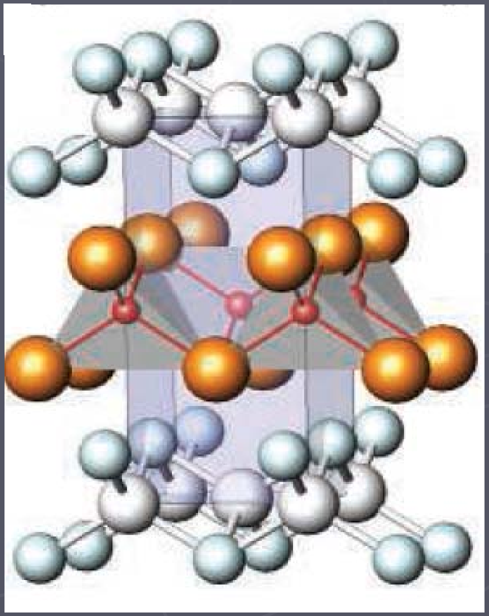
Spin fluctuation pairing in Fe-based superconductors and its consequences

P. Hirschfeld, U Florida
S. Graser, V. Mishra, L. Kemper, H.-P. Cheng, C. Cao,
T. Maier, D.J. Scalapino, I. Vekhter, A. Vorontsov

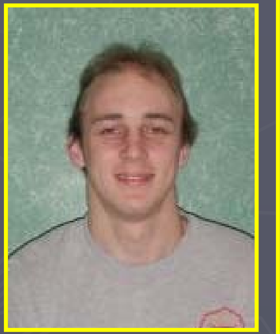


ICMR, July 2009

Collaborators

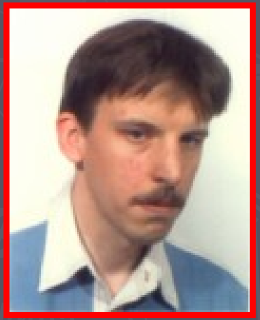
from U. Florida Dept. of Physics:

Vivek Mishra



Lex Kemper

Hai-Ping Cheng



Siggi Graser

Chao Cao

Greg Boyd

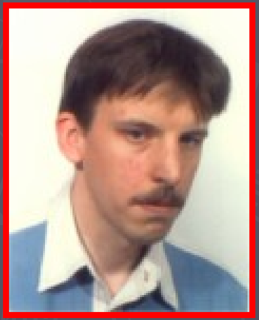
Collaborators

from U. Florida Dept. of Physics:

Vivek Mishra

Lex Kemper

Hai-Ping Cheng

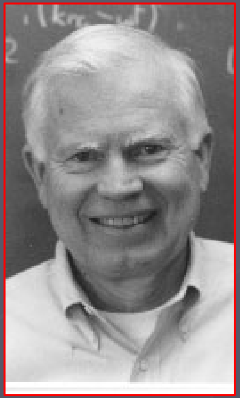


Siggi Graser

Chao Cao

Greg Boyd

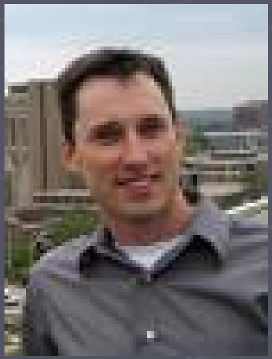
from rest of world:



Doug Scalapino
UCSB

Thomas Maier
ORNL

Ilya Vekhter
Louisiana State

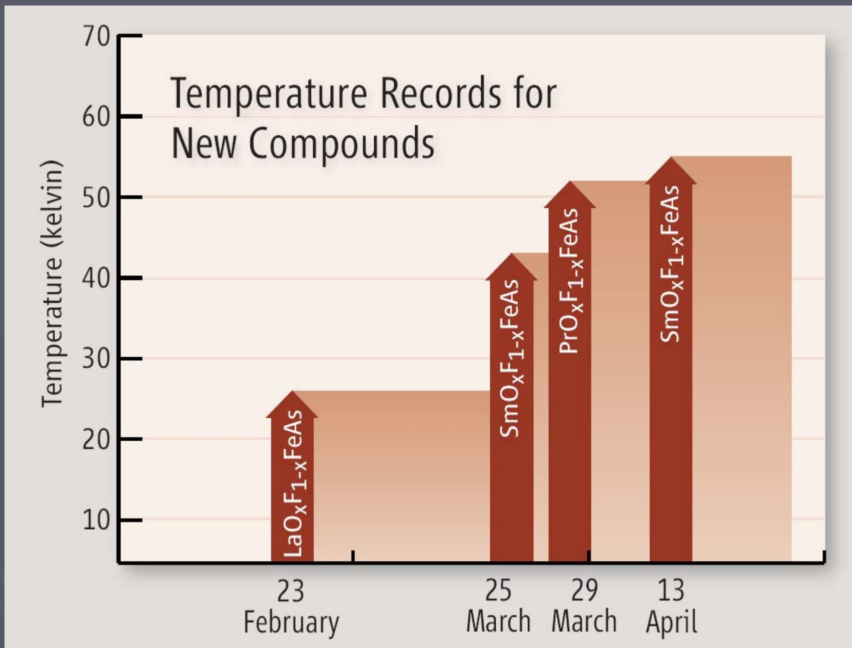


Anton Vorontsov
Montana State

Outline

- Review of Fe-based superconductivity
- Electronic structure/minimal band model
- "contradictory" experiments
- Theory: spin fluctuation pairing
- Disorder in generalized s-states
- Theory of thermal conductivity
- $\Rightarrow$ higher Tc?

First family of ferropnictide SC



Smaller c ↑

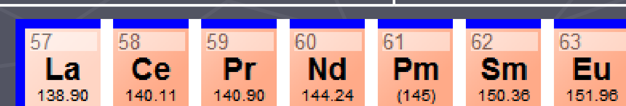
$SmF_xO_{1-x}FeAs$ $x\sim0.2$ d)	Tc=55K, cm/0803.3603 a=3.933A, c=8.4287A
$PrF_xO_{1-x}FeAs$ c)	Tc=52K, cm/0803.4283 a=3.985A, c=8.595A
$CeF_xO_{1-x}FeAs$ b)	Tc=41 K, cm/0803.3790 a=3.996A, c=8.648A
$LaF_xO_{1-x}FeAs$ a)	Tc=26 K, JACS-2008 a=4.036A, c=8.739 A
$La_{1-x}Sr_xOFeAs$	Tc=25K, cm/0803.3021, a=4.035A, c = 8.771A

a) Y. Kamihara et.al., Tokyo, JACS
b) X.H. Chen, et.al., Beijing,arXiv: 0803.3790
c) Zhi-An Ren, Beijing, arXiv: 0803.4283
d) Zhi-An Ren, Beijing, arXiv: 0804.2053.

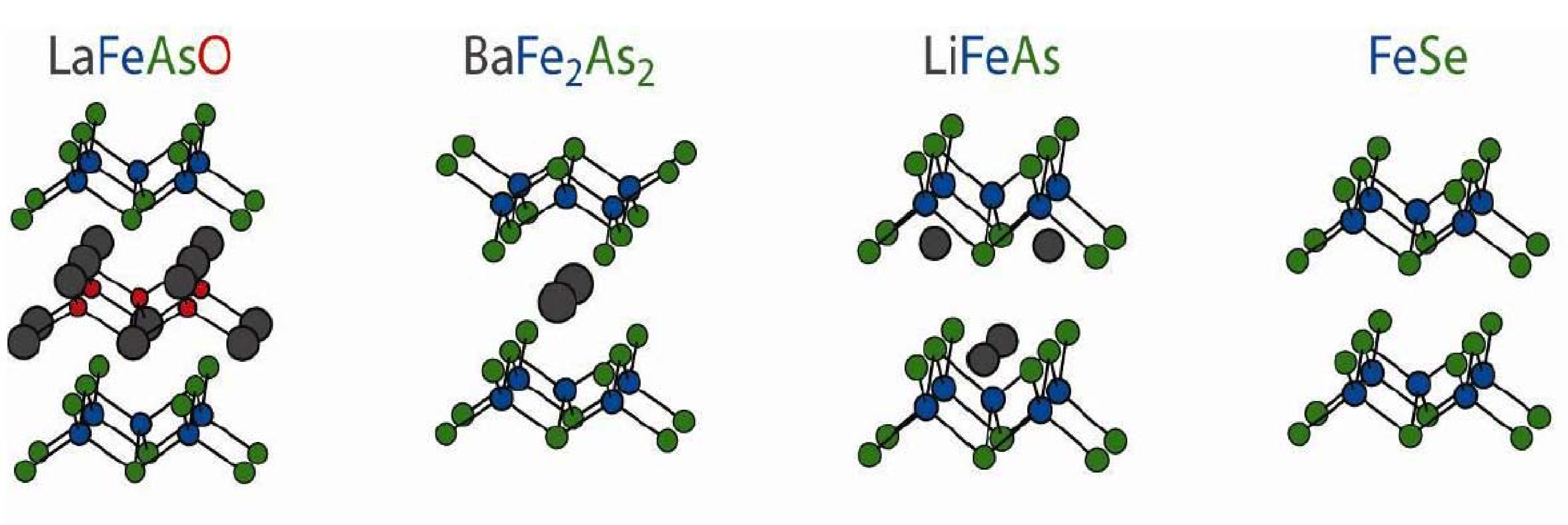
also:

LOFFA under pressure: T_c=43K
(Takahashi et al Nature 453 376 (2008))

Rare earths:



1111 vs. 122 vs. 111 vs. 11 materials



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 arXiv: 0806.4688

T_c=8K

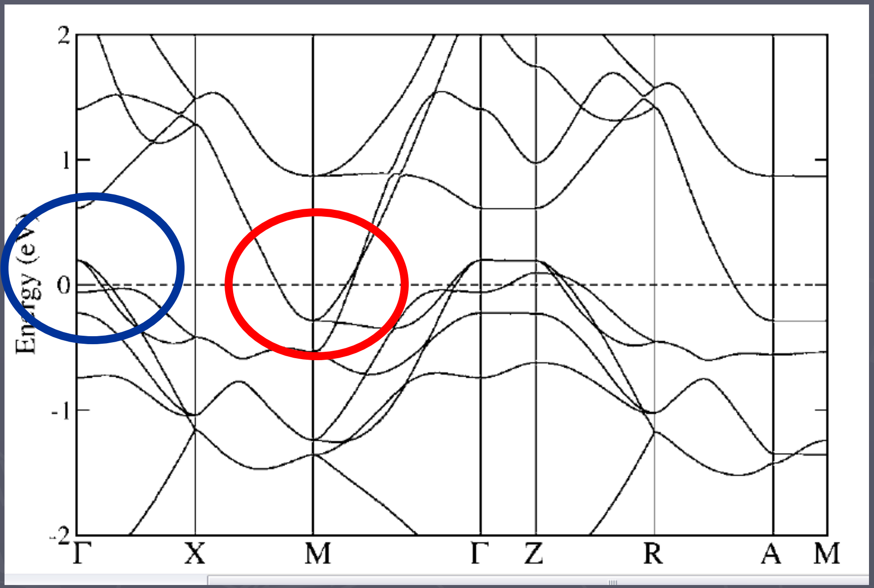
Hsu et al arXiv:0807.2369

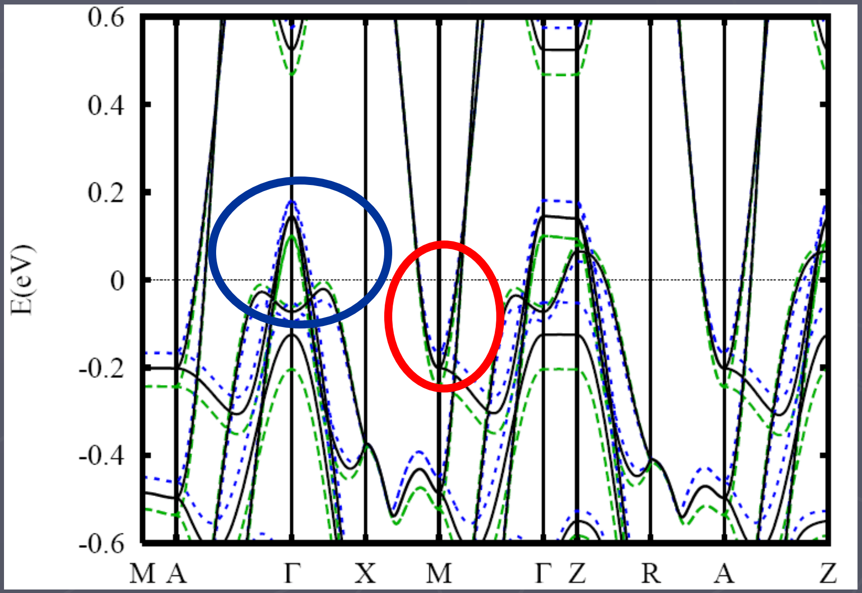
No arsenic ☺!

Electronic structure calculations

LOFP Lebegue 2007 T_c=6K

LOFA Singh & Du 2008 T_c=28K

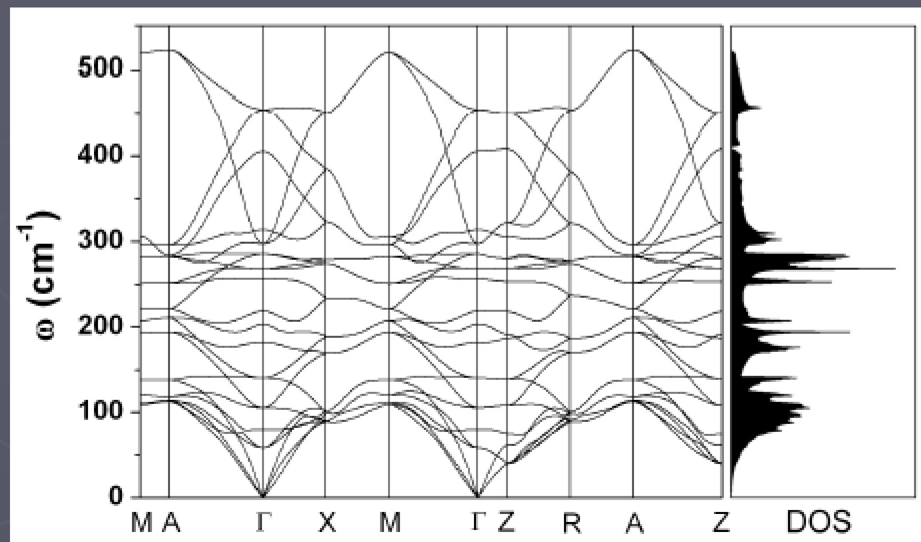




Band structures for 2 materials nearly identical!
Hole pocket near Γ, electron pocket near M

What accounts for factor 5 difference in T_c?

Further conclusions of electronic structure calculations: e-ph coupling is *weak*



Singh & Du PRL 2008

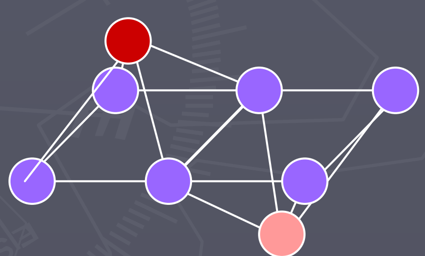
We have calculated *ab initio* the electron-phonon spectral function, $\alpha^2 F(\omega)$, and coupling, λ, for the stoichiometric compound [9]. Some moderate coupling exists, mostly to As modes, but the total λ appears to be ~ 0.2, with $\omega_{log} \sim 250$ K, which can in no way explain $T_c \gtrsim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

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

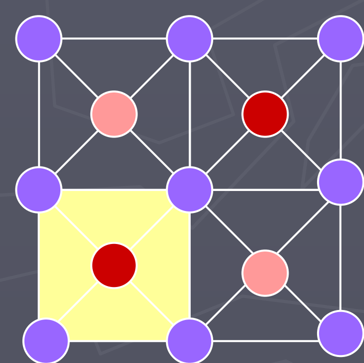
Understanding electronic structure

Band structure – Fe-As-Fe vs. Fe-Fe unit cell

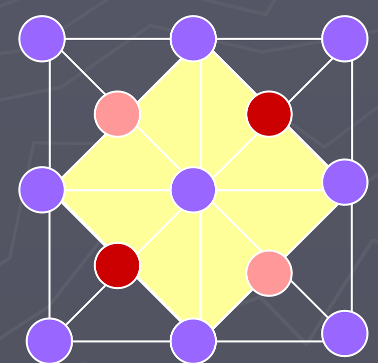
Real unit cell consists of 2 Fe and 2 As atoms, but due to the high degeneracy of the two As positions it is convenient to look at an effective unit cell with only 1 Fe and 1 As atom



