scattering in 2-band $s_{+/-}$ system

Inter-



mixes + and –
gaps, breaks pairs

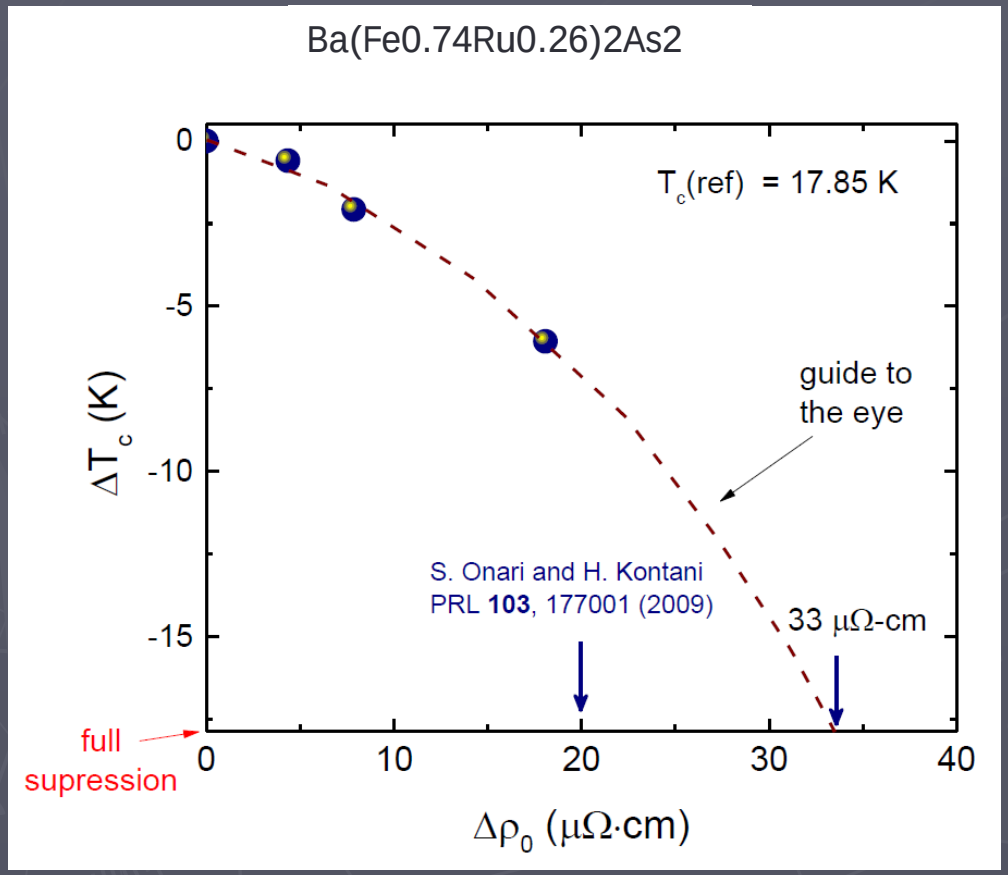
Intra-

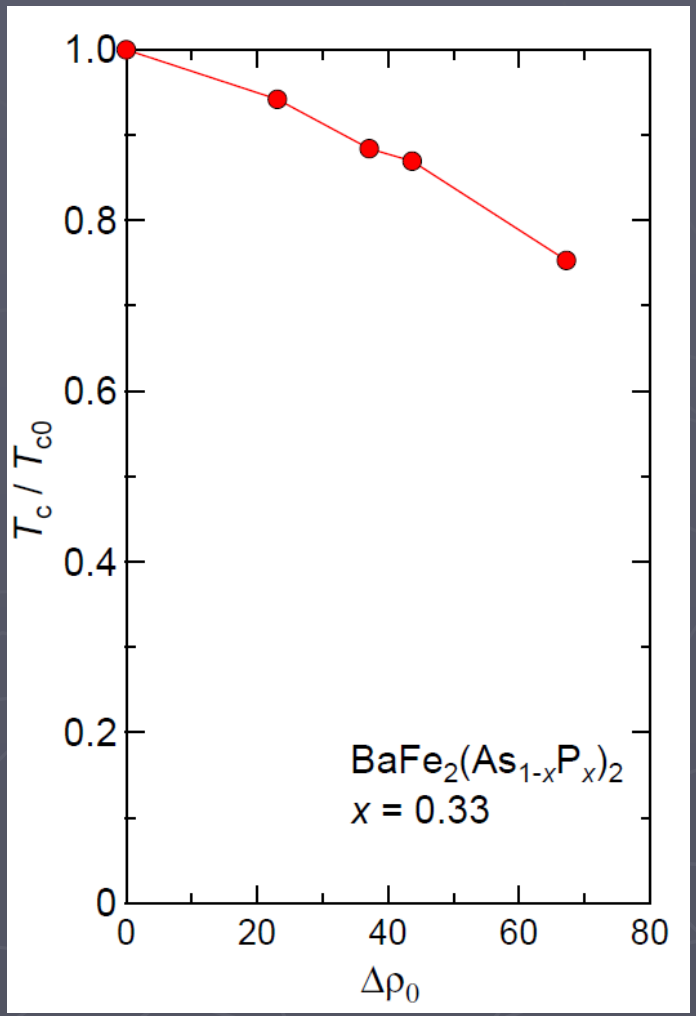


no mixing of +/-
no pairbreaking

e- irradiation experiments

(Prozorov, Shibauchi)





