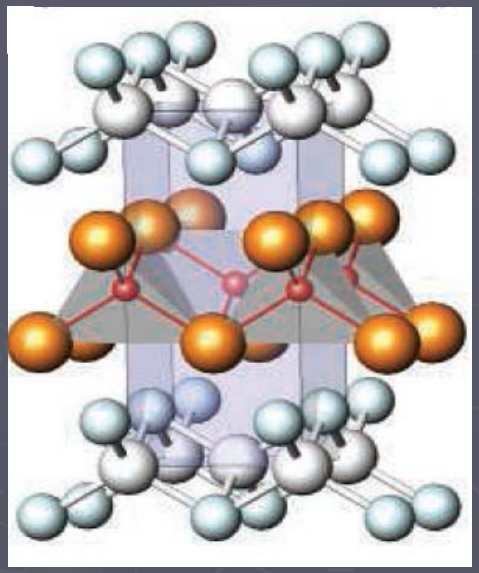
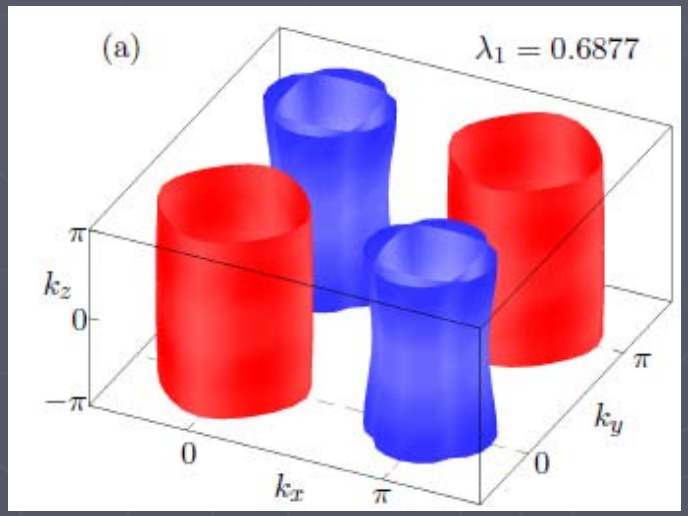
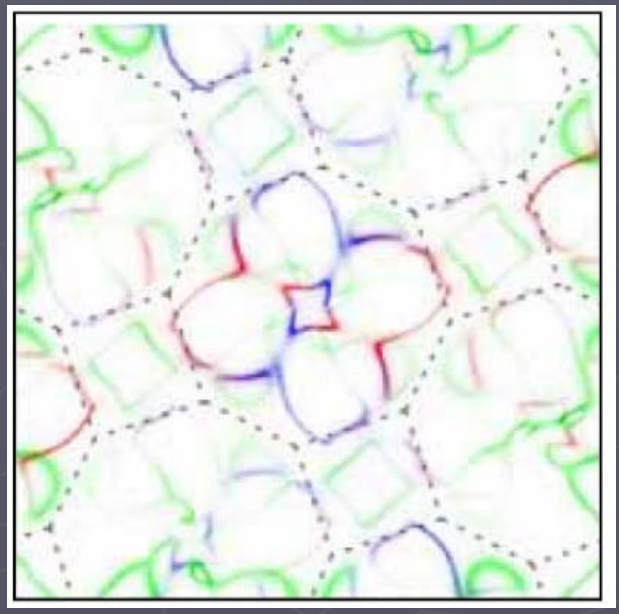
I. Review of Fe-based Superconductivity
II. Disorder effects in unconventional sc

P. Hirschfeld, U. Florida







PH, M.M. Korshunov and I.I. Mazin, Rep. Prog. Phys. 74, 124508 (2011)

Maglab Theory Winter School January 2013

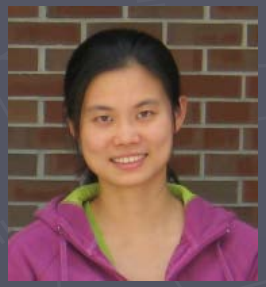
Collaborators

from U. Florida Dept. of Physics:

Tom Berlijn

Andreas Kreisel

Yan Wang



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Harald Jeschke
U. Frankfurt

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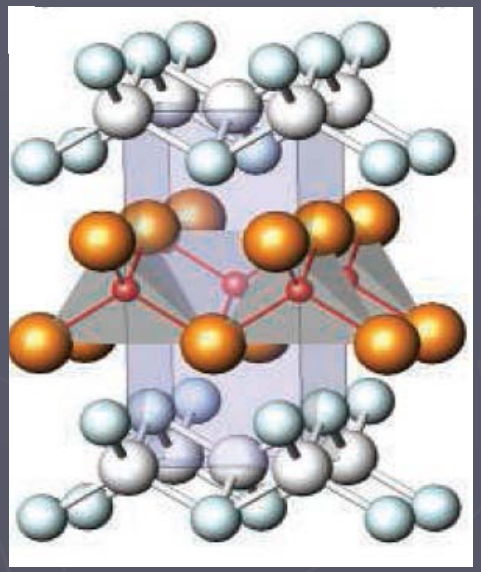
U. Frankfurt

Wei Ku, Brookhaven

I. Review: Superconductivity in Fe-based SC

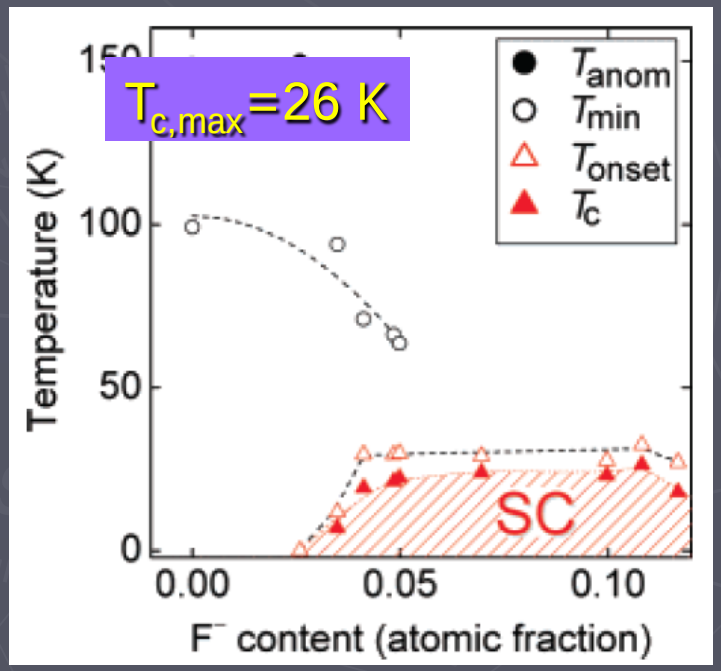


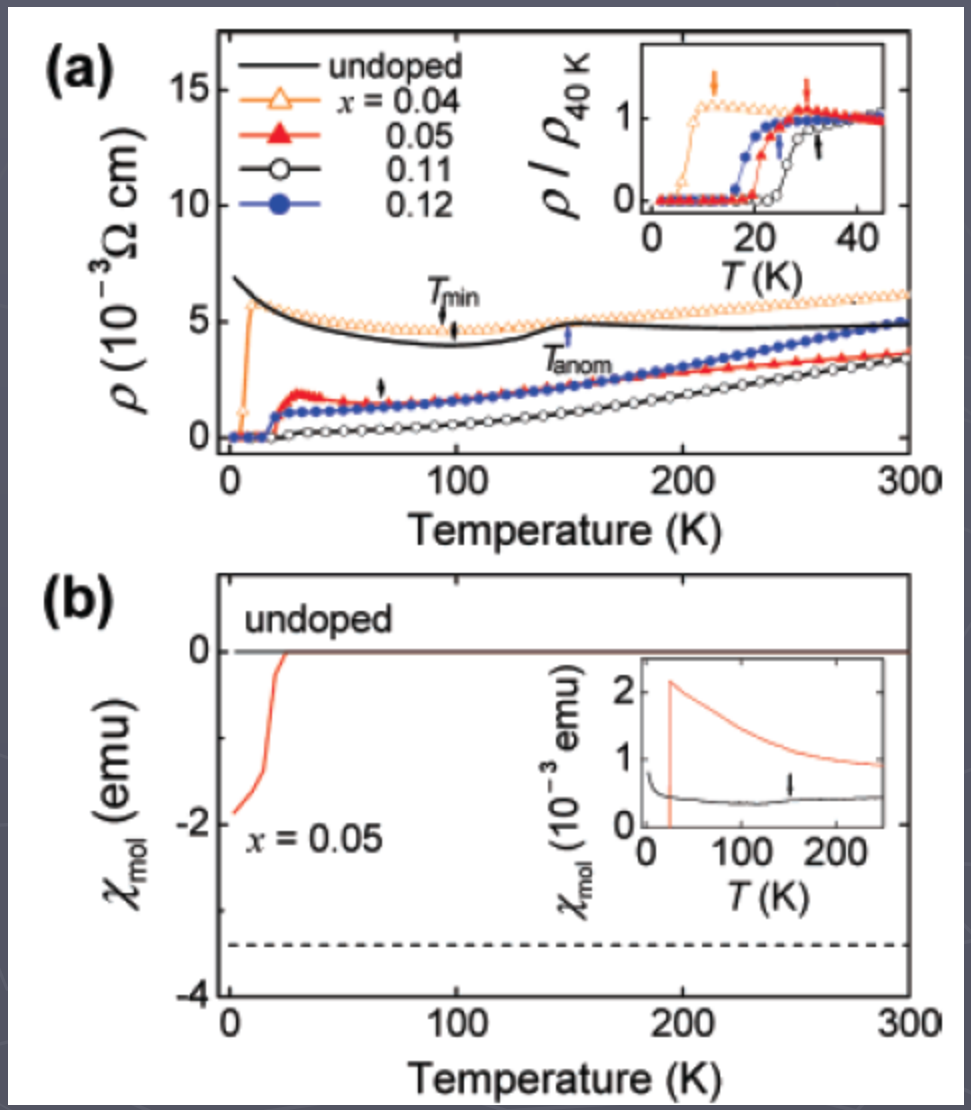
- review of normal state
- review of sc state
- standard model
- new materials & directions

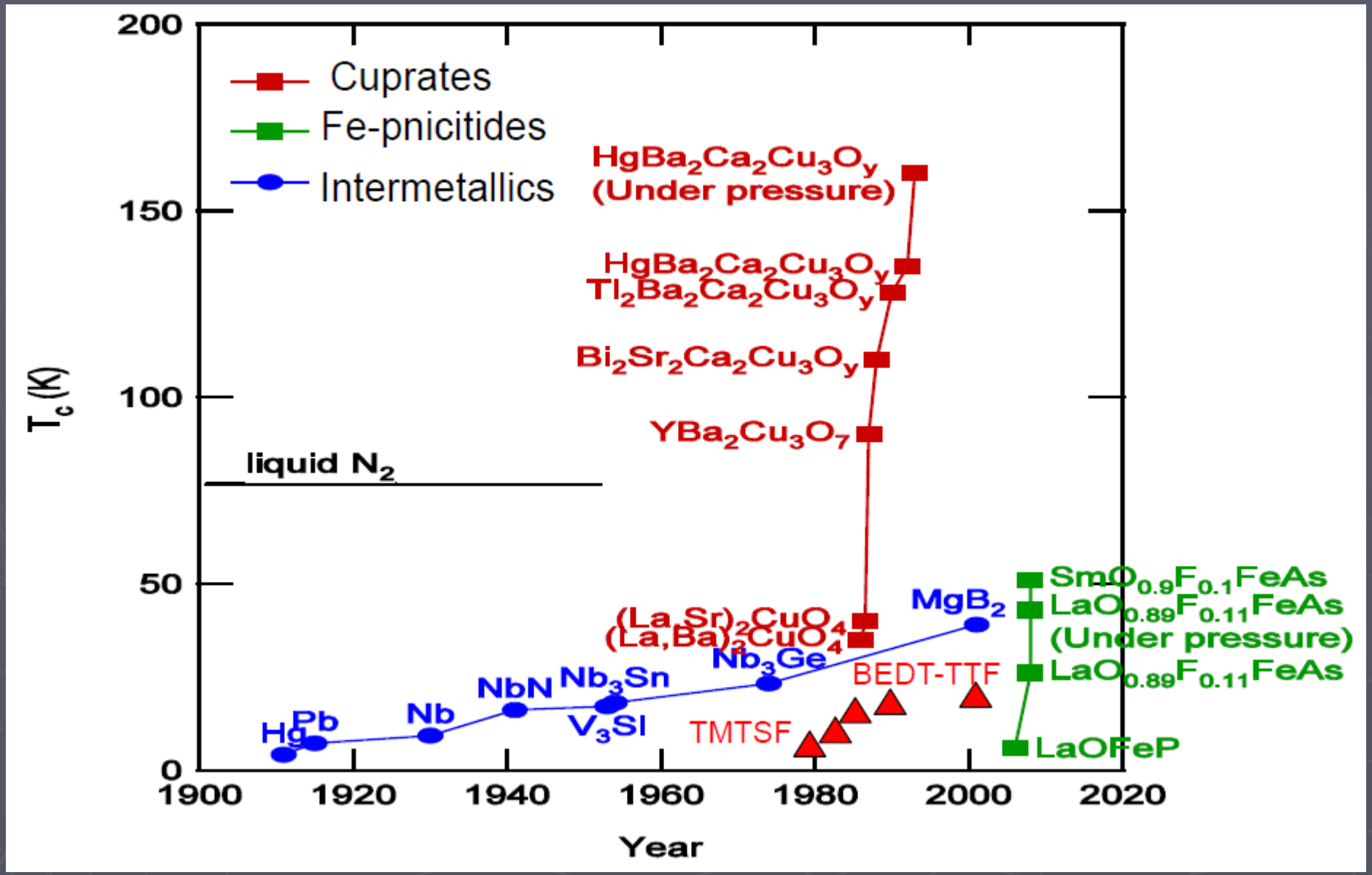
Discovery of $LaO_{1-x}F_xFeAs$

Kamihara et al JACS 2008

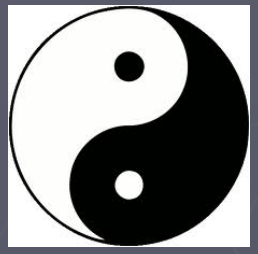
H. Hosono






Cuprates
Fe-pnicitides
Intermetallics
$HgBa_2Ca_2Cu_3O_y$ (Under pressure)
$HgBa_2Ca_2Cu_3O_y$
$Tl_2Ba_2Ca_2Cu_3O_y$
$Bi_2Sr_2Ca_2Cu_3O_y$
$YBa_2Cu_3O_7$
liquid N_2
$(La,Sr)_2CuO_4$
$(La,Ba)_2CuO_4$
MgB_2
Nb_3Ge
Nb_3Sn
NbN
Nb
Pb
Hg
V_3Si
BEDT-TTF
TMTSF
$SmO_{0.9}F_{0.1}FeAs$
$LaO_{0.89}F_{0.11}FeAs$ (Under pressure)
$LaO_{0.89}F_{0.11}FeAs$
LaOFeP
T_c (K)
Year
0
50
100
150
200
1900
1920
1940
1960
1980
2000
2020

Comparison with cuprates



Strong vs. weak coupling?

Single vs. multibands?

2D vs. 3D?

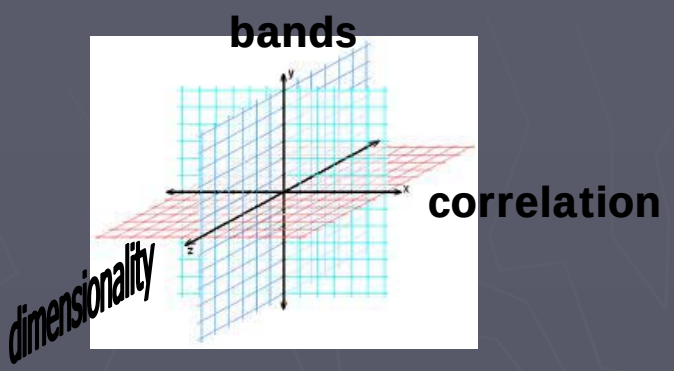


Table 1 | Properties of different classes of superconductor

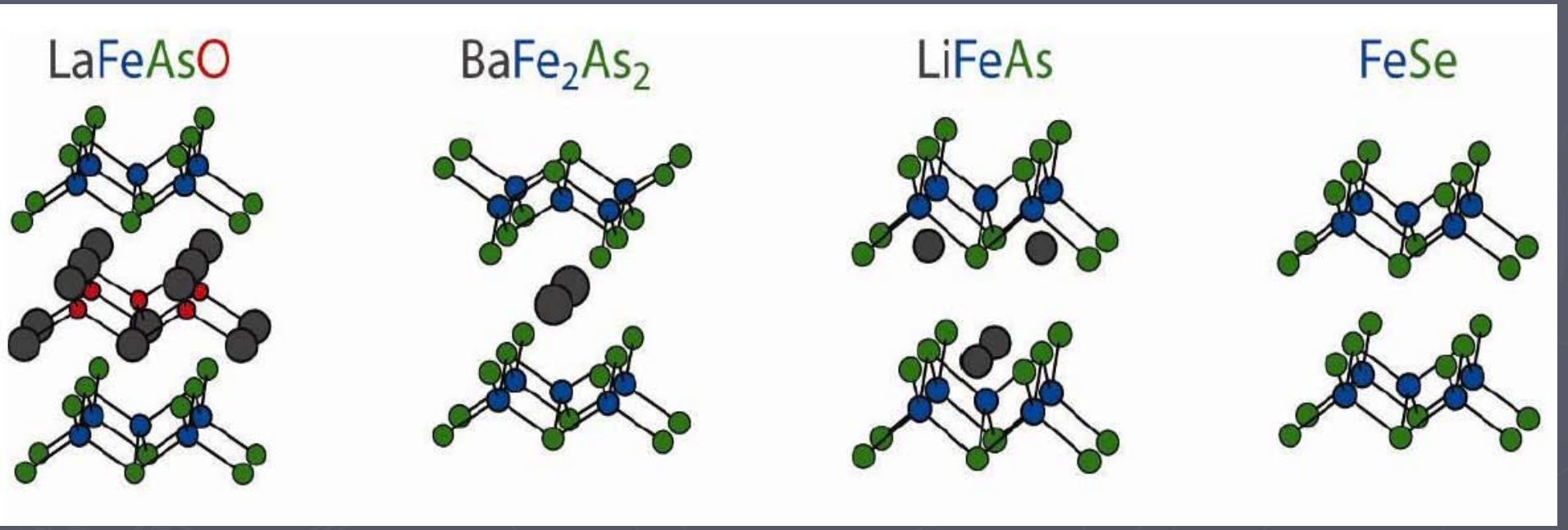
Property	Conventional superconductors	Copper oxides	MgB_2	Iron-based superconductors
T_c (maximum)	<30 K	134 K	39 K	56 K
Correlation effects	None (nearly-free electrons)	Strong local electronic interaction	None (nearly-free electrons)	Long-range (non-local) magnetic correlations
Relationship to magnetism	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?

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

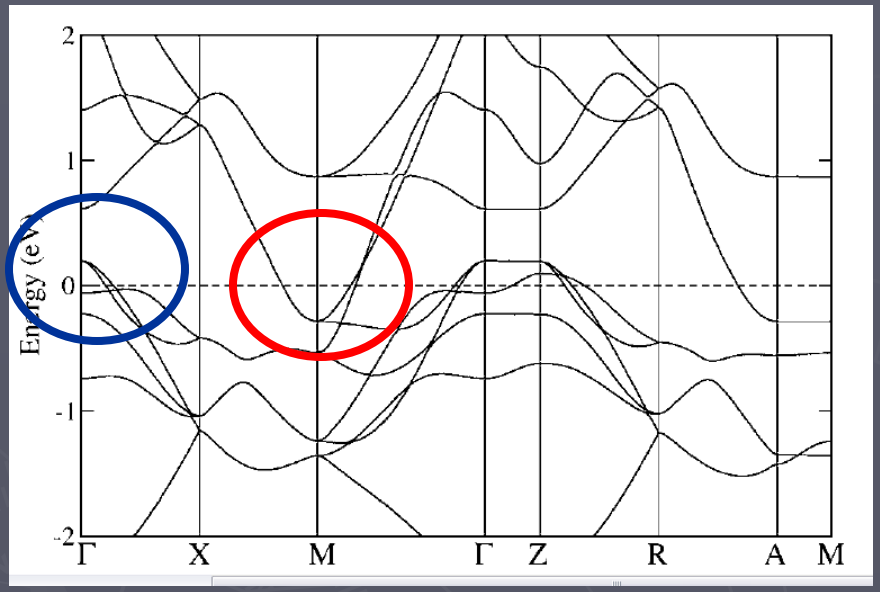
T_c=8K

Hsu et al
PNAS 2008

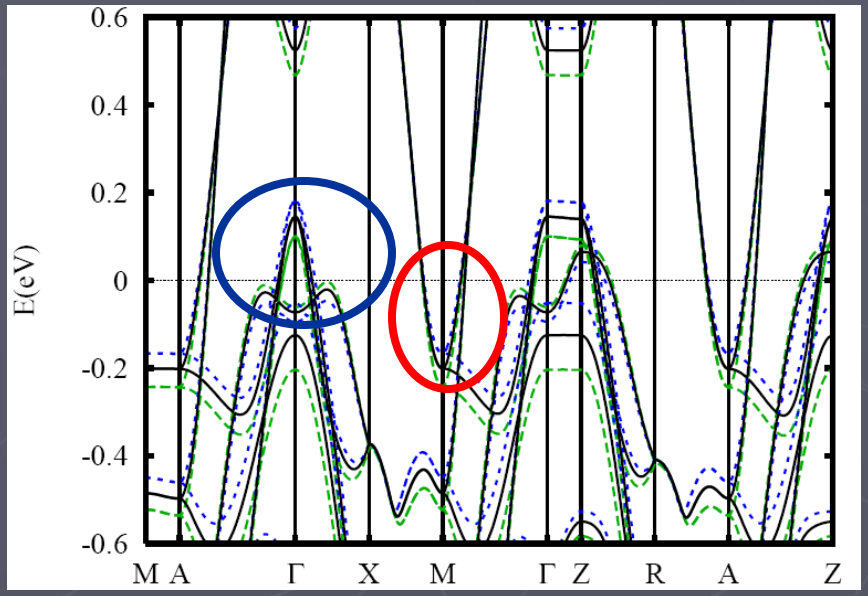
No arsenic ☺!

Electronic structure calculations

LOFP Lebegue 2007 (T_c=6K)

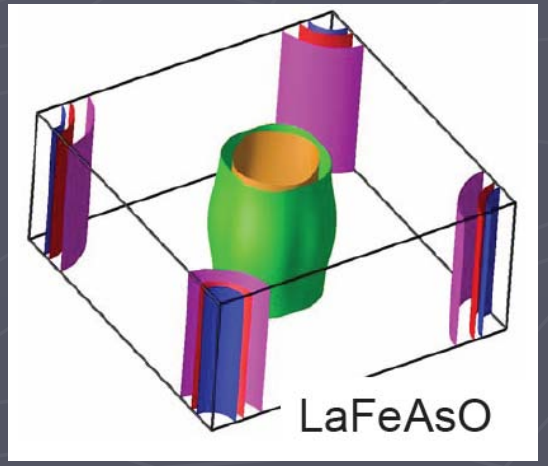


LOFA Singh & Du 2008 (T_c=26K)



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

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



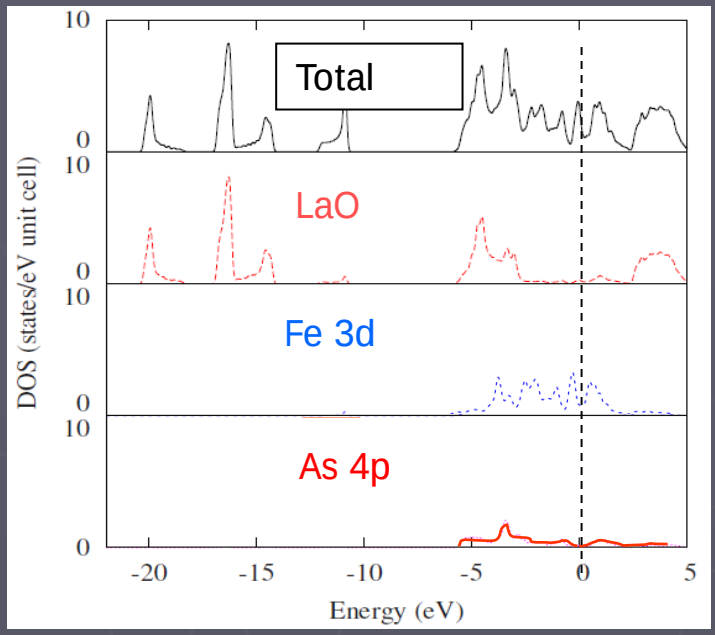
2D!

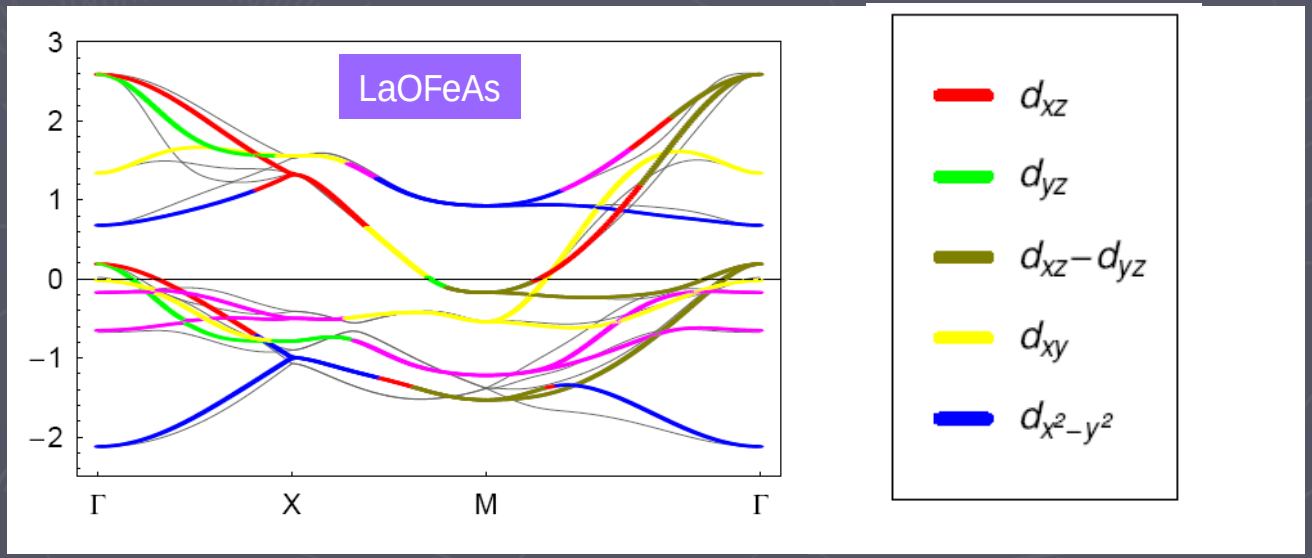
Multiorbital physics

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

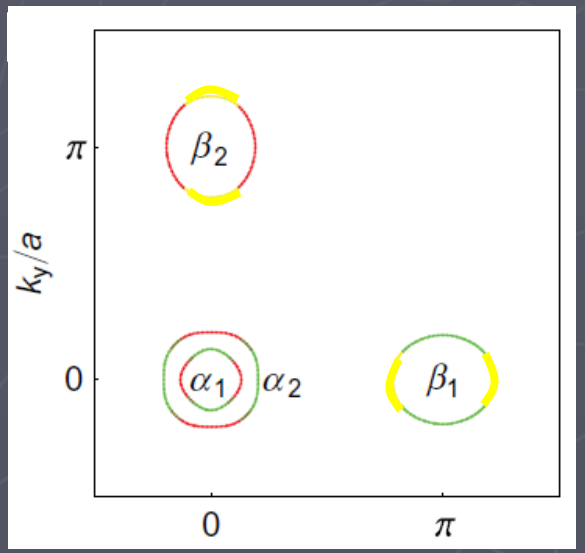
Complications: calculations will be harder

Novelty: surprising new aspects of multiorbital/ multiband physics





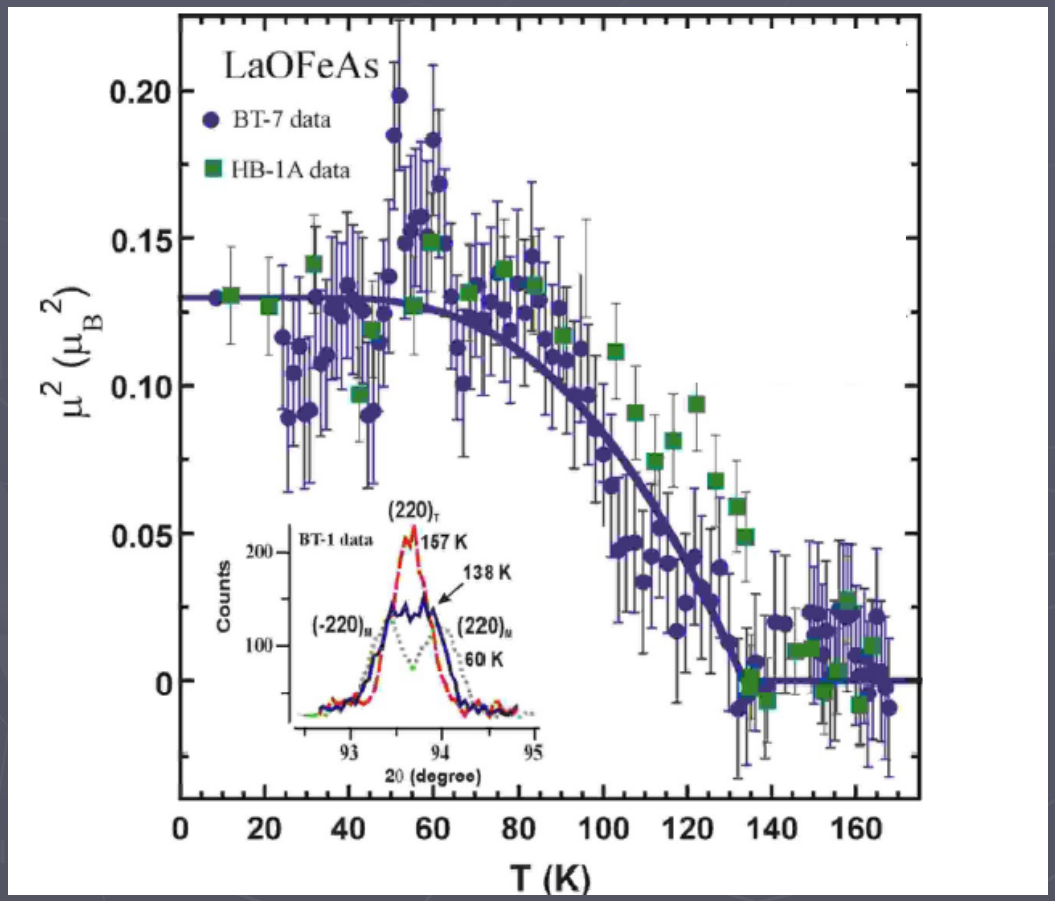
Band structure

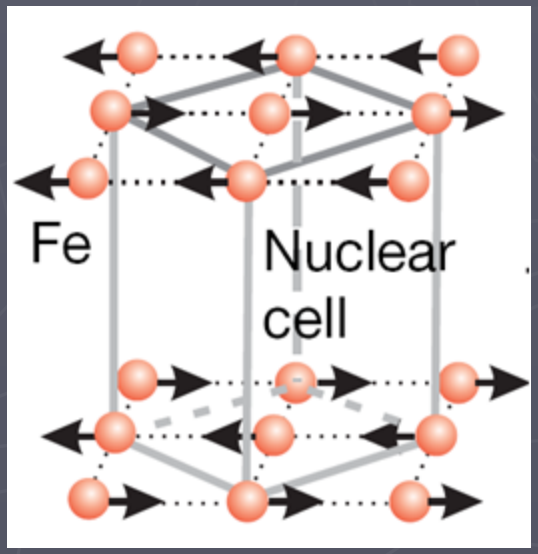


Fermi surface

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 moment 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*	-			

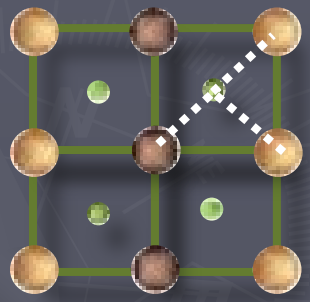
"double stripe" q=(π/2,π/2)

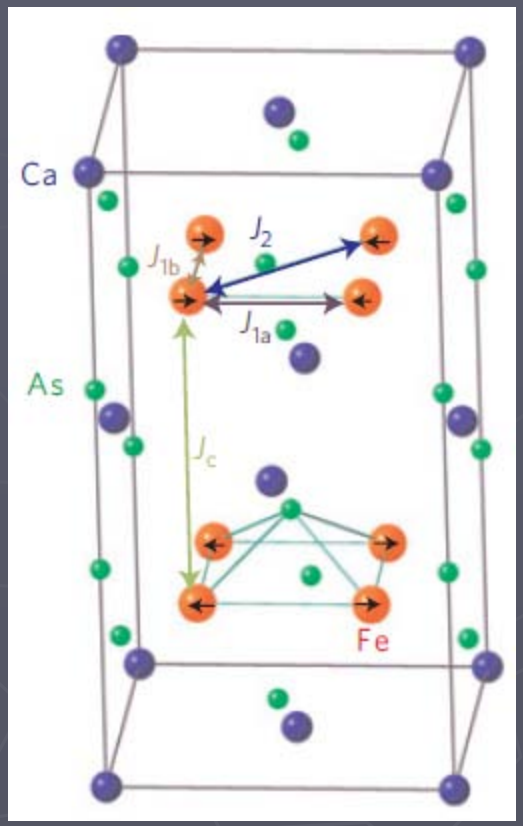
Lynn, Dai 2009

Weak coupling/strong coupling picture of magnetism?