Fe-Fe cell
„effective“ unit cell



Fe-As-Fe cell
„real“ unit cell

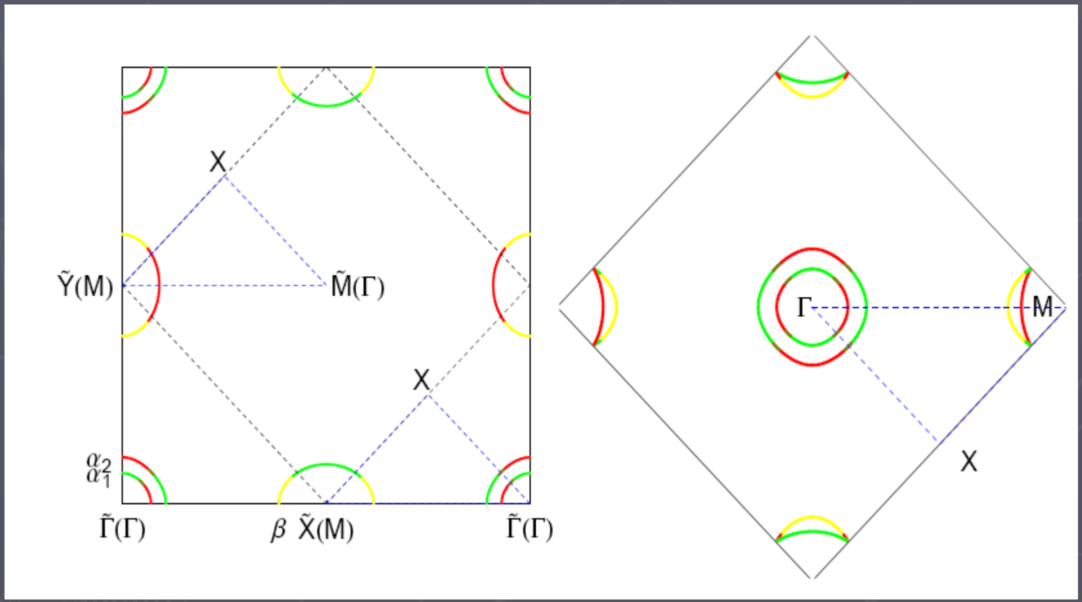


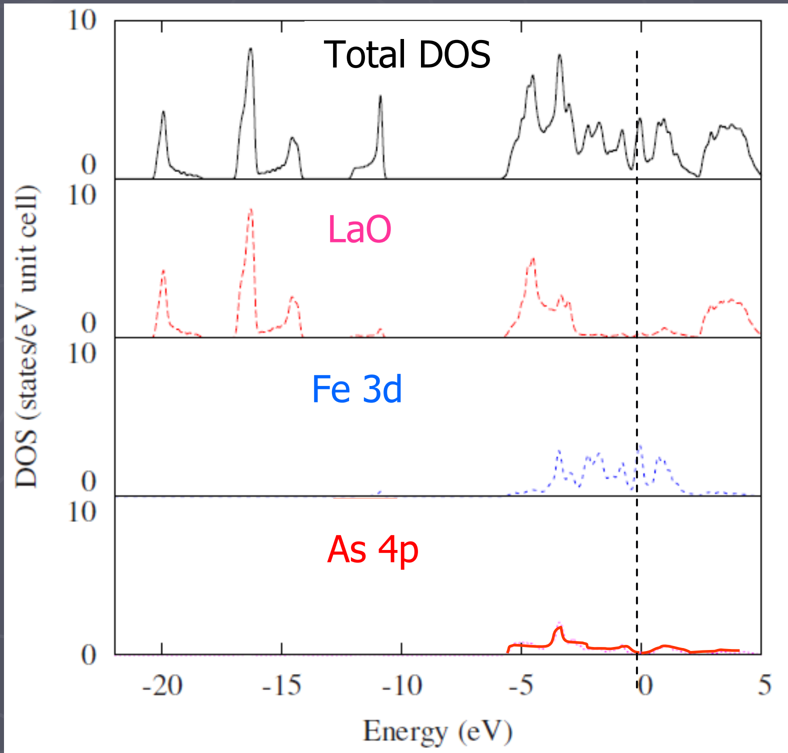
Understanding electronic structure

Fe-As-Fe vs. Fe-Fe unit cell

As DOS at Fermi level negligible: use „effective“ Fe-Fe cell.

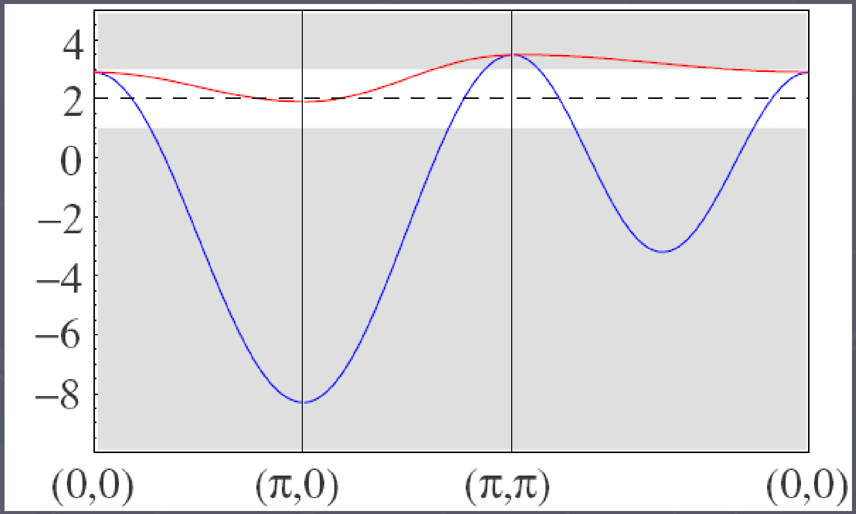
Advantage: We can write down an effective 5 band Fe-Fe model Hamiltonian



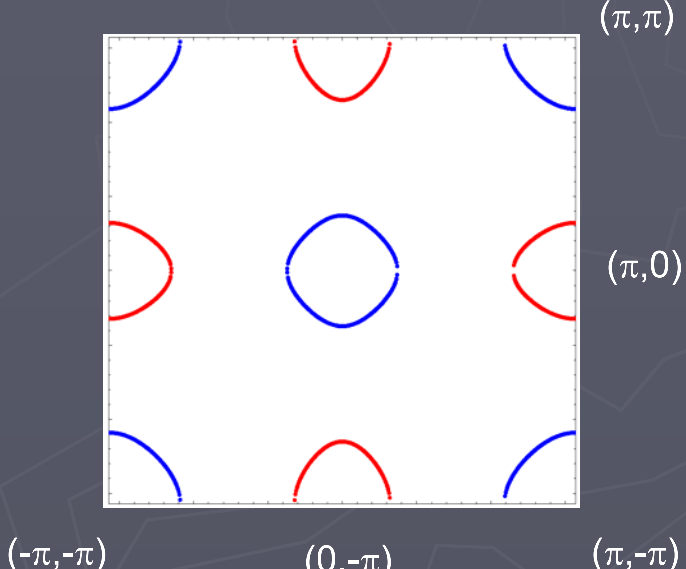


Band structure – Two-band approximation

Assumption (many authors): Most important inter- and intra-orbital hopping between the Fe d_{xz} and d_{yz} orbitals mediated by As p_x and p_y orbitals



Band structure



FS sheets

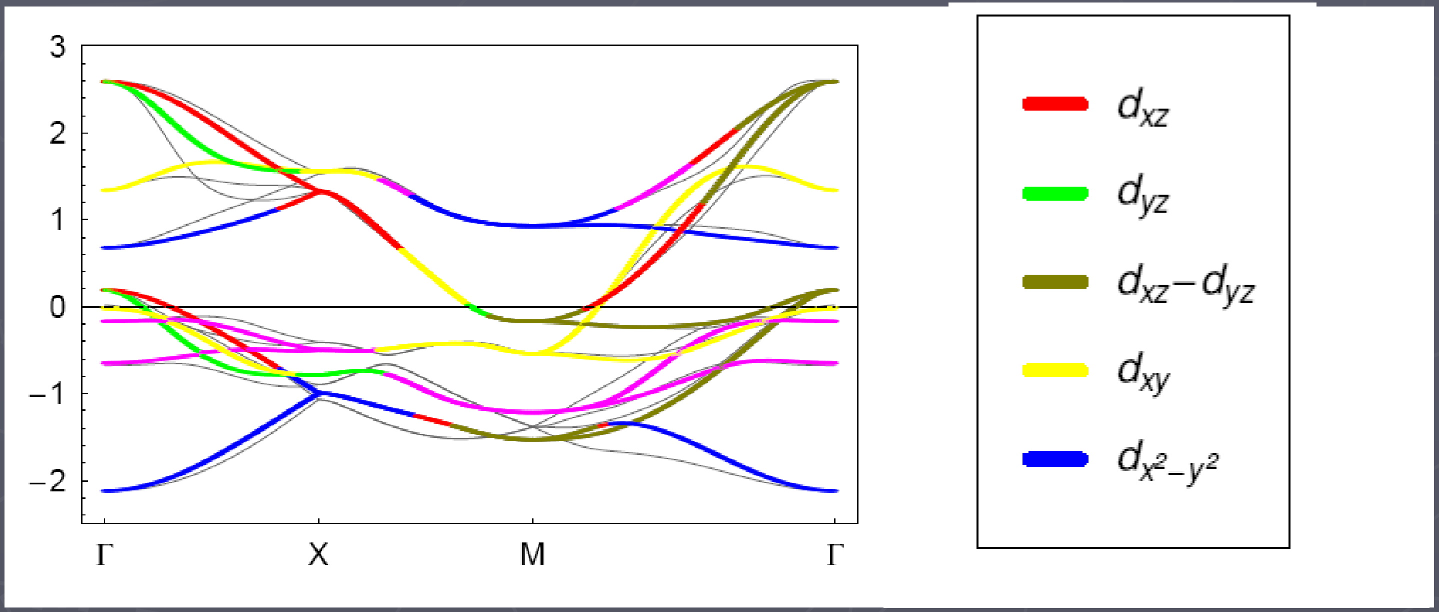
BUT: There should be no FS sheet around (π,π) in the extended „effective" BZ, instead both α FS sheets should be around (0,0)

⇒ 2-band models can produce right folded FS topology, but wrong band character, Fermi velocities, ...

Band structure – Five band model

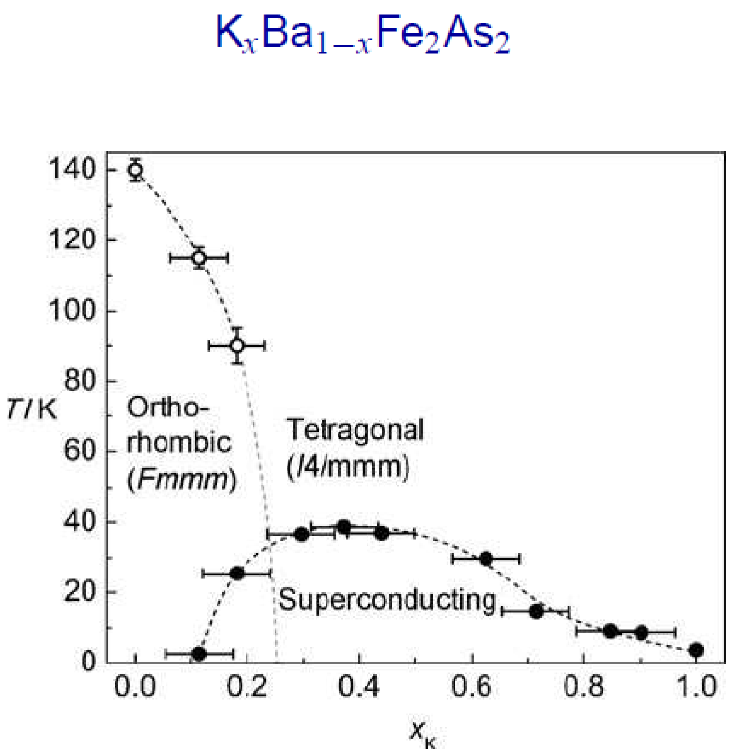
Graser et al. NJP 2009

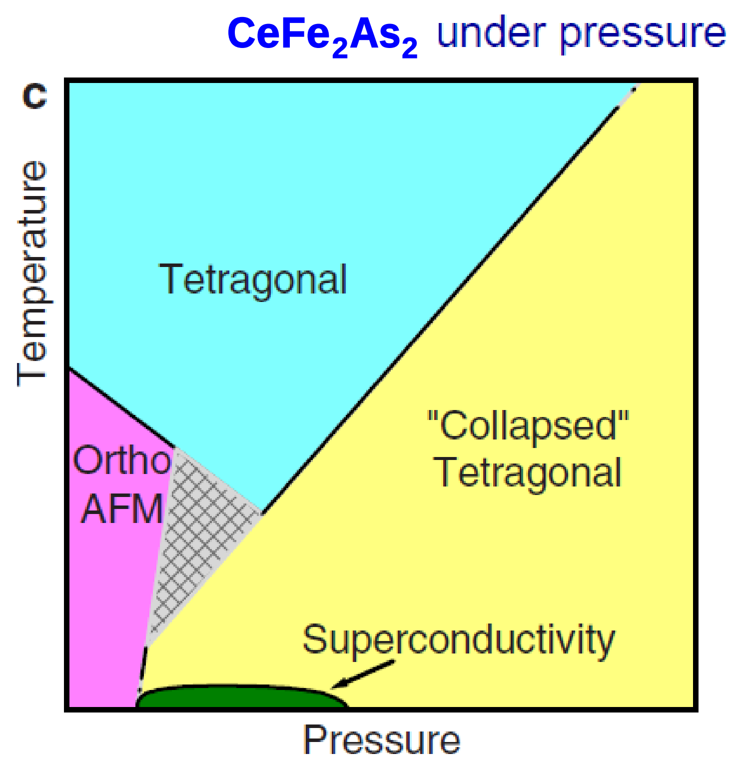
Fit to *Cao et al* PRB 77, 220506 (2008) see also *Kuroki et al* PRL **101**, 087004 (2008)



Notes on 122 materials

- T_c up to 38 K
- good crystals which cleave well—ARPES, STM
- dope with K or Co, or apply pressure to obtain superconductivity
- properties are more 3D than 1111 materials



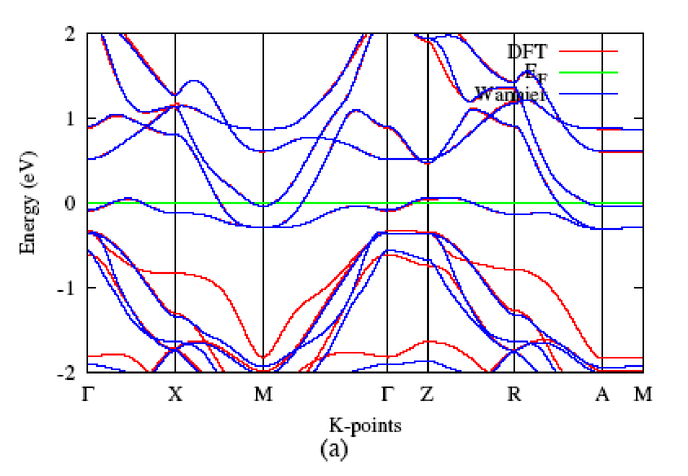


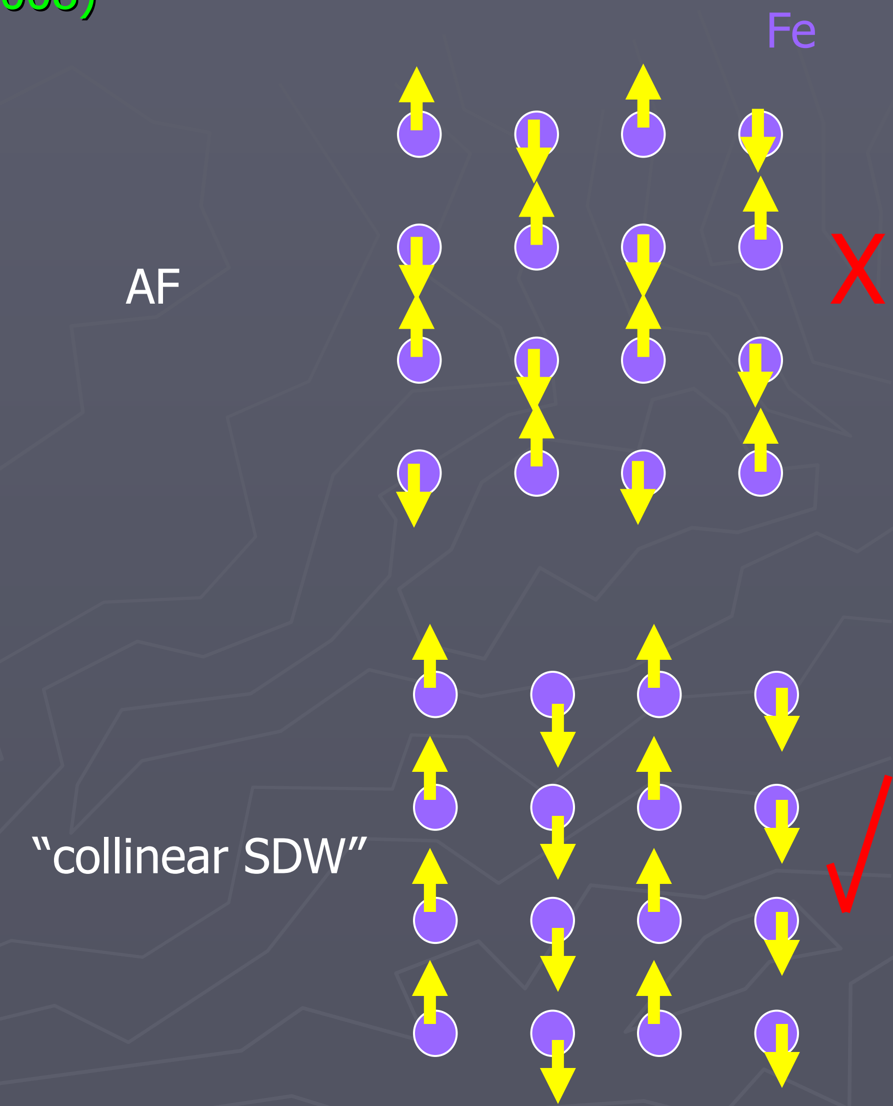
Rotter *et al.* Ang. Chem., **47** 7949 (2008)

Kreyssig *et al.* PRB **78**, 184517 (2008)

Parent compounds are ordered antiferromagnets

Cao et al. Phys. Rev. B 77, 220506 (2008)



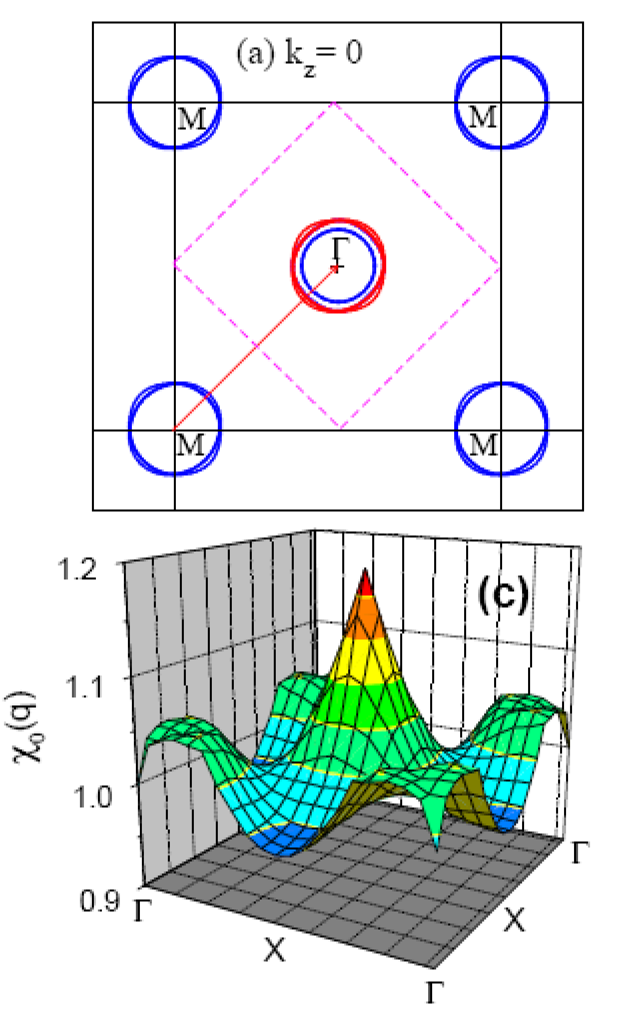


State with AF order is ~40meV lower in energy than paramagnetic state.