New directions in FeSC

Three materials which don't quite fit the "standard" paradigm

LiFeAs: stoichiometric 18K superconductor with

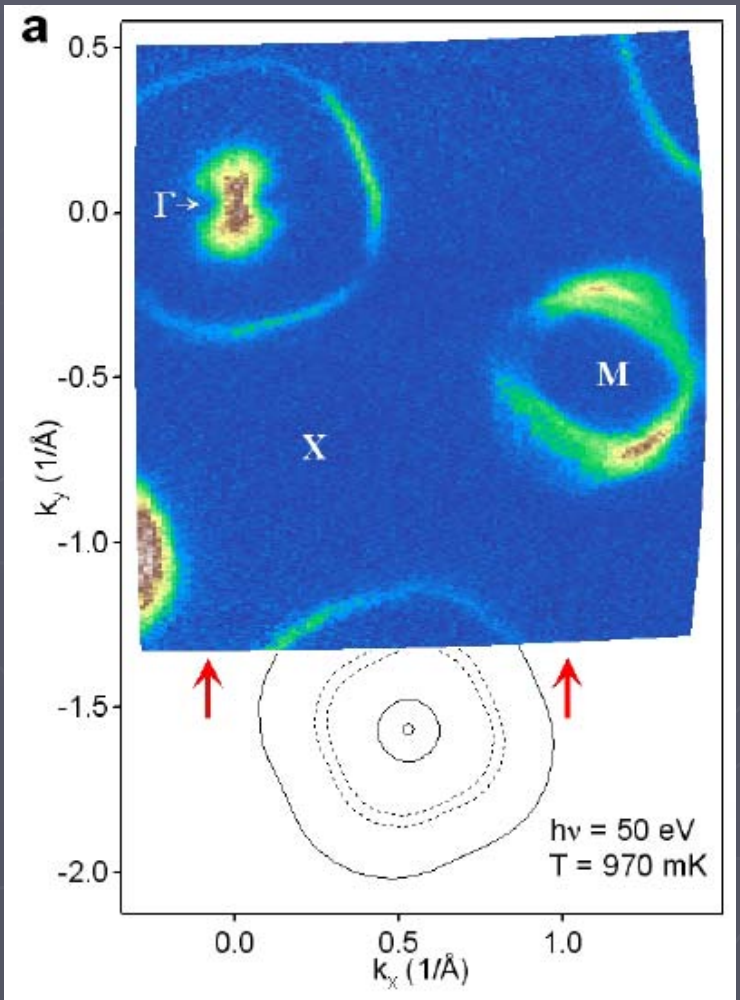
clean, nonpolar surfaces
nonmagnetic, no FS nesting

$KFe_{2-x}Se_2$: 31K superconductor with

$3\mu_B$ ordered magnetic moment,
ordered Fe vacancies,
parent compound may be *insulating*

FeSe under stress: 43K SC intercalated with Li amide, ammonia
40K SC under 10 GPa pressure
?? 65K SC single layer on STO