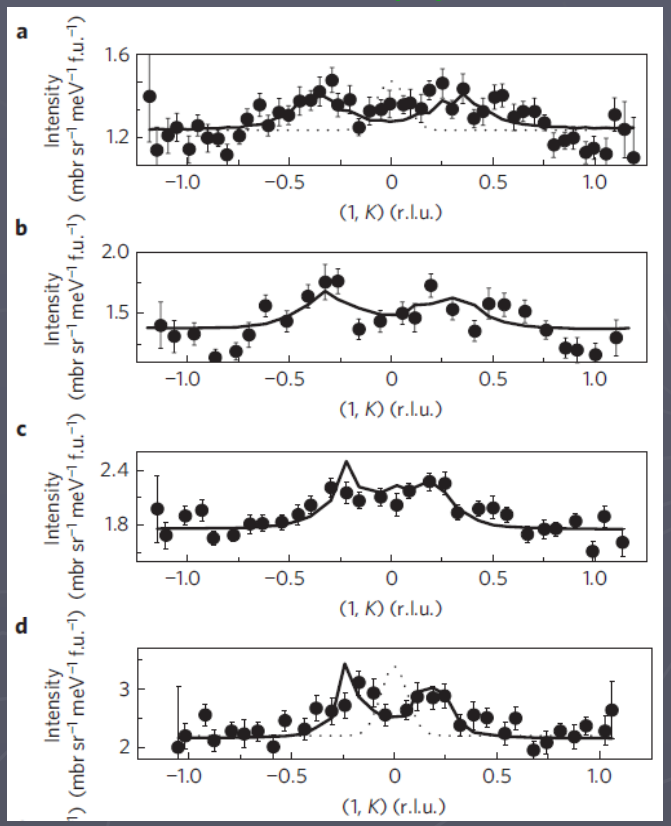
Early theories proposing strong coupling: Yildrim 08; Fang et al 08, Cvectovic & Tesanovic 08, Abrahams & Si 08, Manousakis et al 08

Stripe order stabilized for large J_2





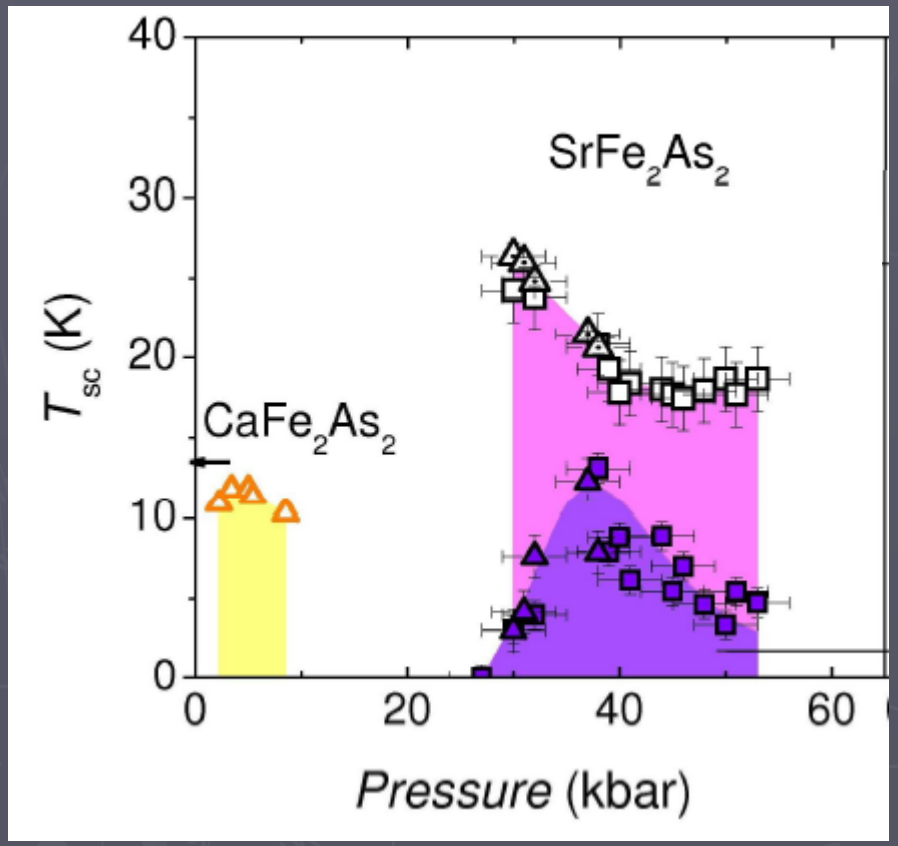
Zhao et al. Natphys 09



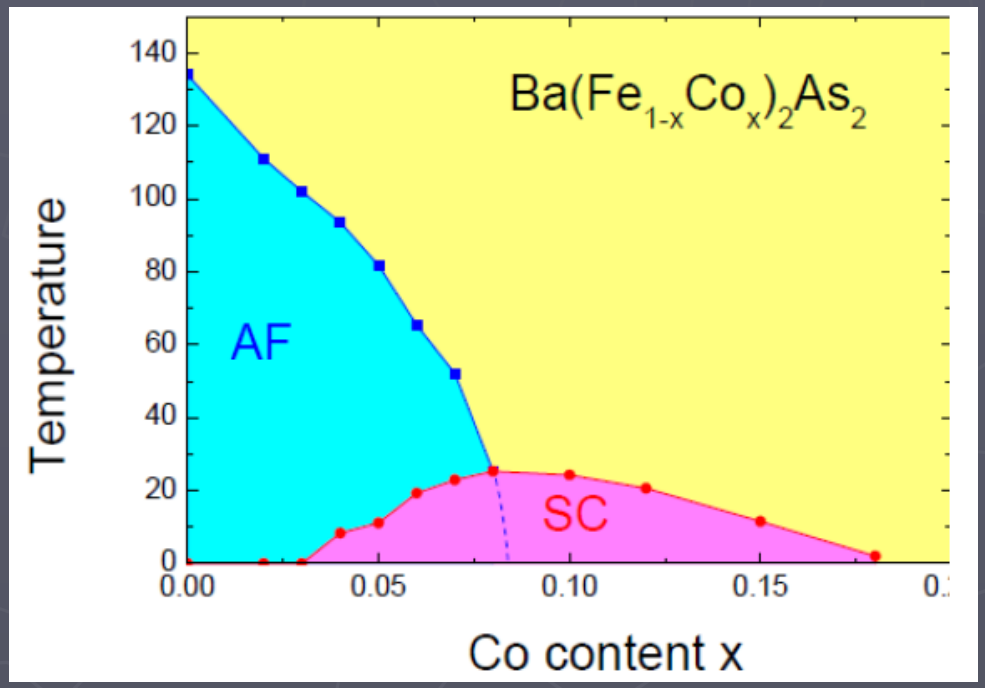
Zhao et al. Natphys 09 spin excitations fit Heisenberg without need for Stoner continuum, but a-b anisotropy hard to understand.
Diallo et al PRL 09: poor fit at higher E, spin waves are damped by p-h excitations; good fit from 1st principles susceptibility

“Doping” the parent compound

Various chemical substituents *or* pressure lead to SC “dome”

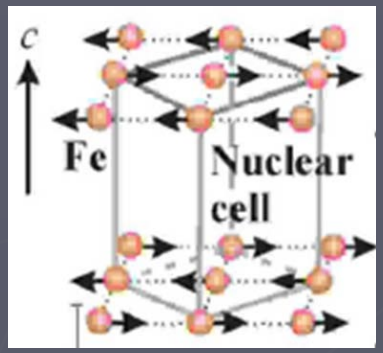


Alireza *et al.* (2008)



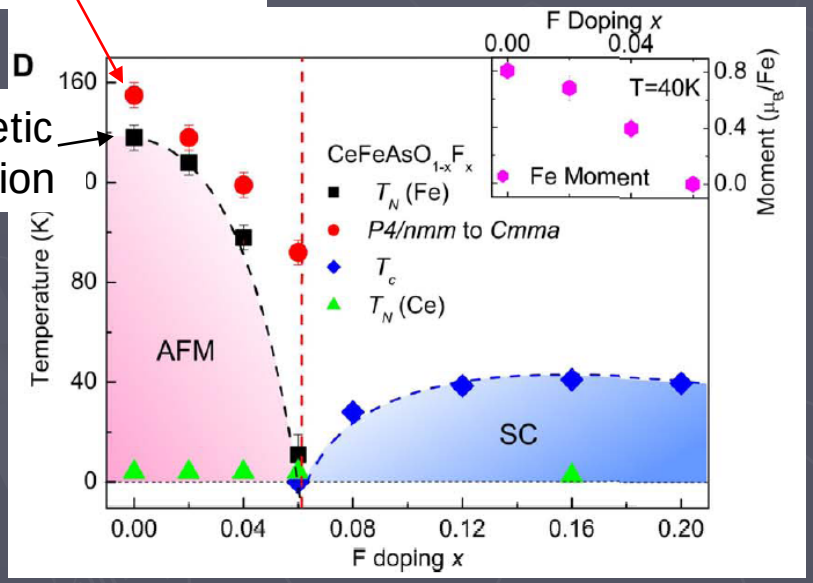
Fang *et al.* (2009)

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

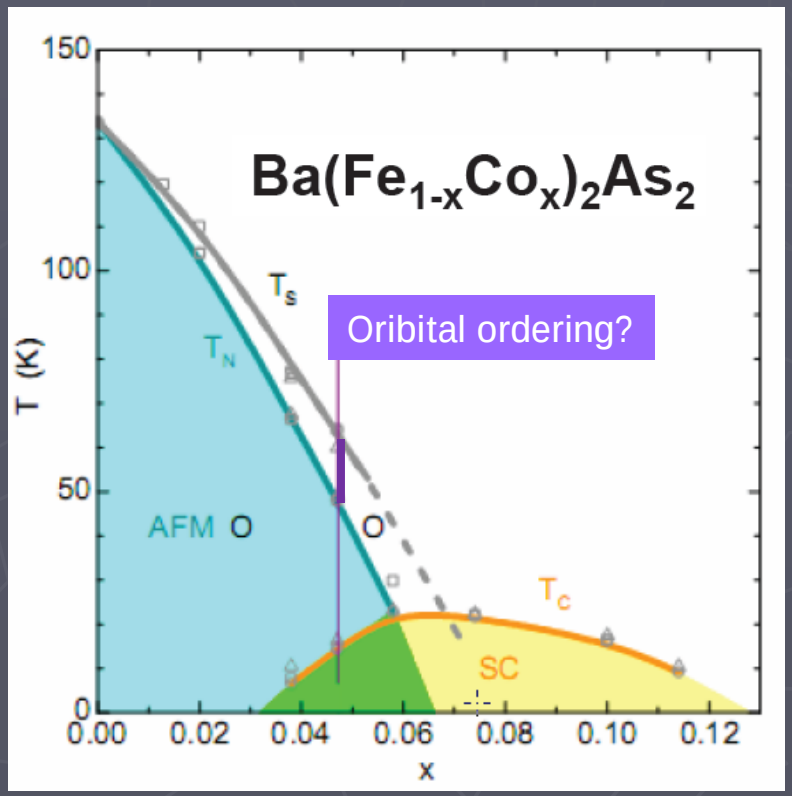


structural transition

magnetic transition



Zhao et al 2008



D.K. Pratt et al 09

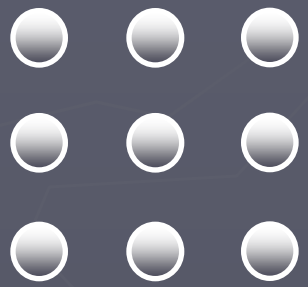
Best guess at present: 1111—NO; 122--YES

Two phase transitions

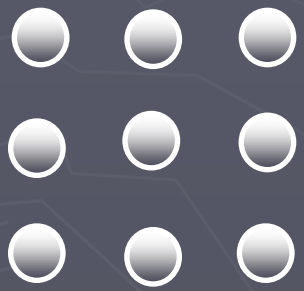
I) Structural Transition

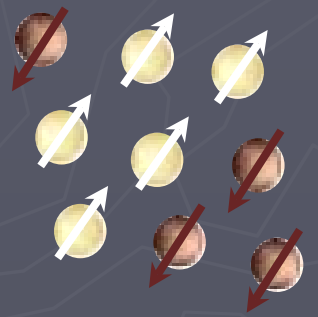
II) Magnetic Transition

122/1111



FeTe

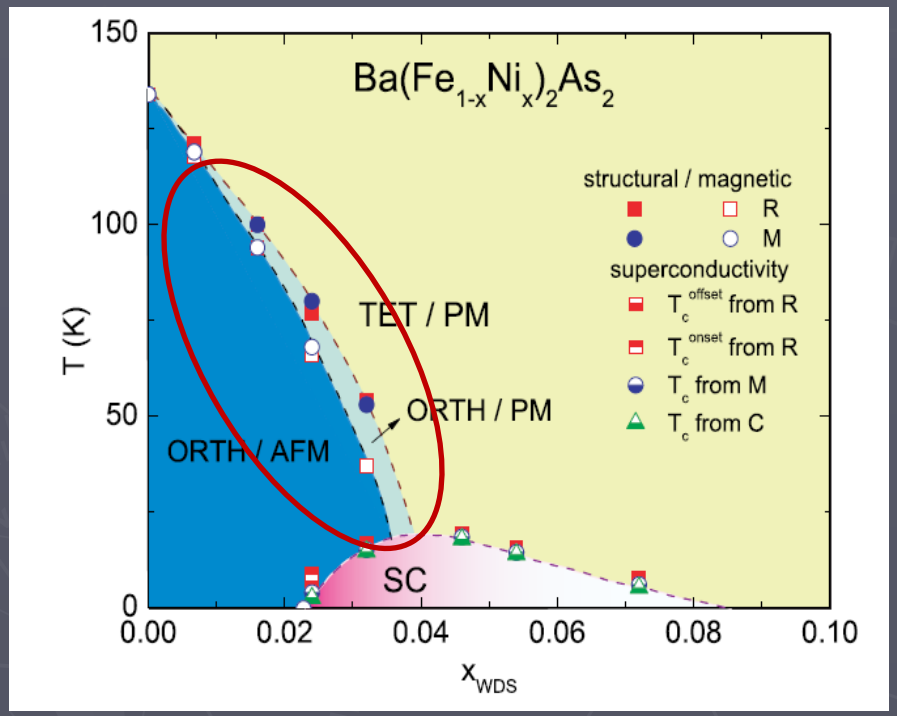




DFT correctly reproduces (or even predicts) correct magnetic and structural ground states, but requires magnetism as a prior condition for distortion

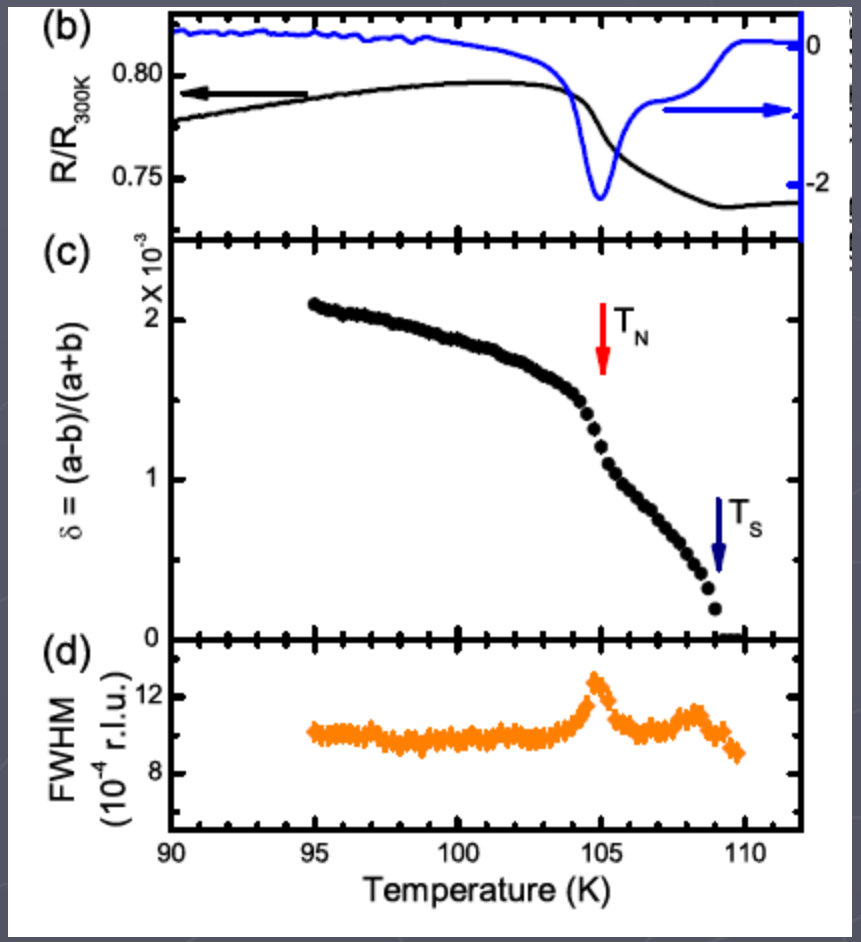
Courtesy of M. Johannes & I. Mazin

structural $T_s \geq$ magnetic T_N



P. Canfield et al 2009

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

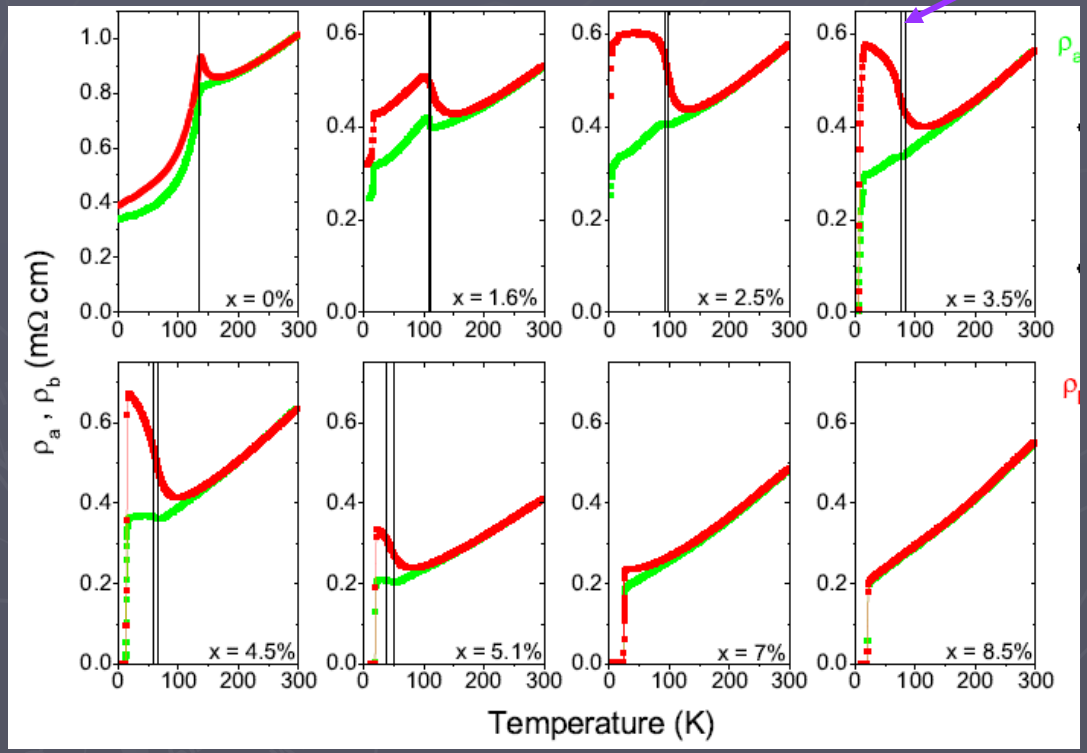


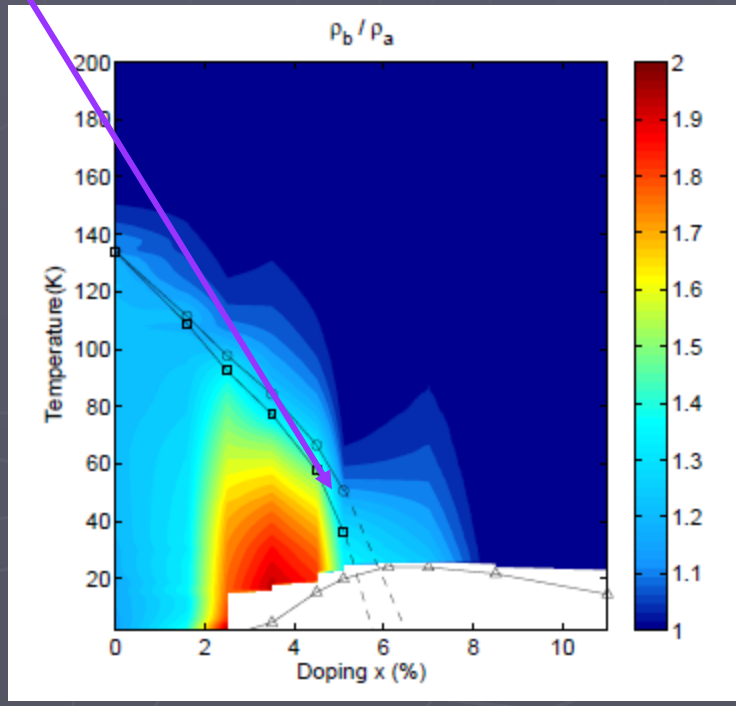
X=0.02

Transition driven by orbital ordering?

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

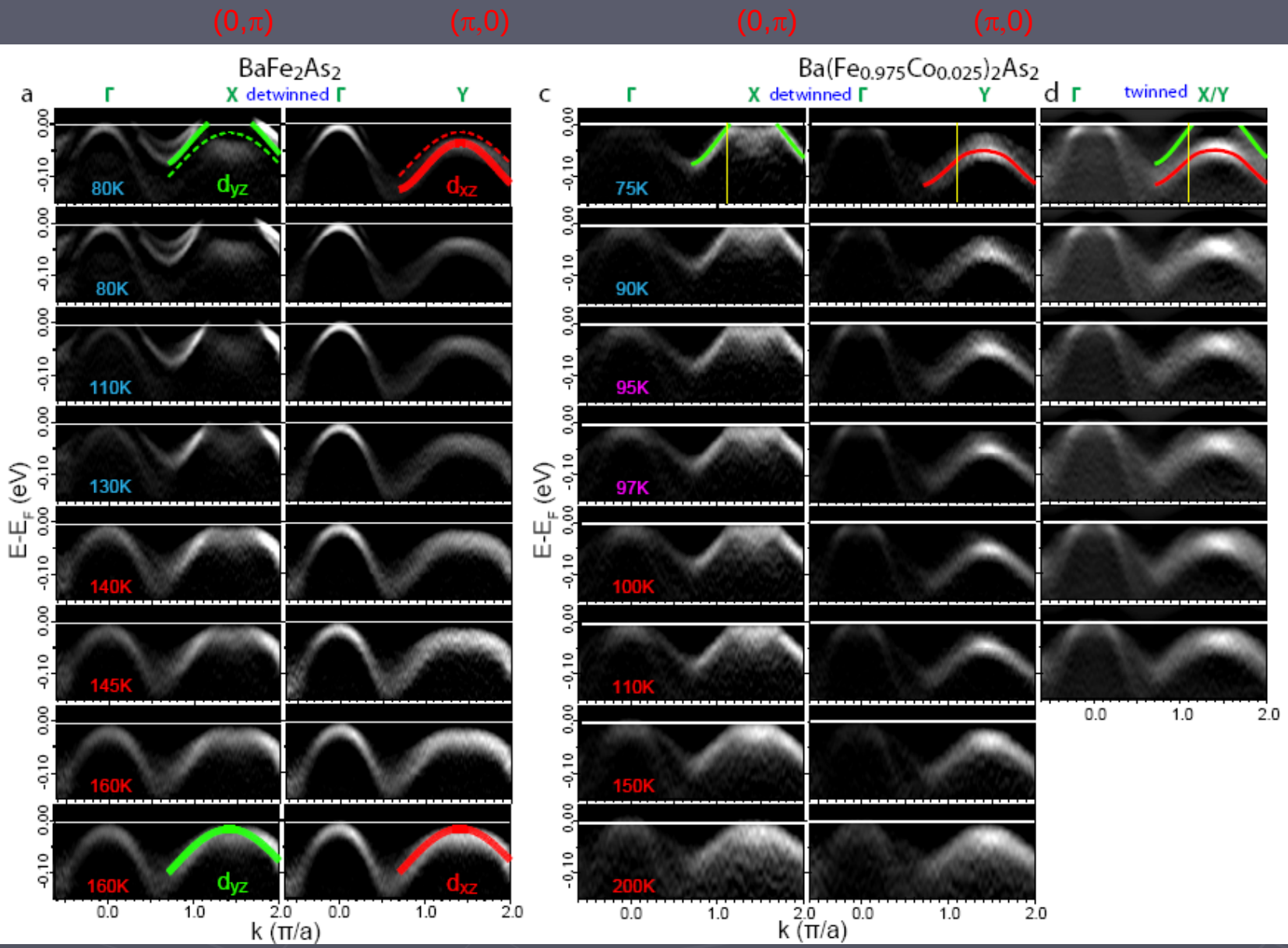
Experiments on untwinned samples: “nematic” susceptibility above T_s?





Implications for superconductivity?

ARPES: orbital ordering



Yi et al PNAS 2011

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?

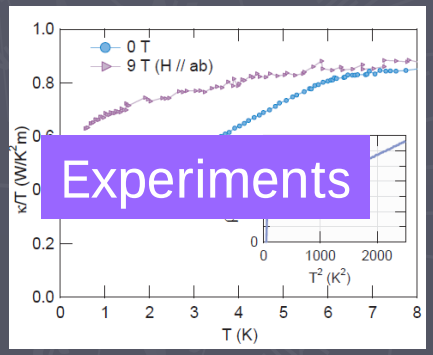
?