But linear SDW state (Dong et al EPL 2008) ~100meV lower!

Both magnetic states found by LDA have ~$2\mu_B$ ordered staggered moment. (exception: Yildrim PRL 2008)

Weak coupling perspective: nesting of FS and susceptibility



Dong et al. EPL 2008

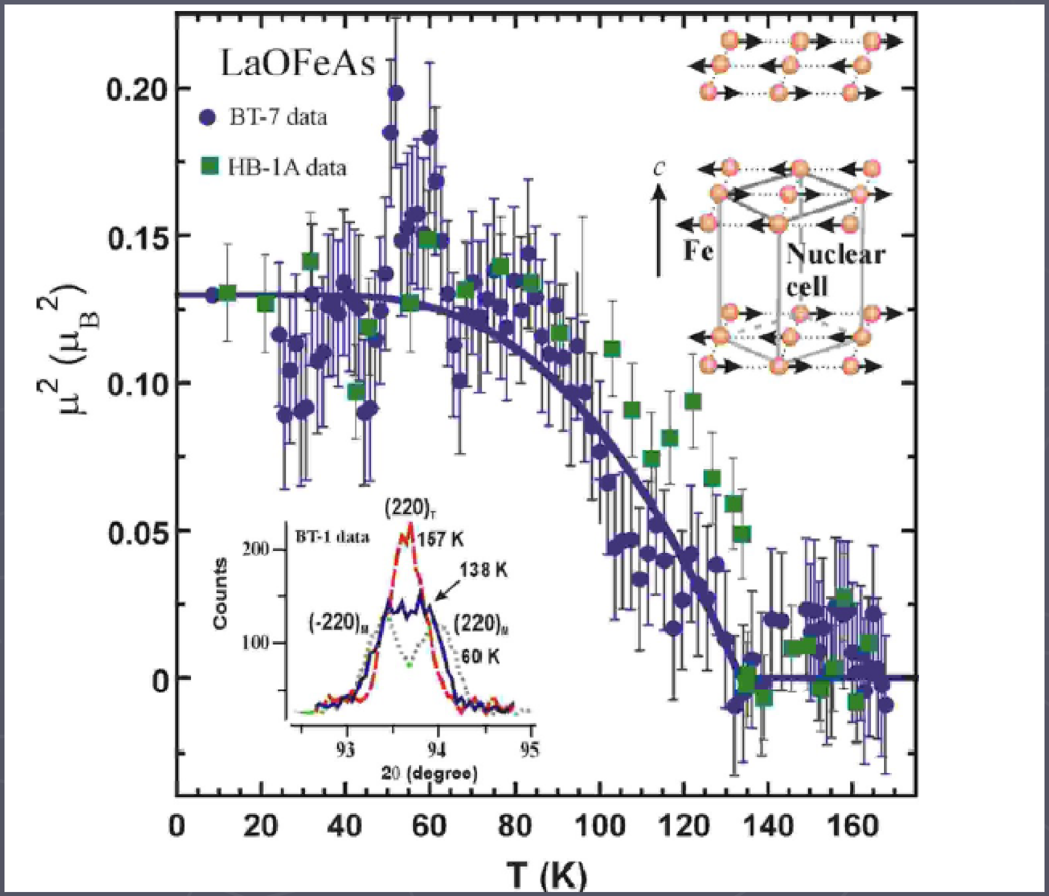
Simple picture put forward by Dong et al:

Small peak in x due to near nesting of FS sheets drives magnetic instability. Doping destroys nesting, kills SDW. Nesting vector is Q=π,π in correct BZ, (or Q =π,0 in effective BZ).

Nesting feature and concomittant susceptibility peak are driving forces for a spin-fluctuation pairing mechanism in several theories.

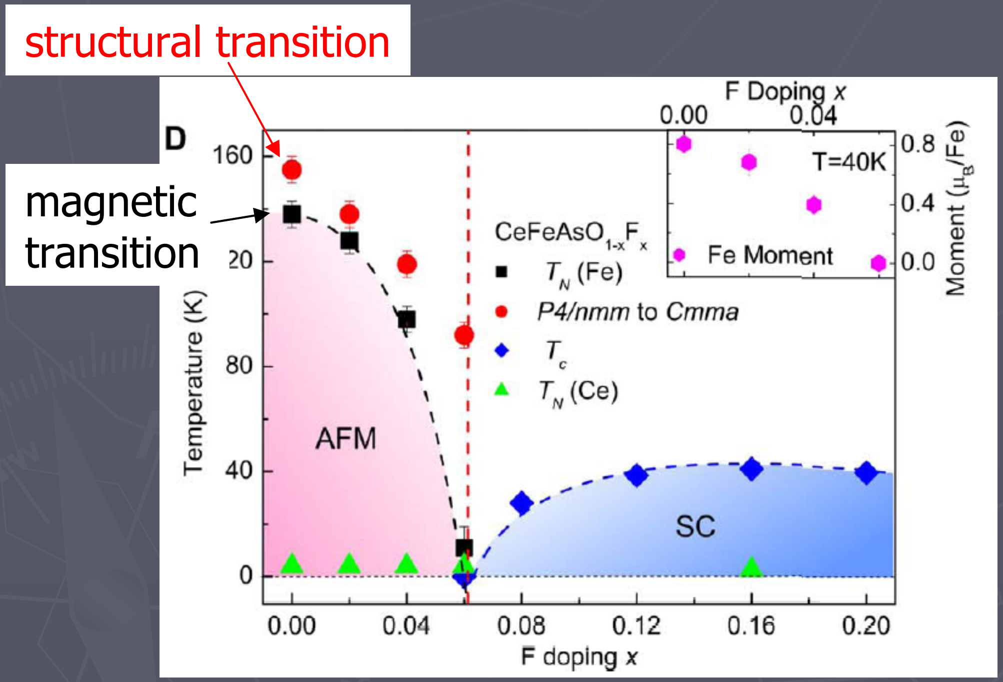
Neutron scattering verifies collinear SDW state

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

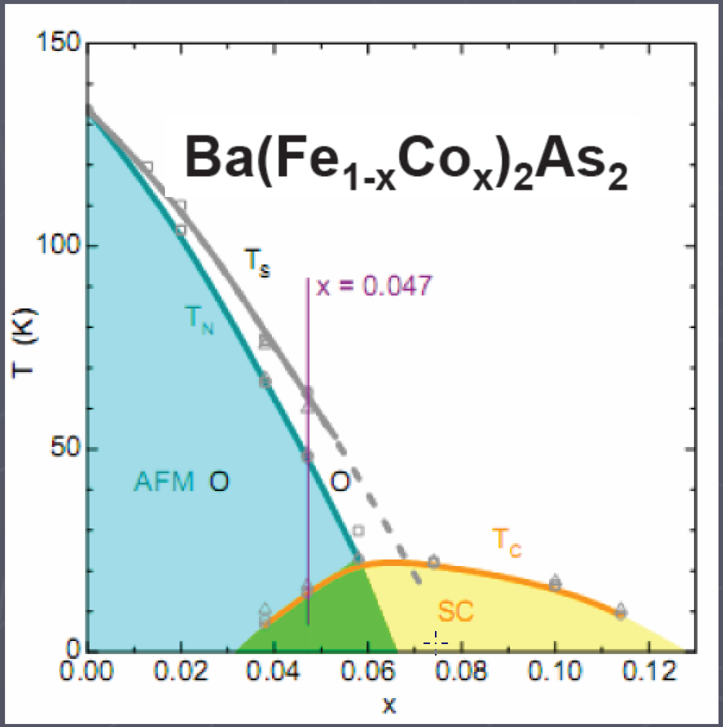


But size of ordered moment is only 0.36 μ_B (others larger)!

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



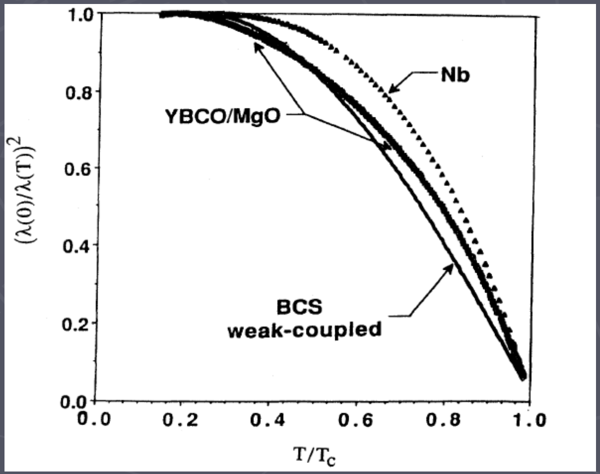
Zhao et al arXiv:0806.2528

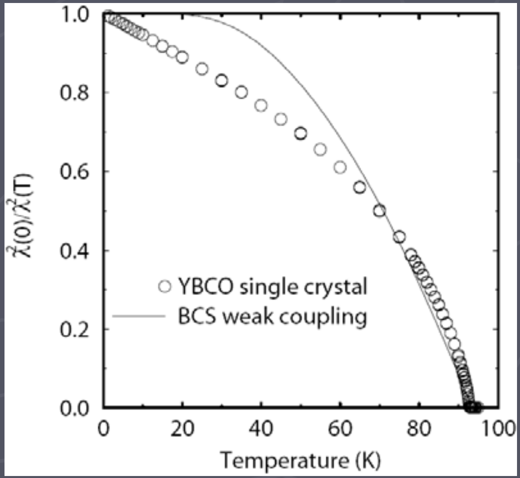


D.K. Pratt et al, aXv 0903.2833

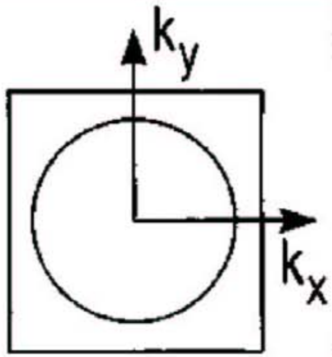
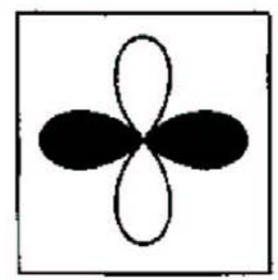
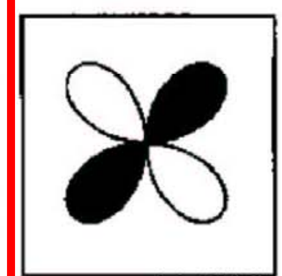
Controversy: symmetry of order parameter?

- Early measurements on powdered LOFFA supported low energy excitations, Andreev surface states, NMR $T_1 \sim T^3 \Leftrightarrow$ nodes.
- Some penetration depth measurements, ARPES suggest isotropic gap
- Recall situation in cuprate field early 90's: lack of understanding of disorder effects, lack of low T data led to wrong conclusions



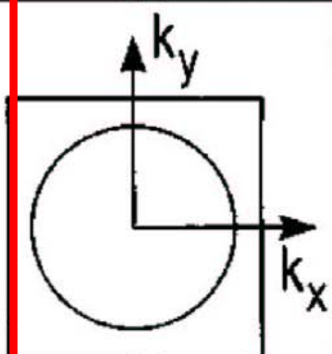
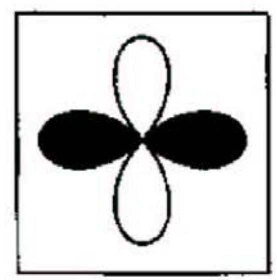
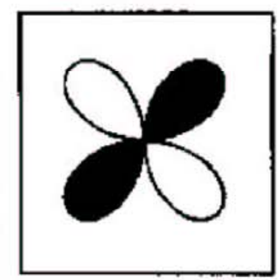


Unconventional superconductors (1-band)

Group-theoretic notation	A_{1g}	A_{2g}	B_{1g}	B_{2g}
Order parameter basis function	constant	$xy(x^2-y^2)$	x^2-y^2	xy
Wave function name	s-wave	g	$d_{x^2-y^2}$	d_{xy}
Schematic representation of Δ(k) in B.Z.				

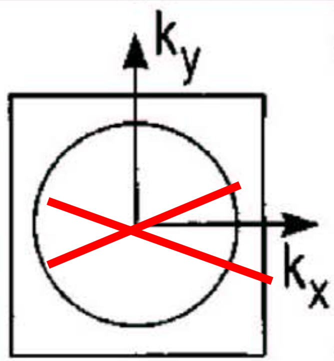
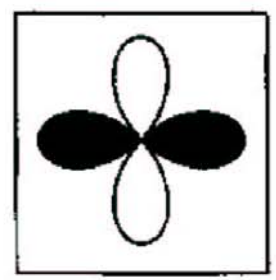
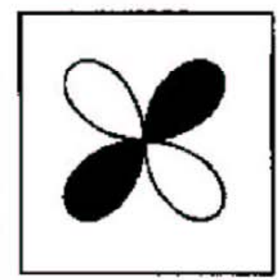
Cuprates

Unconventional superconductors (1-band)

Group-theoretic notation	A_{1g}	A_{2g}	B_{1g}	B_{2g}
Order parameter basis function	constant	$xy(x^2-y^2)$	x^2-y^2	xy
Wave function name	s-wave	g	$d_{x^2-y^2}$	d_{xy}
Schematic representation of $\Delta(k)$ in B.Z.				

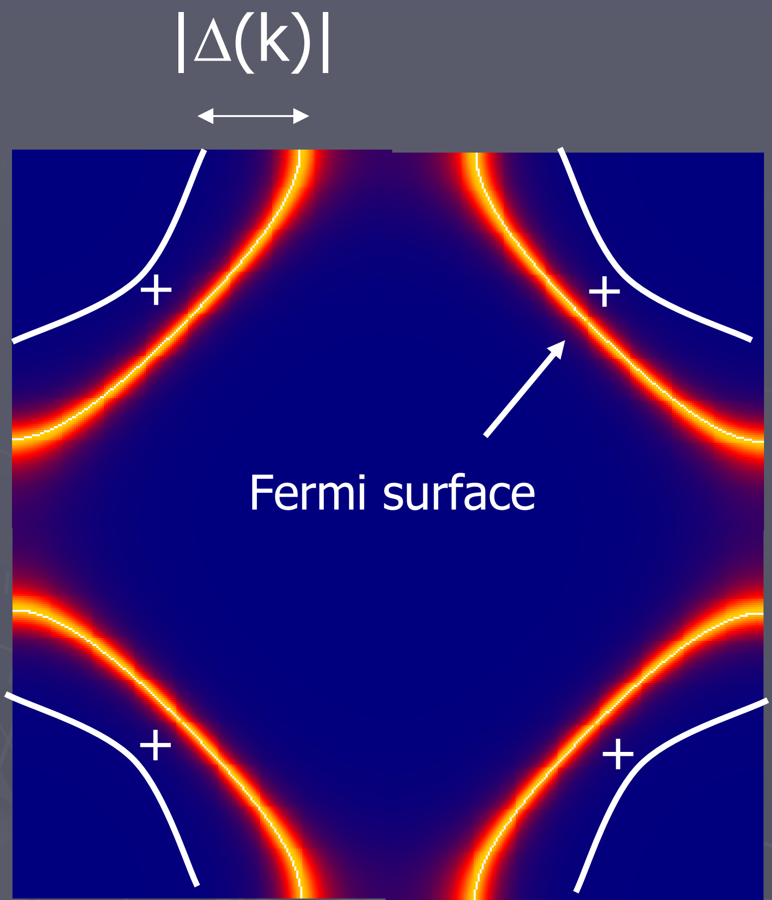
Pnictides??