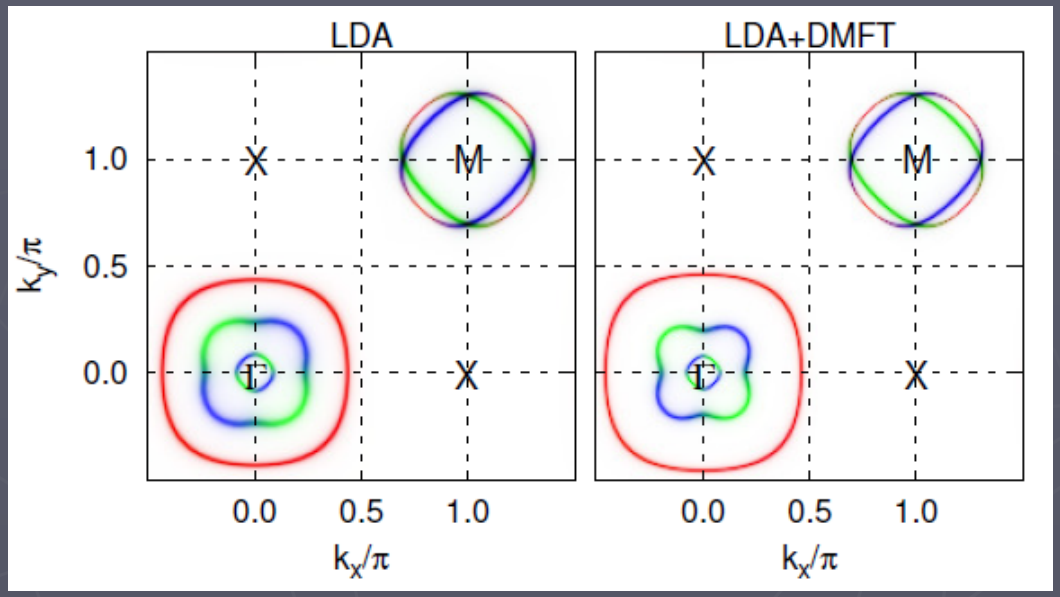
LiFeAs



Borisenko et al PRL 2010

Importance of correlations?

$k_z=0$



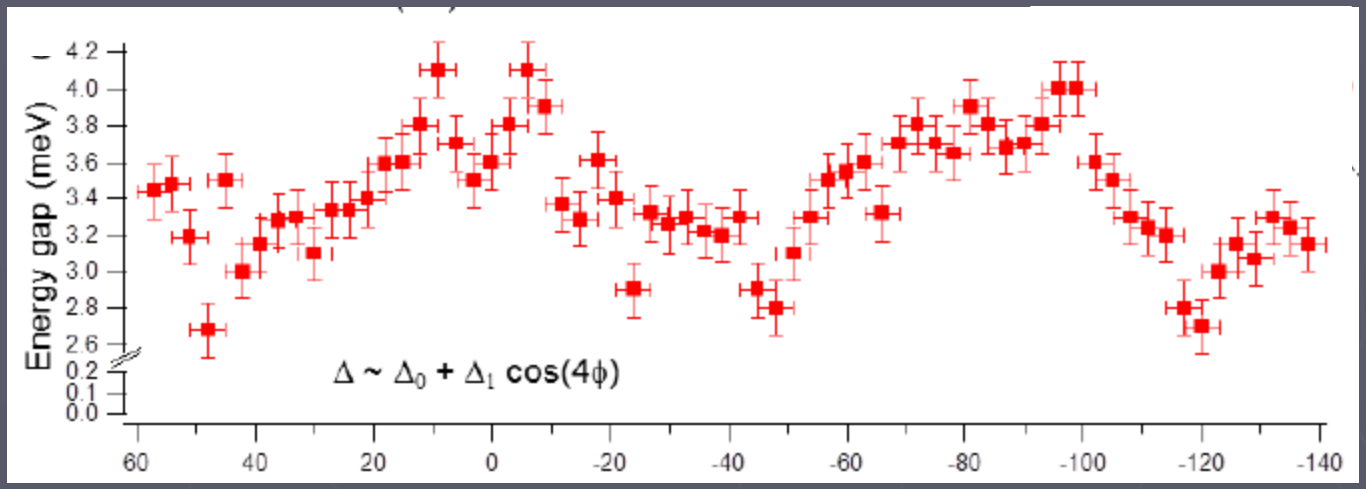
Yin et al 2011 Nat Mat, Ferber et al PRB 2012

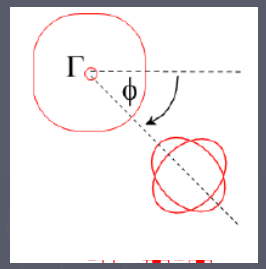
LDA+DMFT: hole pockets shrink, electron pockets unaffected

see also Lee et al, PRL 2012

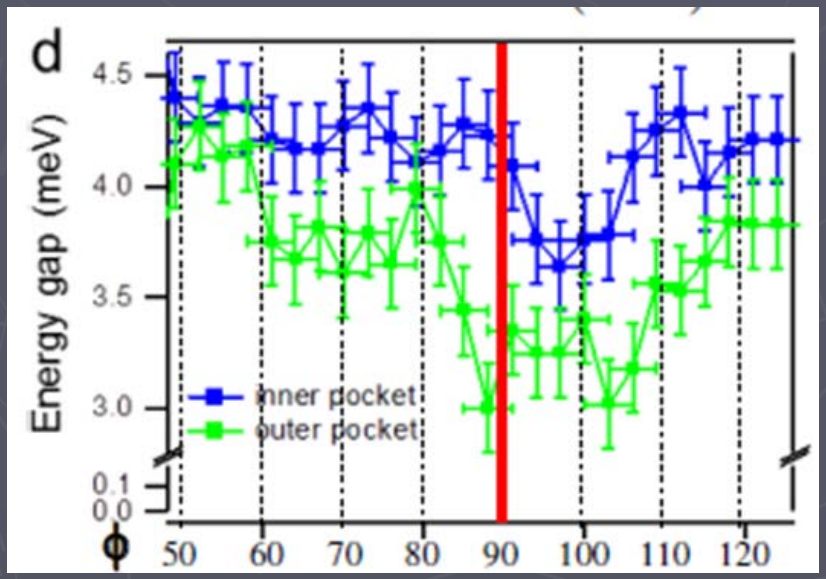
ARPES results for SC gap function (Dresden group)