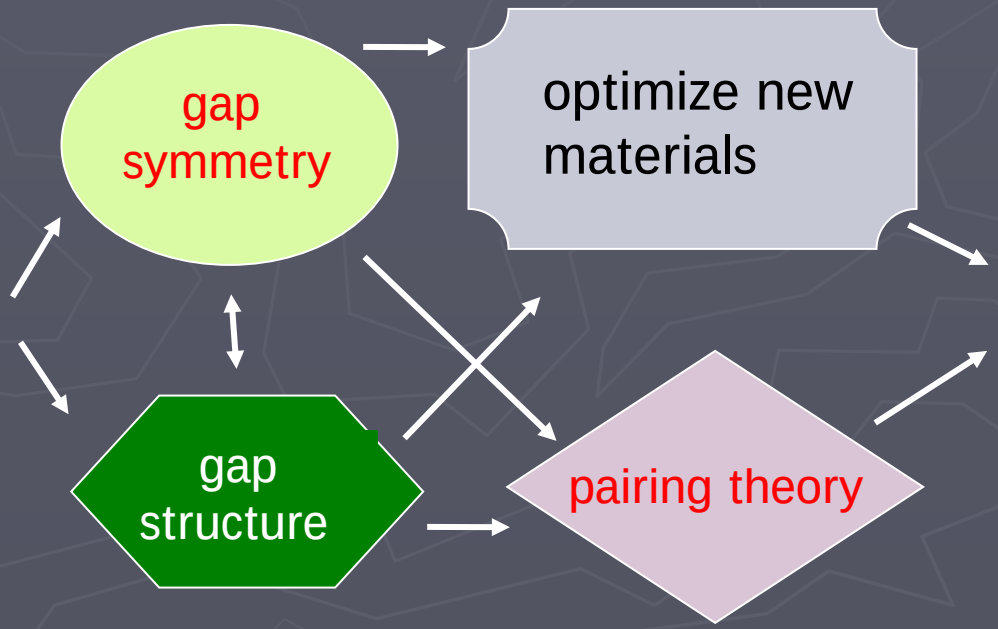
Courtesy of A. Chubukov

Controversies in SC state:

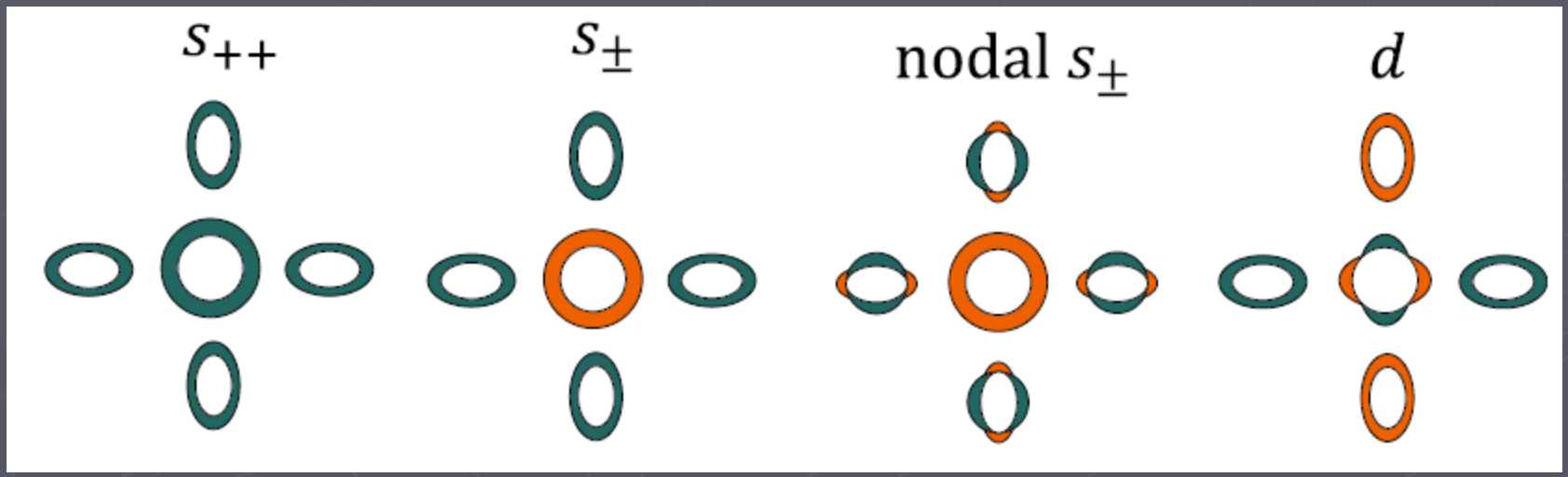
1) *k*-space structure of gap?
2) origin of pairing

- Hope:



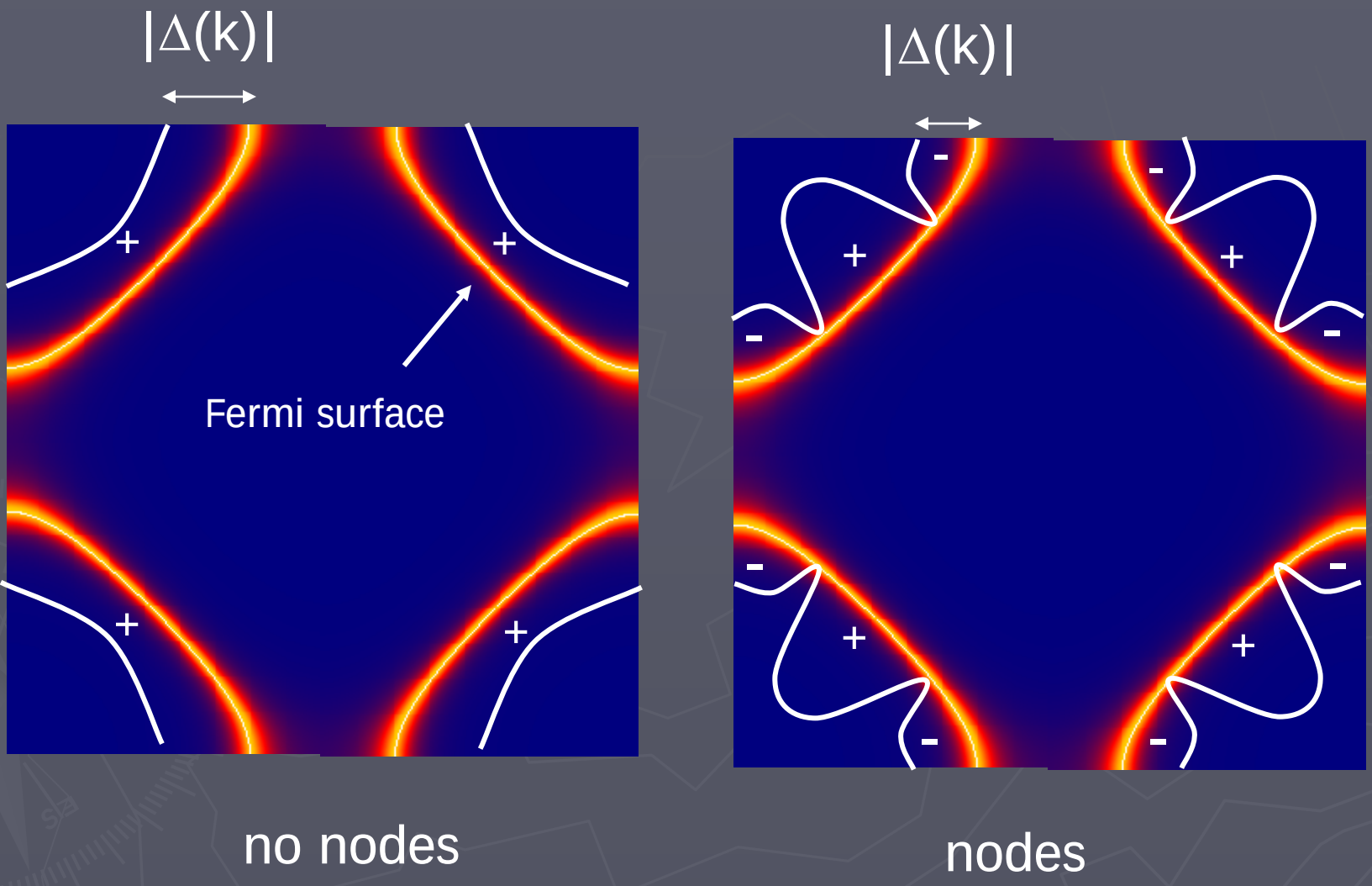


Gap symmetry vs. structure

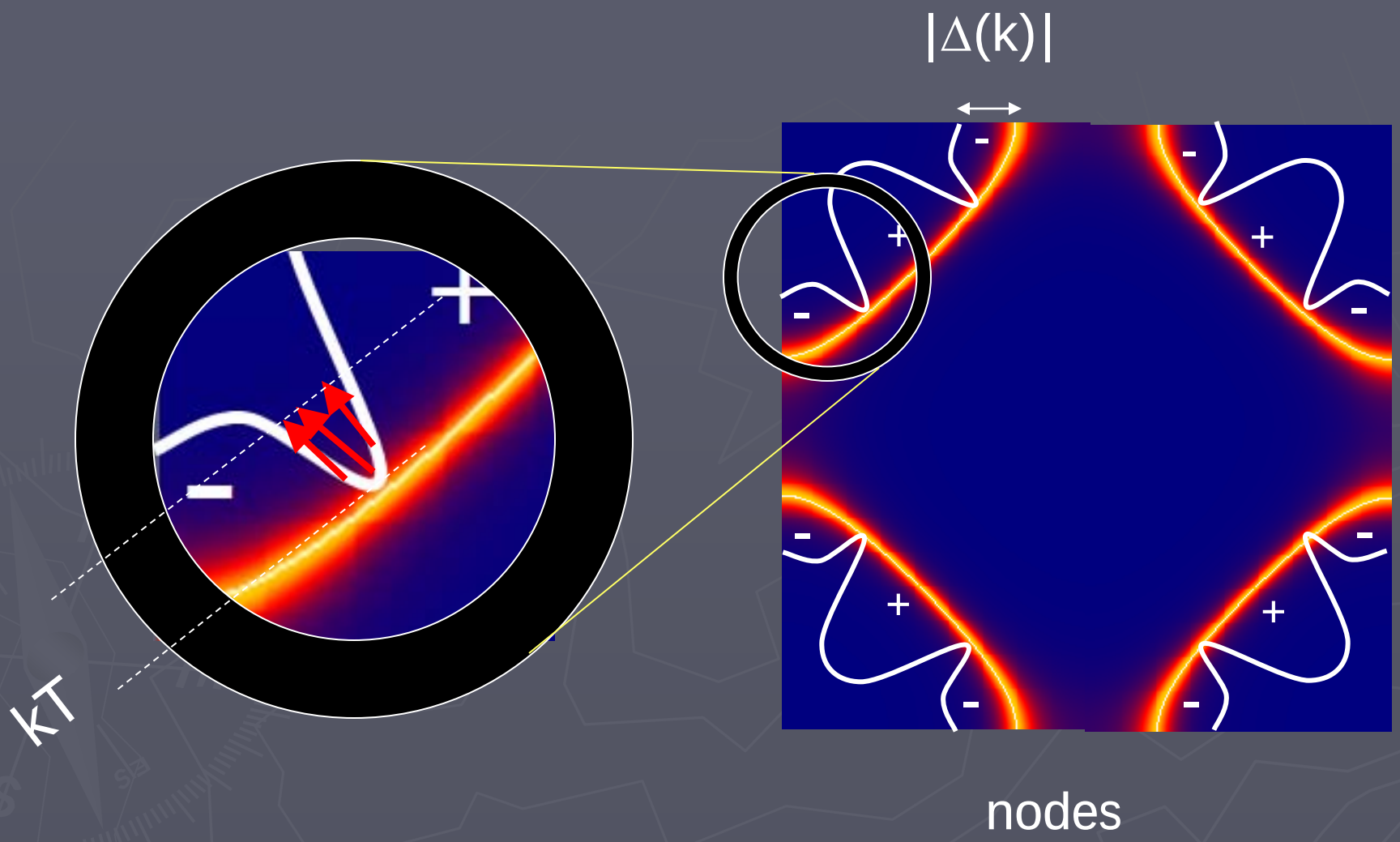


A_{1g} B_{1g}

Order parameter $\Delta(k)$ shape in A_{1g} representations—1 band

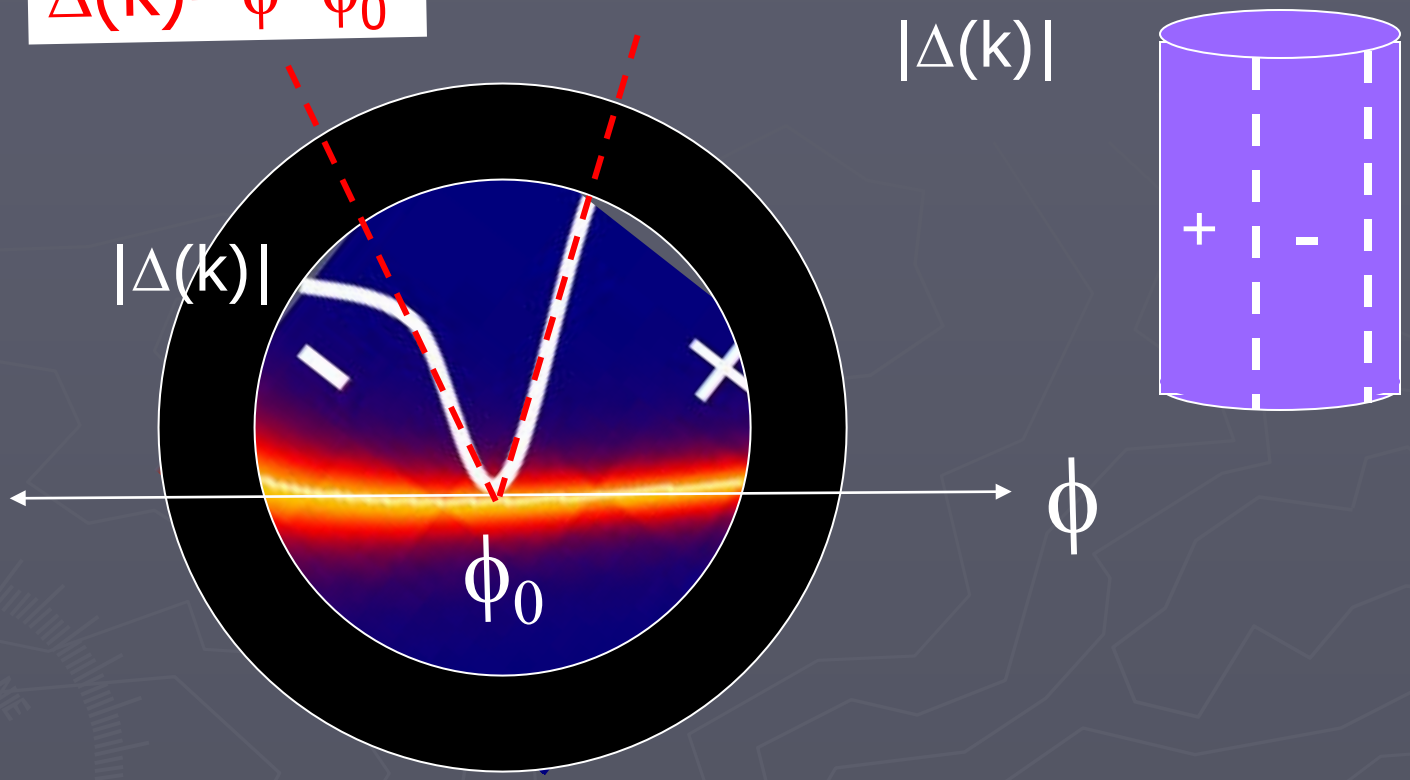


Nodal excitations dominate low T properties

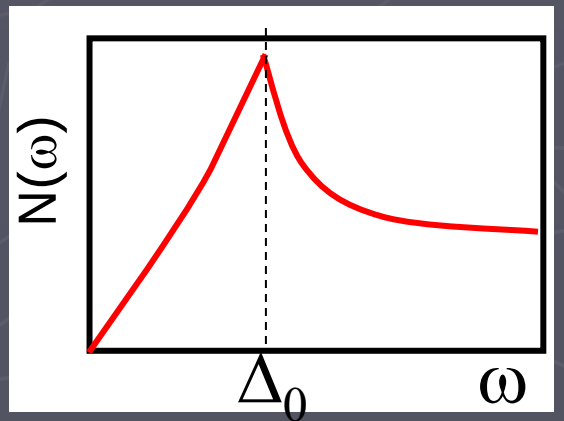


Linear DOS from *line* nodes

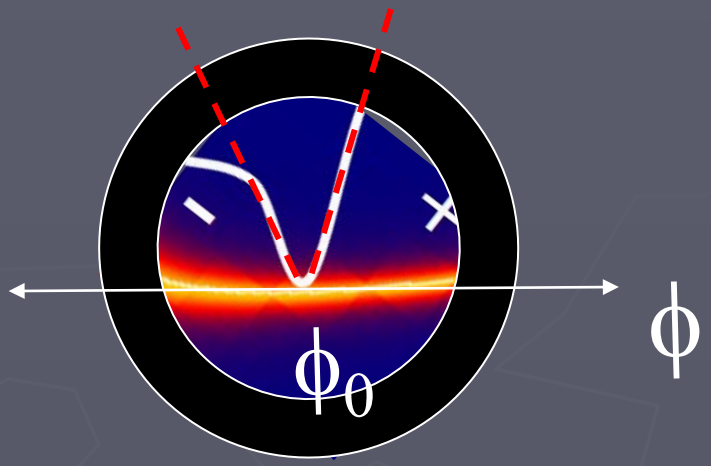
$\Delta(k) \sim \phi - \phi_0$



$$N(\omega) = \int \frac{d\phi}{2\pi} \mathrm{Re} \frac{\omega}{\sqrt{\omega^2 - \Delta_0{}^2 (\phi - \phi_0)^2}} \approx \frac{\omega}{\Delta_0}$$



Example: T^2 specific heat from line nodes



$$N(\omega) \approx \frac{\omega}{\Delta_0}$$

excitations

energy/ excitation

Estimate for energy of free Fermi gas:

$$E = \int d\omega\, \omega N(\omega) f(\omega) \simeq N_0 \int d\omega\, \omega f(\omega) \sim \left(\frac{T}{E_F}\right) \cdot T \sim \frac{T^2}{E_F}$$

$$C = \frac{dE}{dT} \sim \frac{T}{E_F}$$

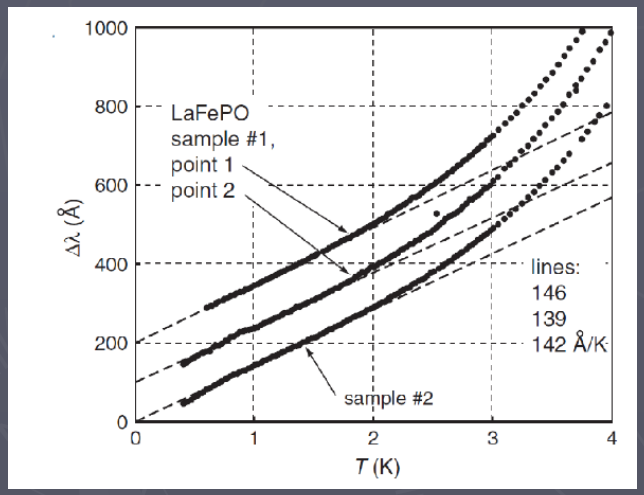
Estimate for energy of d-wave SC:

$$E = \int d\omega\, \omega N(\omega) f(\omega) \simeq N_0 \int d\omega \left(\frac{\omega}{\Delta_0}\right) \omega f(\omega) \sim \left(\frac{T^2}{\Delta_0 E_F}\right) \cdot T \sim \frac{T^2}{E_F}$$

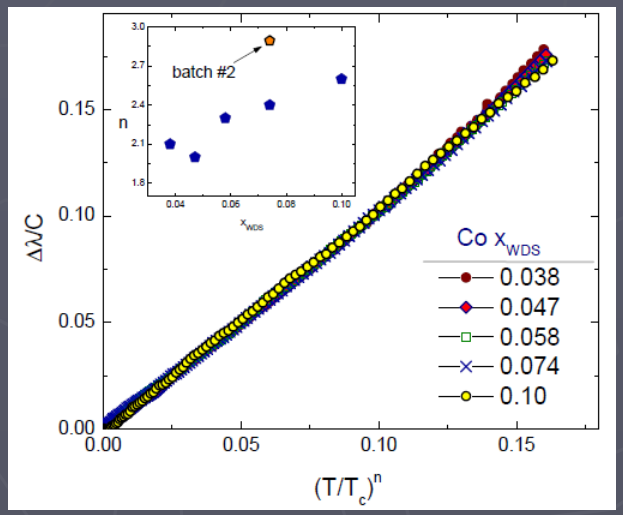
$$C = \frac{dE}{dT} \sim \frac{T^2}{\Delta_0 E_F}$$

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

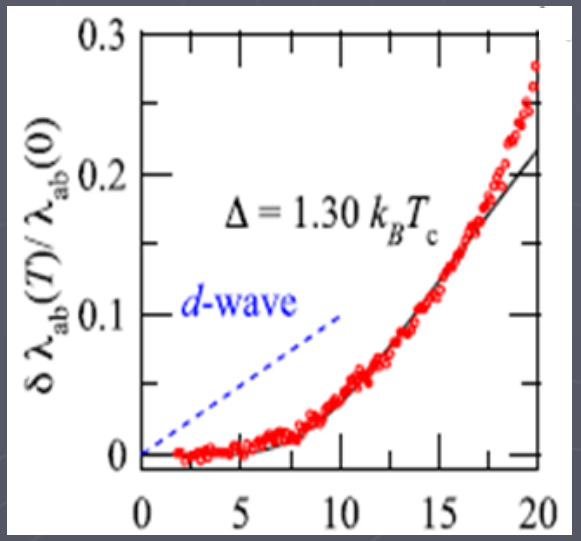
Hicks et al 2008
LaFePO T_c=6K



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*

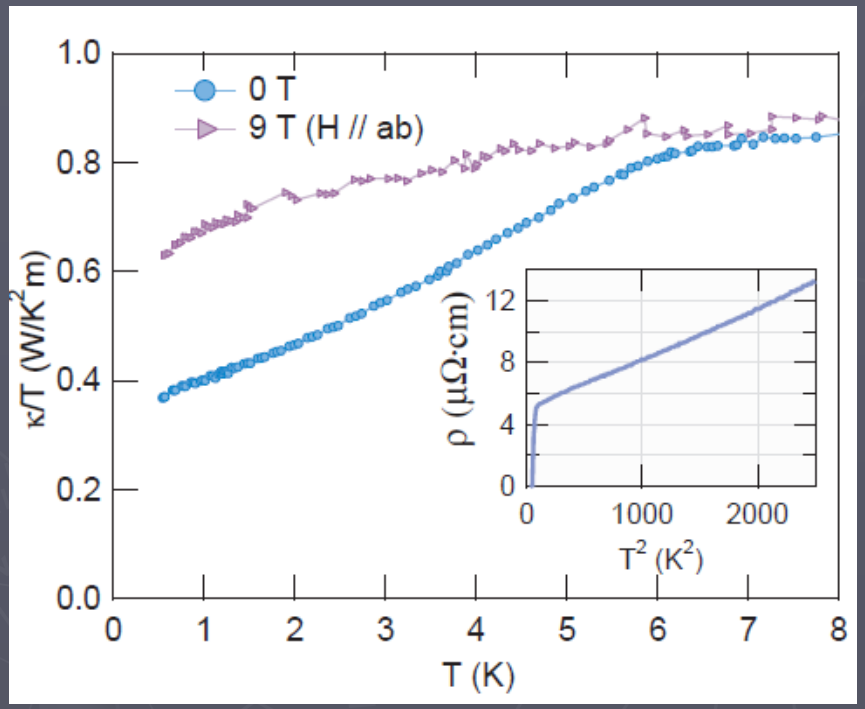
so $\Delta\lambda \simeq \begin{cases} T^2 & \text{dirty} \\ T & \text{clean} \end{cases}$

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

Thermal conductivity (H=0)

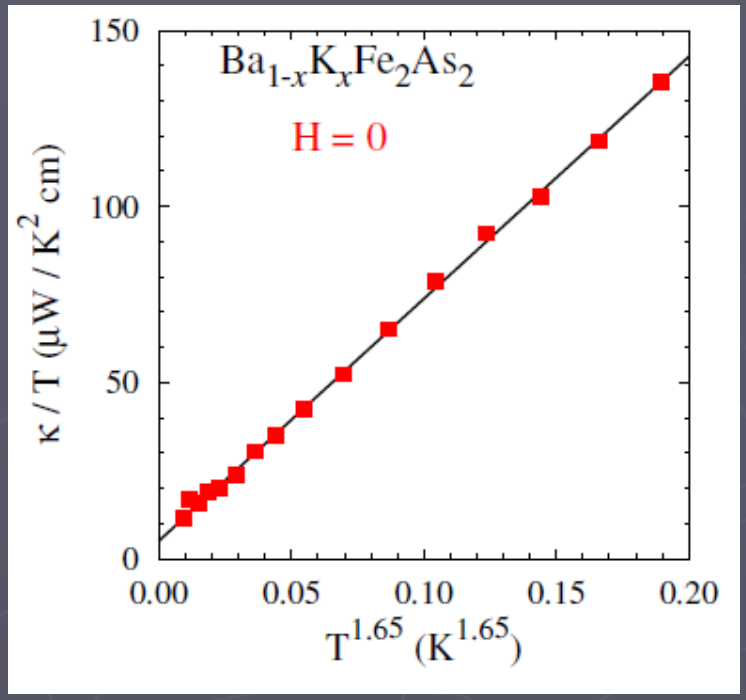
(bulk probe, lowest temperatures thus far)

LaFePO: Yamashita et al aXv:0906.0622



Big linear T term

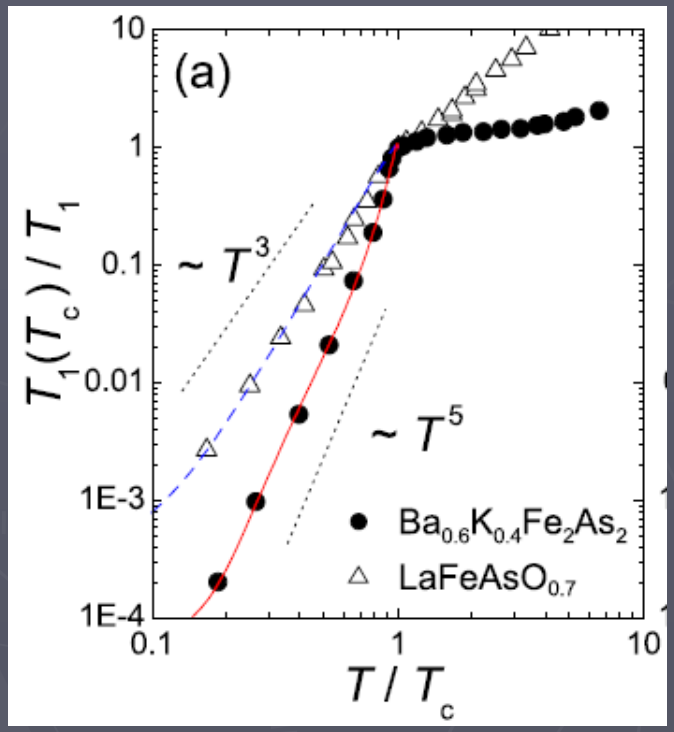
K-doped Ba-122: Luo et al aXv:0904.4049



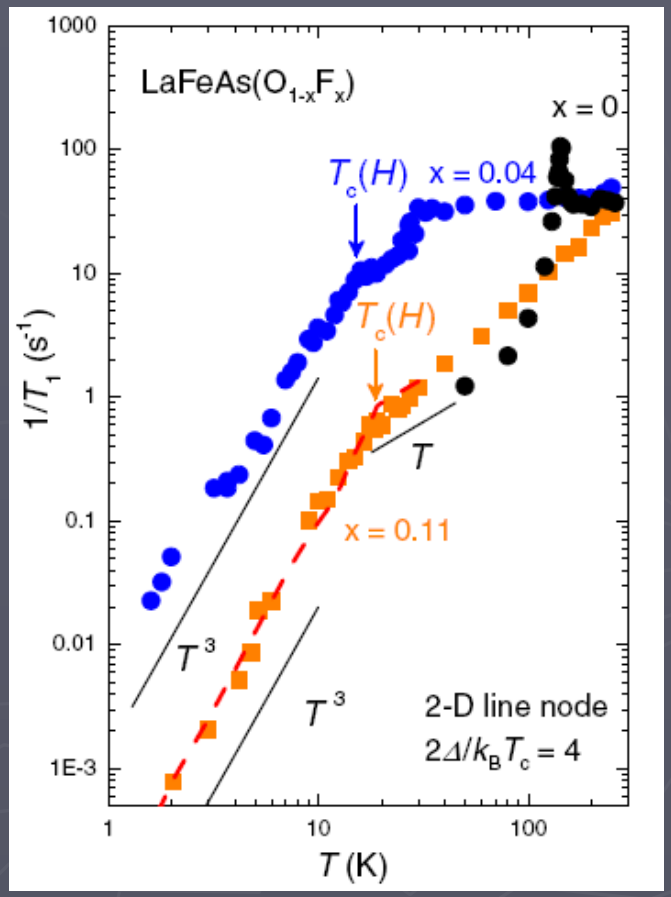
Tiny or zero linear T term

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)

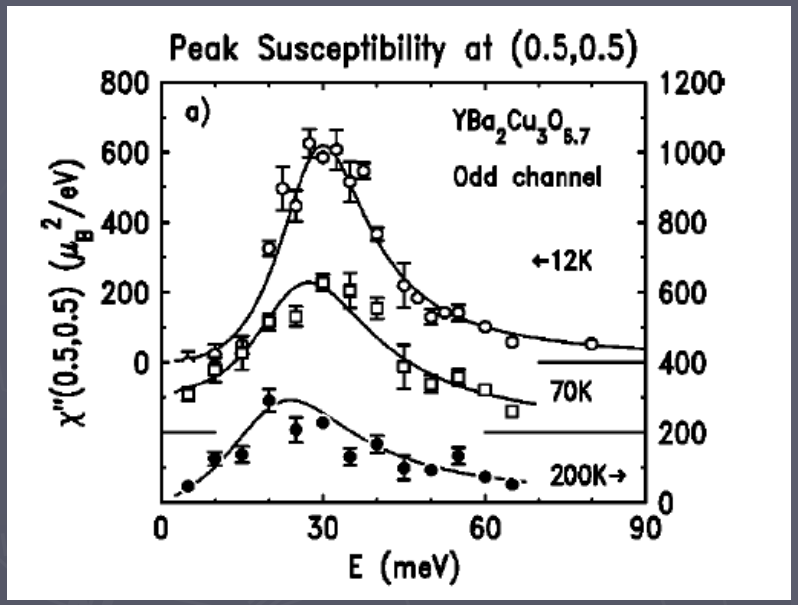
$$\frac{T_1^{-1}}{(T_1^{-1})_N} = 2\frac{T}{T_c}\int_0^\infty d\omega \left[\frac{-\partial f}{\partial \omega}\right]\left[\frac{N(\omega)}{N_0}\right]^2$$

$\longleftrightarrow$

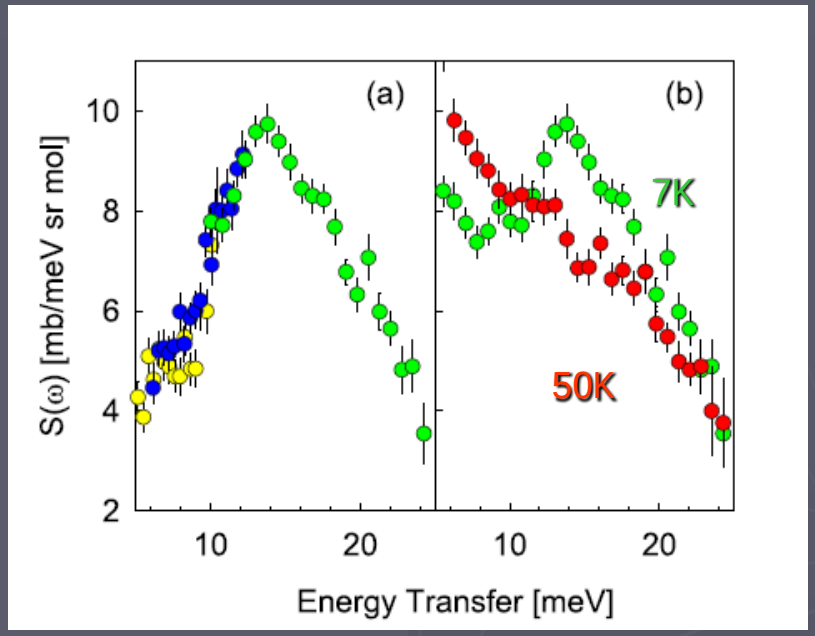
line nodes $\Rightarrow N(\omega) \sim \omega \Rightarrow T^3$!