Unconventional superconductors ~~(1-band)~~

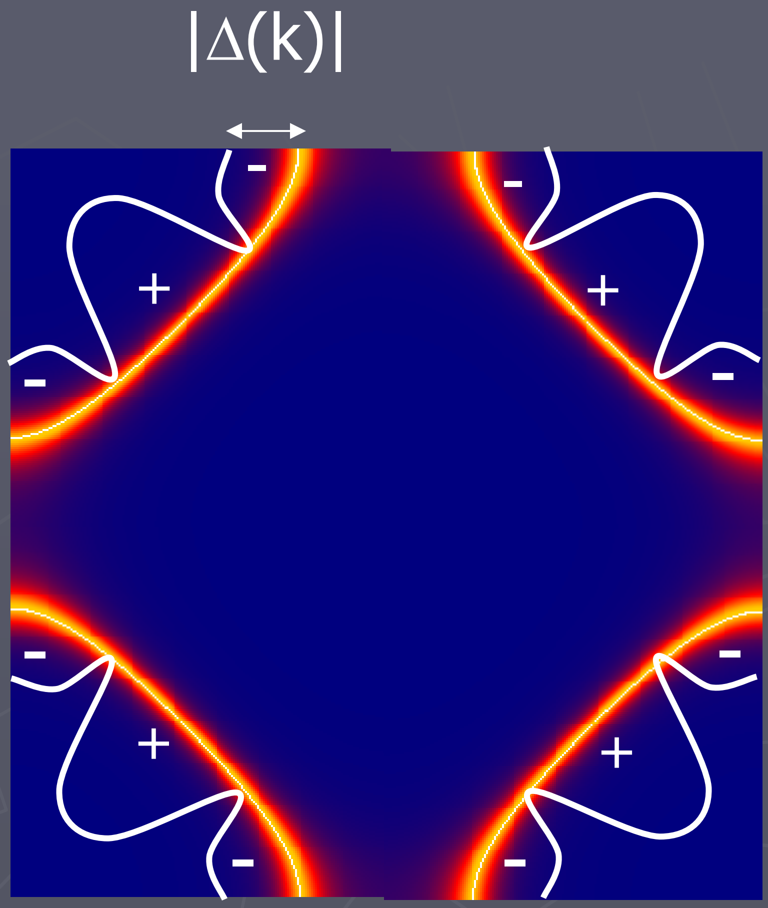
Group-theoretic notation	A_{1g}	A_{2g}	B_{1g}	B_{2g}
Order parameter basis function	~~constant~~	$xy(x^2-y^2)$	x^2-y^2	xy
Wave function name	"s-wave"	g	$d_{x^2-y^2}$	d_{xy}
Schematic representation of $\Delta(k)$ in B.Z.				

Pnictides??

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

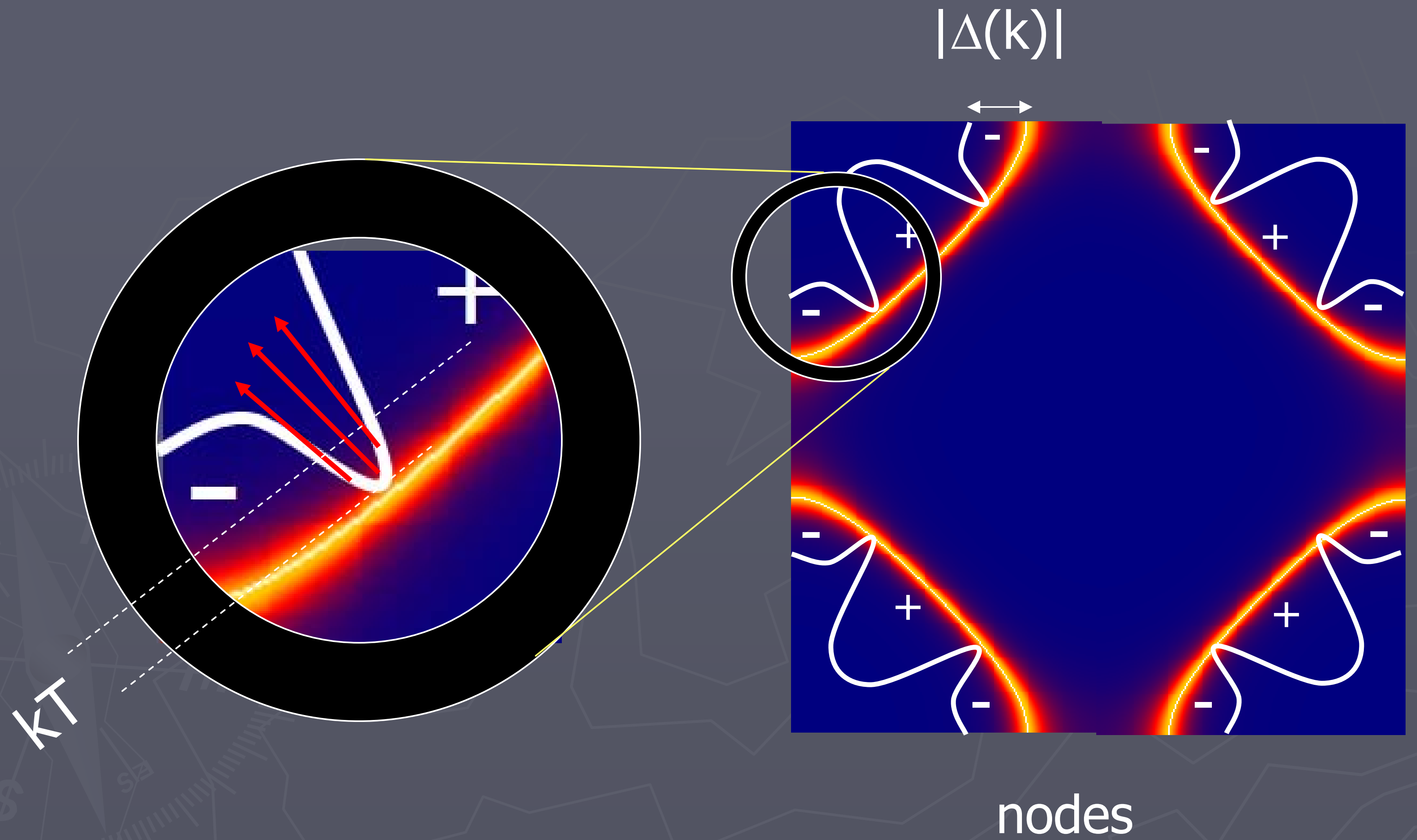


no nodes

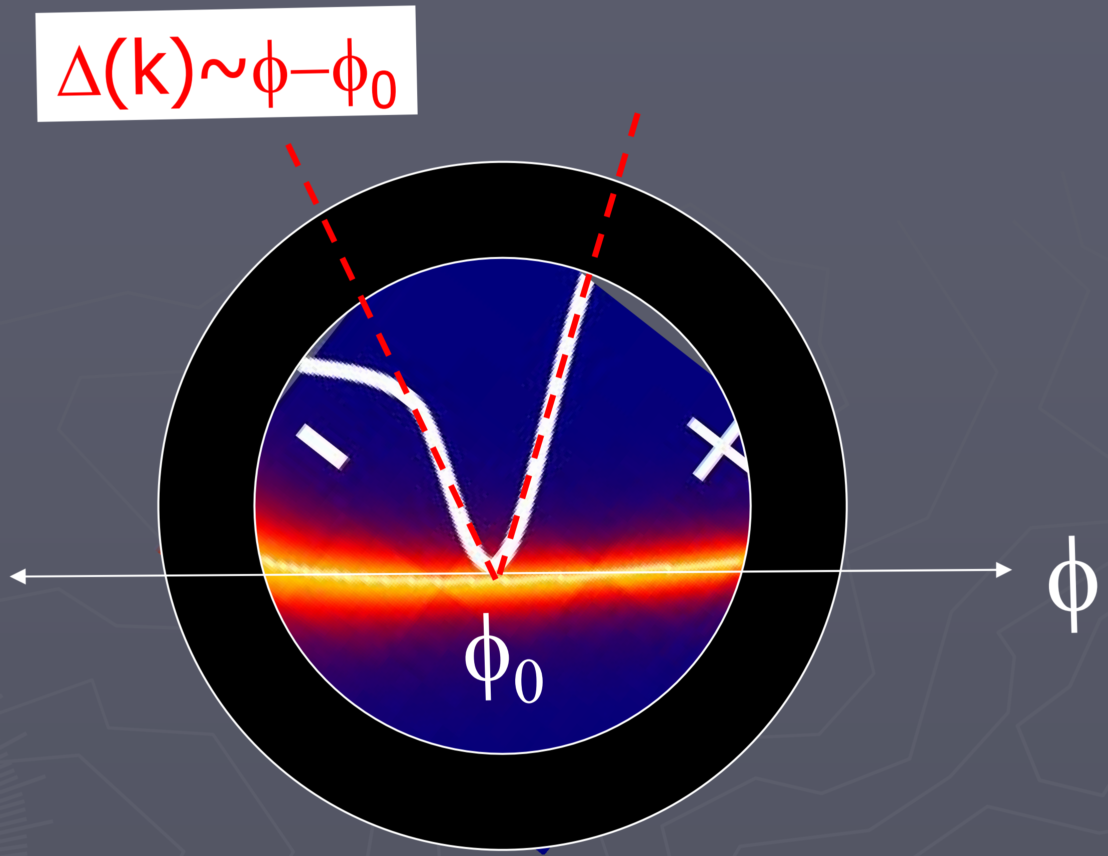


nodes

Nodal excitations dominate low T properties



Linear DOS from line nodes

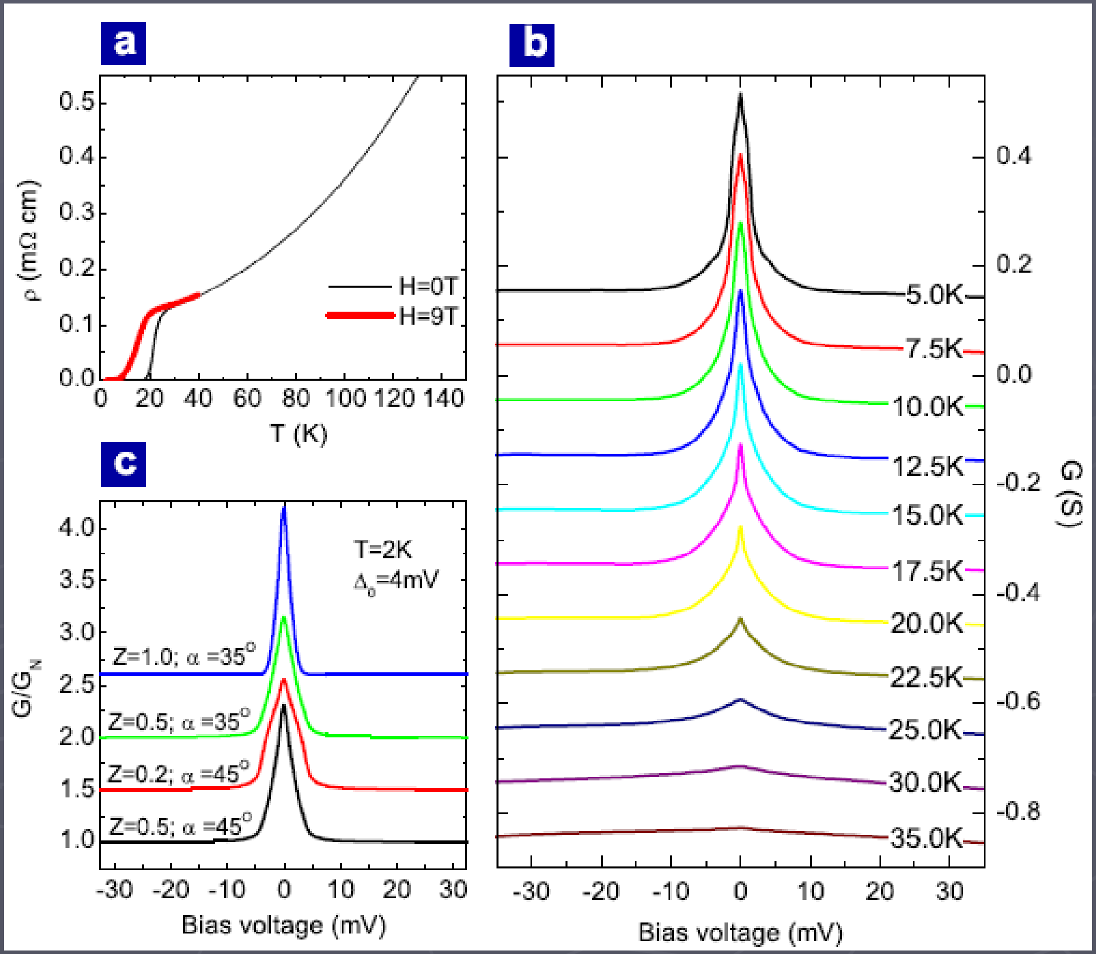


$$N(\omega) = \int \frac{d\phi}{2\pi} \mathrm{Re} \frac{\omega}{\sqrt{\omega^2 - \Delta_0{}^2 (\phi - \phi_0)^2}} \approx \frac{\omega}{\Delta_0}$$

Early evidence for nodes 1: Andreev pt contact spectroscopy

Shan et al EPL 2008

LOFFA



expt

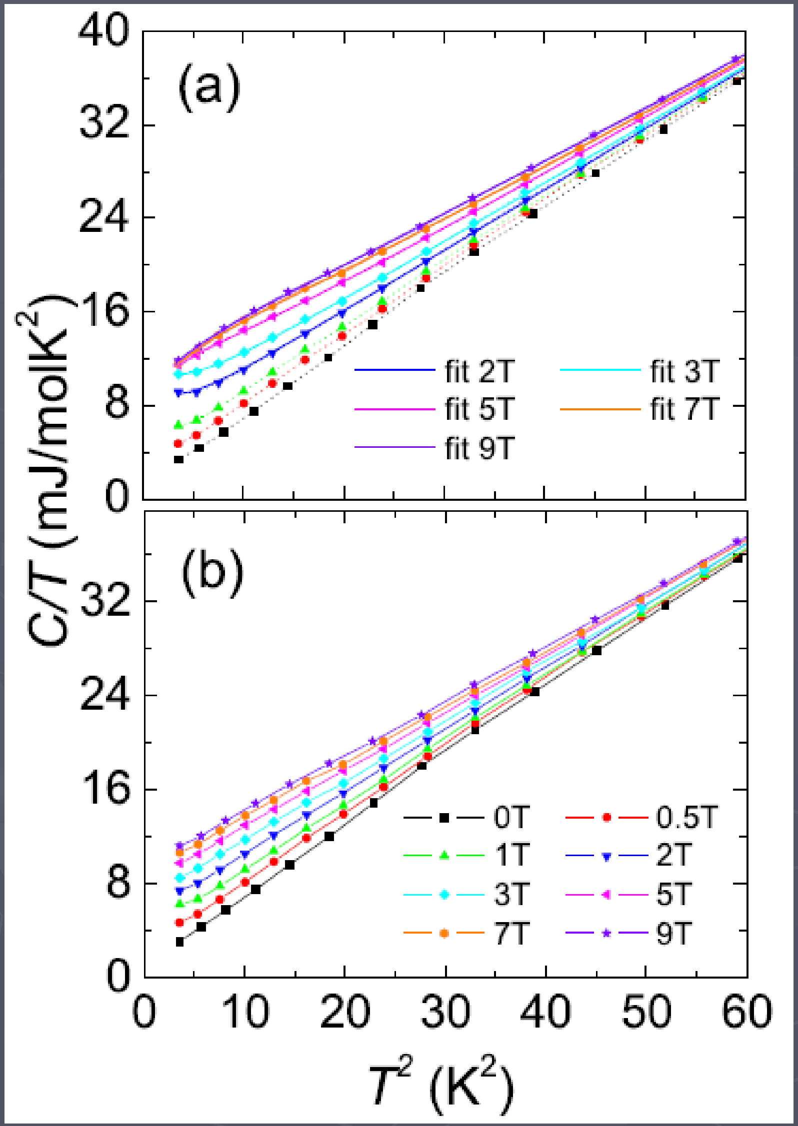
BTK theory

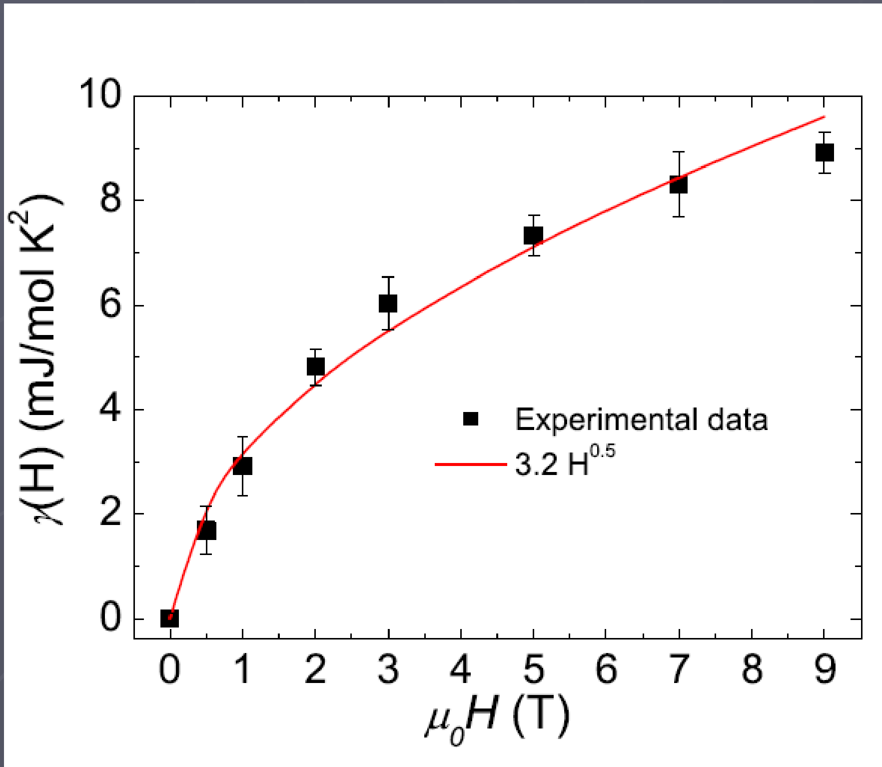
(similar to d-wave)