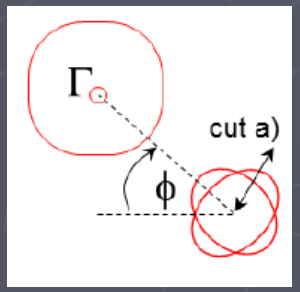
γ hole pocket



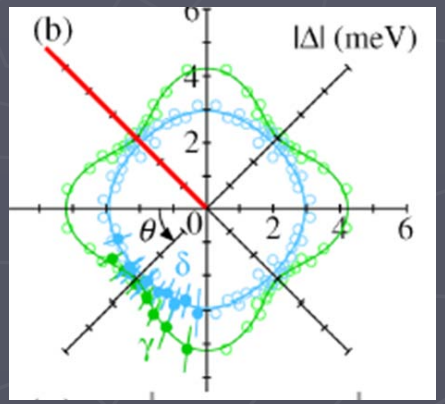


β electron pocket



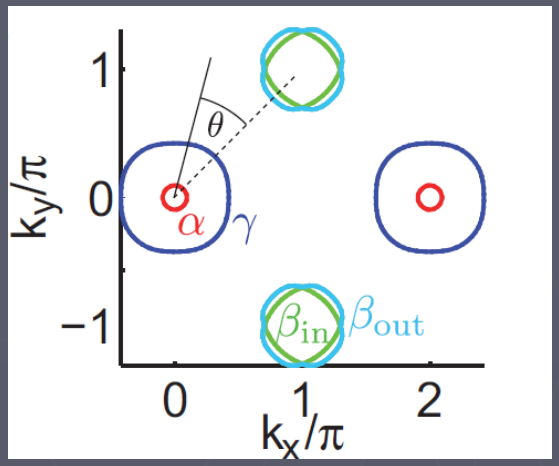


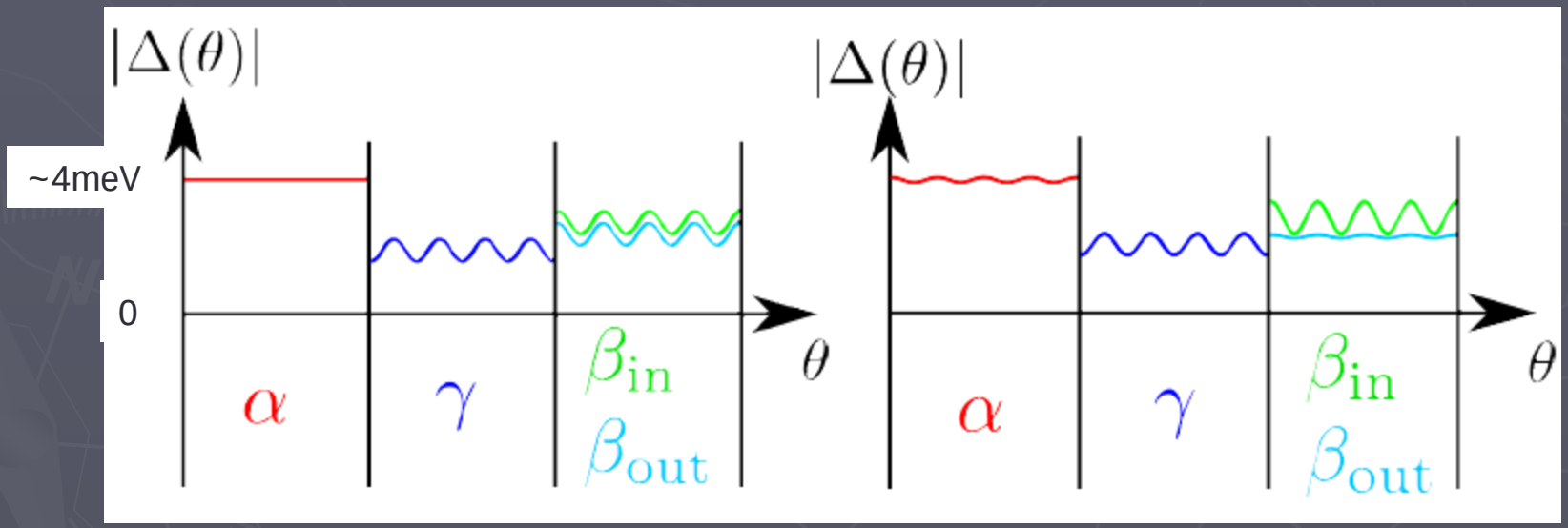
See also
K. Umezawa et al 2012



Borisenko et al Symmetry 2012

Experimental data (Disney version)