Resonant mode in inelastic neutron scattering

Reminder: cuprates: Fong et al PRB 2000



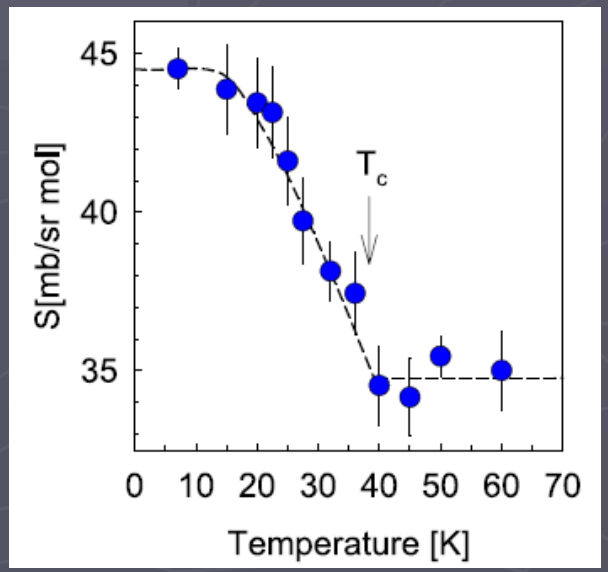
$Ba_{0.6}K_{0.4}Fe_2As_2$: Christianson et al Nature 2008



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

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

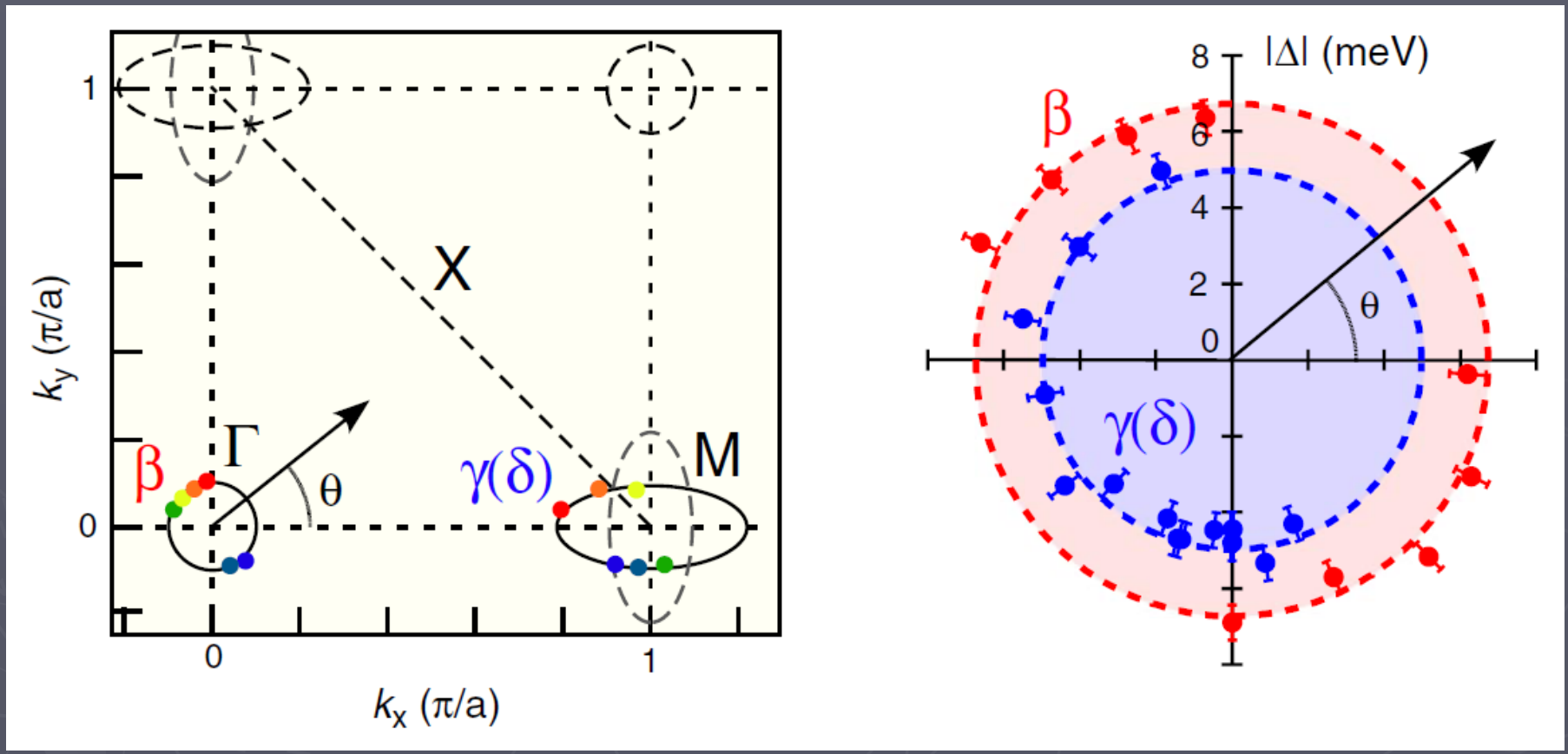
$\Delta_{k+Q} = -\Delta_k \Rightarrow$ sign change of order parameter



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

Mystery: ARPES

$BaFe_{1.85}Co_{0.15}As_2$



K. Terashima et.al. PNAS 2009

Many ARPES measurements, almost *none* find highly anisotropic gap*

* More discussion to come!

ARPES “paradox”

On many samples thermodynamics & transport indicate nodes, whereas ARPES finds isotropic gaps

Possible resolutions:

- electronic structure changes near surfaces, inducing π,π pocket
  Kemper et al 2010
- intraband scattering from rough surfaces smears out gap anisotropy, “lifts” nodes
- ARPES resolution at electron pockets is poor, averages over angular dependence of β_1 and β_2 pockets

questions

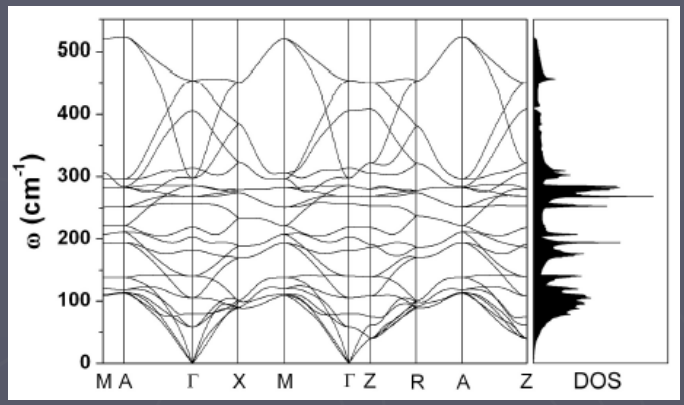
- What is the symmetry of SC order parameter?
- What controls whether Fe-based material is nodal or gapped superconductor?
- Why are these systems' superconducting states nonuniversal?

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

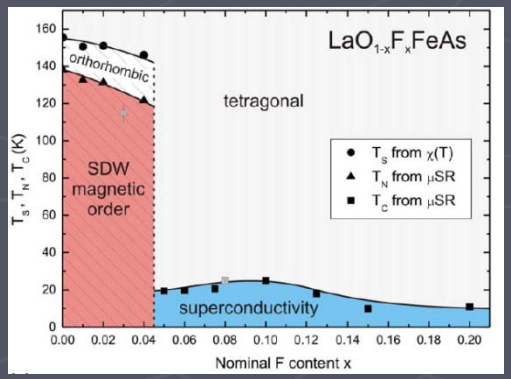


Singh & Du PRL 2008

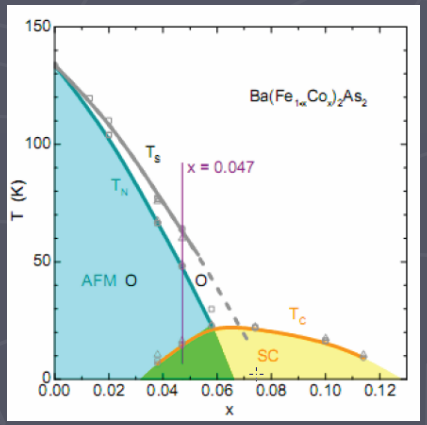
2) Magnetism is usually nearby:

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

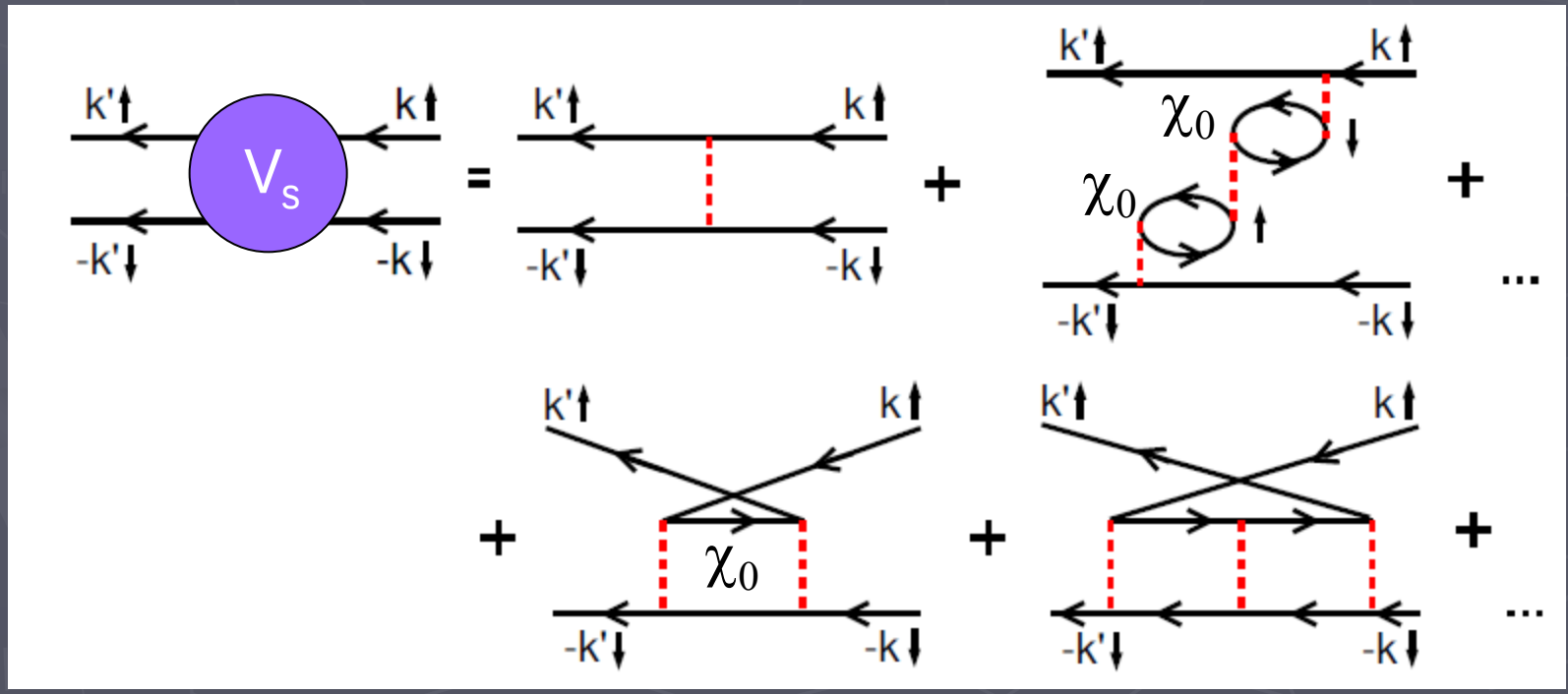
No magnetism ⇒ low T_c

Spin fluctuation theories of pairing

Effective interaction from spin fluctuations (Berk-Schrieffer 1966)

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

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



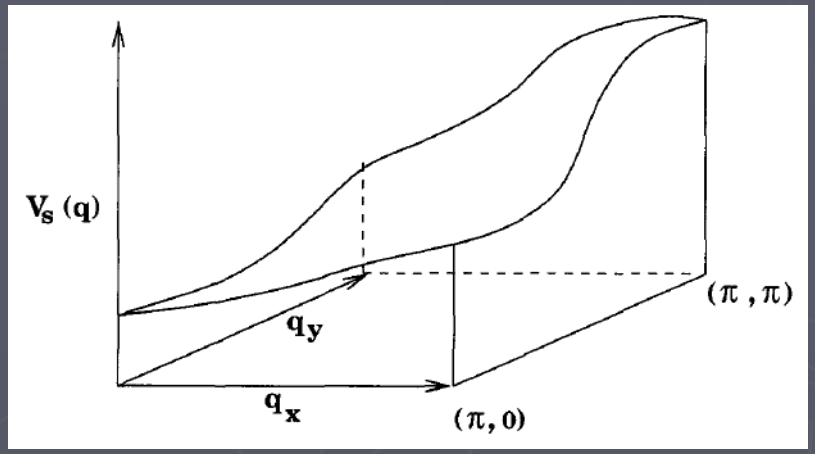
Spin fluctuation theories of pairing

Effective interaction from spin fluctuations (Berk-Schrieffer 1961)

paradigm: *d*-wave in cuprates from antiferromagnetic spin fluctuations

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

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

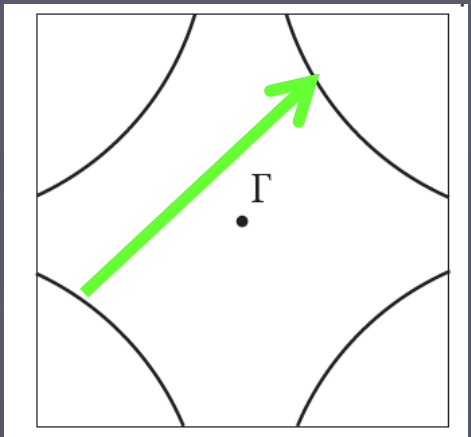


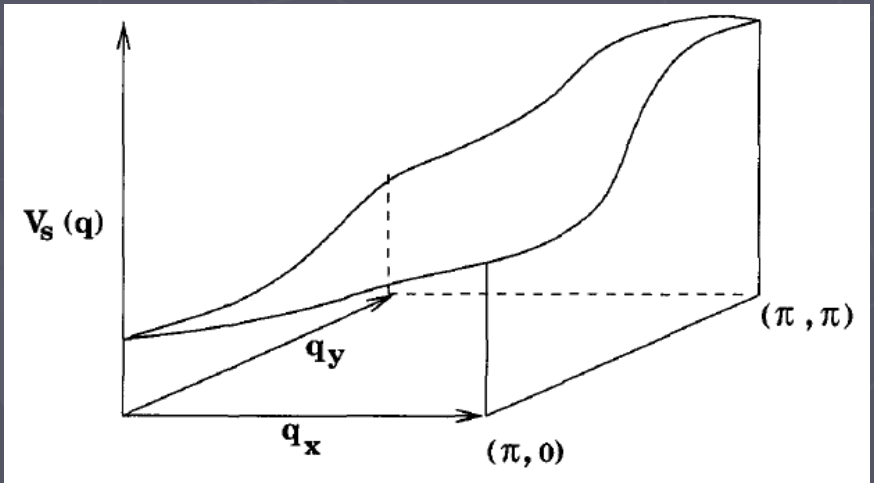
$$\Delta_p = -\sum_{p'}\frac{V(p-p')\Delta_{p'}}{2E_{p'}}$$

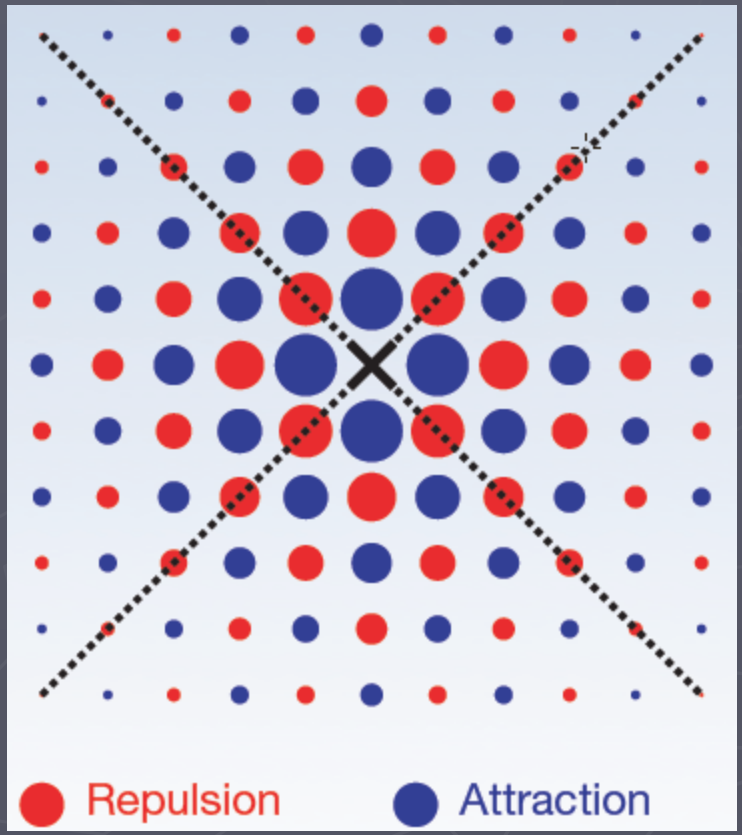
d-wave takes advantage of peak in spin fluct. interaction at π,π!

$$\Delta_{p+(\pi,\pi)} = -\Delta_p$$

remember at least some interactions attractive in order to form Cooper bound state







k-space:
$V_s(k-k') \sim V_0 + V_2 \phi_d(k)\, \phi_d(k') + \ldots$

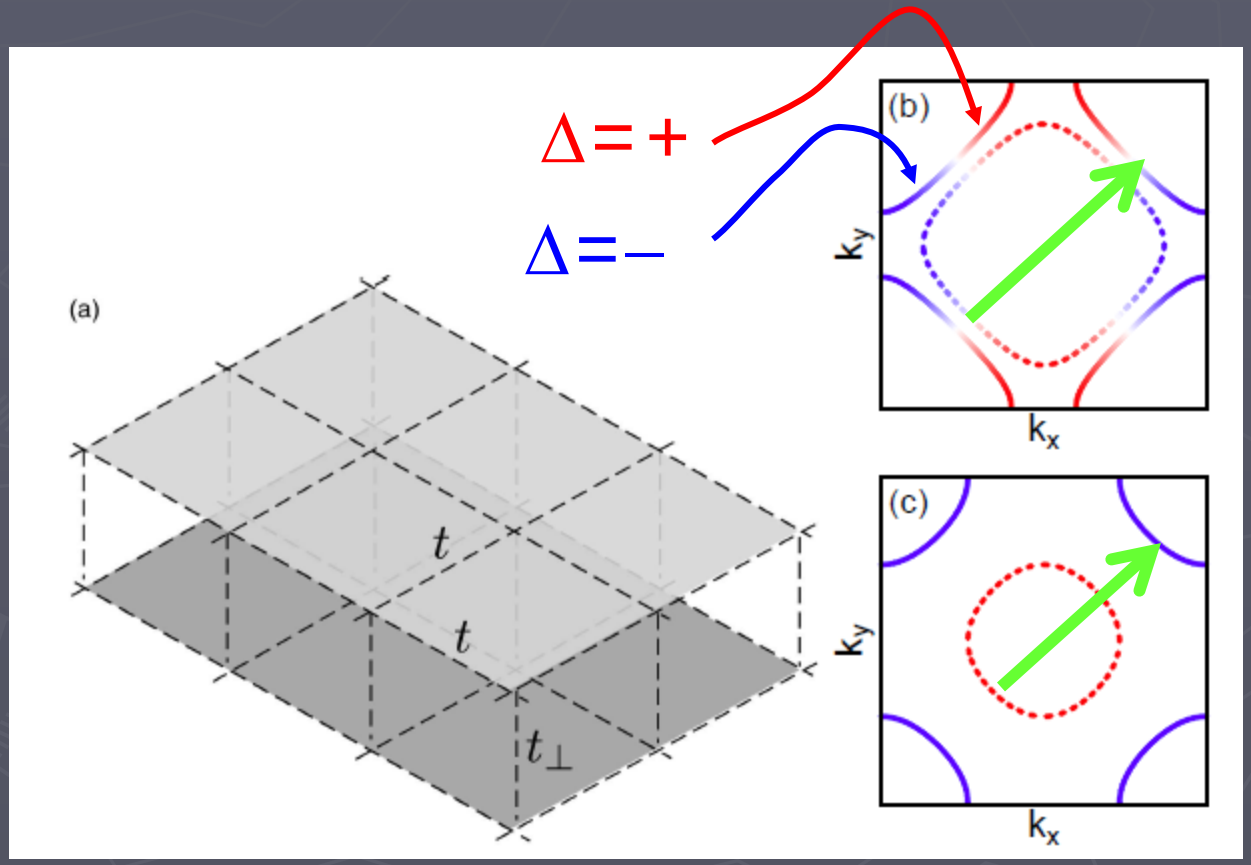
r-space

bilayer Hubbard model: sign changing s state

N Bulut, D J Scalapino and R T Scalettar Phys. Rev. B 45. 5577 (1992) (QMC)

A. I. Liechtenstein, I.I. Mazin, and O. K. Andersen, Phys. Rev. 74, 7306 (1995) (phenomenology)

H. Zhai, F.Wang and D.-H. Lee, Phys. Rev. B 80, 064517(2009) (fRG)



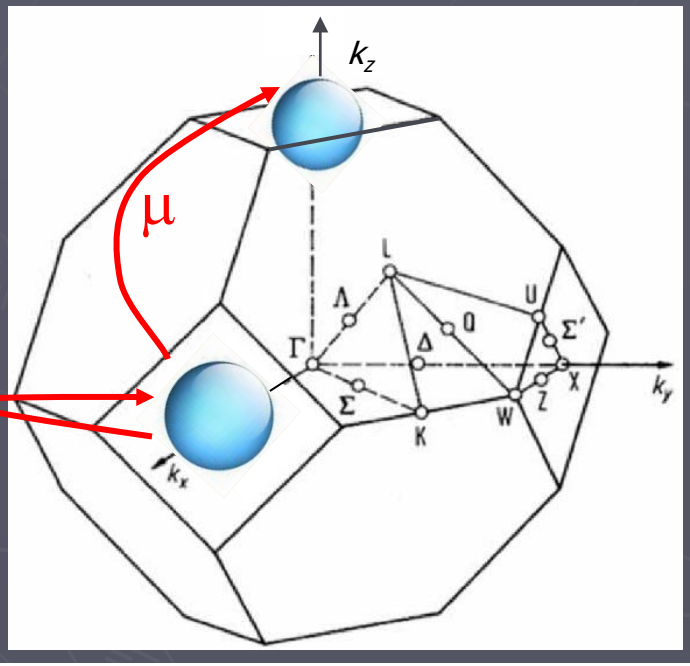
d_{x2-y2}

$s_{+/-}$

From T.A. Maier, D.J. Scalapino arXiv:1107.0401

Unconventional pairing from multiple Fermi pockets around high symmetry points

D. F. Agterberg , V. Barzykin, L.P. Gor'kov PRB 80, 14868 (1999)



$$\lambda_{\alpha\beta} = \lambda\,\delta_{\alpha\beta} + \mu(1-\delta_{\alpha\beta})$$

possible singlet BCS solutions:

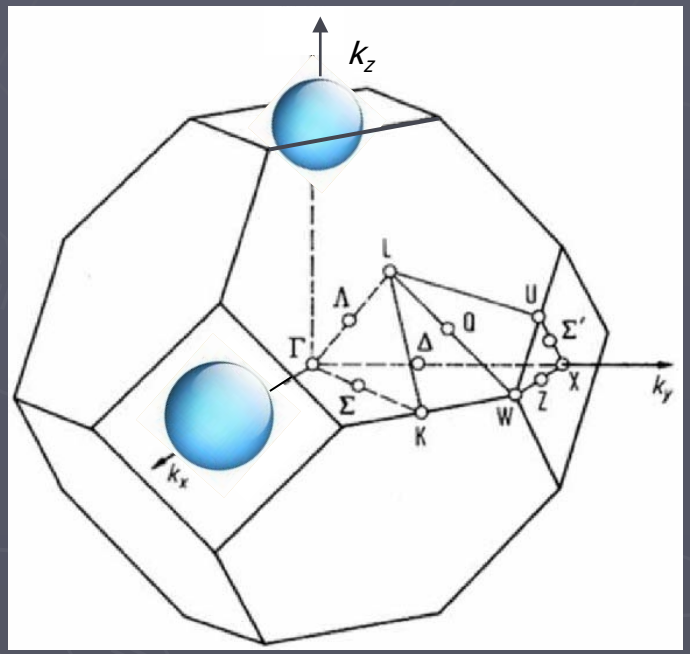
1D: A_{1g} s-wave
3D: E_{1g} d-wave

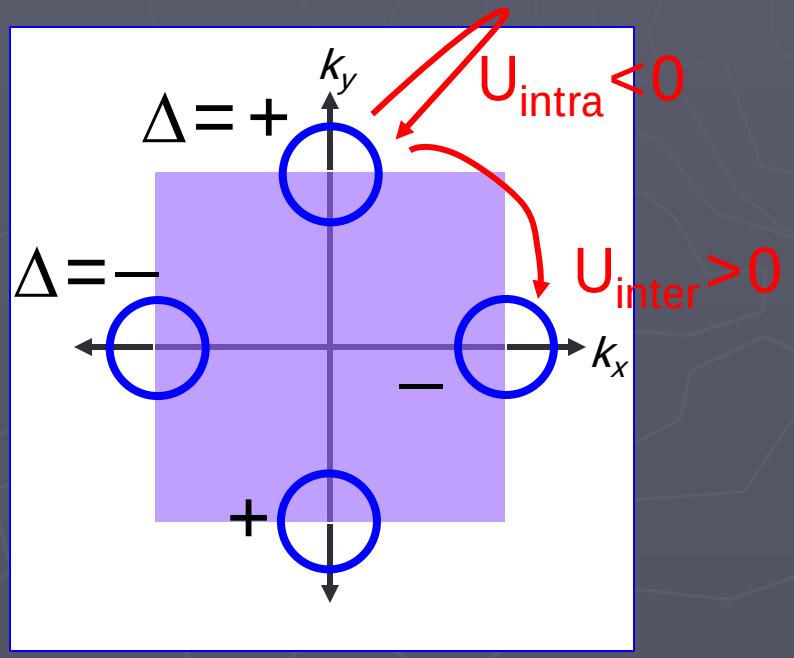
"The nontrivial 3D representation is stable if $\lambda - \mu < 0$ and $\mu > 0$, i.e., if the interaction is *attractive* for each pocket alone, while it is *repulsive* between two different pockets."

Unconventional pairing from multiple Fermi pockets around high symmetry points

D. F. Agterberg , V. Barzykin, L.P. Gor'kov PRB 80, 14868 (1999)

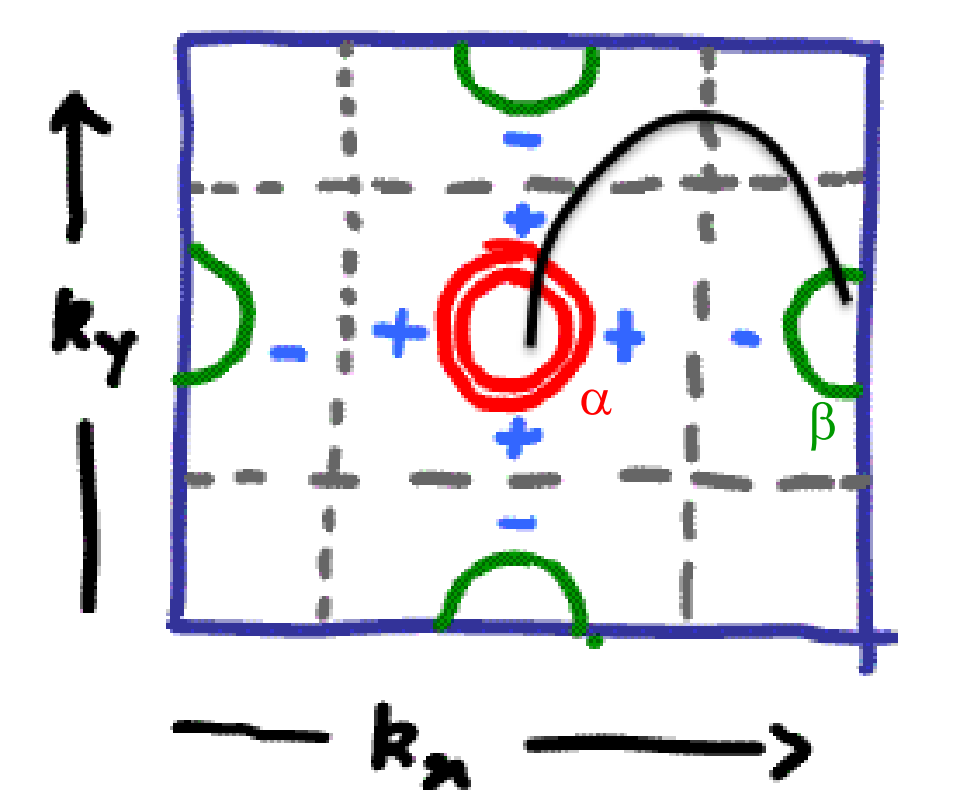
Same idea, only in 2D

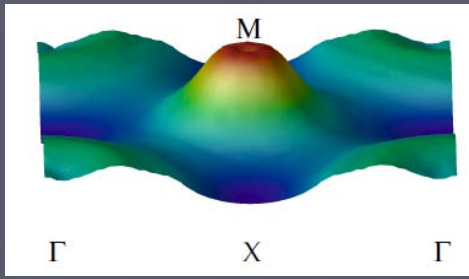




(nodeless) d-wave

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

Early electronic structure calculations show $\lambda_{e\text{-}ph}$ *weak*

Early calculations of spin-fluctuation pairing :

- Kuroki et al PRL 2008
- Cvetkovic et al EPL 2009
- Wen-Lee aXv:0804.1739
- Mazin et al PRL 2008
- Zhang et al PRL 2008
- Wang et al 2008
- Y. Bang et al 2008
- Seo et al PRL 2008
- Graser et al NJP 2009
- Zhang et al PRB 2009
- Ikeda et al PRB 2009

Many others since:

- Maier et al PRB 2009
- Chubukov et al PRB 2009
- Kuroki et al PRB 2009
- Thomale et al PRB 2009
- Thomale et al aXv 2010
- Wang et al aXv 2010
- Graser et al aXv 2010
- Kemper et al aXv 2010
- Ikeda et al PRB 2010

⇓

Tight-binding model +interactions investigated by most authors:

$H=H_0+H_{int}$ 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!

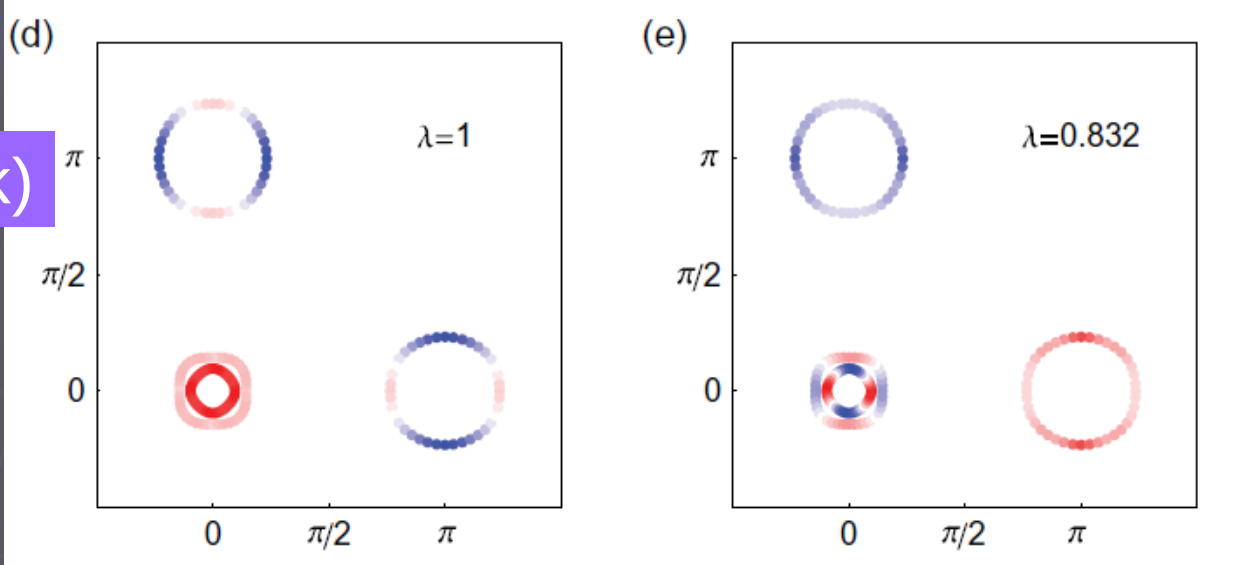
Realistic theories: gaps display strong anisotropy/ nodes

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

"anisotropic extended-s"-wave

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

$\Delta(k)$



similar:

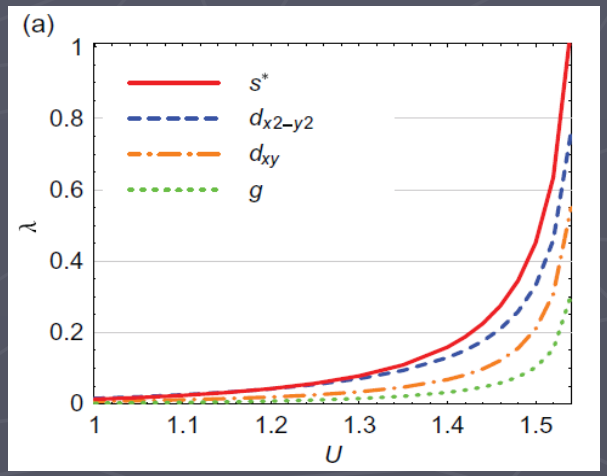
Kuroki et al '08, '09,
Ikeda et al '09, '10,
Graser et al 09,10,
Wang et al. 08,09

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

Two pairing channels nearly degenerate

a) Can different FeAs materials have different symmetries?