Early evidence for nodes II: Volovik effect

Mu et al Chin.Phys.Lett. (2008)

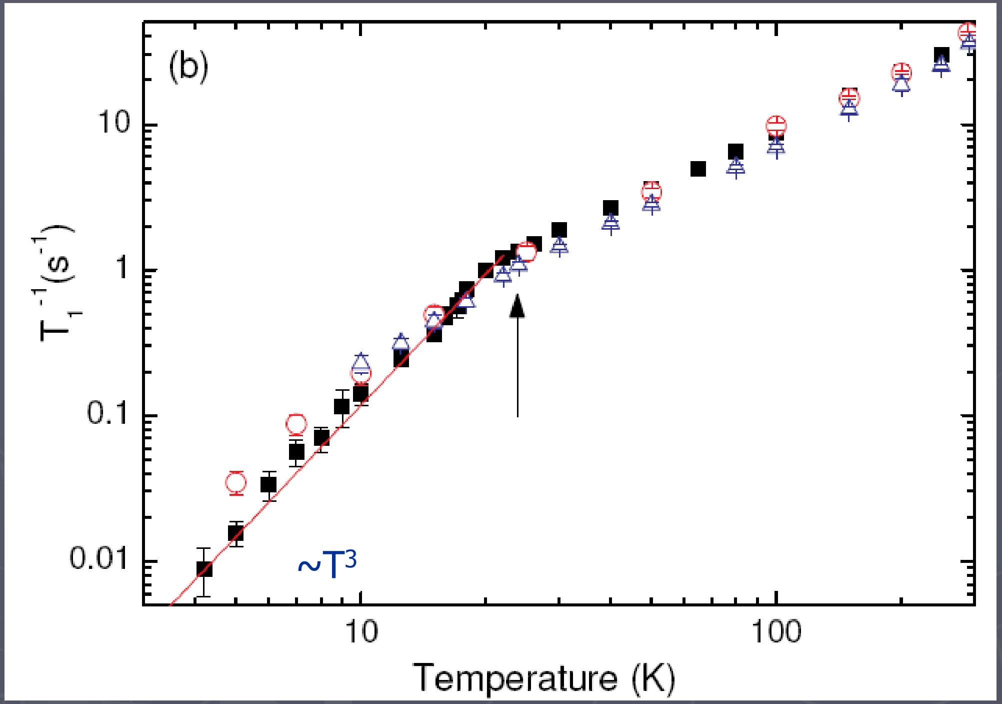
LOFFA

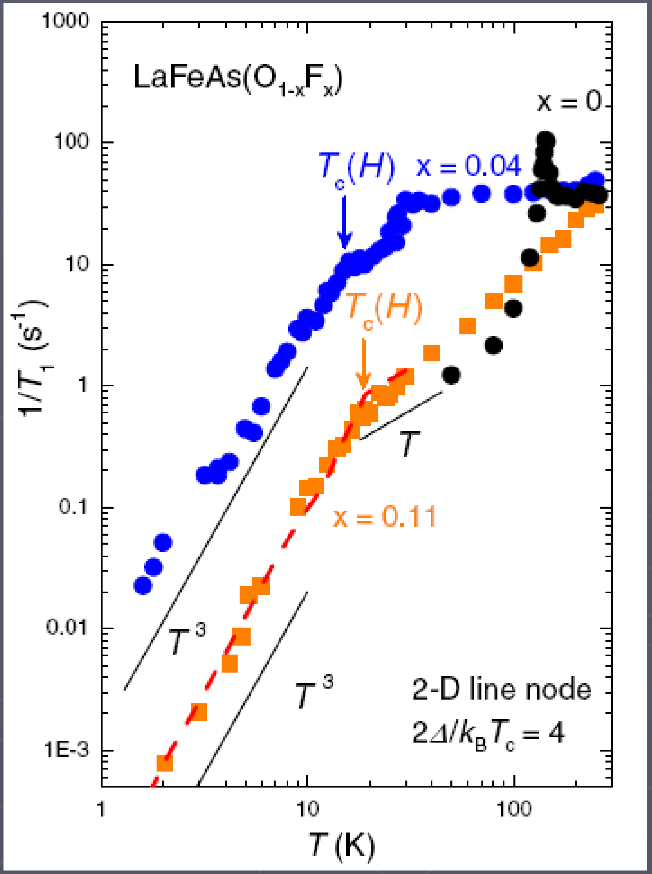




Early evidence for nodes III: NMR

LOFFA





Grafe et al PRL (2008)

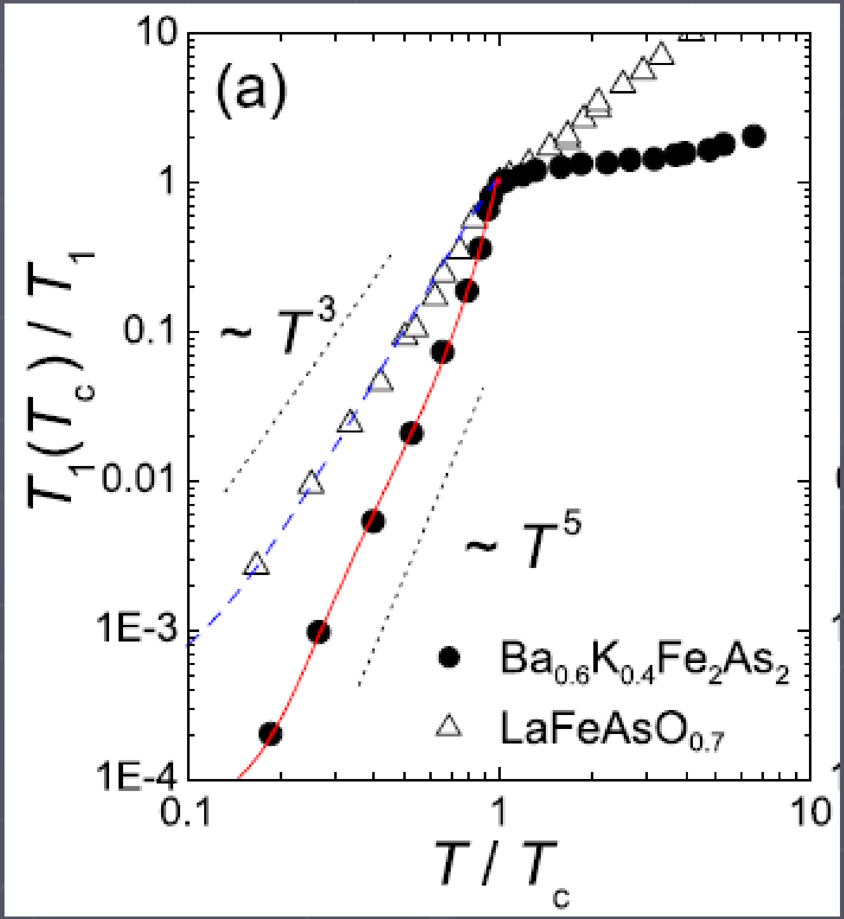
Nakai et al. JPSJ (2008)

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

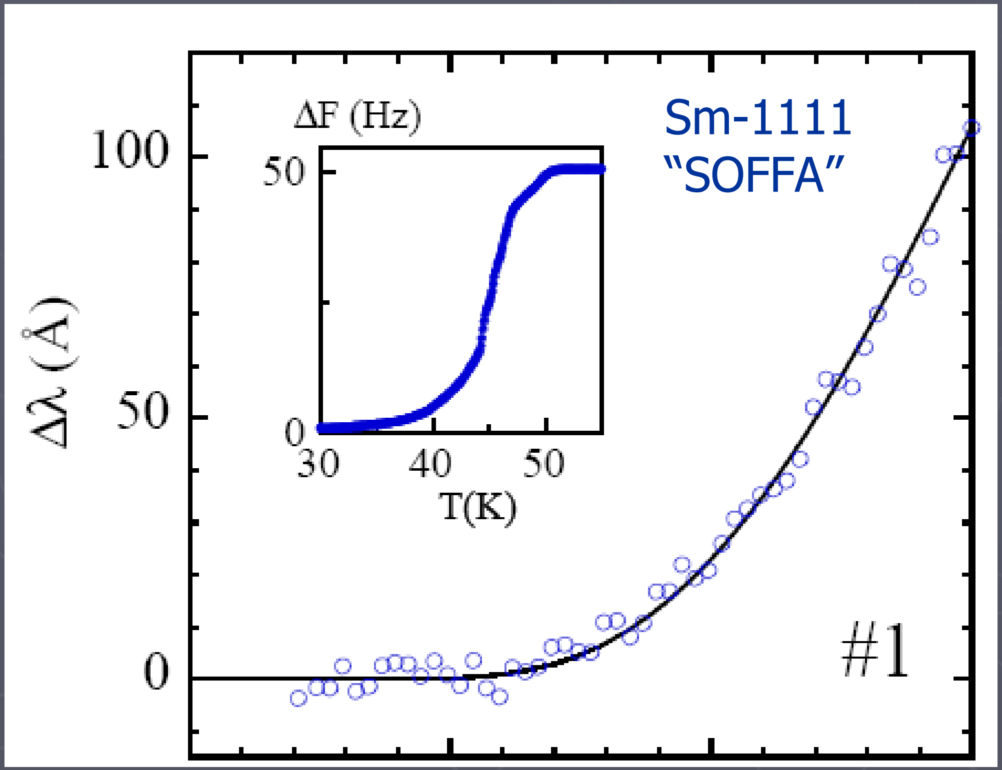
PH et al 1988 ⟵⟶ line nodes ⇒ $N(\omega) \sim \omega$ ⇒ T^3 !

NMR on K-doped Ba-122

Yashima et al arXiv:0905.1896



Early penetration depth experiments reported *exponential* λ(T) (⇒ full gap)

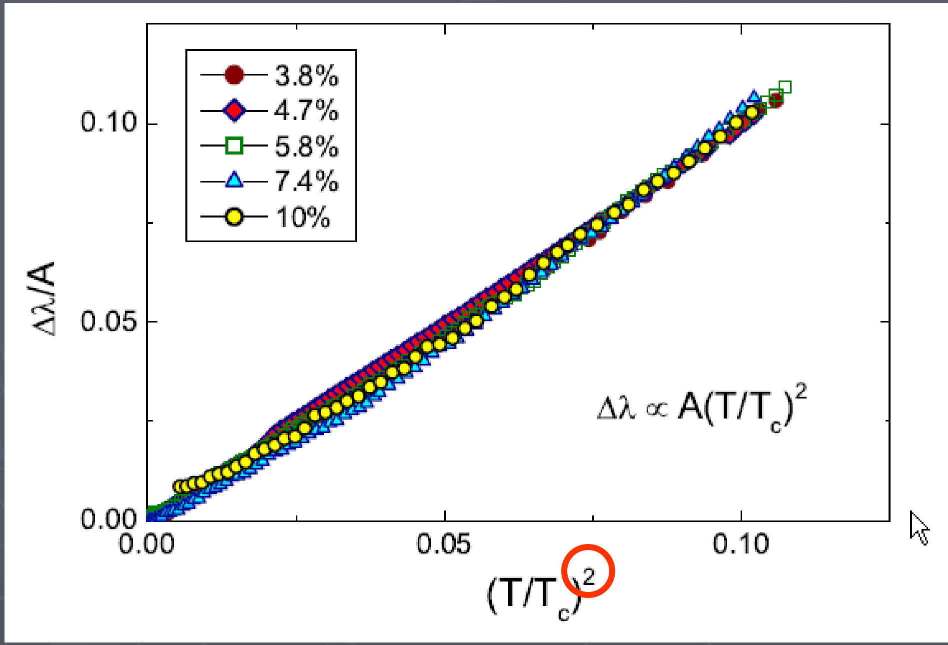


Malone et al Phys. Rev. B 2009

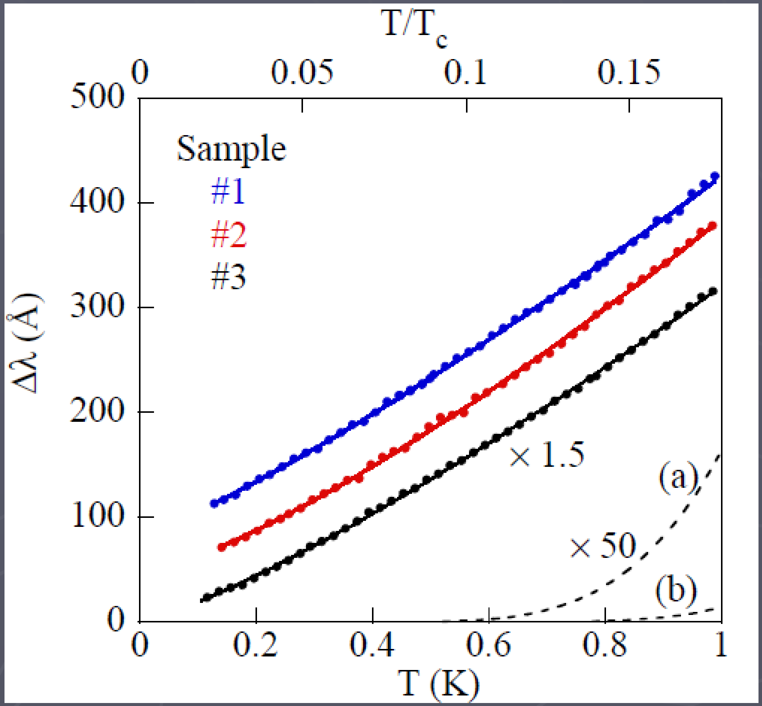
Caution: magnetism of rare earth ions

Other pen. depth experiments

Gordon et al 2008 $Ba_{1-x}Co_xFe_2As_2$ $T_{c,max}$=38K



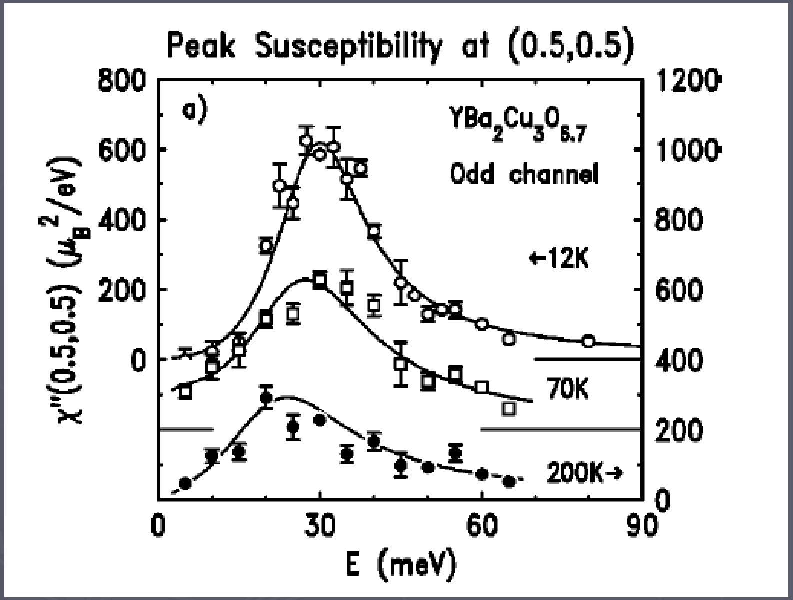
Fletcher et al 2008 LaFePO T_c=6K



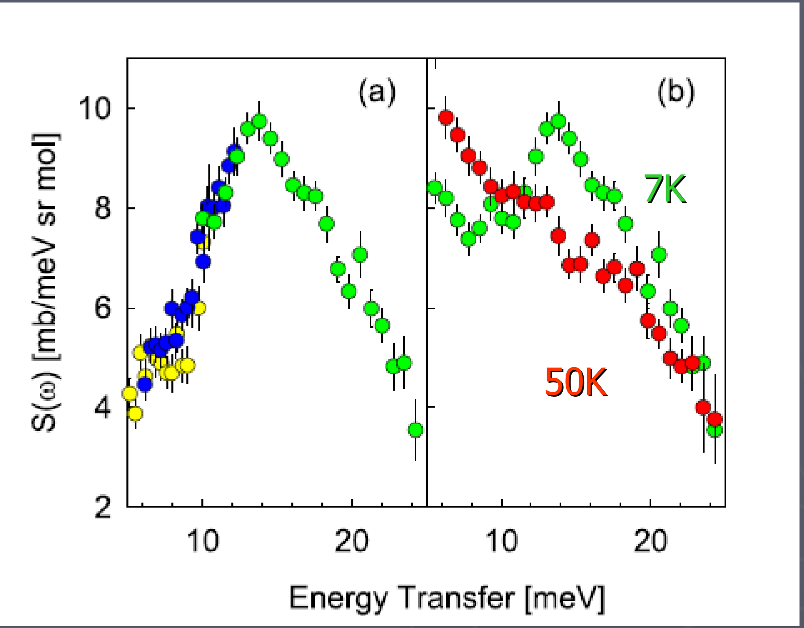
Recall $\Delta\lambda \simeq \int d\omega \left(-\frac{\partial f}{\partial \omega}\right) N(\omega)$ and for dirty / clean nodal SC $N(\omega) \simeq N_0 + a\omega^2$ / $N(\omega) \simeq \omega$ so $\Delta\lambda \simeq \begin{cases} T^2 & dirty \\ T & clean \end{cases}$