Borisenko et al 2012

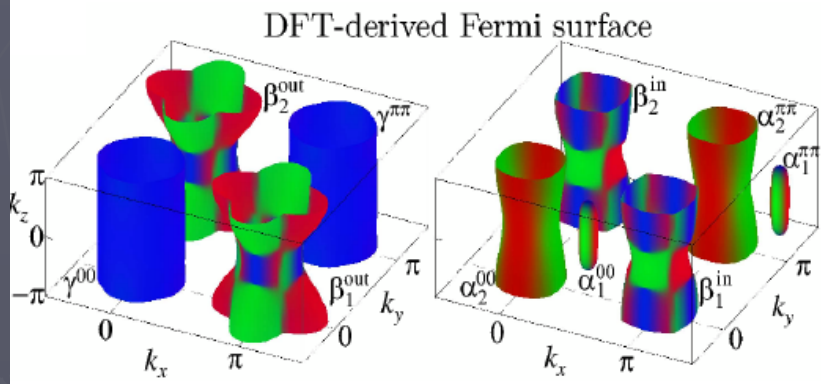
Umezawa et al 2012

Results of 3D spin fluctuation calculations I

Leading pairing eigenstate 10-orbital DFT-based or ARPES-fit bands

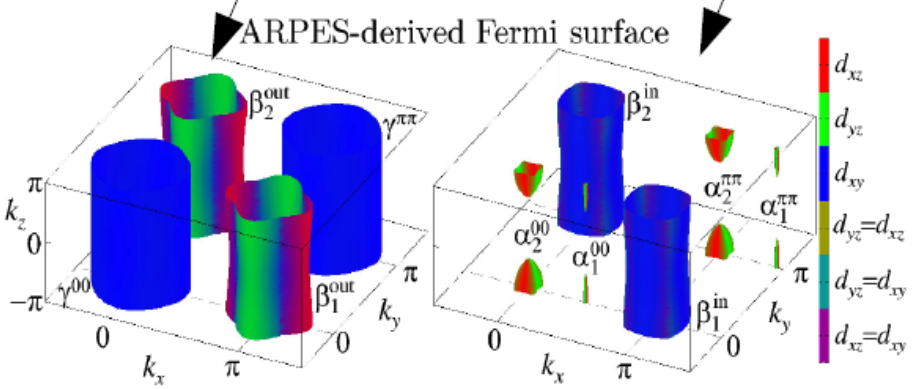
Wang et al PRB 2013

- Fermi surface



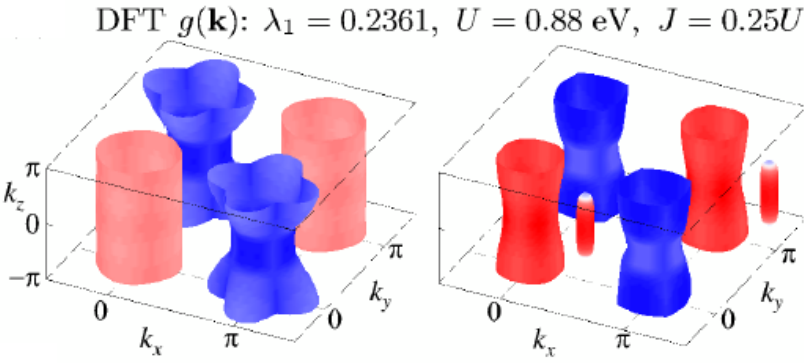
outer sheets

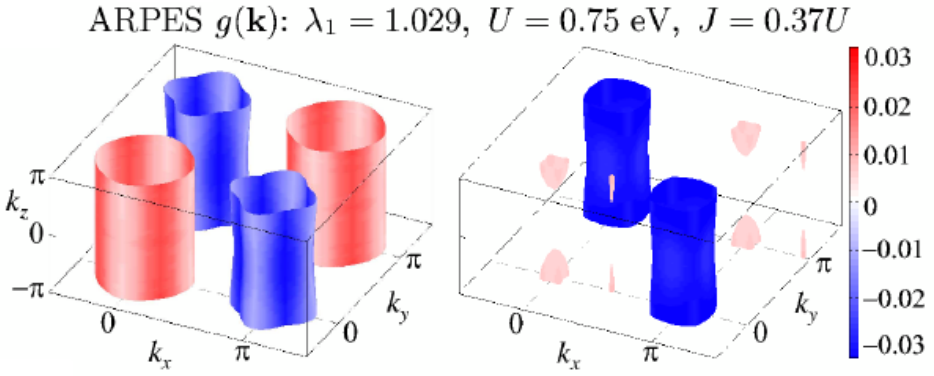
inner sheets



- gapfunction

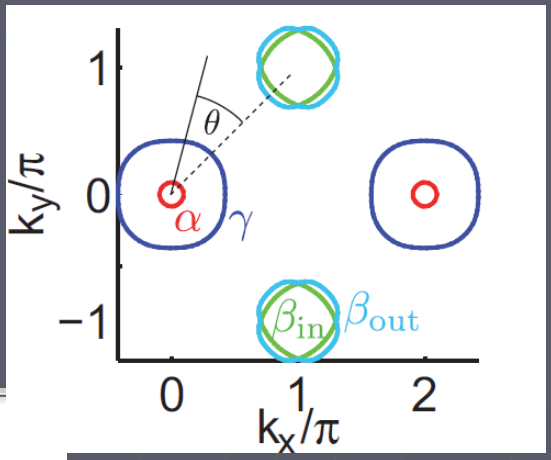
Fit provided by
S. Borisenko V. Zabolotnyy