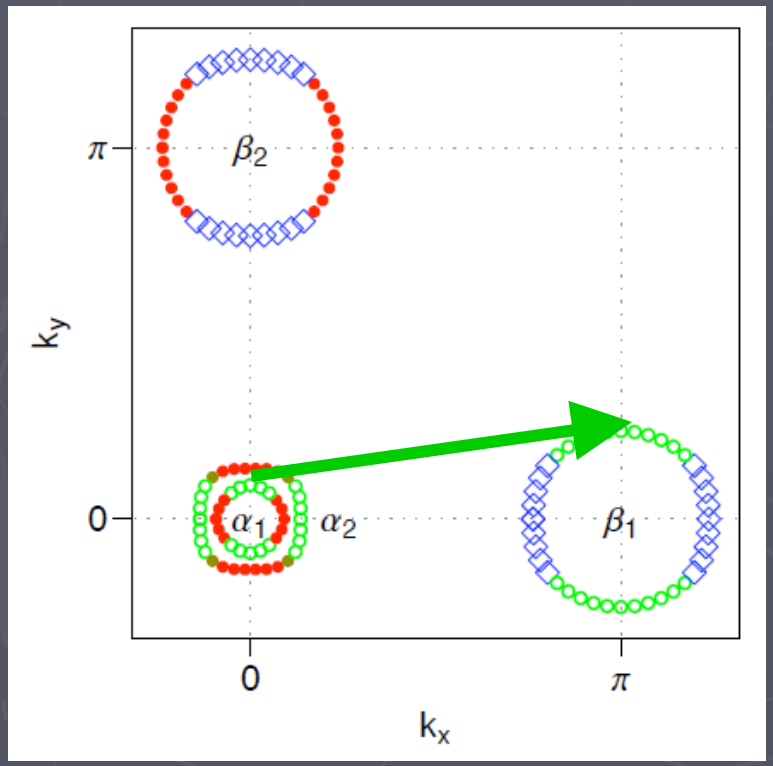
b) More likely: s-wave *symmetry*, differing gap *structures* for different materials



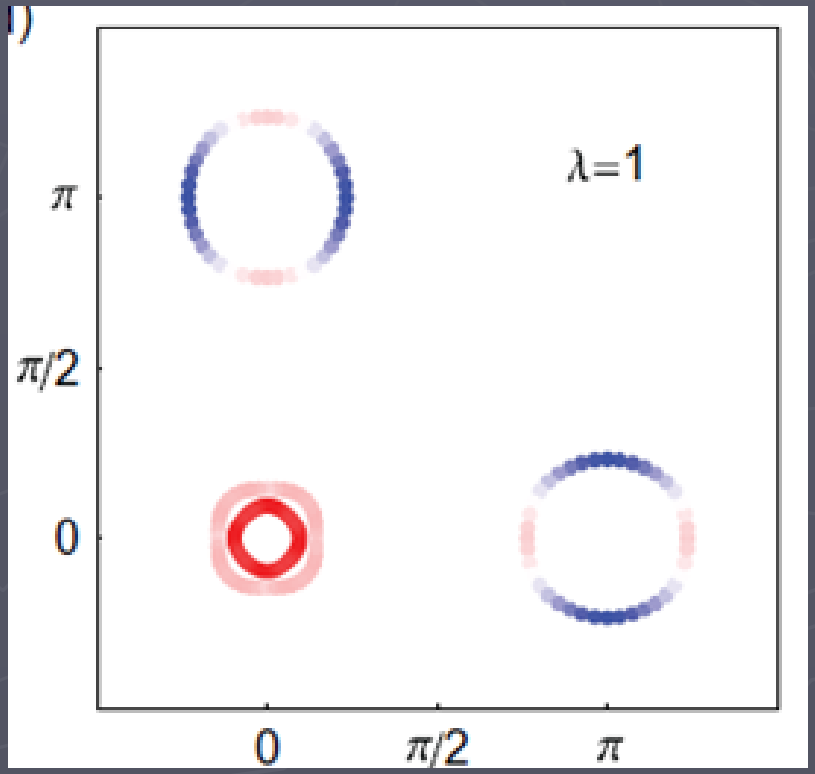
What is the origin of the gap anisotropy [Maier et al PRB 09]?

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

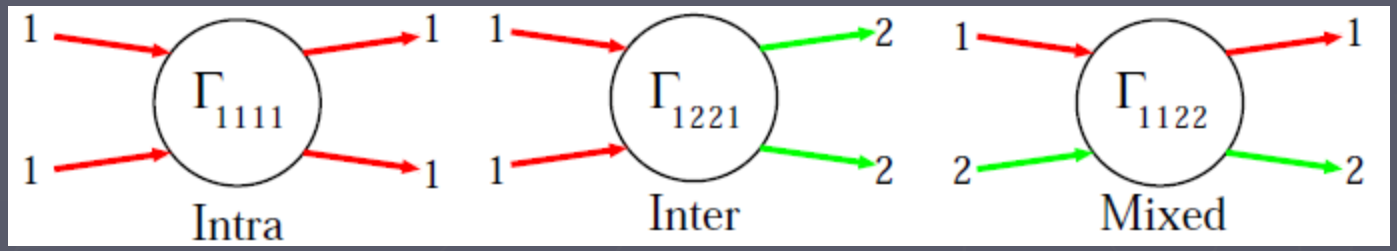


Fermi surface w/ orbital character



Gap

Intra- vs. interorbital pairing: RPA analytical results



$$\Gamma_{ij}(k-k') = \sum_{l_1,l_2,l_3,l_4} a^{l_3}_{\nu_i}(k) a^{l_2}_{\nu_i}(-k) \mathrm{Re}\left[\Gamma_{l_1,l_2,l_3,l_4}(k-k',\omega=0)\right] a^{l_1}_{\nu_j}(k') a^{l_4}_{\nu_j}(-k')$$

intra

$$\Gamma_{1111} = \Gamma_{2222} = \frac{3}{4}\left[\frac{(\bar{U}+\bar{J})^2\chi_0}{1-(\bar{U}+\bar{J})\chi_0} + \frac{(\bar{U}-\bar{J})^2\chi_0}{1-(\bar{U}-\bar{J})\chi_0}\right]$$

Largest- driven by U,J

inter

$$\Gamma_{1221} = \Gamma_{2112} = \frac{3}{4}\left[\frac{(\bar{U}'+\bar{J}')^2\chi_0^{12}}{1-(\bar{U}'+\bar{J}')\chi_0^{12}} - \frac{(\bar{U}'-\bar{J}')^2\chi_0^{12}}{1-(\bar{U}'-\bar{J}')\chi_0^{12}}\right]$$

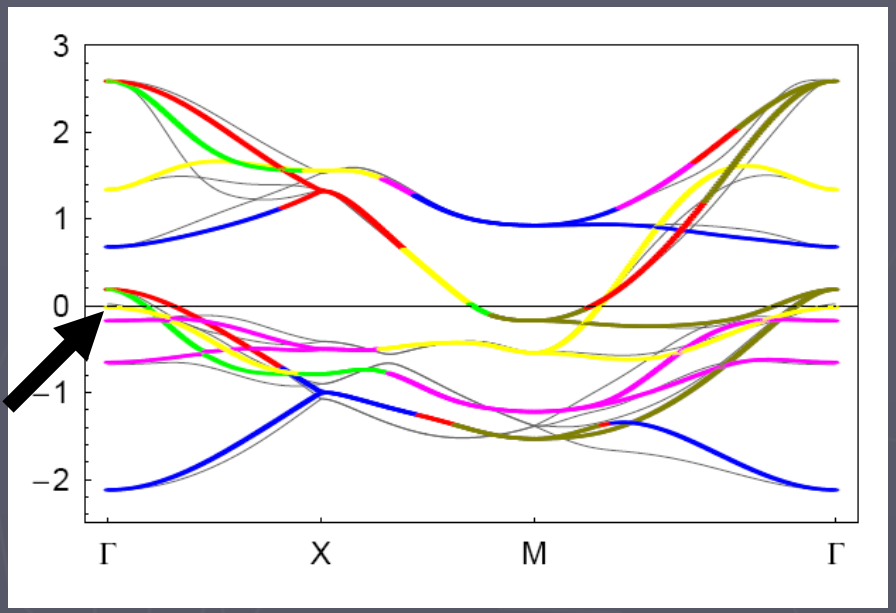
U',J' drive instability

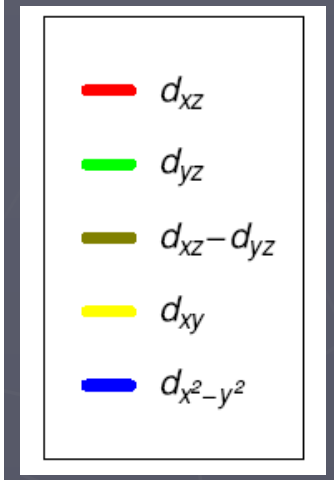
mixed

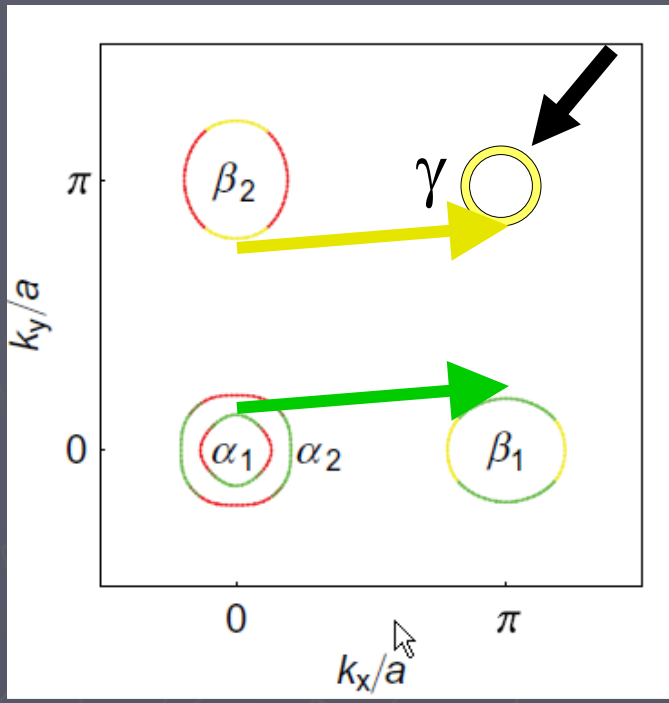
$$\Gamma_{1122} = \Gamma_{2211} = \frac{3}{4}\left[\frac{(\bar{U}+\bar{J})^2\chi_0}{1-(\bar{U}+\bar{J})\chi_0} - \frac{(\bar{U}-\bar{J})^2\chi_0}{1-(\bar{U}-\bar{J})\chi_0}\right]$$

small due to mat elts.

Importance of γ (π,π) pocket







Kuroki et al 2009 found that pocket at (π,π) promotes a nodeless gap

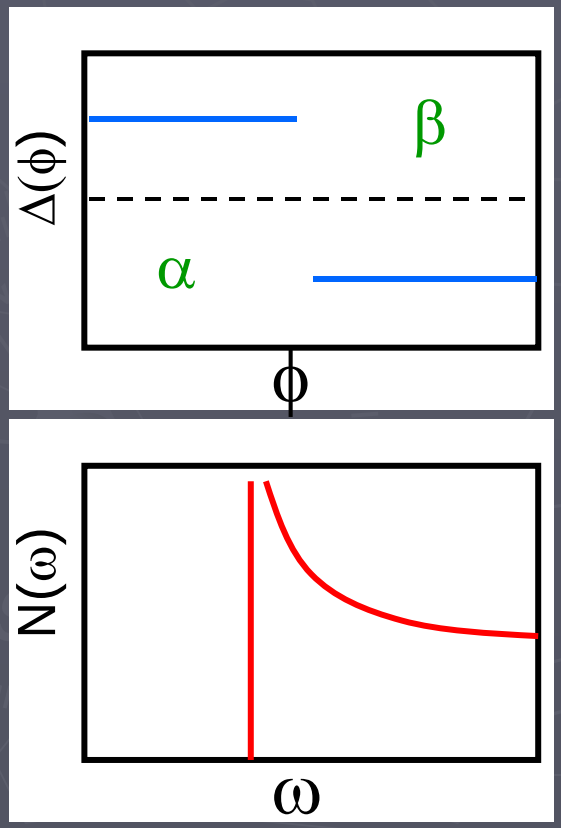
Presence of pocket can be controlled by doping AND by tuning the height of As above the Fe plane

Tendency of hole-doped systems to be more isotropic

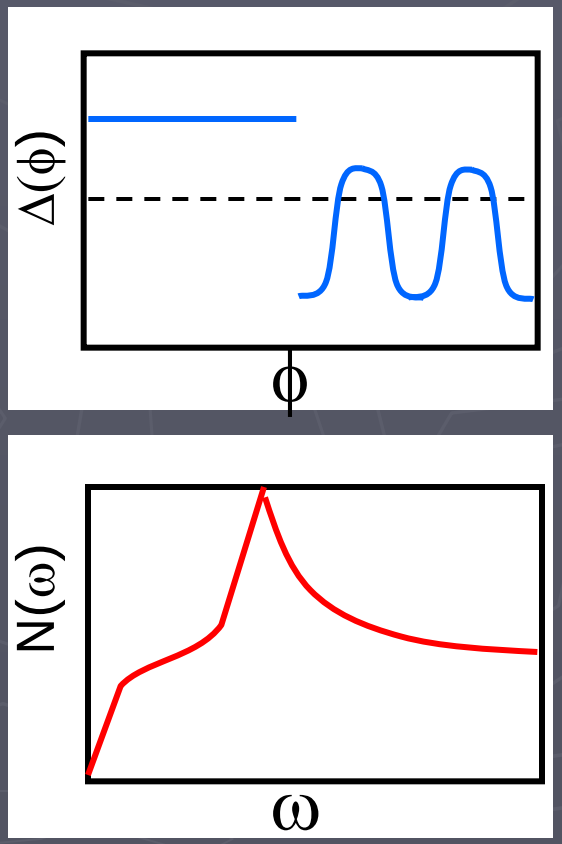
“sensitivity” to small changes in electronic structure, disorder

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

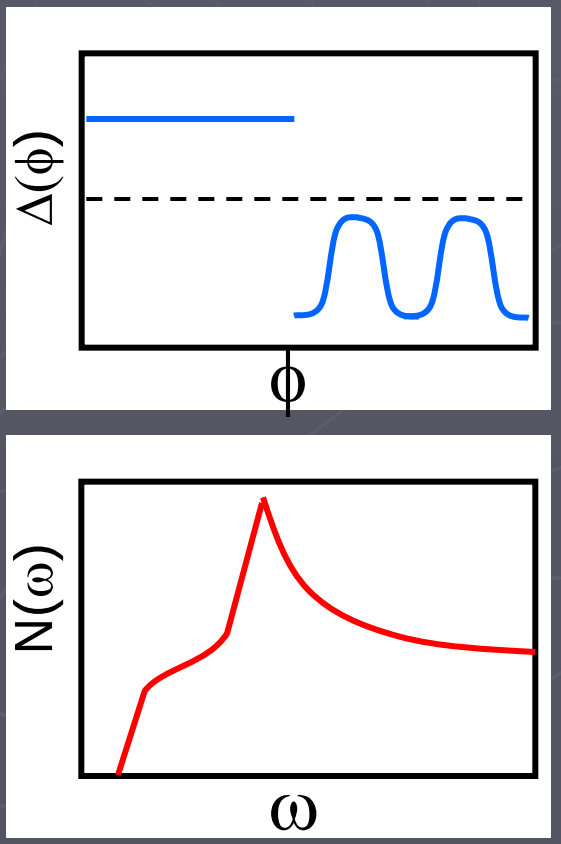
a) isotropic $s_{+/-}$



b) nodes



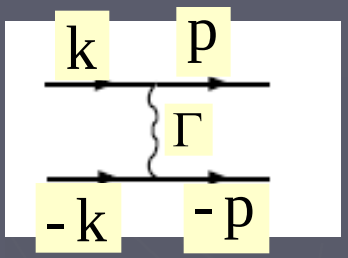
c) deep minima

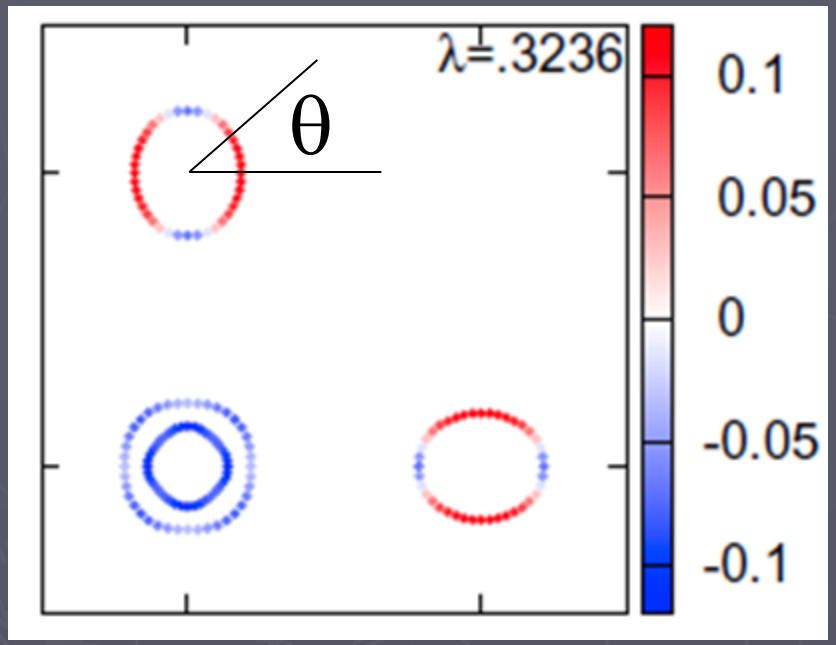


Angular harmonic representation of RPA results

Maiti et al 2011

S-wave (A_{1g}) channel





$$\Gamma(k,p) = \sum_{n,m} \Gamma_{n,m}\, \psi_n(k)\, \psi_m(p)$$

$$\psi_n(k) = \cos k_x + \cos k_y, \quad \cos k_x \cos k_y \ldots$$

$$\psi_{n,m}(\pm k_x, \pm k_y) = \psi_{n,m}(\pm k_y, \pm k_x)$$

Near k=0, pure s-wave

$$\psi_n(k) = A_n + B_n \cos 4\varphi + C_n \cos 8\varphi + \ldots$$

φ along hole FS

Near p=(π,0) ,

$$\psi_n(p) = (\tilde{A}_n + \tilde{B}_n \cos 4\theta + \tilde{C}_n \cos 8\theta + \ldots) \pm (D_n \cos 2\theta + E_n \cos 6\theta + \ldots)$$

θ along electron FS

keep only the leading terms in the series:

$$\psi_n(k) = A_n + B_n \cos 4\psi + C_n \cos 8\psi + \ldots \Rightarrow A_n$$

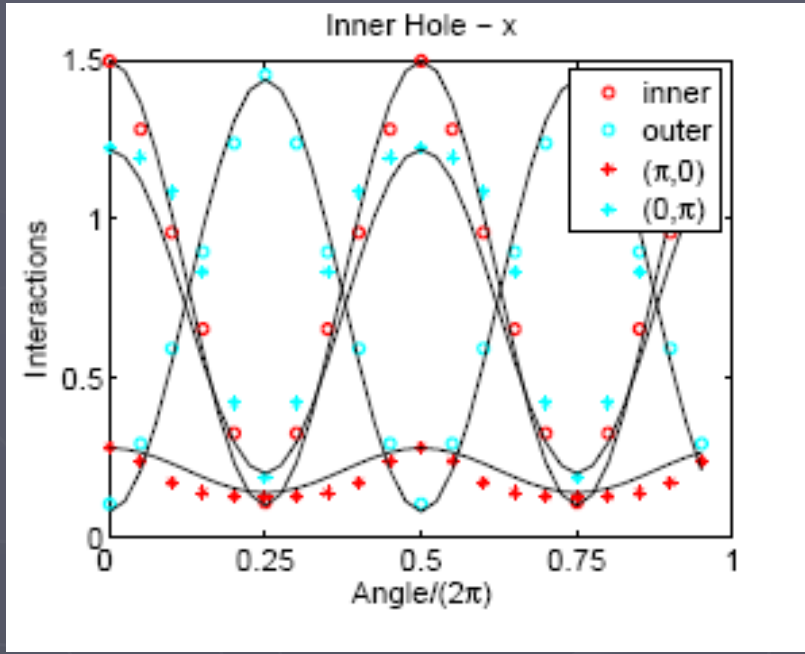
$$\psi_n(p) = \tilde{A}_n + \tilde{B}_n \cos 4\theta + \tilde{C}_n \cos 8\theta + \ldots$$
$$\pm(\tilde{D}_n \cos 2\theta + \tilde{E}_n \cos 6\theta + \ldots) \Rightarrow \tilde{A}_n \pm \tilde{D}_n \cos 2\theta$$

effective interactions:

$$\Gamma_{h,h}(k,p) = u_{h,h}, \quad \Gamma_{e,h}(k,p) = u_{e,h}\,(1 \pm 2\alpha_{he} \cos 2\theta),$$
$$\Gamma_{e1,e1}(k,p) = u_{e,e}\,(1 + 2\alpha_{ee}\,(\cos 2\theta_1 + \cos 2\theta_2) + 4\beta_{ee} \cos 2\theta_1 \cos 2\theta_2$$

$\Rightarrow$ solve gap equation analytically

fits to RPA



determine direct band interaction coefficients in “harmonic space”

	$u_{h_1h_1}$	$u_{h_2h_2}$	$u_{h_1h_2}$	u_{h_1e}	α_{h_1e}	u_{h_2e}	α_{h_2e}	u_{ee}	α_{ee}	β_{ee}
NSF	0.8	0.76	0.78	0.46	−0.24	0.4	−0.30	0.77	0.14	0.09
SF	2.27	2.13	2.22	4.65	−0.34	2.29	−0.22	3.67	0.15	0.04

Results of harmonic analysis (2D)

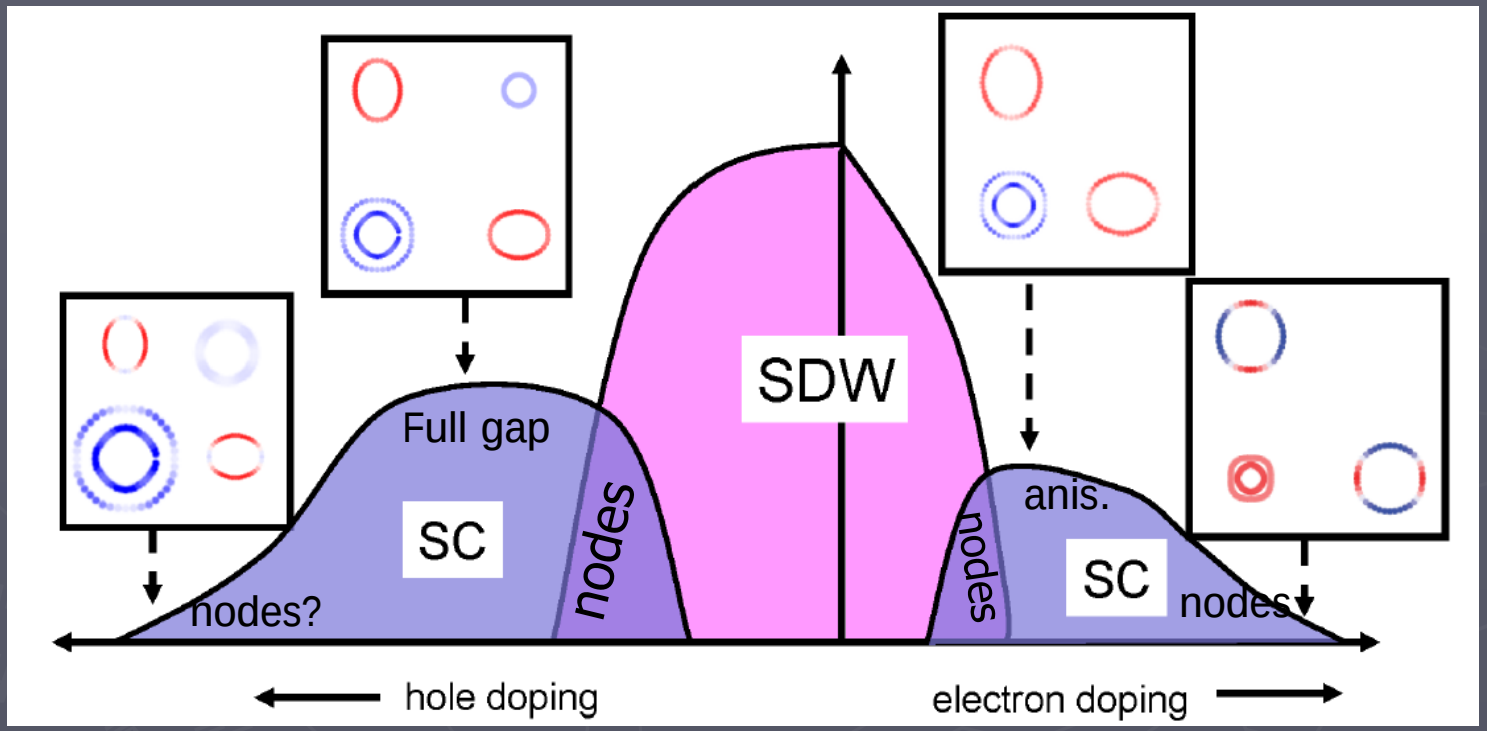
- Generic case: as long as both hole and electron pockets are present, the driving force is electron-hole interaction. Poor nesting suppresses isotropic s+/- away from optimal doping

- for strongly electron doped FeSCs, strong direct d-wave attraction between electron pockets develops (Graser et al, Wang et al, Das/Balatsky 2011)

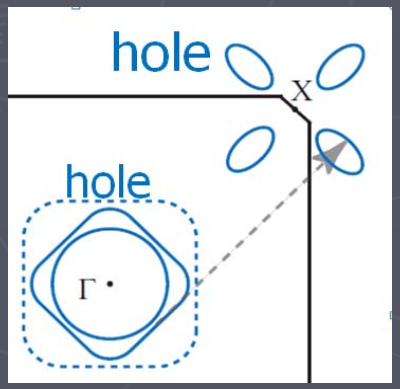
- for strongly hole-doped FeSCs, d-wave channel again wins. There is d-wave attraction within hole pocket at (π,π) and strong attraction between the two hole pockets at (0,0), both effects lead to $\lambda_d > 0$ (Thomale et al 2011)

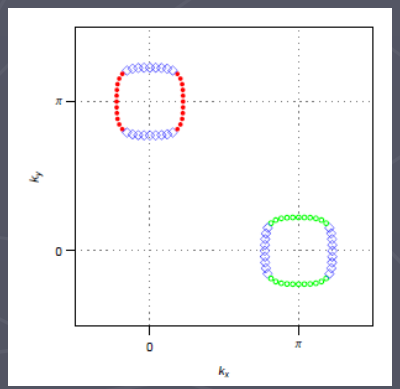
Big picture: evolution of gap with doping

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



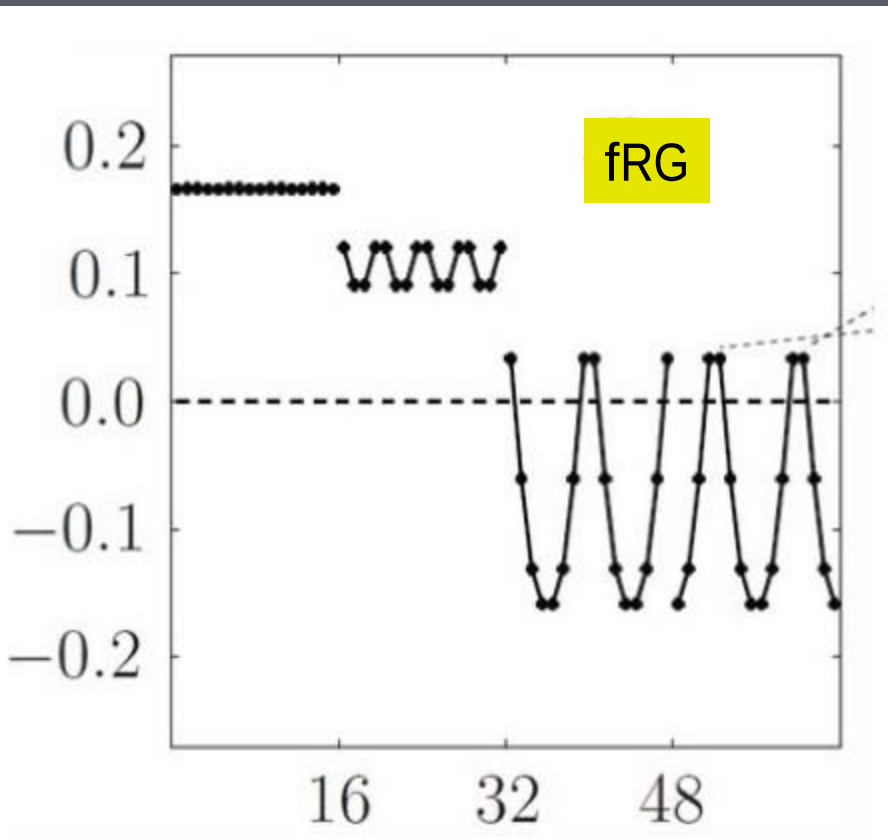
KFe_2As_2:
No electron pockets: d-wave?
Thomale et al

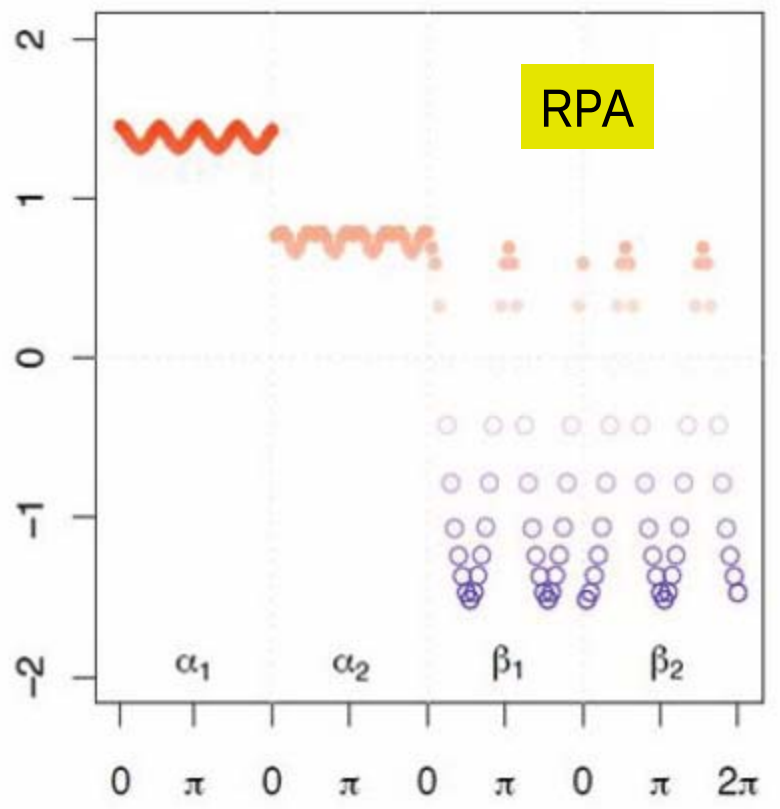




KFe_2Se_2:
No hole pockets: d-wave?
Wang et al
Graser et al
s-wave?
Mazin, Fang et al

Different implementations of spin fluctuation theory





Thomale et al 2009

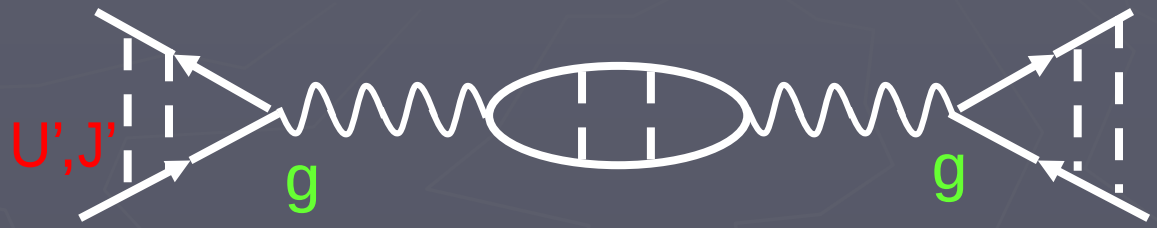
Maier et al 2009

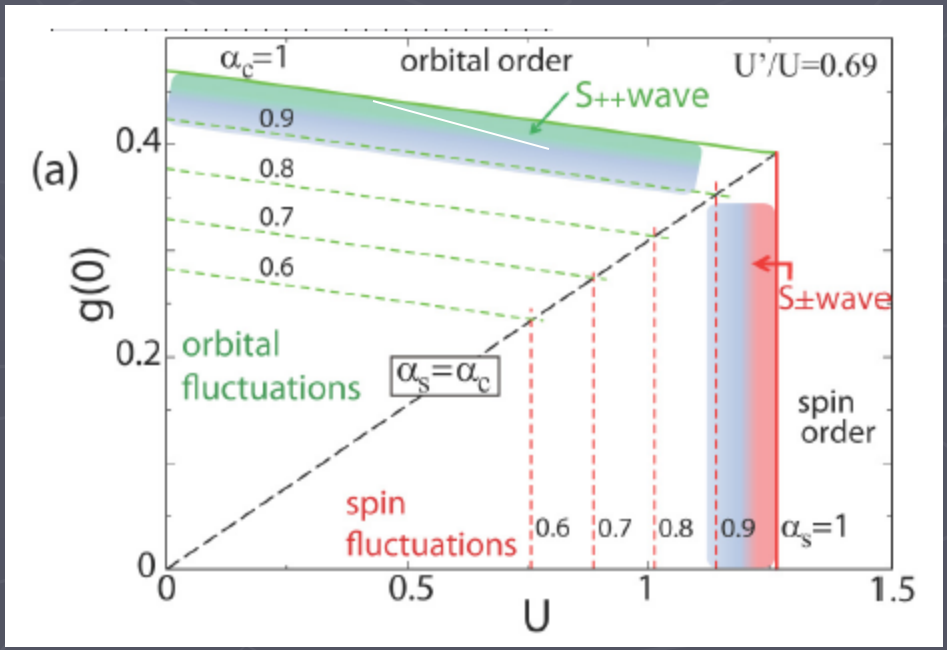
FLEX also similar: Ikeda, Kuroki...