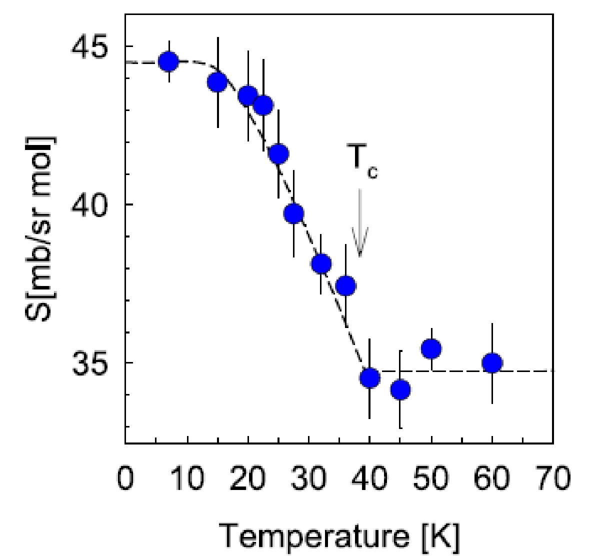
Resonant mode in inelastic neutron scattering

Reminder: cuprates: Fong et al PRB 2000



$Ba_{0.6}K_{0.4}Fe_2As_2$: Christianson et al aXv:0807.3932





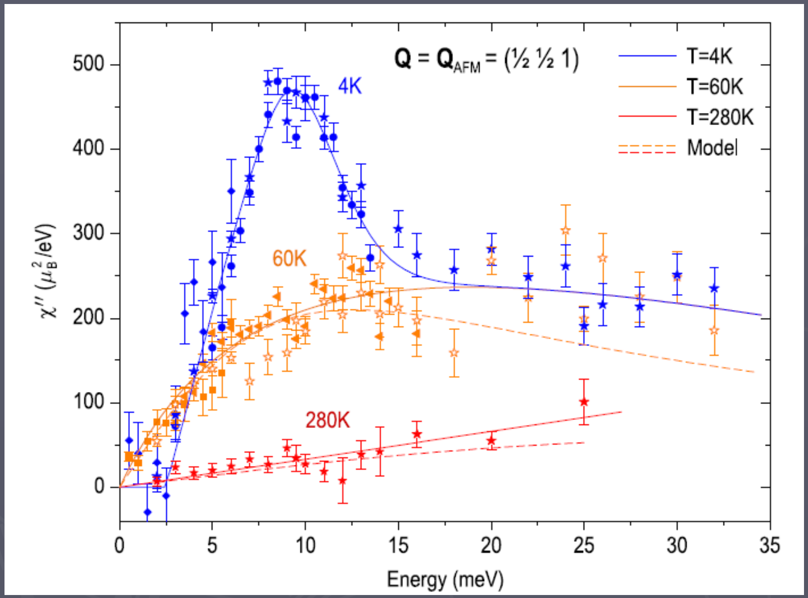
In Ba-122 resonance observed near Q=π,π (folded BZ)

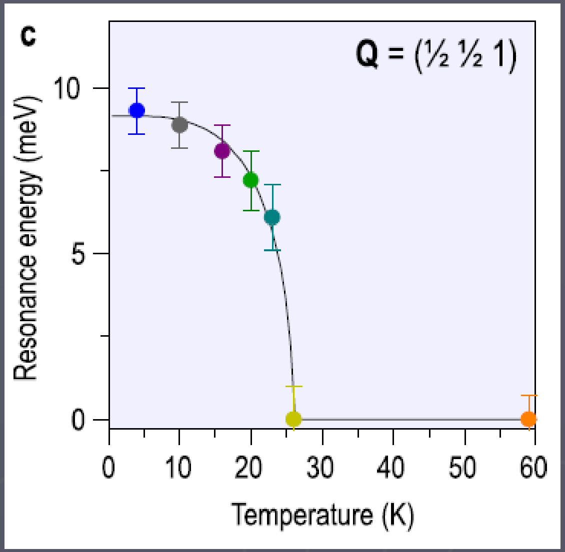
Appears only in SC state (like opt. doped cuprates)

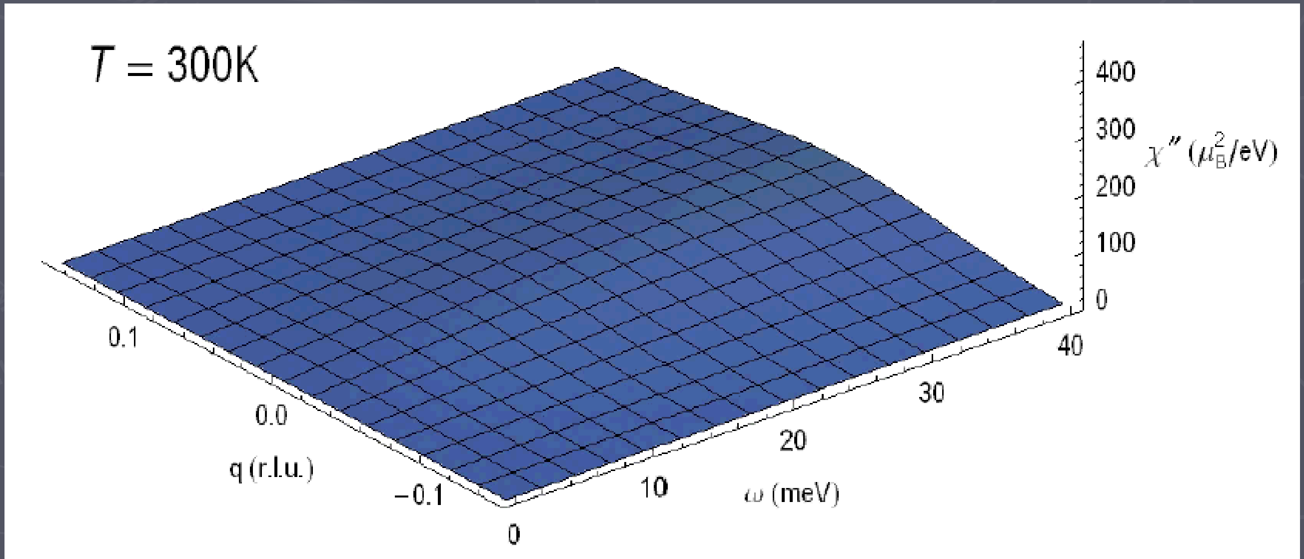
In 1-band models ⇒ $\Delta_{k+Q} = -\Delta_k$ ⇒"unconventional"

Neutron response/resonant mode II

Inosov et al arXiv:0907.3632



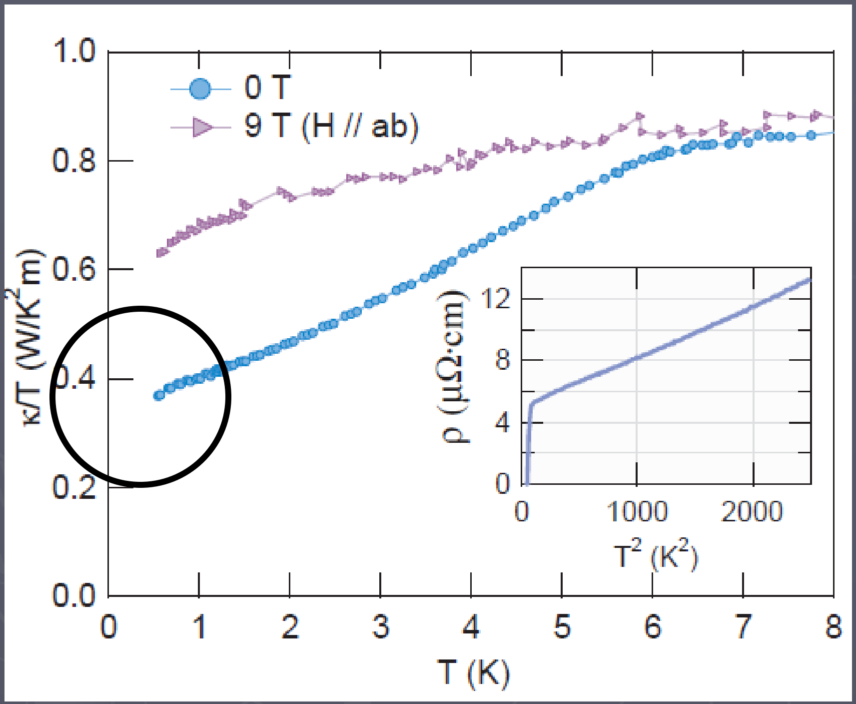




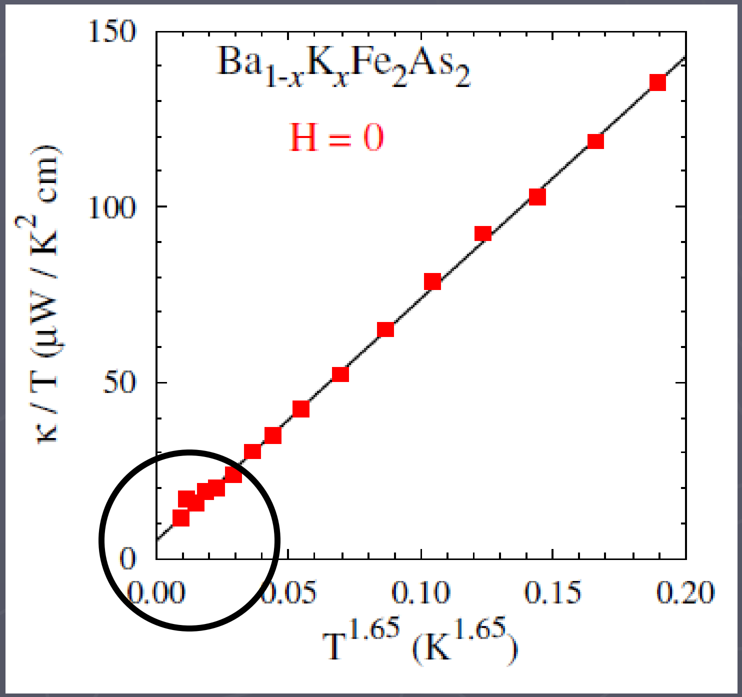
Thermal conductivity (H=0)

(bulk probe, lowest temperatures thus far)

LaFePO: Yamashita et al aXv:0906.0622



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



Big linear T term

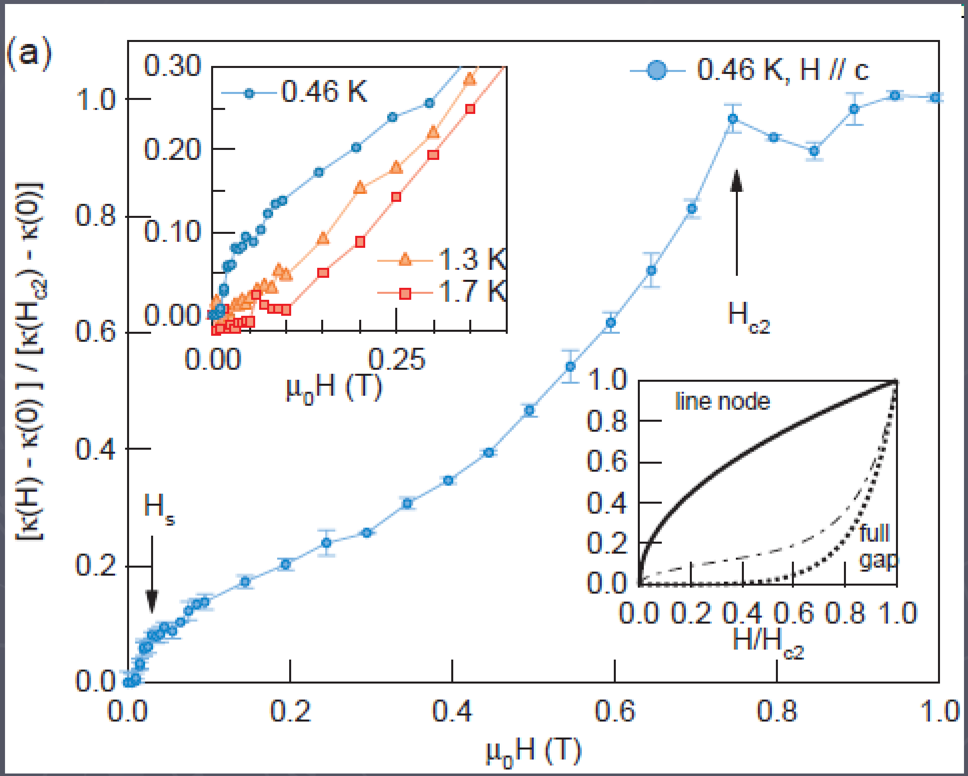
Tiny or zero linear T term

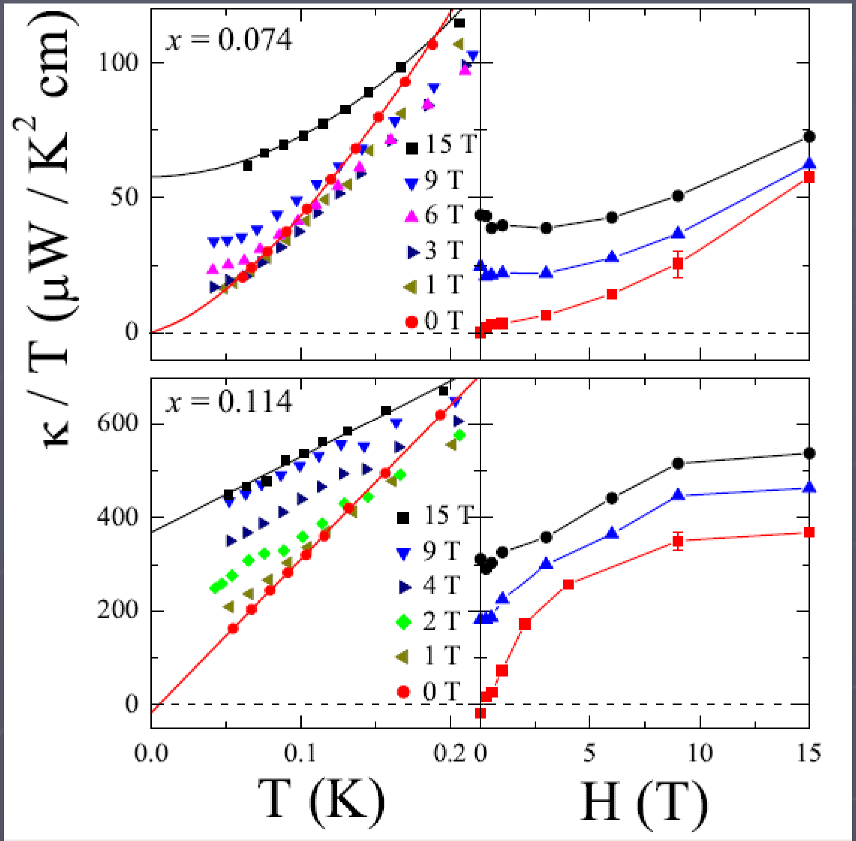
Recall in theory of nodal SC linear T term ⇒ residual qp excitations (metallic-like) for d-wave superconductor this term is "universal" $\kappa \sim N_0 v_F^2/\Delta_0$

Thermal conductivity (H>0)

LaFePO: Yamashita et al aXv:0906.0622

Co-doped Ba-122: Tanatar et al aXv:0904.4049

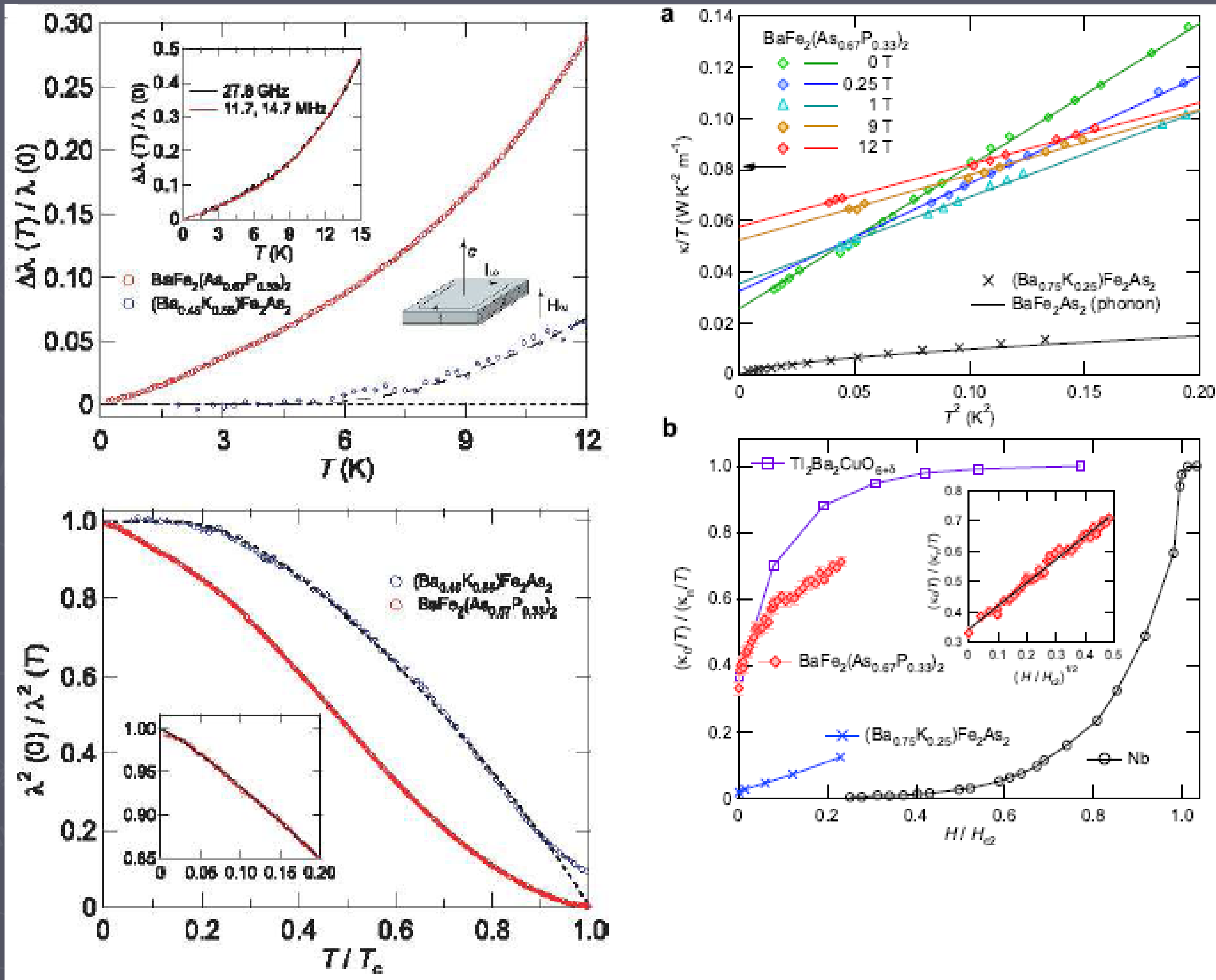




Nodal superconductivity in 122 system!