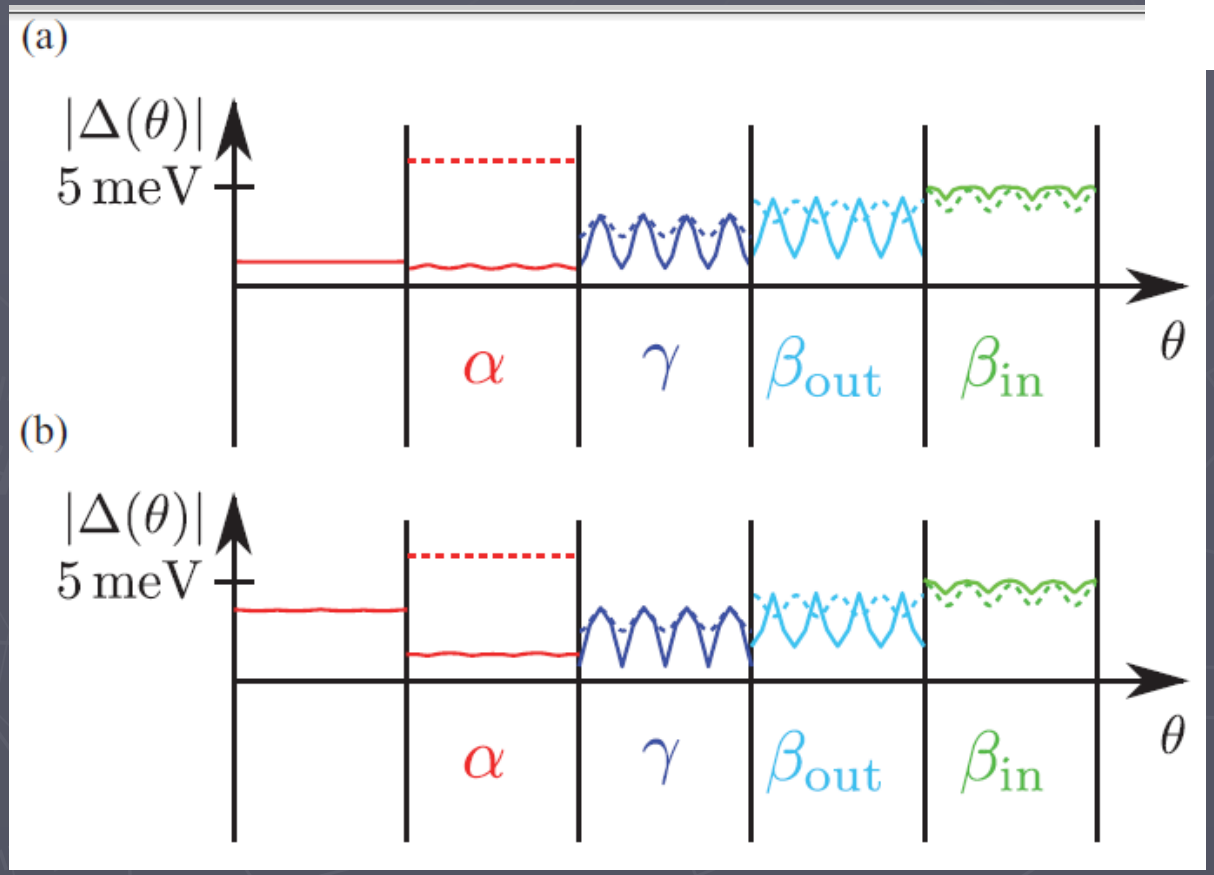




Comparison theory/expt

Y. Wang, A. Kreisel, V. B. Zabolotnyy, S. V. Borisenko,
B. Büchner, T. A. Maier, PJH, D. J. Scalapino, PRB 2013



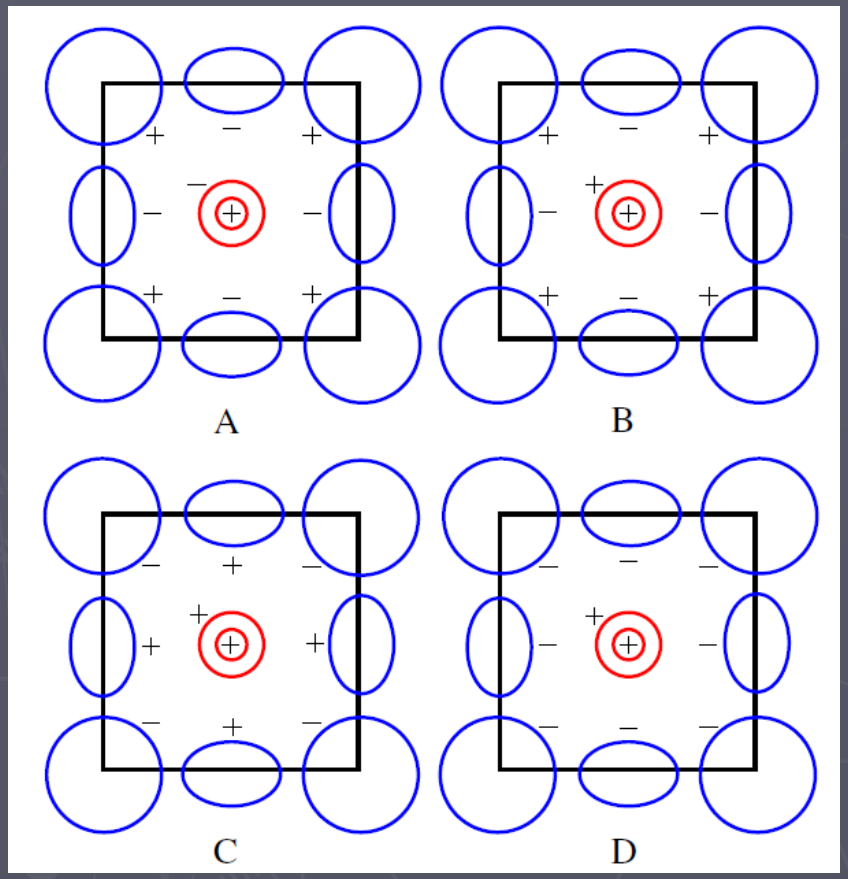


Conclusion: s+/- pairing from spin fluctuations despite lack of Fermi surface nesting

LiFeAs ``ab initio" pairing theory: success or failure?