Can charge/orbital fluctuations pair?

Case of attractive interpocket interaction: s_{++} state

Concrete realization: Hubbard-Holstein approach, Kontani-Onari 2010,...

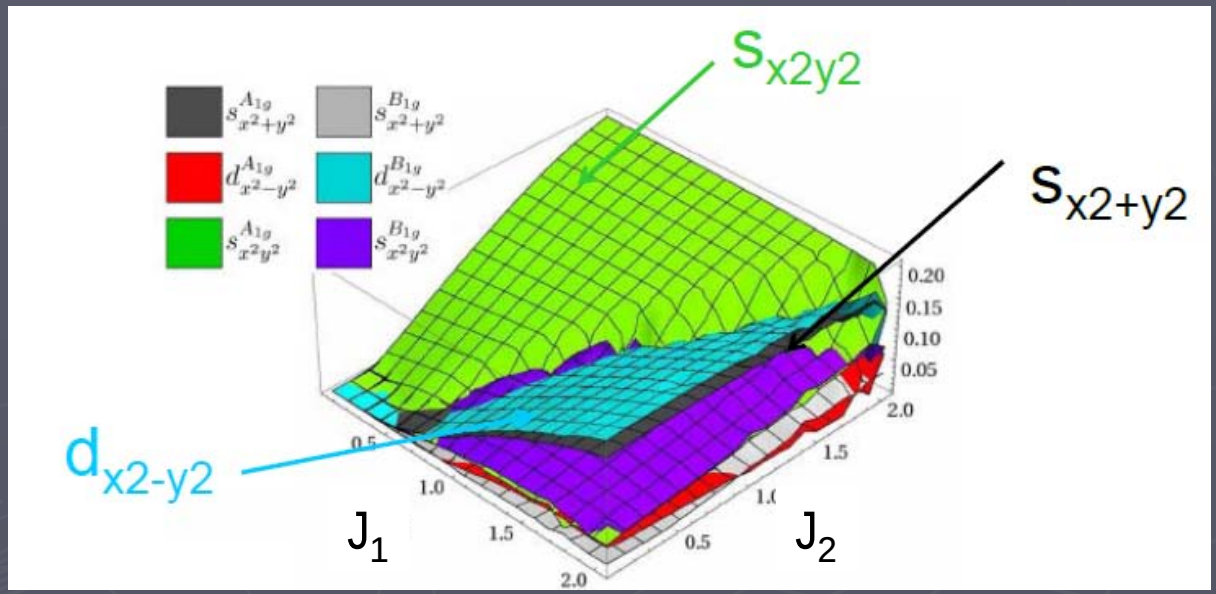




Onari et al 2010

“Strong coupling” theories of SC

e.g. Seo et al 2008, P. Goswami et al (2010): decouple exchange terms in t-J_1-J_2 model

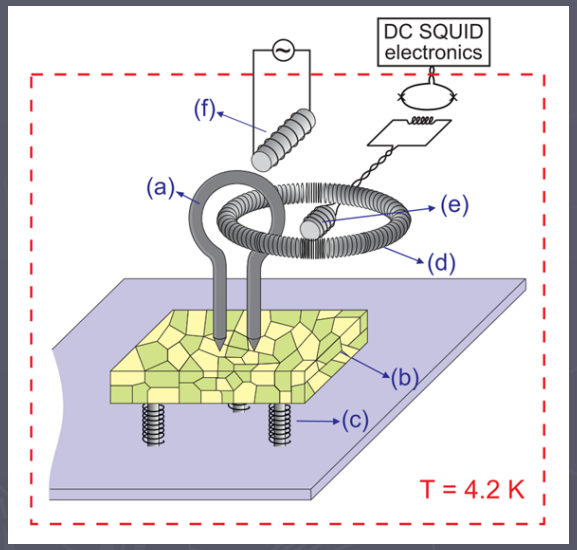


Also gives similar results to weak coupling approach, *but*

- *artificially separates itinerant electrons & local moments*
- *not derivable from Hubbard-type model (t not projected)*
- *band calculations map onto Heisenberg + biquadratic exchange, ring exchange*
- *mean field decoupling ⇒ nodes fixed in BZ*

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

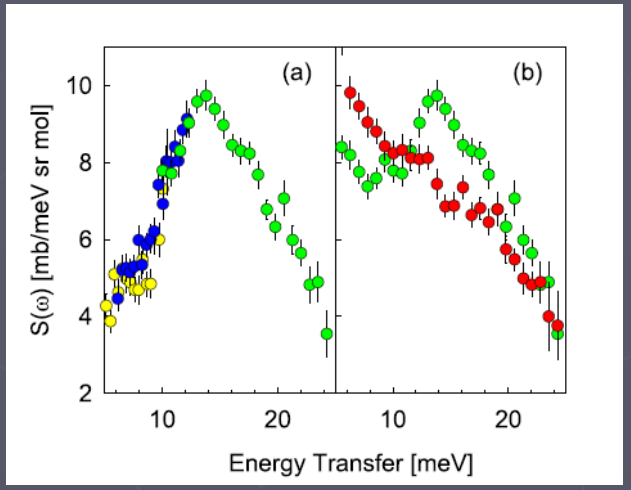
Chen et al, Nature 2010



$NdFeAsO_{0.88}F_{0.12}$

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

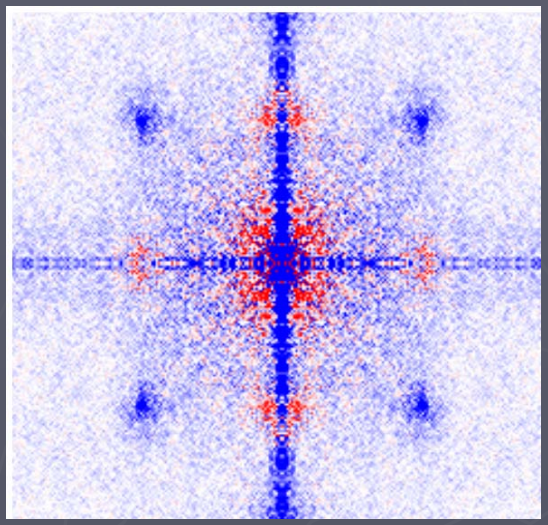
Christianson et al Nature 2008



$Ba_{0.6}K_{0.4}Fe_2As_2$

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

Hanaguri et al Science 2010



Fe(Se,Te)

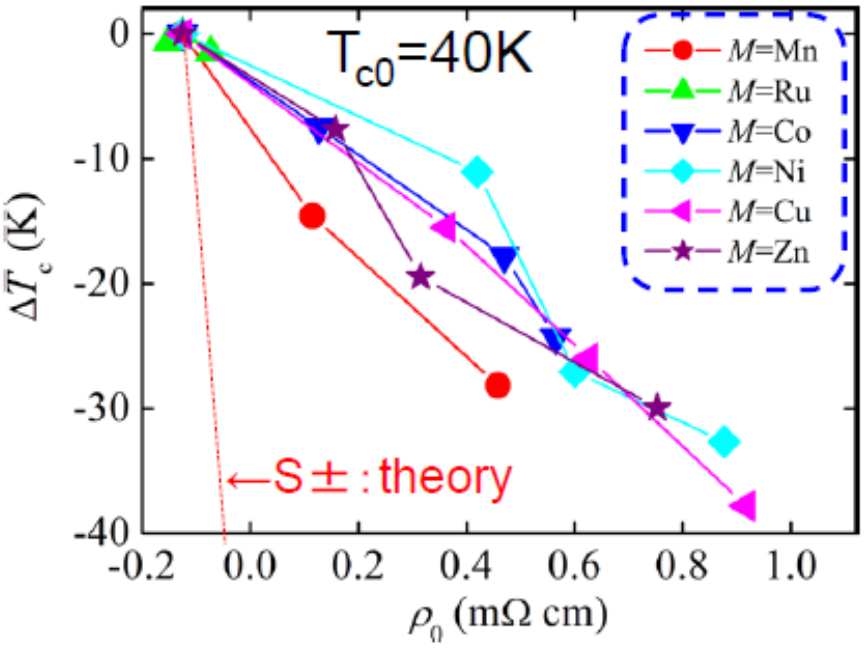
Field dependence of quasiparticle interference peaks depends on order parameter sign

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

?

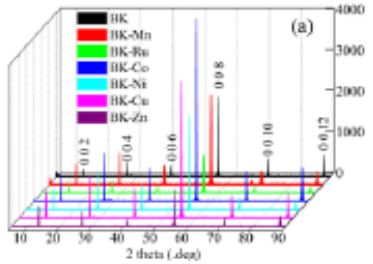
impurity effect in single crystal $(Ba,K)Fe_2As_2$

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
$\rho_{imp} > 500\mu\Omega cm$
$[l_{imp} \sim 3\,Å]$

⇔

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

local impurity
on Fe-sites

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*

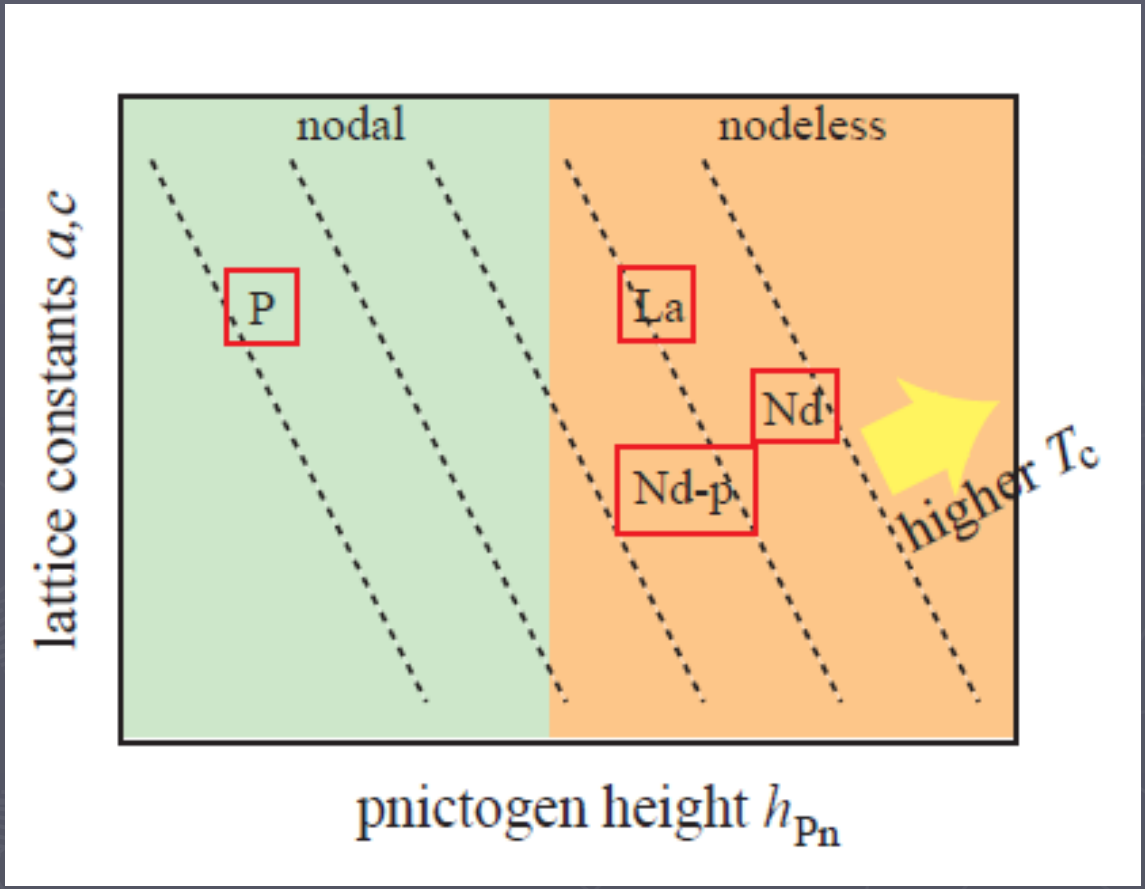
FeSe under stress: 43K SC intercalated with Li amide, ammonia
40K SC under 10 GPa pressure
?? 65K SC single layer on STO

Goal: towards materials-specific theory of unconventional SC

- Traditional condensed matter theory prejudice:
  impossible to calculate T_c from microscopic principles
- Some success within Eliashberg/DFT framework in
  case of *conventional* electron-phonon superconductors
  (Cohen, Pickett, Gross...)
- Needed: similar theories for *unconventional* SC
- Use calculations of trends of T_c within families of uSC
  (e.g. doping sequences, pressure, ...) to identify
  essential ingredients of high-T_c

Higher Tc

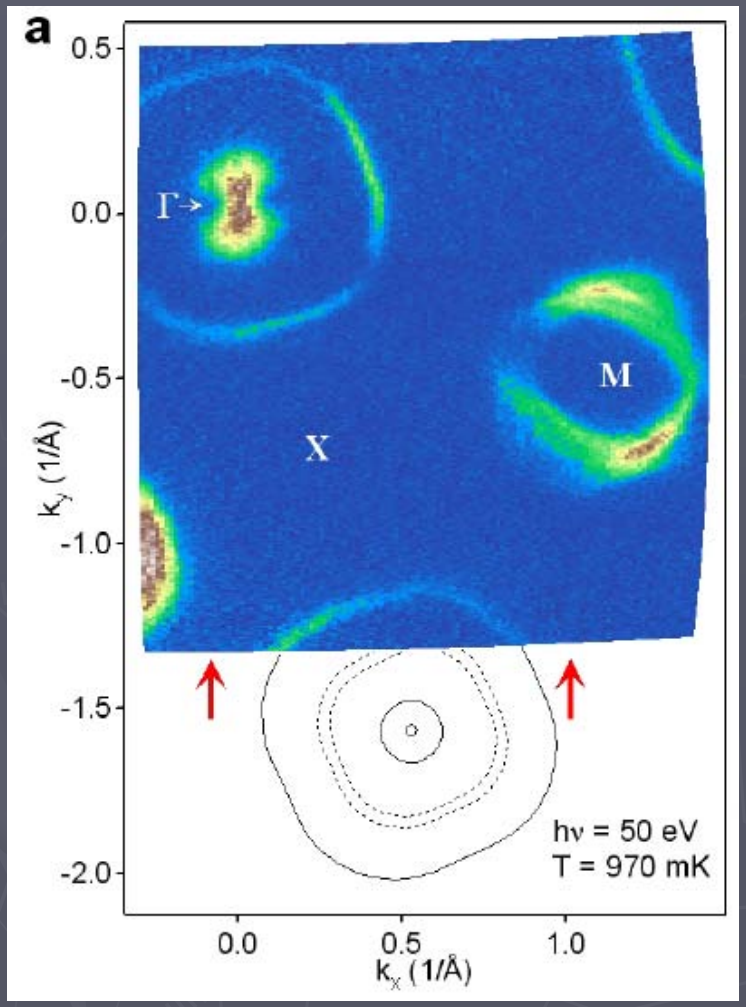
Kuroki et al. PRB '09: spin fluctuation theory for 1111 materials



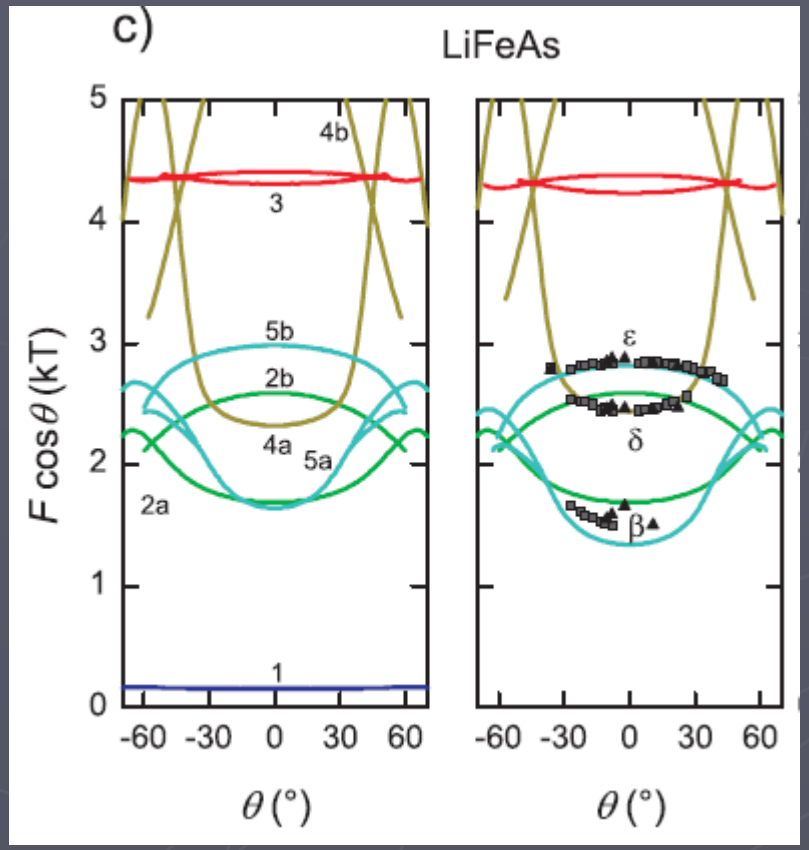
Tc, pair structure trends from band structure changes alone

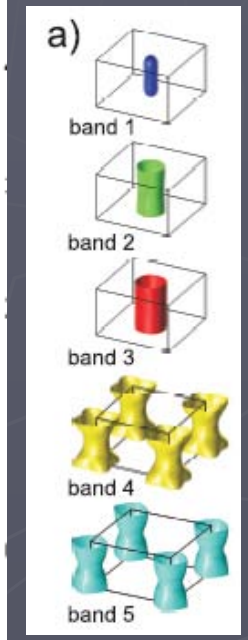
Analogy: T_c of 1-layer cuprates vs. apical oxygen height? (Pavarini et al 2001)

LiFeAs



Borisenko et al PRL 2010

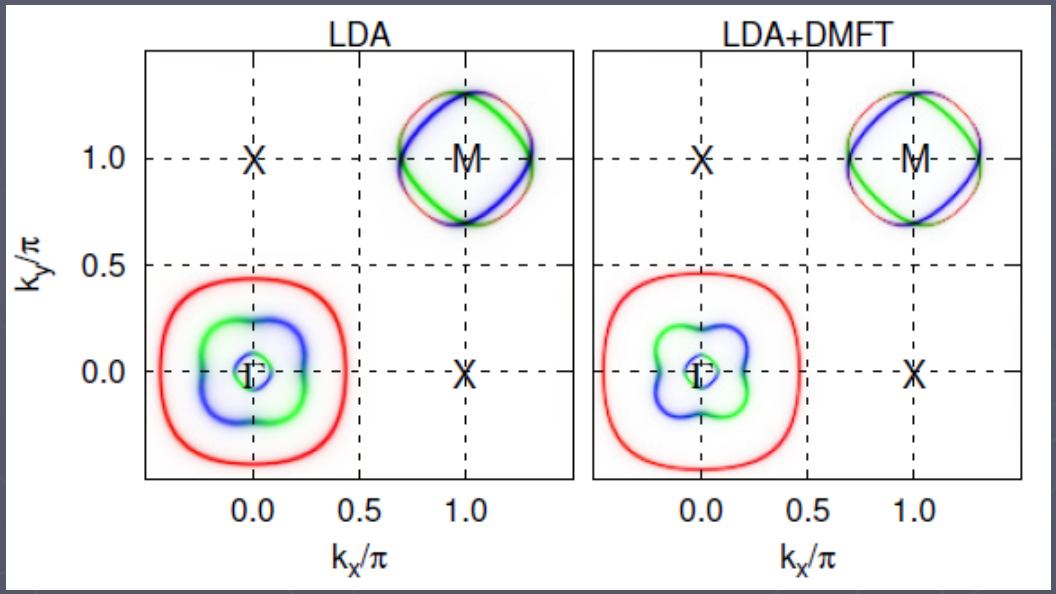




Putzke et al PRL 2012

Importance of correlations?

$k_z=0$

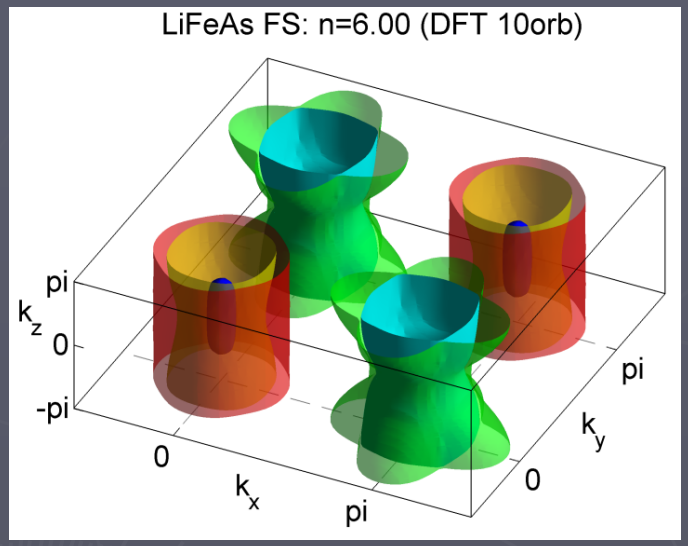


Yin et al 2011 Nat Mat, Ferber et al PRB 2012

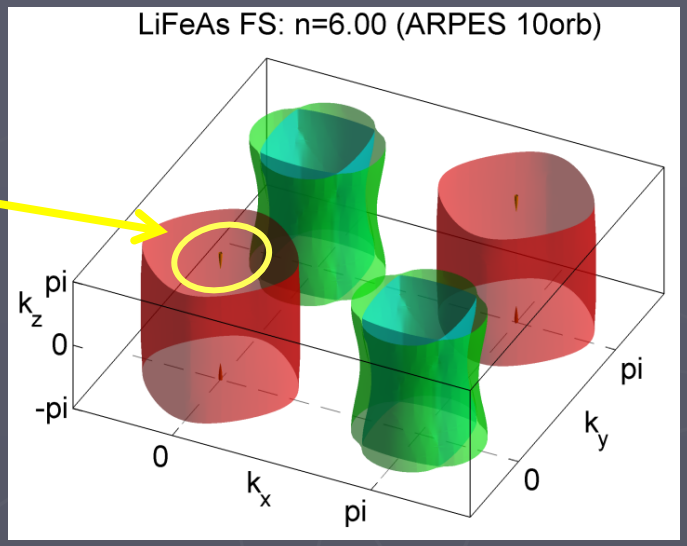
LDA+DMFT: hole pockets shrink, electron pockets unaffected

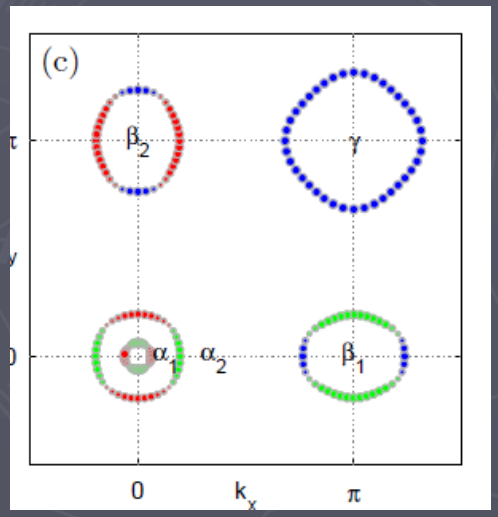
see also Lee et al, PRL 2012

Comparison of DFT with ARPES derived tight binding fit
(in collaboration with Borisenko group, Dresden [unpublished])

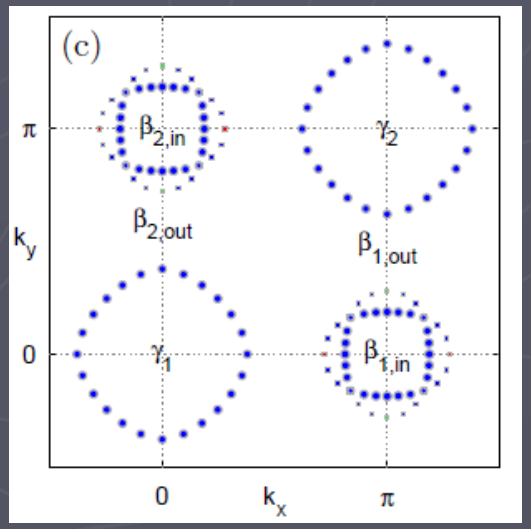


$\alpha_{1,2}$



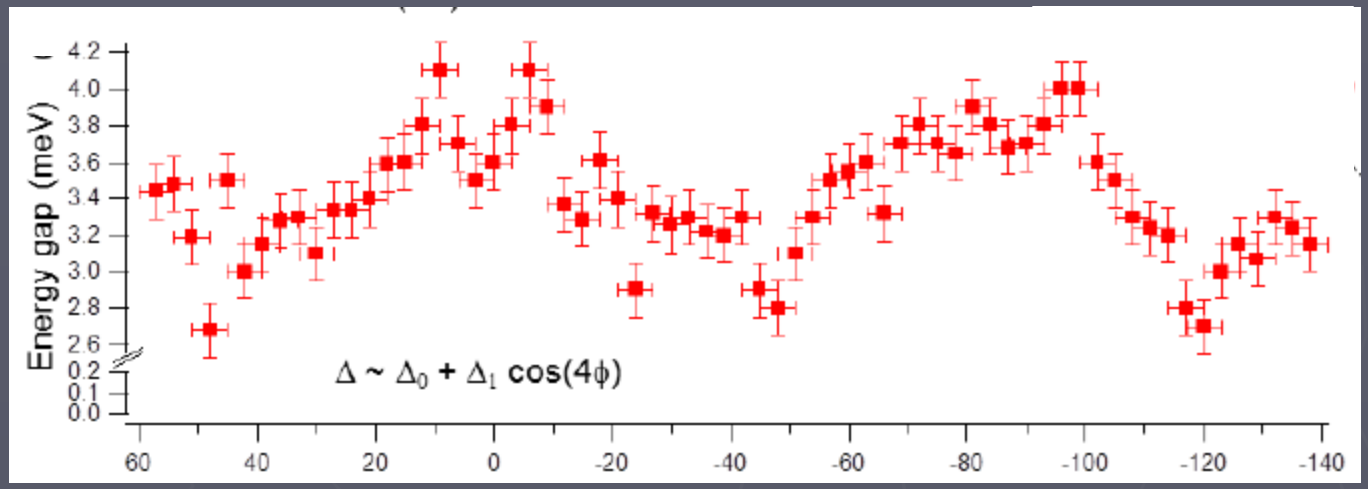


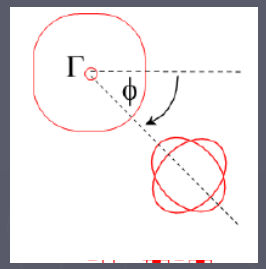
k_z=0



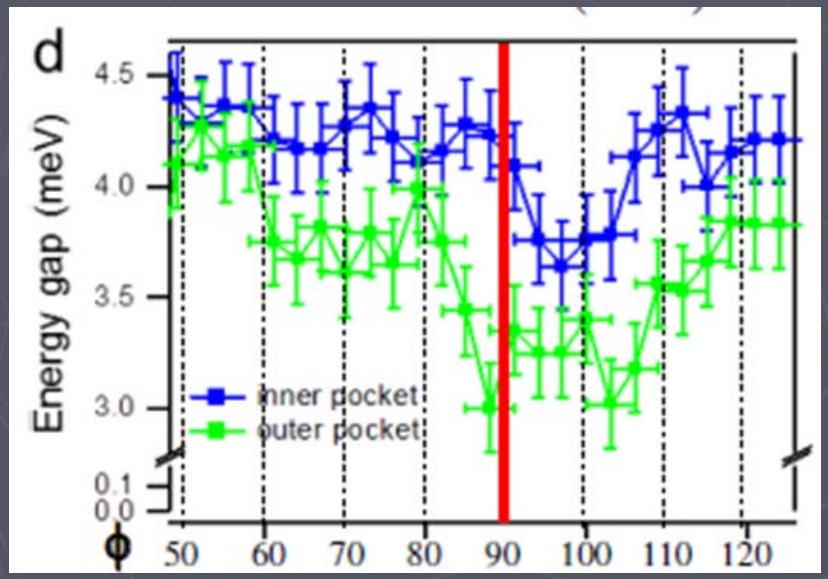
ARPES results for SC gap function (Dresden group)