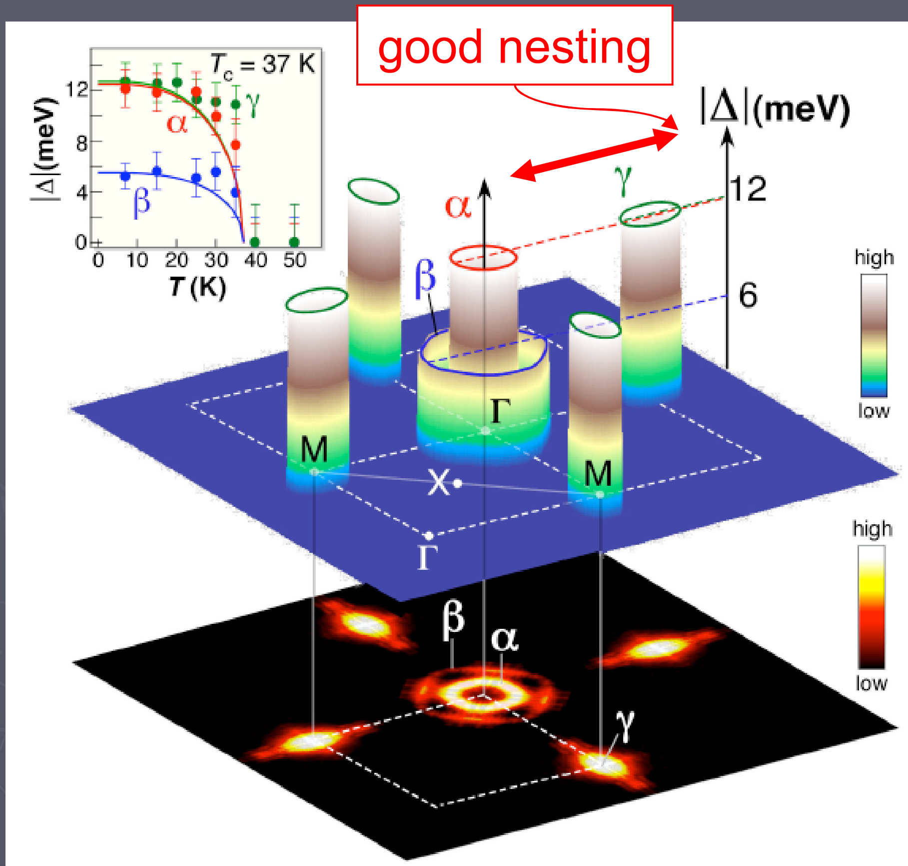
$$BaFe_2(As_{1-x}P_x)_2$$

Hashimoto et al arXiv 0907.4399

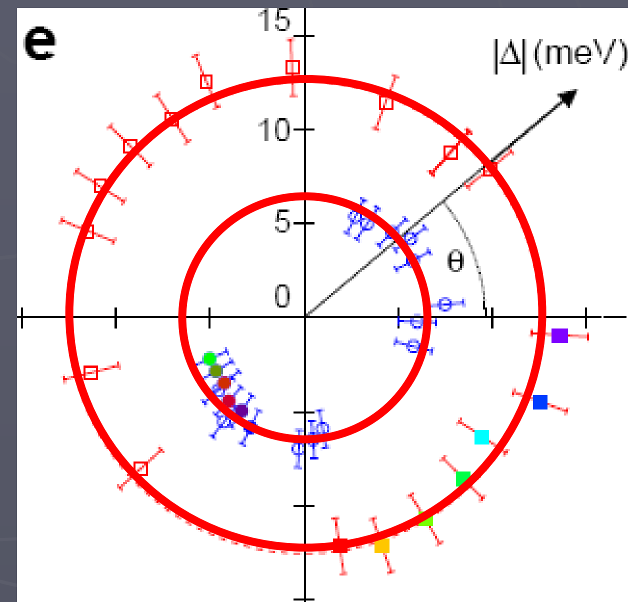


ARPES

$Ba_{0.6}K_{0.4}Fe_2As_2$



Gap size



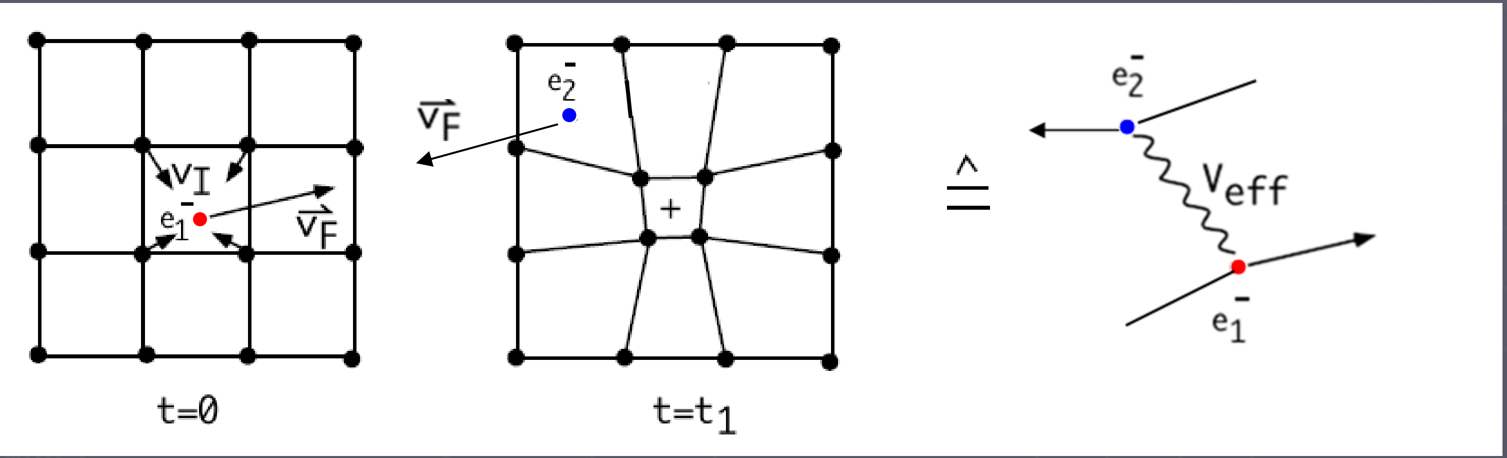
H. Ding et.al.,
Europhys. Lett. 83, 47001 (2008).

Many ARPES measurements, none find highly anisotropic gap

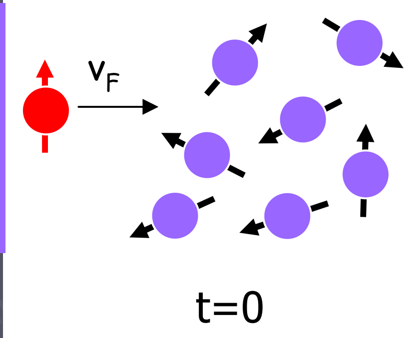
Spin fluctuation theories of pairing

Effective interaction from spin-fluctuations (Berk-Schrieffer 1961)

e-ph
conv SC
retarded



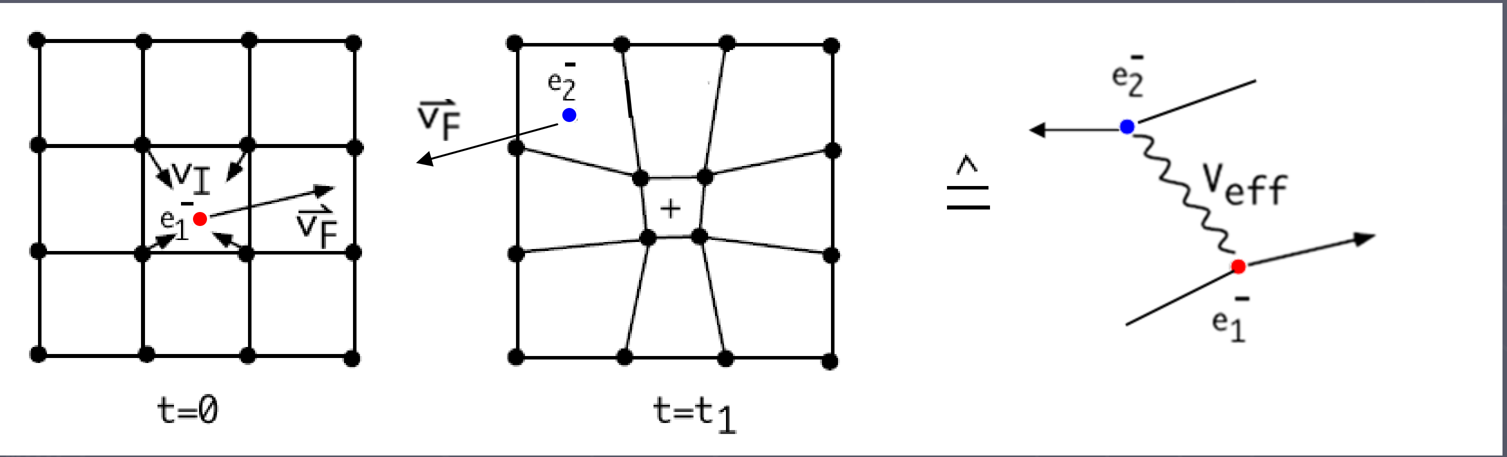
ferro spin
fluct.
^{3}He,…
retarded?



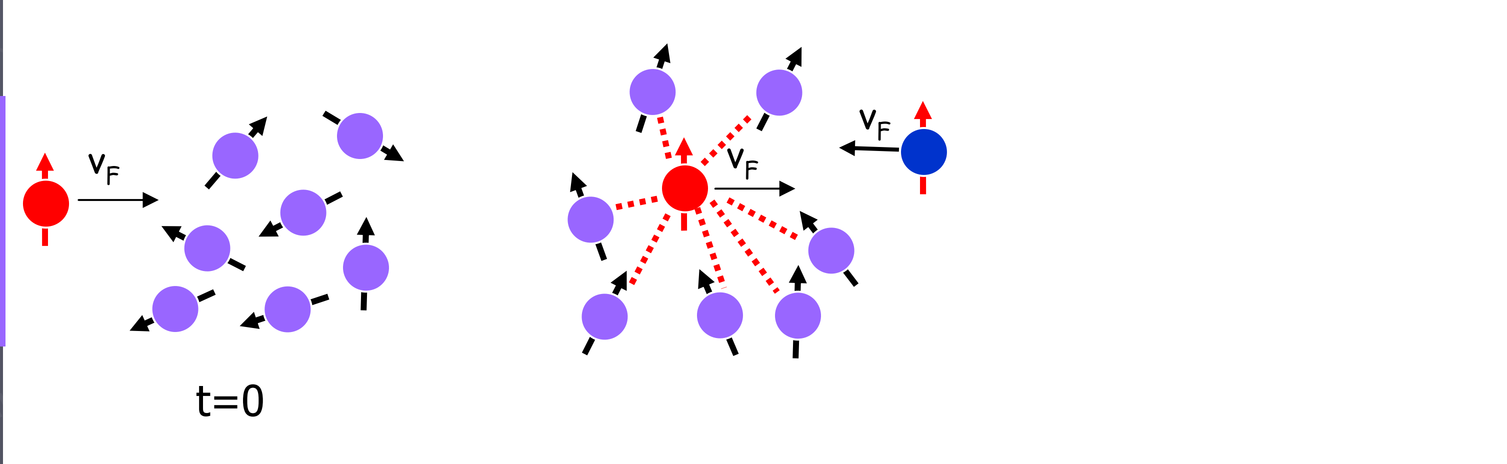
Spin fluctuation theories of pairing

Effective interaction from spin-fluctuations (Berk-Schrieffer 1961)

e-ph
conv SC
retarded



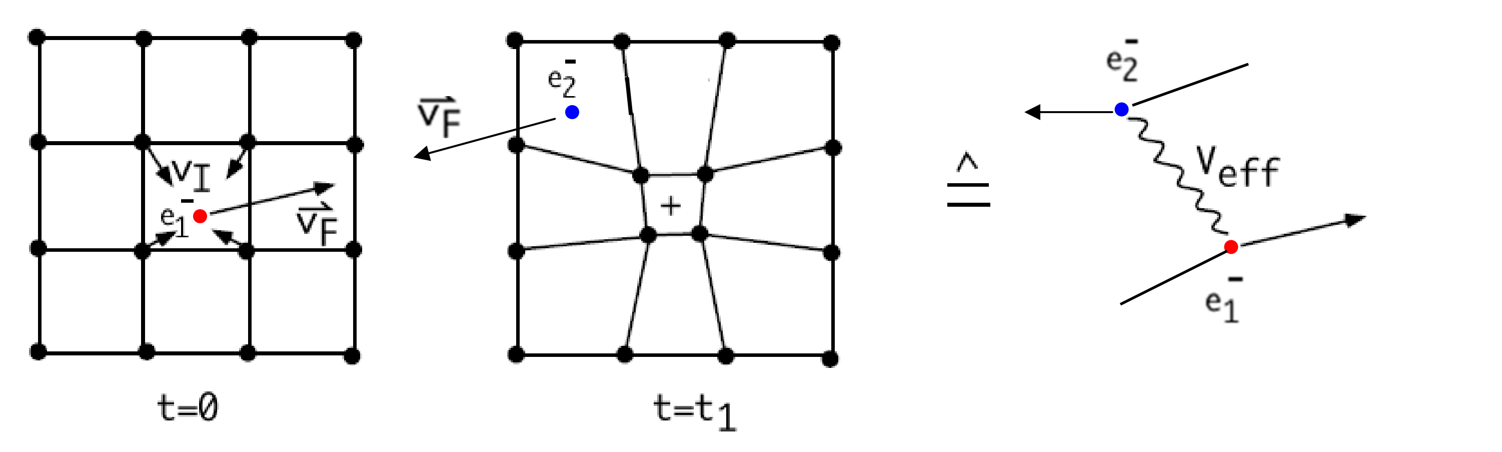
ferro spin
fluct.
^{3}He,…
retarded?



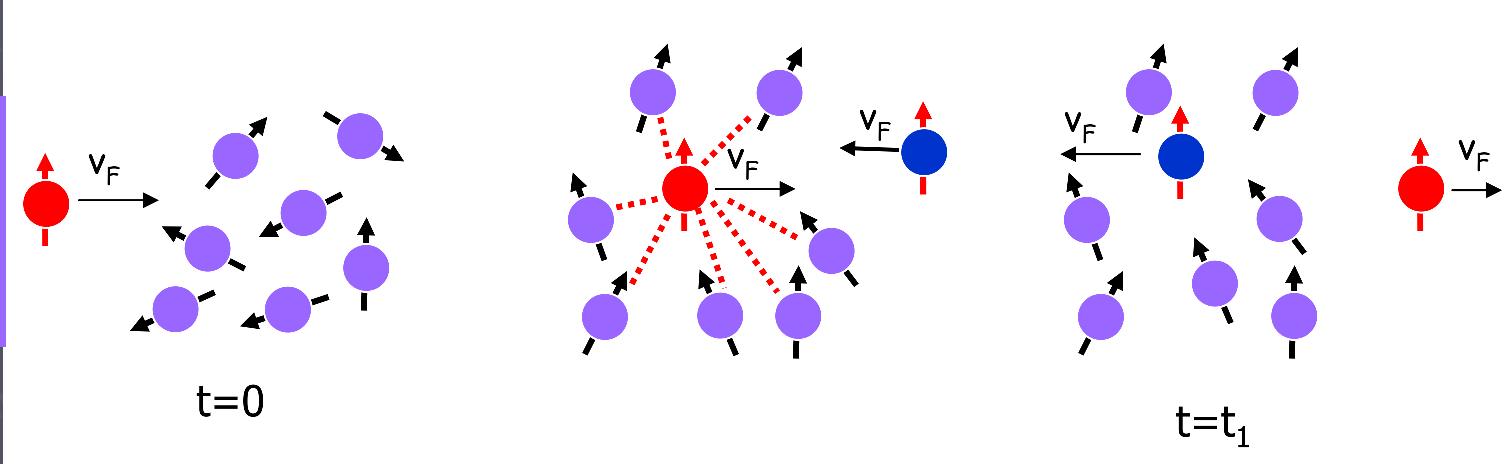
Spin fluctuation theories of pairing

Effective interaction from spin-fluctuations (Berk-Schrieffer 1961)

e-ph
conv SC
retarded



ferro spin fluct.
^{3}He,…
retarded?



timescales for response of pairing "glue" not obviously different from particles in pair!