Comparison with experiment

IV. Ahn et al aXv: '14 I. Wang et al. PRB '13

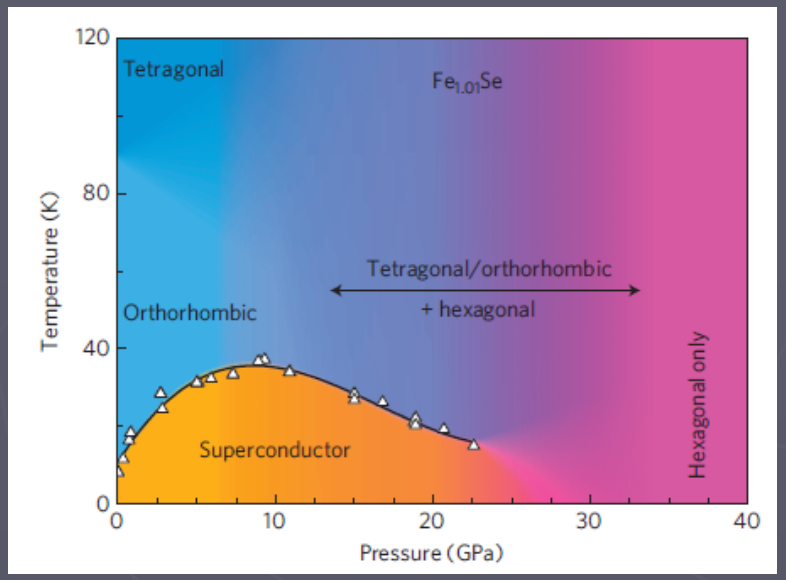


	I	II	III	IV
Bands	ARPES*	LDA+DMFT	ARPES*	ARPES*
Full gap	yes	no	yes	yes
Ratios of gaps on large pockets	yes	?	yes	possible
Gap size on α pockets	"no"	?	yes	possible
Phase of gap on β pockets	yes	yes	yes	possible