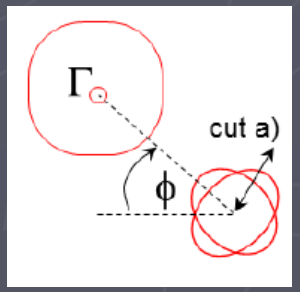
γ hole pocket



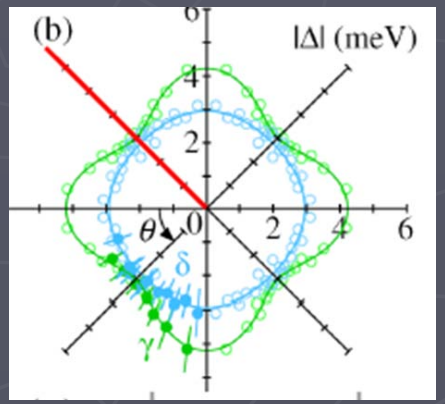


β electron pocket





See also
K. Umezawa et al 2012

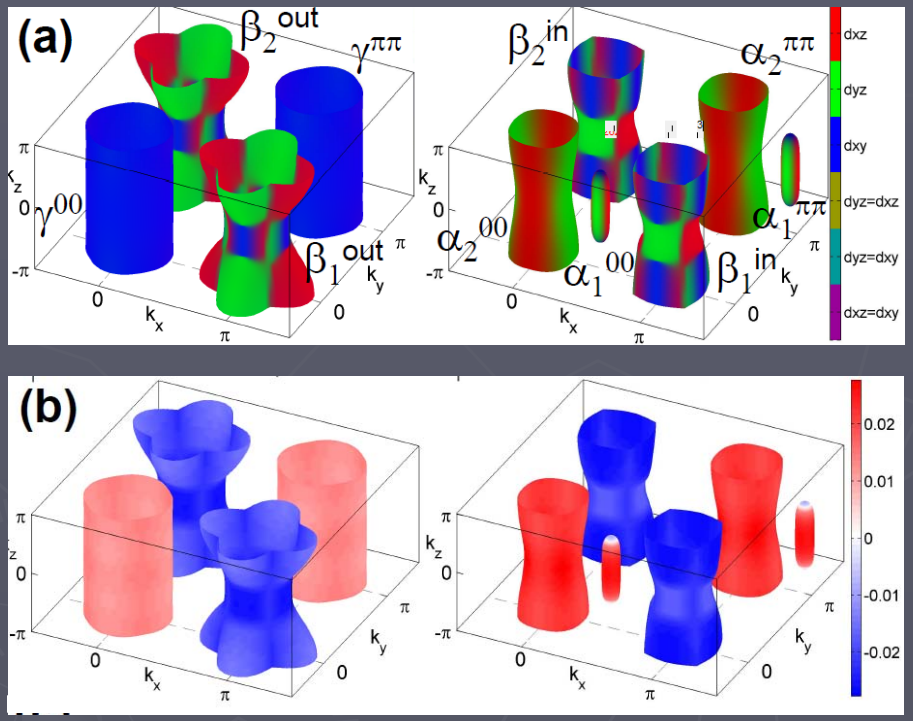


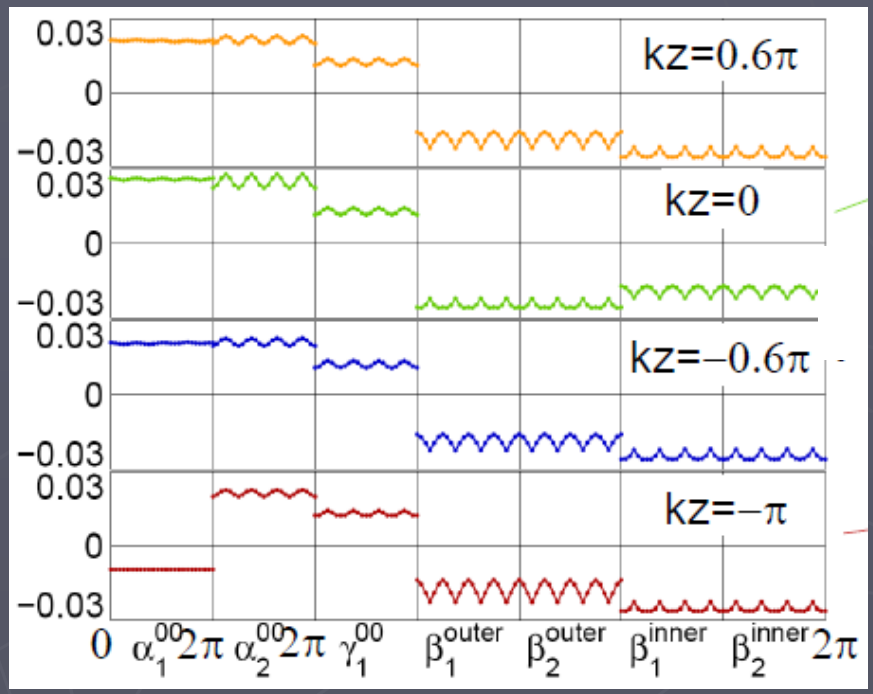
Borisenko et al Symmetry 2012

Results of 3D spin fluctuation calculations I

Leading pairing eigenstate 10-orbital DFT-based bands

λ_1=0.23613,U=0.88,J=0.25U (LiFeAs 10orbDFT)



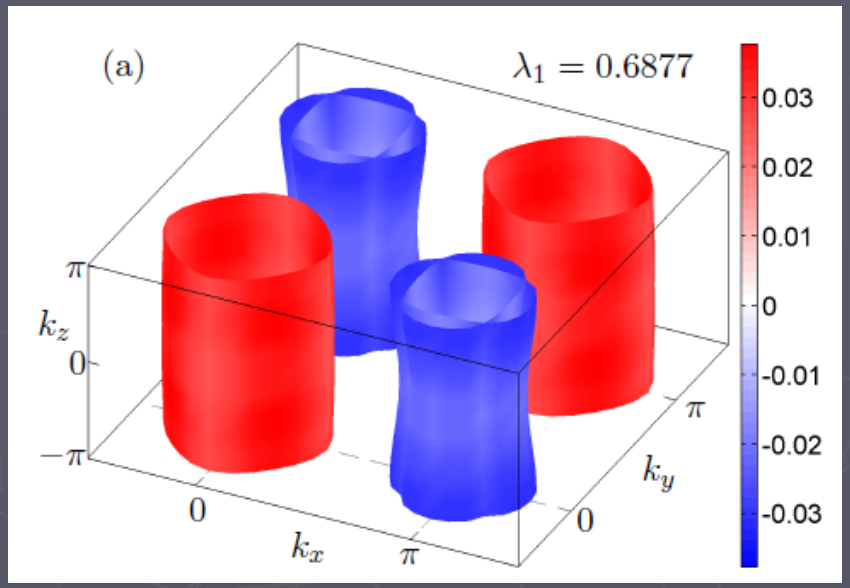


- Largest, isotropic gap on α pocket √
- Intermediate size oscillatory γ pocket √

- Gap minima along Fe-Fe bond √
- Intermediate size oscillatory β pocket √
- β pocket gaps out of phase X

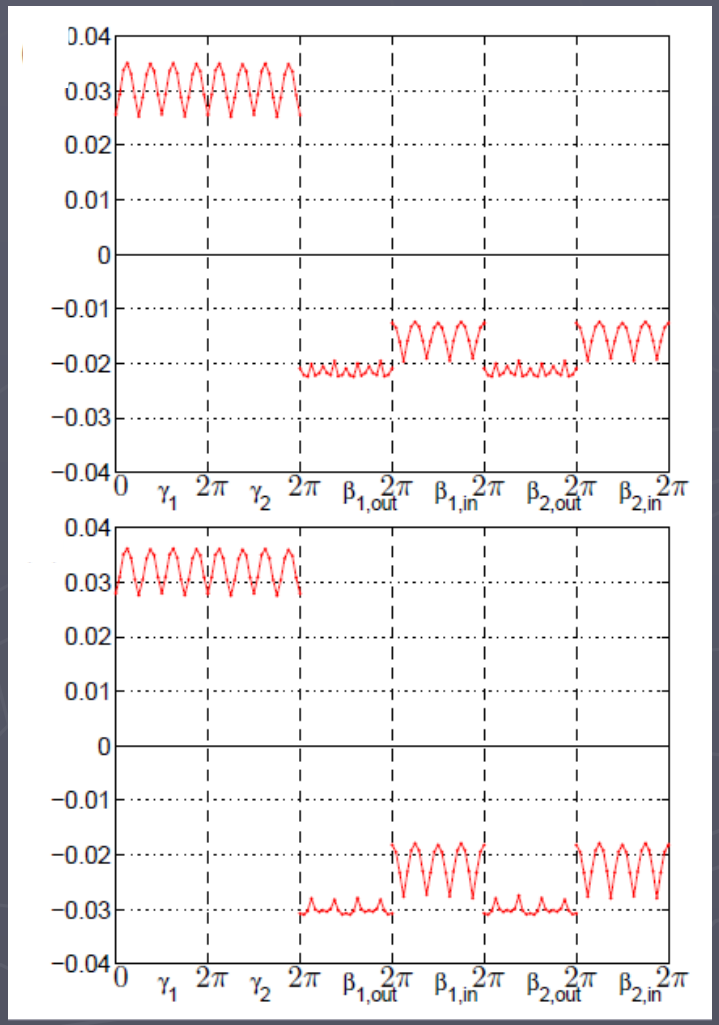
Results of 3D spin fluctuation calculations II

Leading pairing eigenstate ARPES-derived bands



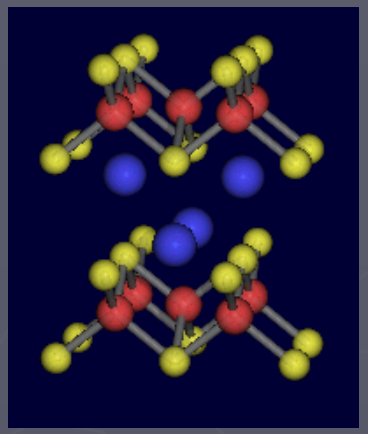
k_z=0

k_z=π



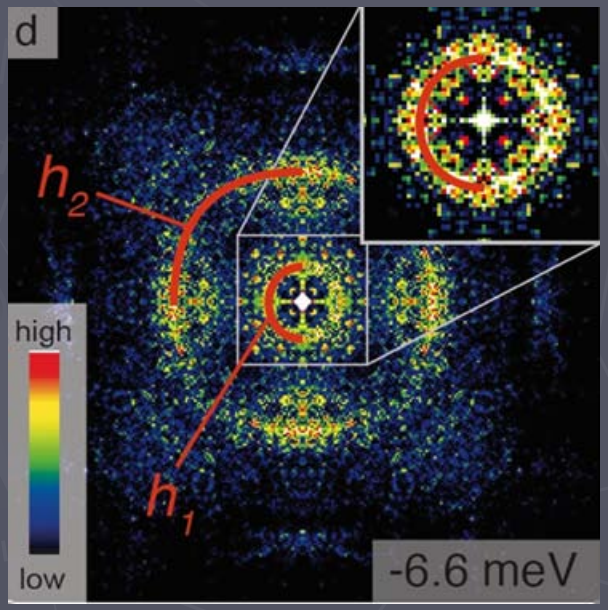
- Small gap on α pocket X
- Intermediate size oscillatory γ pocket √
- Gap minima along Fe-Fe bond √
- Intermediate size oscillatory β pocket √
- β pocket gaps out of phase √

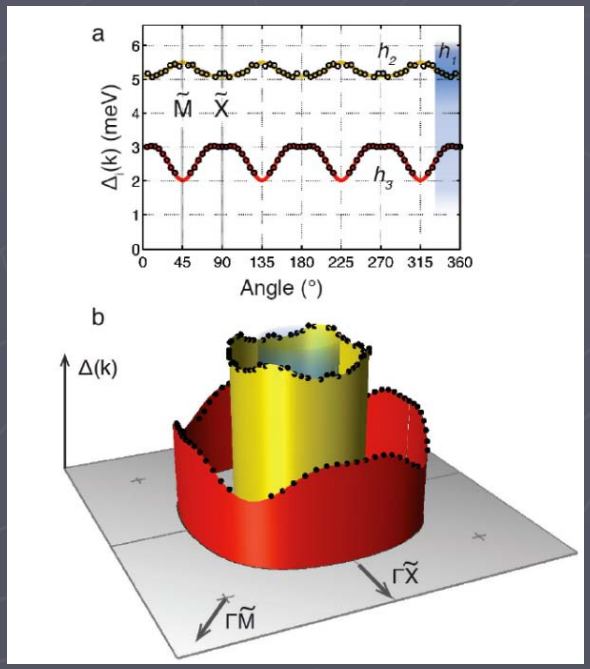
STM quasiparticle interference experiments on high quality LiFeAs surfaces



- Quasiparticle interference measurement
- Find smallest, oscillatory gap with minima along Fe-As bond – γ pocket?
- Find larger, isotropic gap with smaller radius – $\alpha 2$ pocket?
- Apparently do not observe β pockets – ?

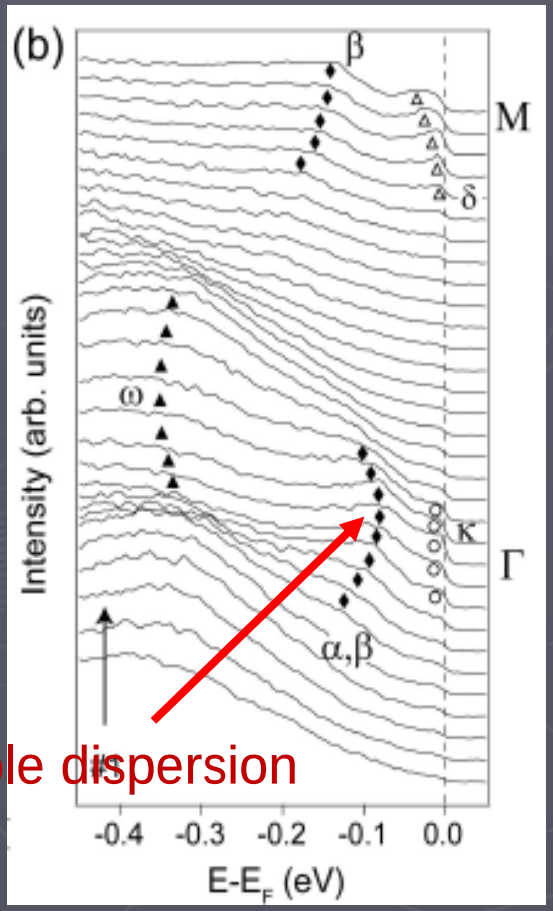
Rost et al 2012



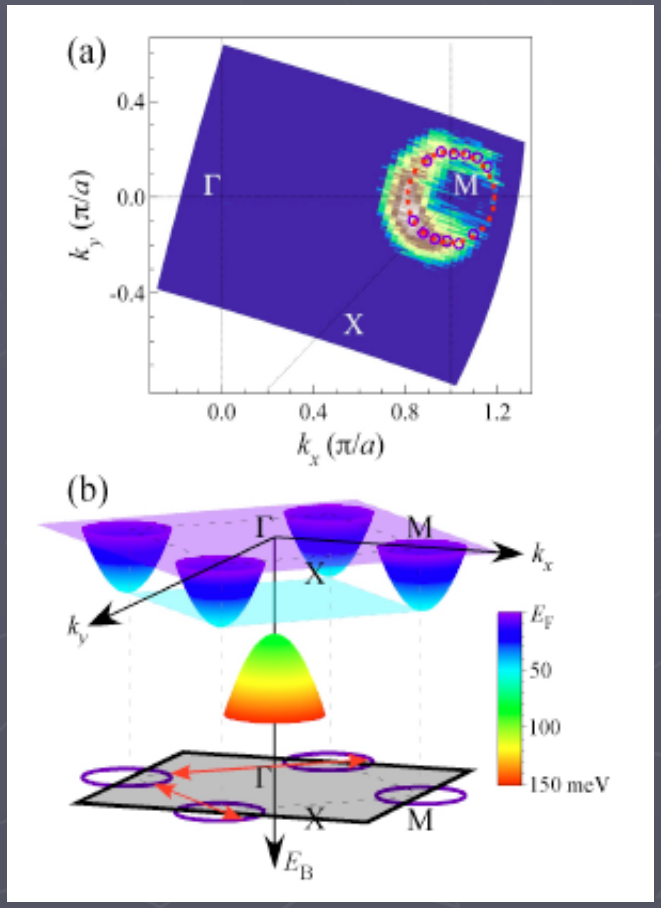


Alkali-intercalated FeSe: "KFe_2Se_2"

ARPES: KFe_2Se_2 strongly e-doped, no h pocket?



Y. Zhang et al



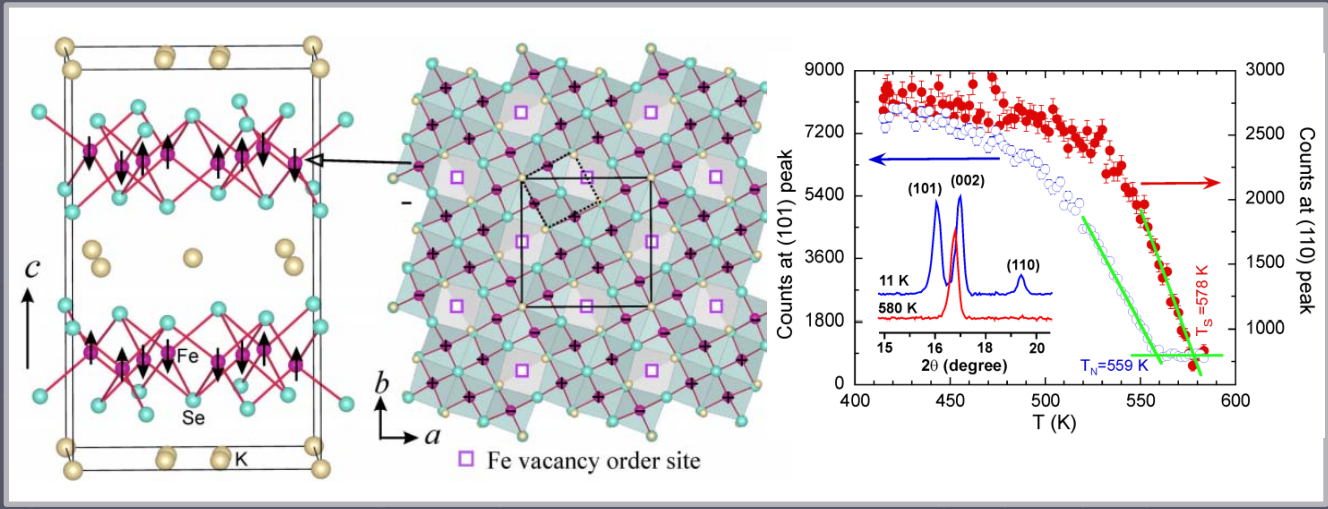
H. Ding et al

W. Bao et al, CPL 2011; F. Ye et al, PRL 2011:

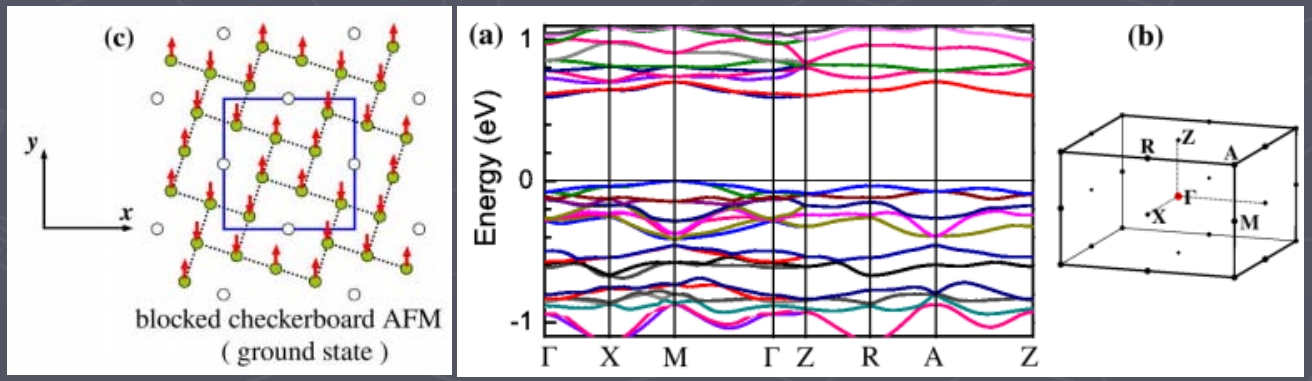
245 Fe vacancy phase

AFM transition: T_N=559K

M=3.31 μB/Fe, Q=(4/5, 2/5, 1)



DFT: Yan et al PRB 2011, Cao et al PRL 2011: block AF semiconductor



ordered vacancies, magnetism present in superconducting samples!

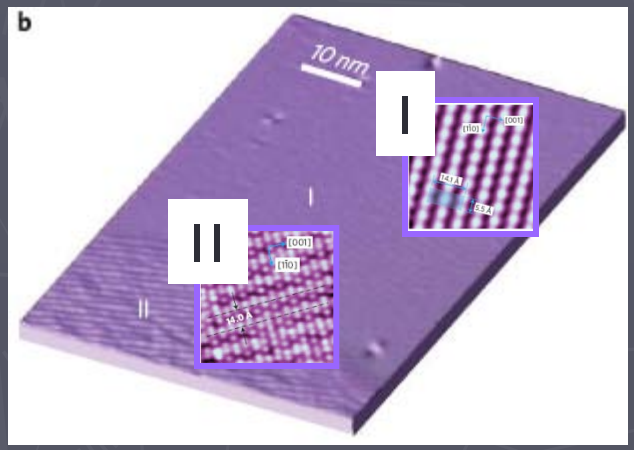
What is correct starting point for description of SC phase?

a) itinerant: Fermi surface w/ no hole pockets as reported by ARPES?
Wang et al 2011, Maier et al 2011, Saito et al 2011 (“weak coupling”)
Yu et al 2011, Fang et al 2011 (“strong coupling”)

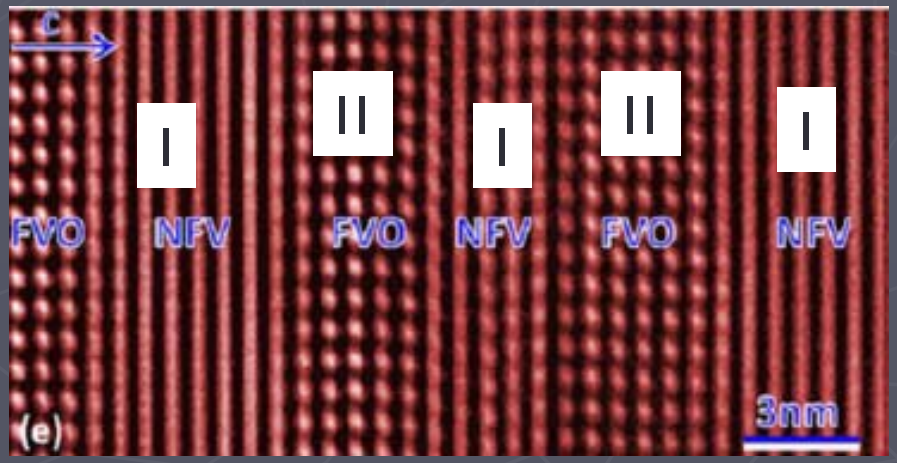
b) itinerant: disordered, paramagnetic vacancy phase?
Berlijn et al 2012

c) SC coexistence with ordered vacancy, magnetic phase?
Das-Balatsky 2011, Huang-Mou 2012

Evidence for inhomogeneity in all samples:



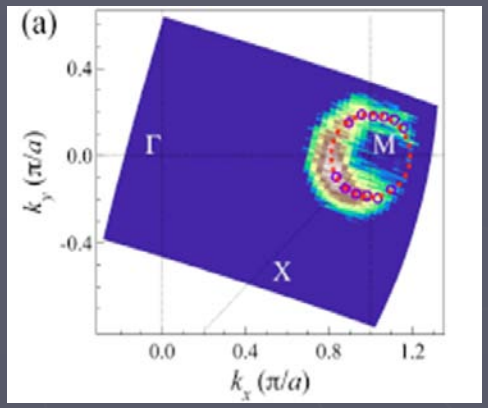
W. Li et al., Nat. Phys. (2011)
Region I: no Fe vacancies (Superconducting)
Region II: ordered Fe vacancies (Insulating)



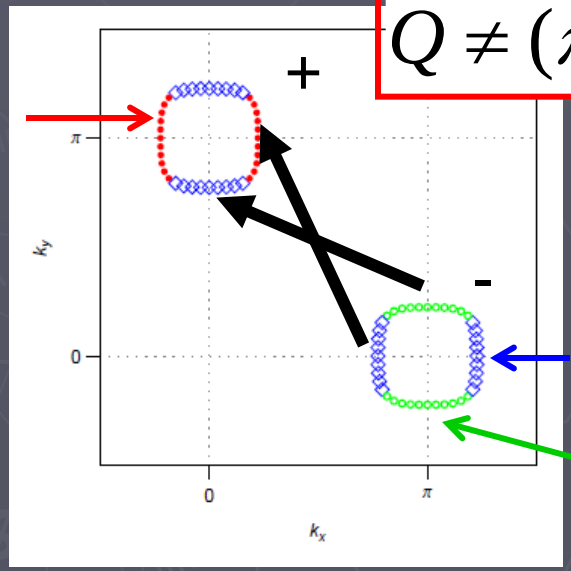
W. Li et al., Nat. Phys. (2011)
Region I: no Fe vacancies
Region II: ordered Fe vacancies

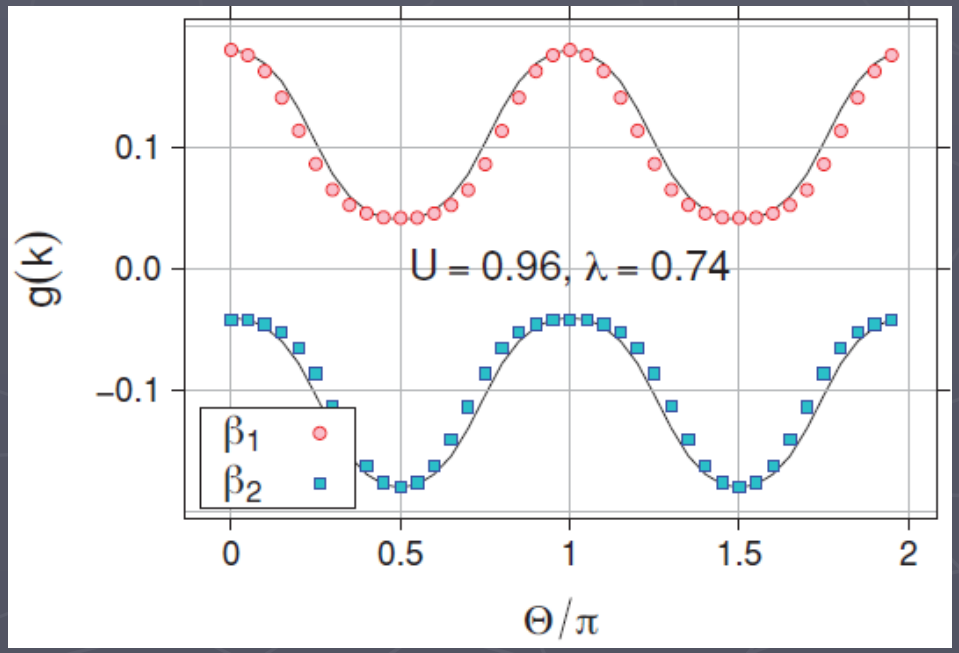
Maier et al PRB 2011 "nodeless" d-wave state for KFe_2Se_2

Similar: F. Wang et al 2011, Das and Balatsky 2011



- Ingredients: DFT calculation for KFe2Se2
  5-orbital tight-binding fit
  Adjustment of hoppings to suppress hole pockets
  "Standard" spin fluctuation calculation



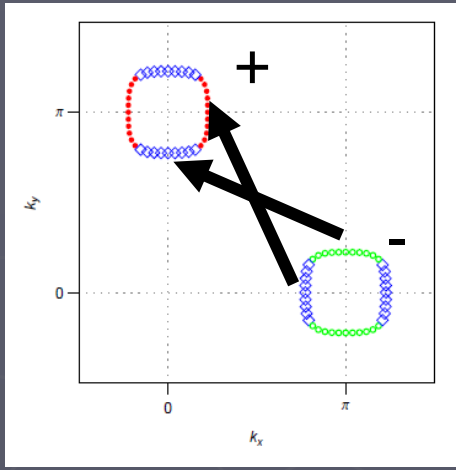


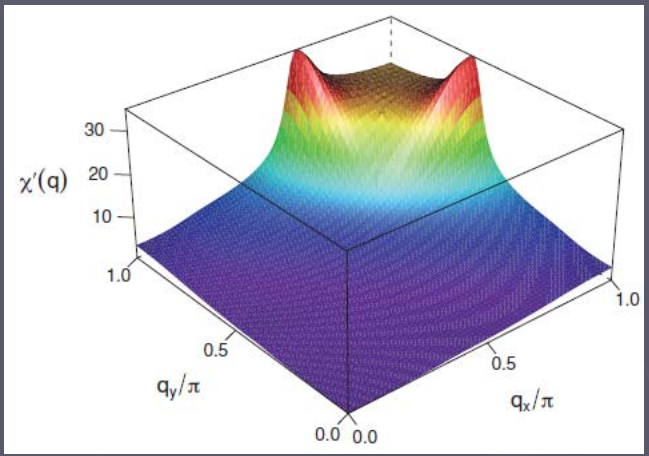
e-e scattering maximized by opposite sign v_F's

Anisotropic but nodeless d-wave

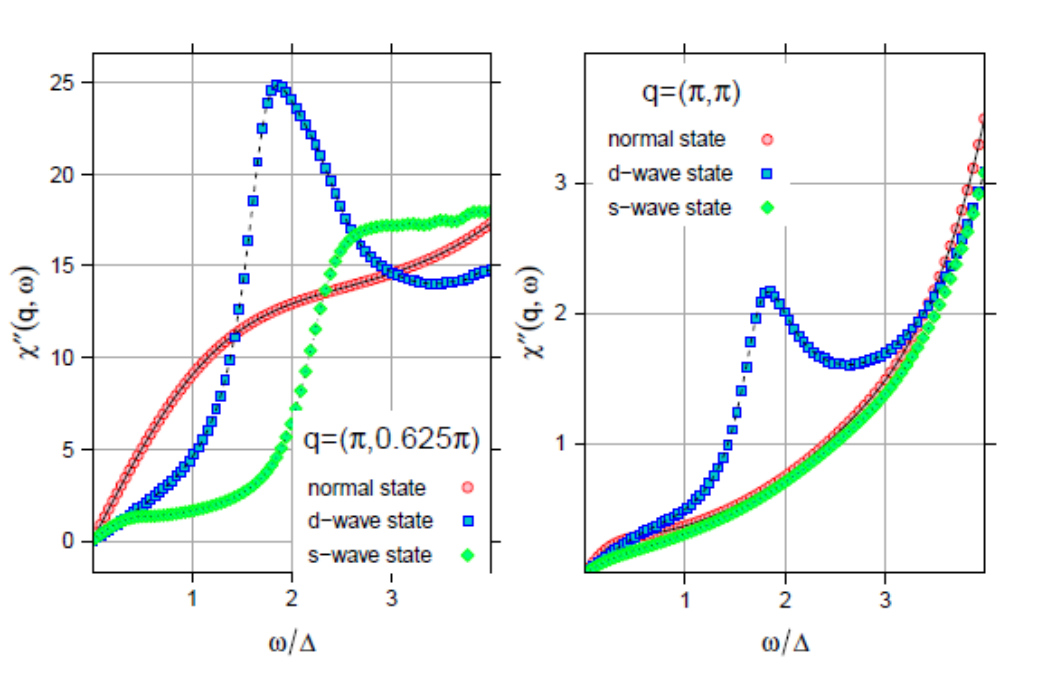
Prediction of neutron scattering resonance near $q=(\pi,0.6\pi)$