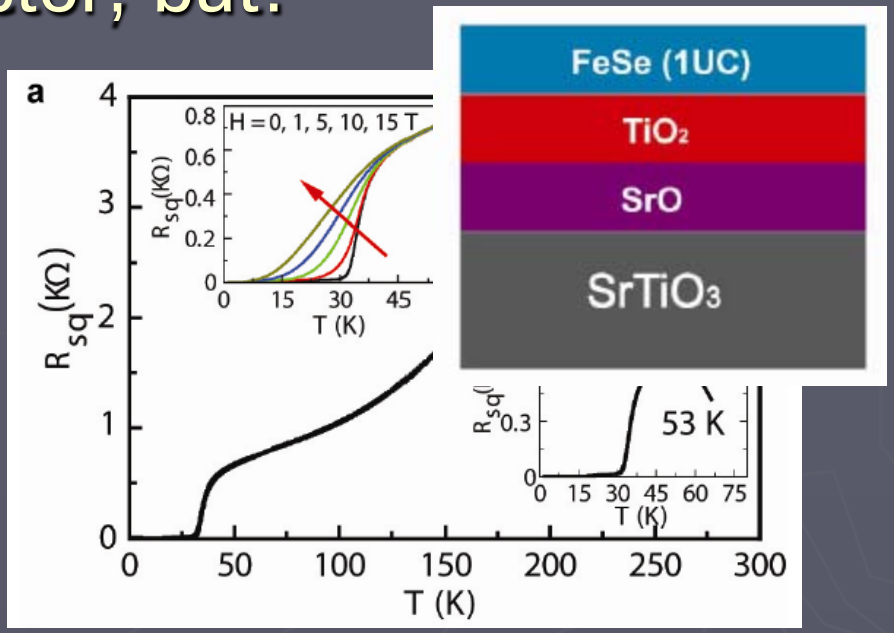
III. Saito et al. aXv: '14 IV. Yin et al. aXv '13

•Some disagreement re ARPES Fermi surface: cf. Chi et al 1308.4413 surfaces, samples?

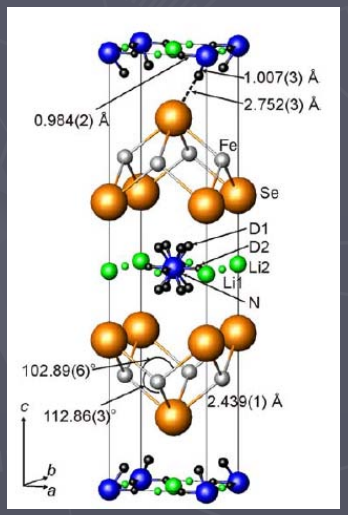
FeSe: 8K superconductor, but:

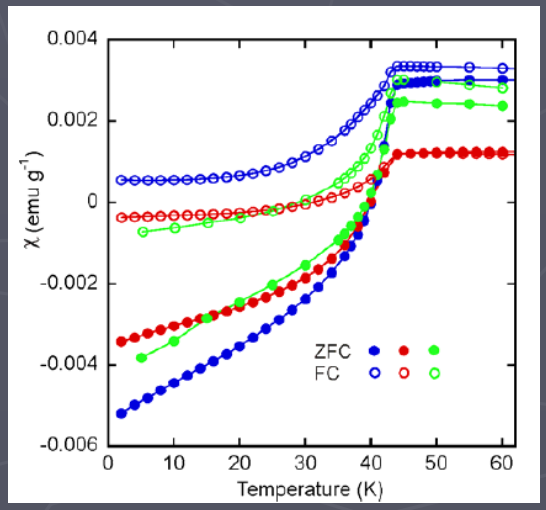


Medvedev et al 2010: Tc→37K under pressure

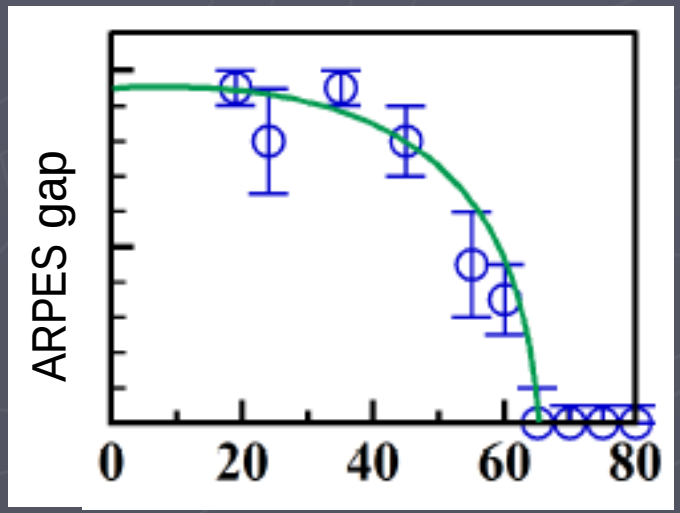


Wang et al. Chin. Phys. Lett. 2012
1 layer Tc→35K under tensile strain





Burrard-Lucas et al 2012
Tc→43K molecular intercalation



S. He et al aXv::1207.6823

Conclusions

- Magnetic and orbital correlations at high T both lead to stripe magnetic order and superconductivity: which are more important?
- repulsive interactions probably lead to s+/- state for "generic" Fe-based SC with hole and electron pockets
- orbital character, intraband Coulomb enhance gap anisotropy. anisotropic $s_{+/-}$ nodal structures show strong sensitivity to small changes in electronic structure (pnictogen height, surfaces, strain, defects)
- spin fluctuation theory explains gap anisotropy of 122's across phase diagram, gets details correct in "generic" FeSC
- "end point compounds" show tendency to d-wave order