Maier et al PRB 2011

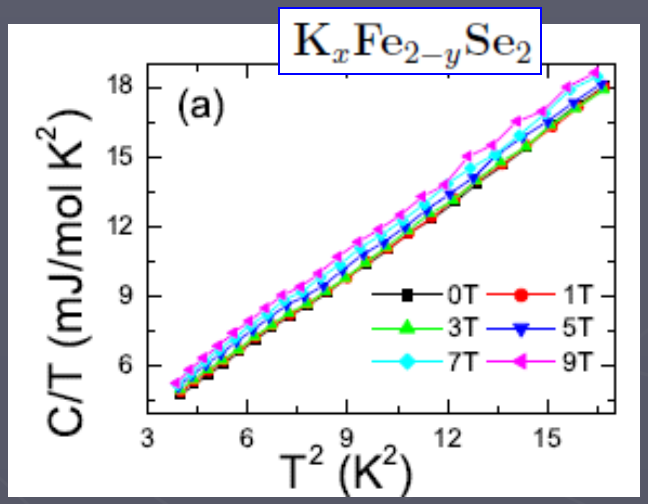




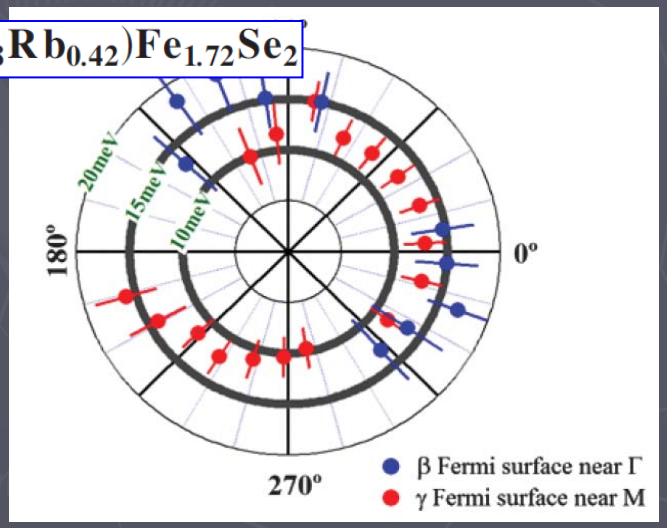
Re $\chi(q,\omega)$



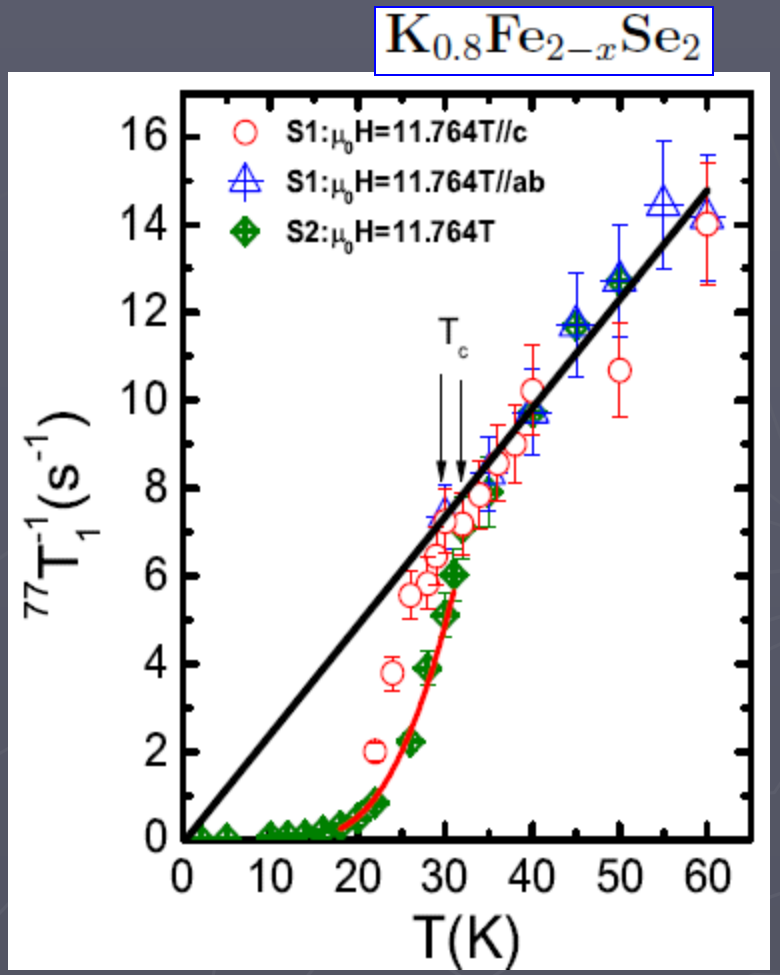
Evidence for fully gapped SC state



Specific heat
Zeng et al 2011



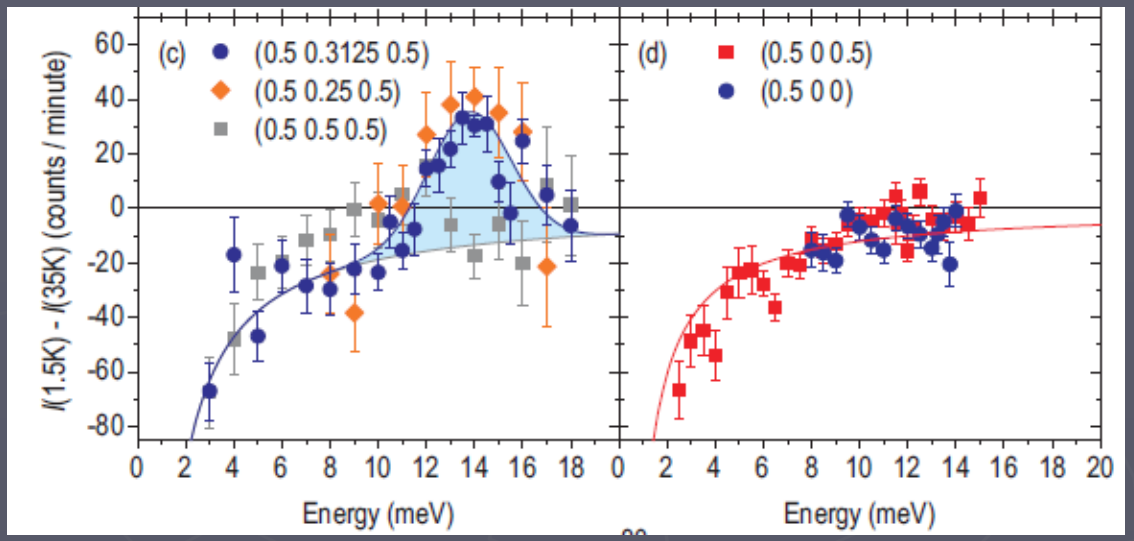
ARPES
Mou et al 2011

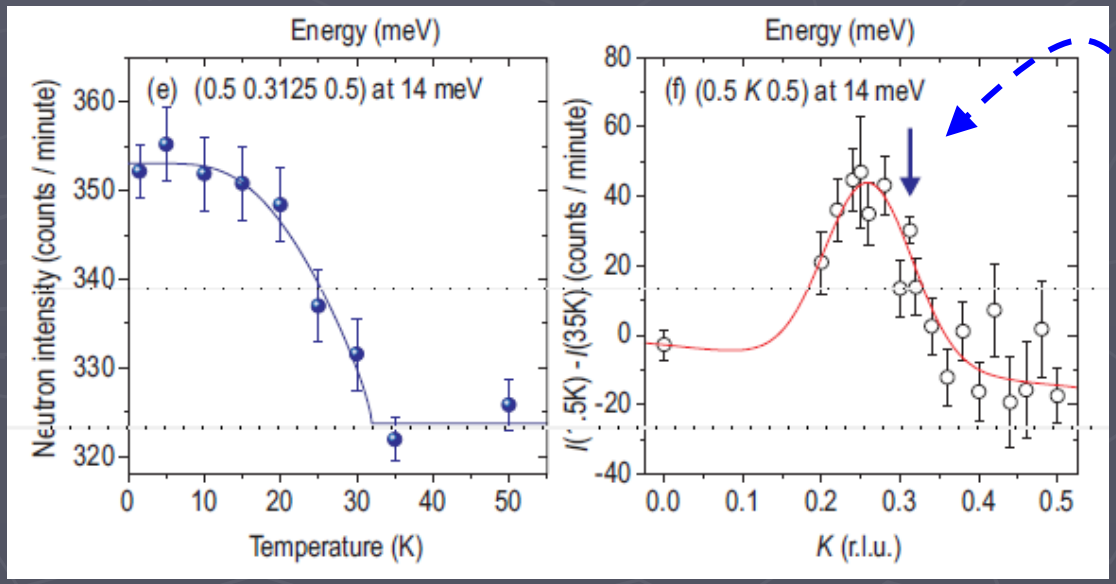


Spin-lattice T_1 ^{77}K
Ma et al 2011

Park et al PRL 2011

$Rb_2Fe_4Se_5$



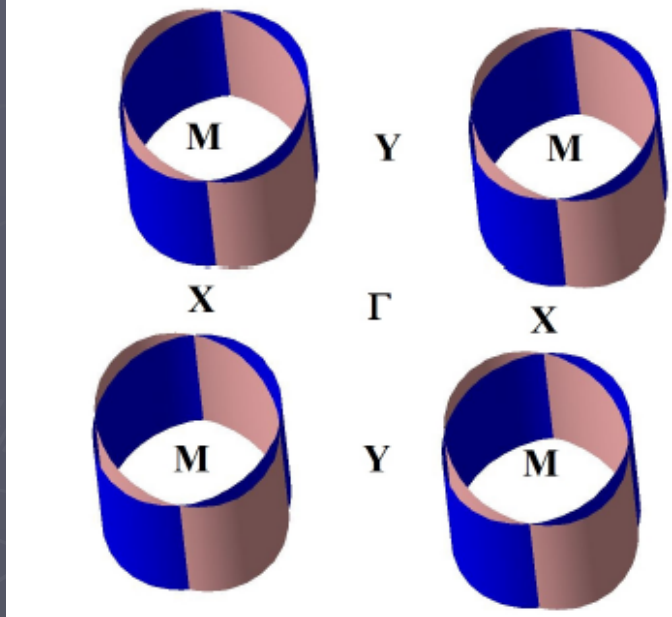


Maier et al prediction

Evidence for sign change of SC gap

d-wave gap nodes & 122 symmetry

I.I. Mazin 2011



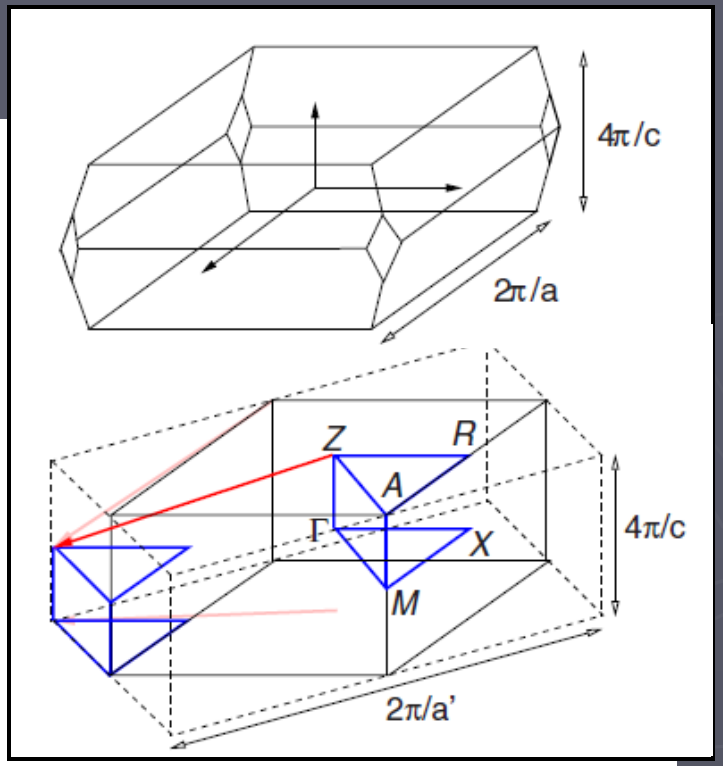
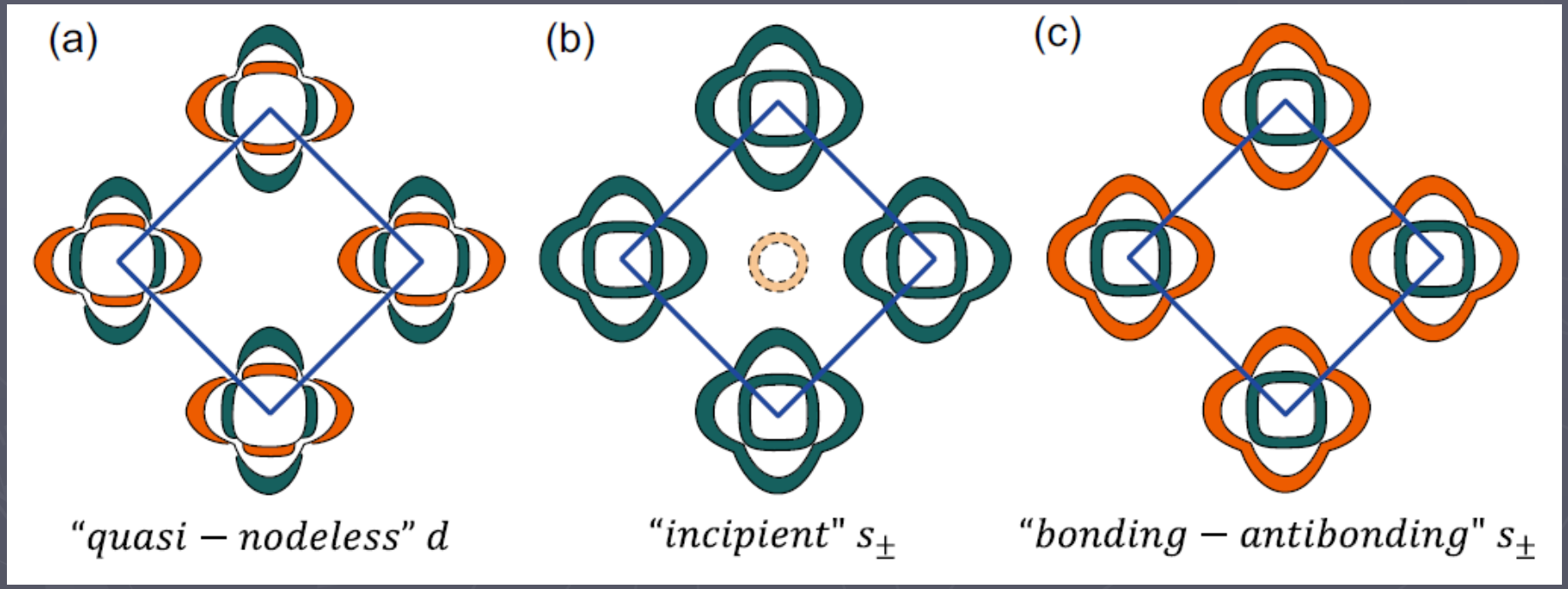


Figure 26. A cartoon showing a folded 3D Fermi surface for an AFe_2Se_2 material, assuming a finite ellipticity, but zero k_z dispersion. Different colors show the signs of the order parameter in a *d*-wave state. Wherever the two colors meet, turning on hybridization due to the Se potential creates nodes in the order parameter.

At best d-wave can be “quasinodeless”: nodes are weighted by strength of hybridization

some alternatives



Fang et al, Maier et al,
Saito et al 2011

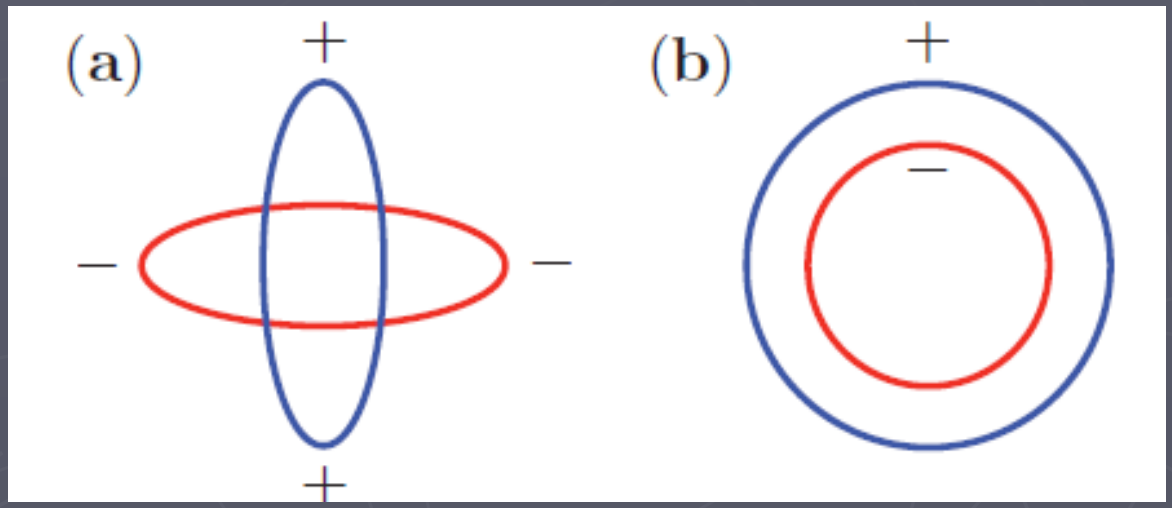
Fang et al 2011

Mazin 2011

modulated d-wave: Das-Balatsky 2011
s++ with orbital fluctuations: Saito et al 2011

Khodas Chubukov 2012

Theory of pairing of electrons on β pockets including interband pairing



d

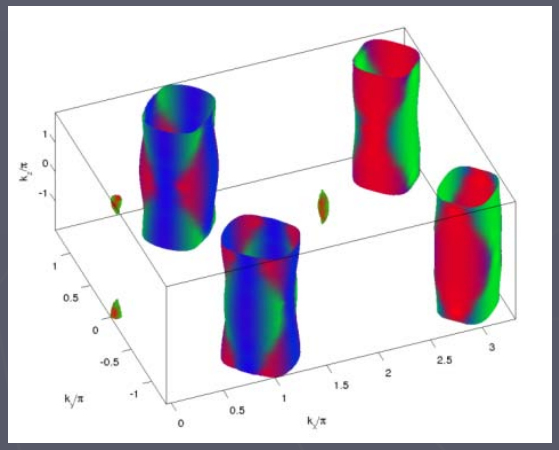
s

hybridization ⟶

Our tentative conclusion: hybridization probably too weak to access s+id, s phases. System remains in d-wave state with quasinodes

10-orbital 3D DFT-based spin fluctuation calculations

Orbital content

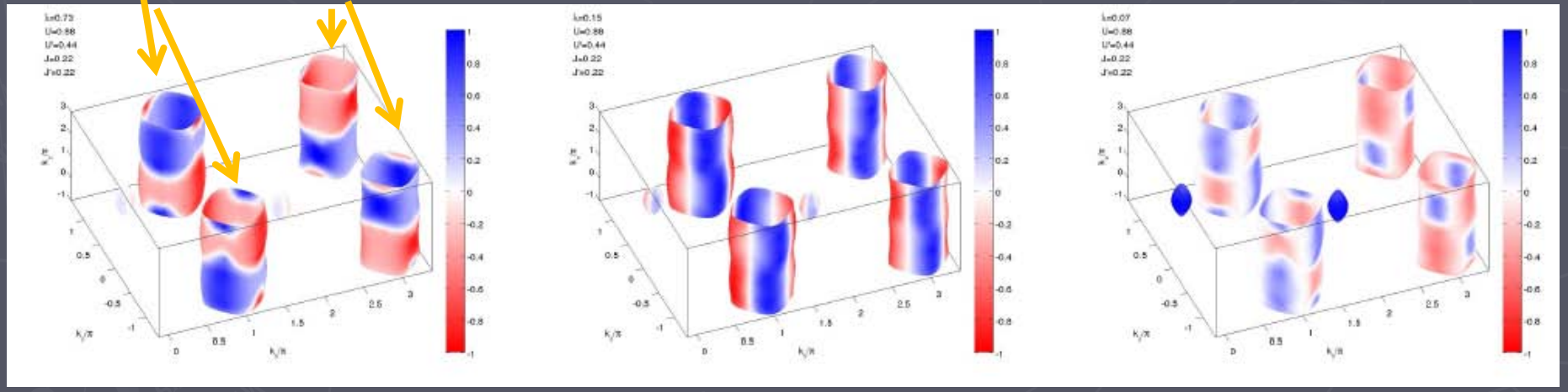


So far:

- d-wave always wins
- vertical or loop nodes depending on doping

outer inner

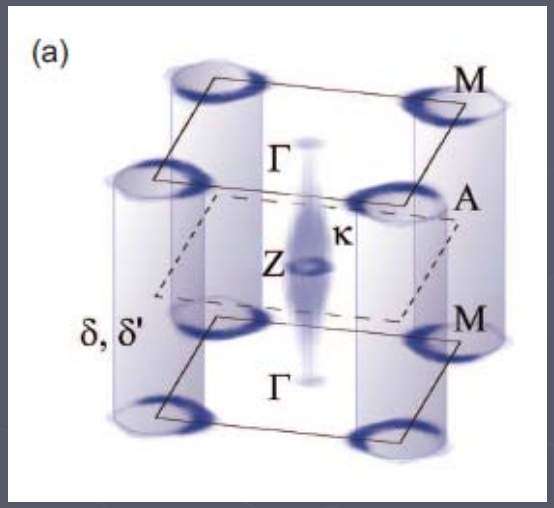
U=0.88 J=0.25U n=6.2

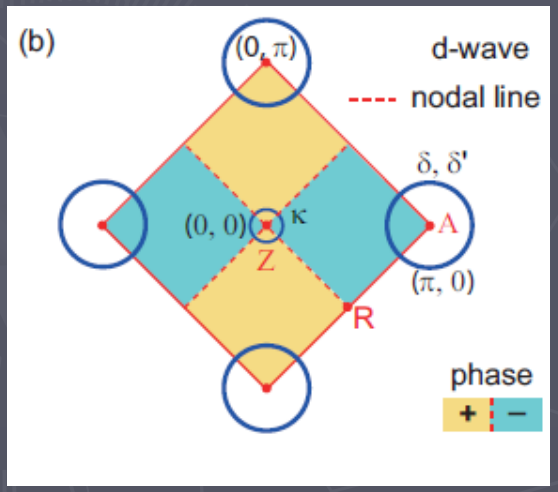


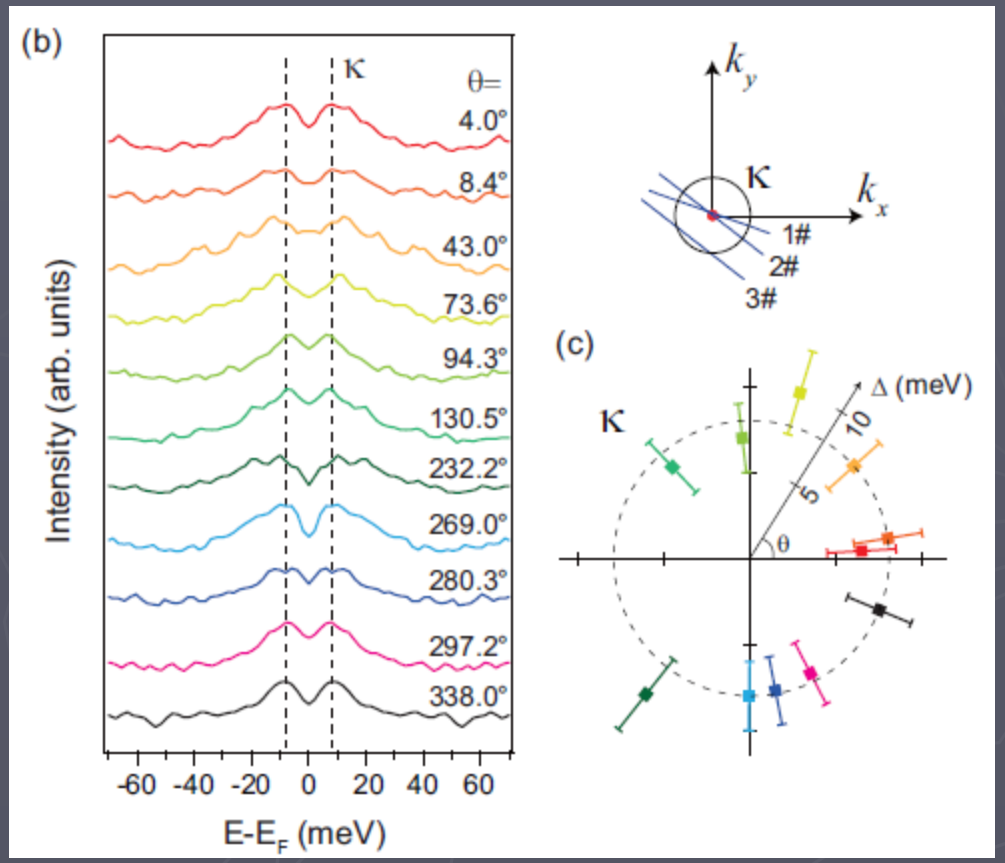
d λ=0.73 d λ=0.15 s λ=0.04

Problem with d-wave scenario: ARPES on Z-centered pocket

Xu et al 2012



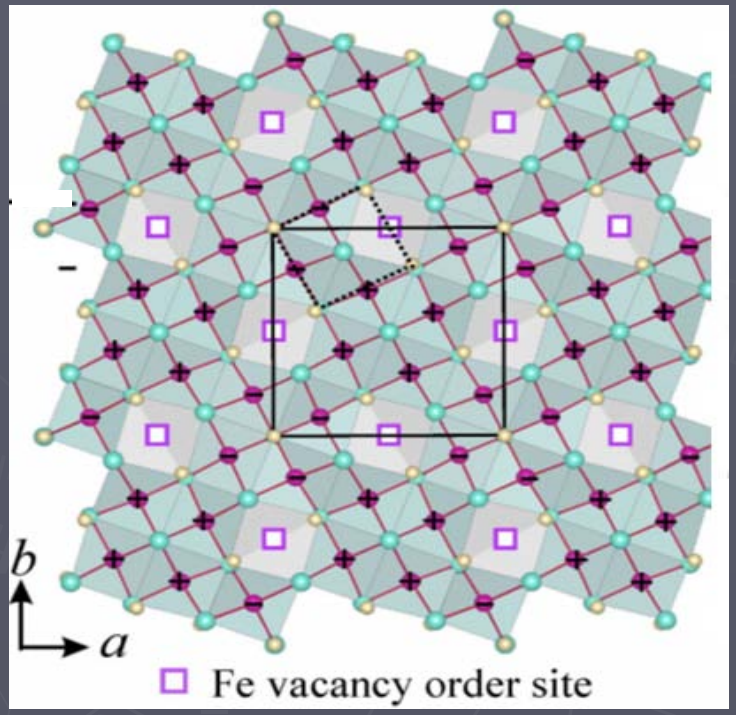




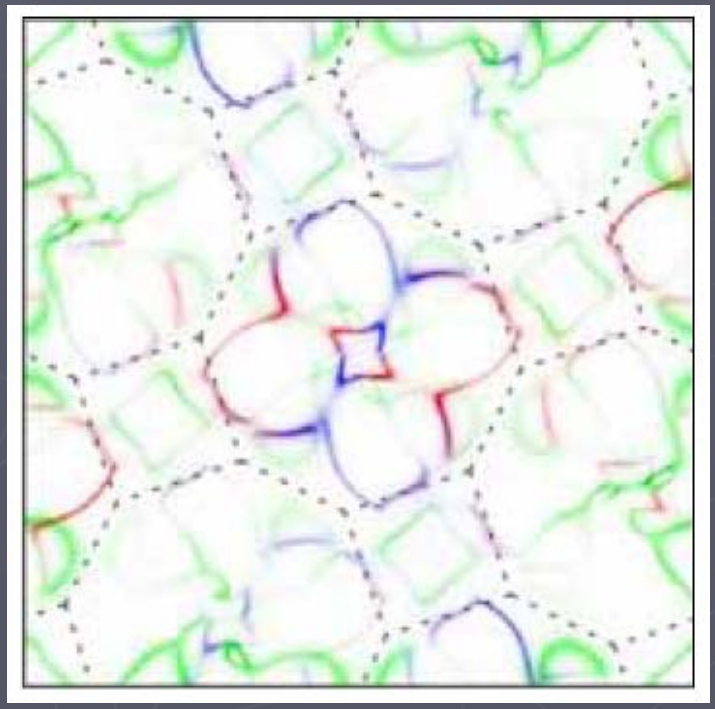
If correct rules out d-wave!

Effect of Fe vacancies?

Han et al 2011: possibility that SC takes place in state with *disordered* vacancies?



W. Bao et al, CPL 2011



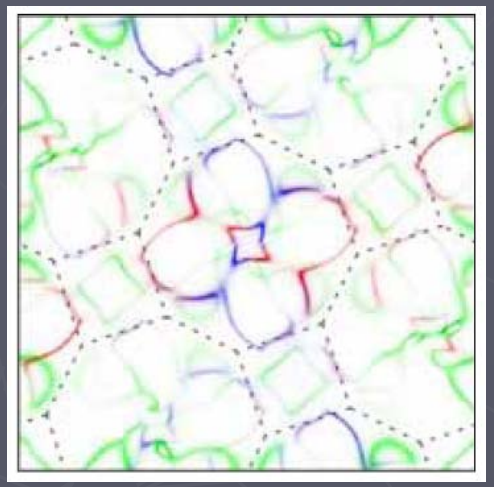
Lin et al, PRL 2011

Fermi surface of paramagnetic
vacancy $\sqrt{5}\times\sqrt{5}$ block state in 1-Fe zone
But: ARPES sees no reconstruction of bands

Effect of Fe vacancies?

Berlijn et al 2012: average over 20 vacancy disorder configurations within effective Hamiltonian method Berlijn et al PRL 2011

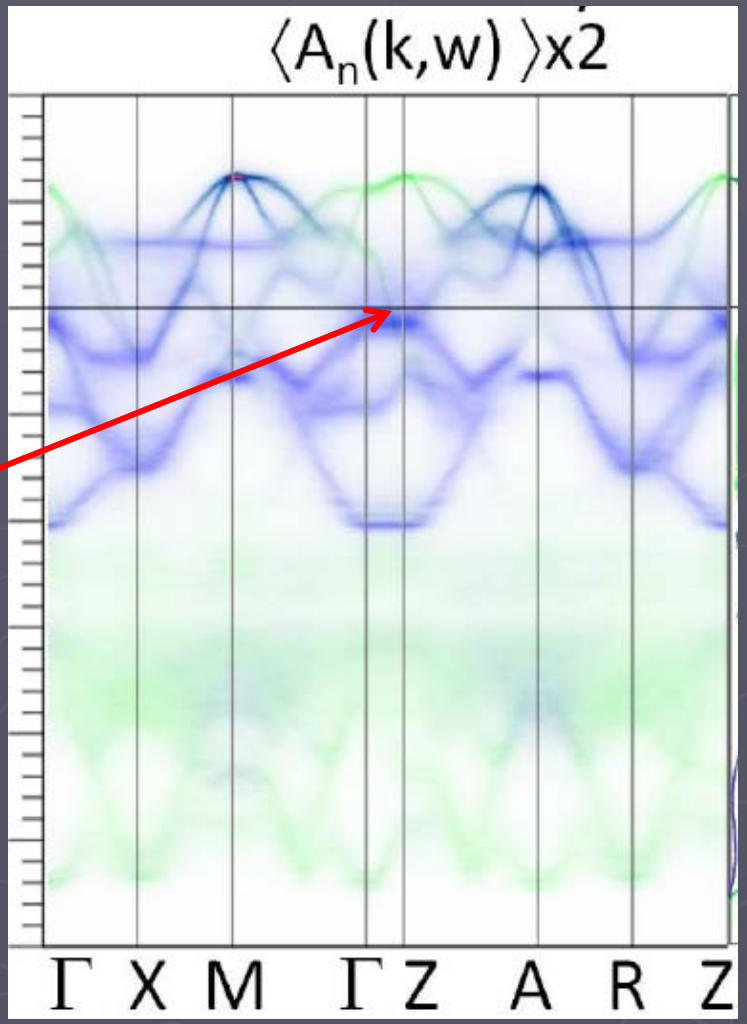
Fermi surface



disorder

Similar to Mou et al

Effective doping: hole pocket shifted below Fermi level



Conclusions

- Magnetic and orbital correlations at high T 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