Spin fluctuation theories of pairing
S. Graser, T. Maier, PH & D.J. Scalapino NJP 2009

Effective interaction from spin-fluctuations (Berk-Schrieffer 1961)

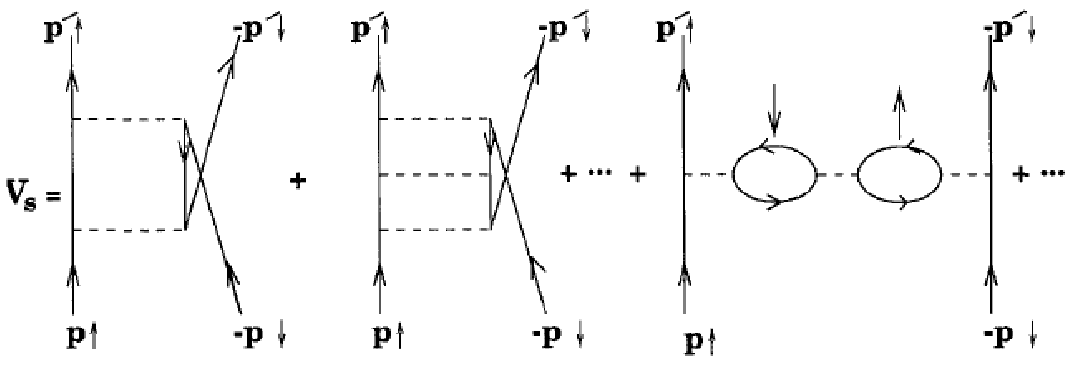


Fig. 1. Diagrams representing the Berk-Schrieffer [1] spin-fluctuation mediated pairing interaction in the singlet channel.

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

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

$$\lambda_{SF} = -\int_0^\infty \frac{\langle ImV_s(q,w)\rangle}{w}\,dw = -Re\,\langle V_s(q,0)\rangle$$

Spin fluctutation pairing theories in Fe-pnictides

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

Several calculations of spin-fluctuation pairing:

- Kuroki et al PRL 2008
- Qi et al aXv:0804.4332
- Wen-Lee aXv:0804.1739
- Mazin et al PRL 2008
- Zhang et al PRL 2008
- Graser et al NJP 2009

Graser et al calculation starting point:

$H=H_0+H_{int}$ H_0=5-band tight-binding model

$$H_{int} = U\sum_{is} n_{i,s\uparrow}n_{is\downarrow} + \frac{V}{2}\sum_{i,s,t\neq s} n_{is}n_{it} - \frac{J}{2}\sum_{i,s,t\neq s} \vec{S}_{is}\cdot\vec{S}_{it} + \frac{J'}{2}\sum_{i,s,t\neq s}\sum_{\sigma} c^\dagger_{is\sigma}c^\dagger_{is\bar{\sigma}}c_{it\bar{\sigma}}c_{it\sigma}$$

orbit

most general 2-body Hamiltonian with intrasite interactions only!

spin fluctuation pairing theories cont'd

Graser et al: start from generalized multiorbital susceptibility:

$$\chi^{p\gamma,q\delta}_{s\alpha,t\beta}(\mathbf{q},i\Omega) = \frac{1}{6}{\chi_1}^{pq}_{st}\vec{\sigma}_{\beta\alpha}\cdot\vec{\sigma}_{\gamma\delta} + \frac{1}{2}{\chi_0}^{pq}_{st}\delta_{\beta\alpha}\delta_{\gamma\delta}$$

then define singlet and triplet pairing vertices

$$\Gamma_0{}^{pq}_{st}(\mathbf{k},\mathbf{k}',i\Omega) = -\frac{1}{2}\left(U_0 - 3U_1\right)^{tq}_{ps}(\mathbf{k}-\mathbf{k}',i\Omega)$$

$$\Gamma_1{}^{pq}_{st}(\mathbf{k},\mathbf{k}',i\Omega) = -\frac{1}{2}\left(U_0 + U_1\right)^{tq}_{ps}(\mathbf{k}-\mathbf{k}',i\Omega)$$

$$U_0{}^{tq}_{ps} = \left[\tfrac{1}{2}\gamma_0 + \gamma_0\chi_0^{\mathrm{RPA}}\gamma_0\right]^{tq}_{ps}$$

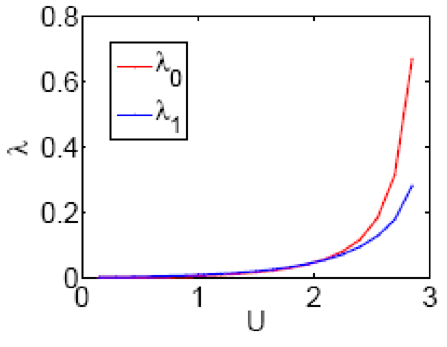
$$U_1{}^{tq}_{ps} = \left[\tfrac{1}{2}\gamma_1 + \gamma_1\chi_1^{\mathrm{RPA}}\gamma_1\right]^{tq}_{ps}$$

linearized gap equation has various eigenvectors g:

$$-\sum_j \oint_{C_j} \frac{dk'_{\parallel}}{2\pi}\frac{1}{2\pi v_F(k')}\Gamma_{ij}(k,k')g_\alpha(k') = \lambda_\alpha g_\alpha(k)$$

Which one wins? dimensionless pairing interaction for each pairing symmetry:

$$\lambda[g(\mathbf{k})] = -\frac{\sum_{i,j}\oint_{C_i}\frac{d\mathbf{k}_{\parallel}}{v(\mathbf{k})}\oint_{C_j}\frac{d\mathbf{k}'_{\parallel}}{v(\mathbf{k}')}g(\boldsymbol{k})\Gamma^{[g]}_{ij}(\boldsymbol{k},\boldsymbol{k}')g(\boldsymbol{k}')}{(2\pi)^2\sum_i\oint_{C_i}\frac{d\mathbf{k}_{\parallel}}{v(\mathbf{k})}g^2(\boldsymbol{k})}$$

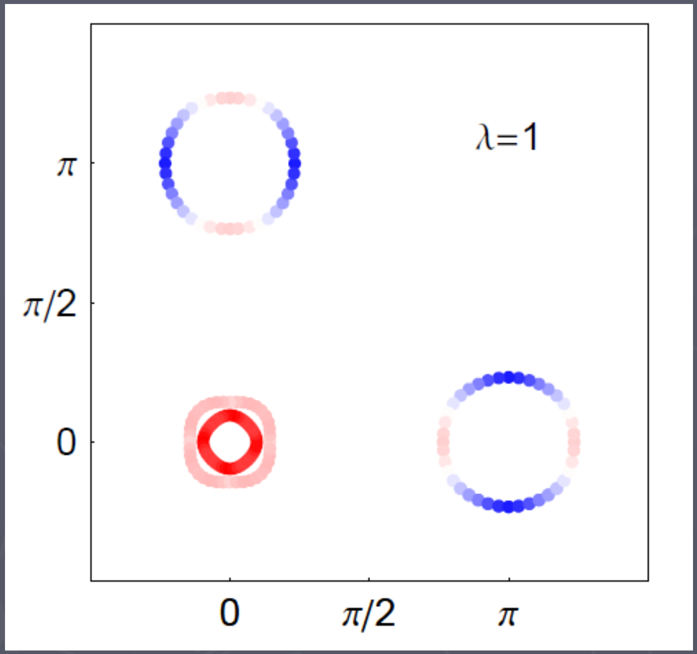


Kuroki et al (nodes)
Zhang et al (aniso)
Graser et al (nodes)

differences in: band structure, effective interaction, method…?

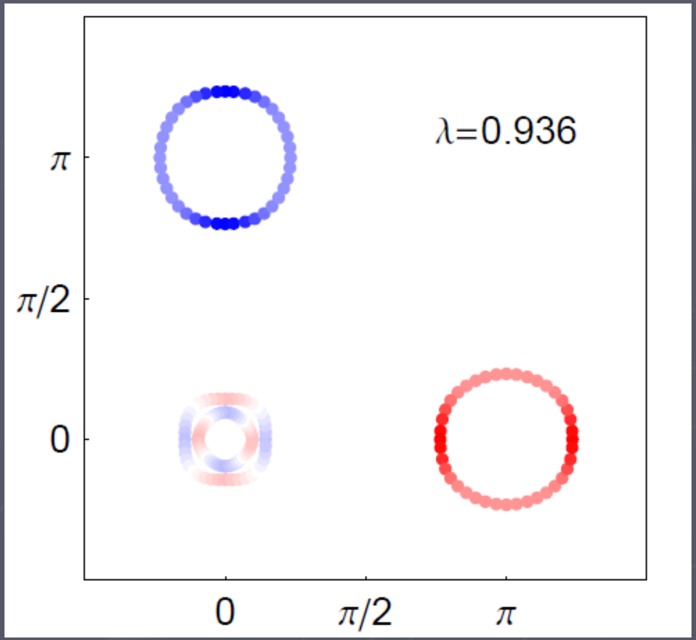
Graser et al: The "winning" pairing functions for $U \to U_c$ display gap nodes!

"anisotropic extended-s"-wave



U=1.73 J=0

nearby: dx_2-y_2



U=1.78 J=U/2

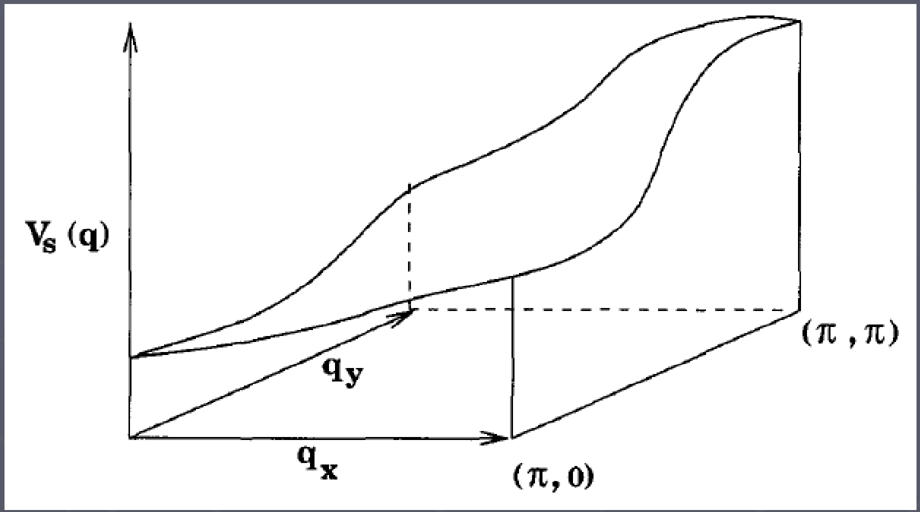
(x=0.125 e-doped)

Two pairing channels appear to be nearly degenerate within this scheme:

a) Can different FeAs materials have different symmetries?
b) New types of excitonic order parameter modes?

see Maier & Scalapino 2009, W-C Lee et al 2009

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



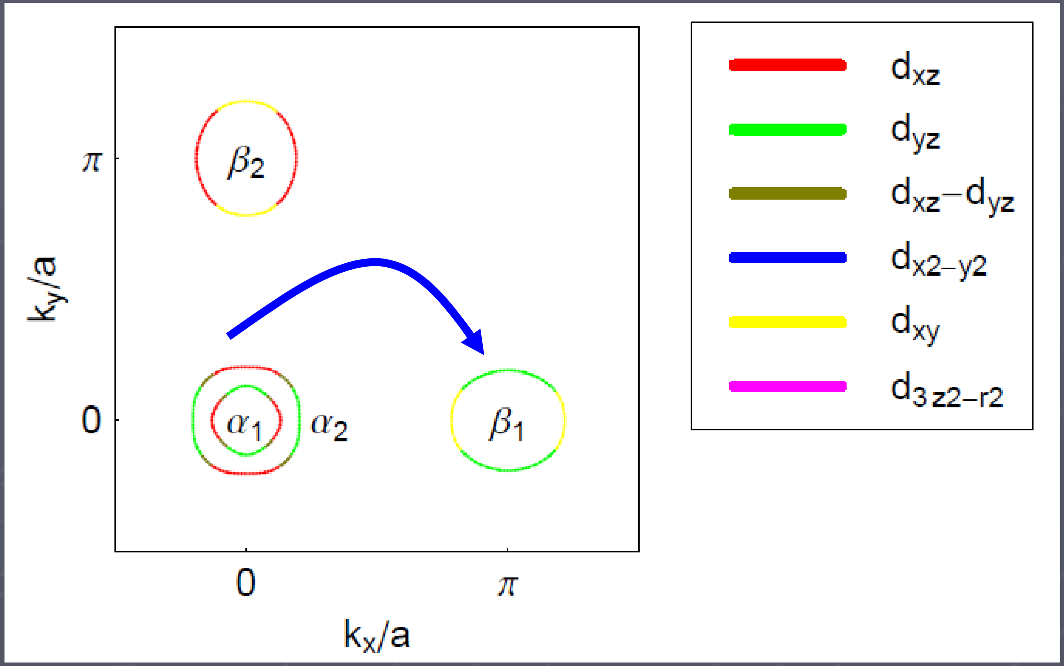
BCS:

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

Δ~cos kx-cosky takes advantage of peak in spin fluctutuation interaction at π,π!

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

Similar argument from Mazin et al PRL 2008 for pnictides: consider only $\alpha-\beta$ pair scattering

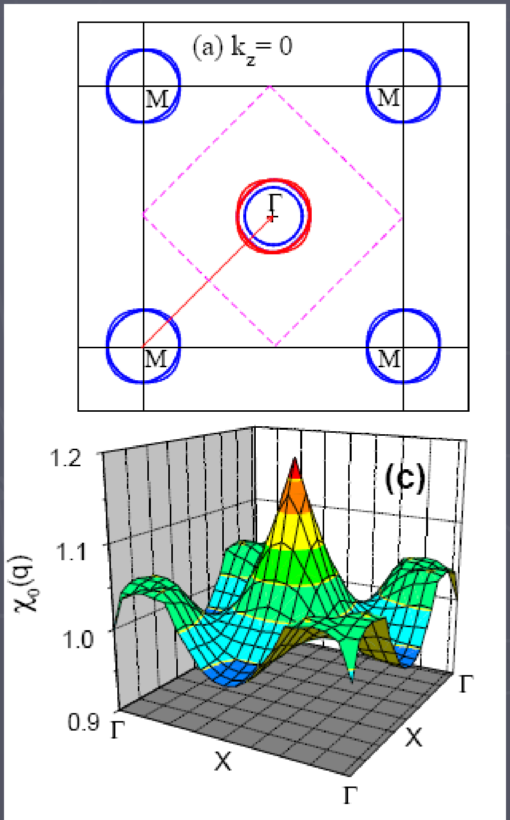


- nesting peaks interaction V_s at π,0 in 1-Fe zone.
- interaction is constant over sheet since they are small.
- therefore *isotropic* sign-changing $s_{+/-}$ state solves gap eqn

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

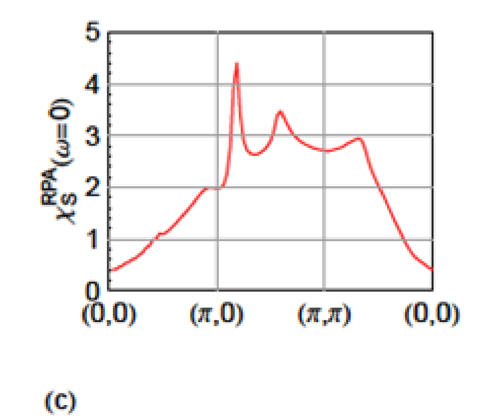
What is the origin of the gap anisotropy [Maier et al PRB 09]?

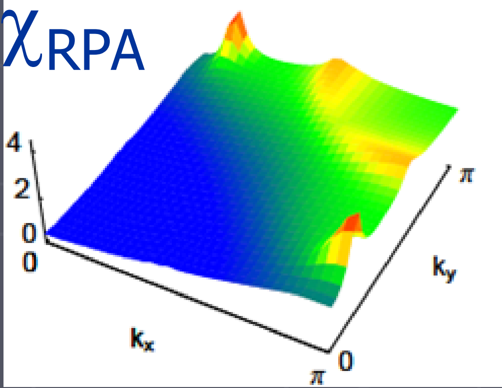
1. importance of orbital character on Fermi sheets
2. scattering between β_1 and β_2 sheets
3. intrasheet coulomb repulsion



Dong et al, Mazin et al 2008: orbital character neglected

$$\chi^{pq}_{st}(q,\omega) = -\frac{1}{N}\sum_{k,\mu\nu} \frac{a^s_\mu(k)a^{p*}_\mu(k)a^q_\nu(k+q)a^{t*}_\nu(k+q)}{\omega + E_\nu(k+q) - E_\mu(k) + i0^+} \times [f(E_\nu(k+q)) - f(E_\mu(k))]$$





Graser et al 2009

Importance of orbital character on Fermi sheets

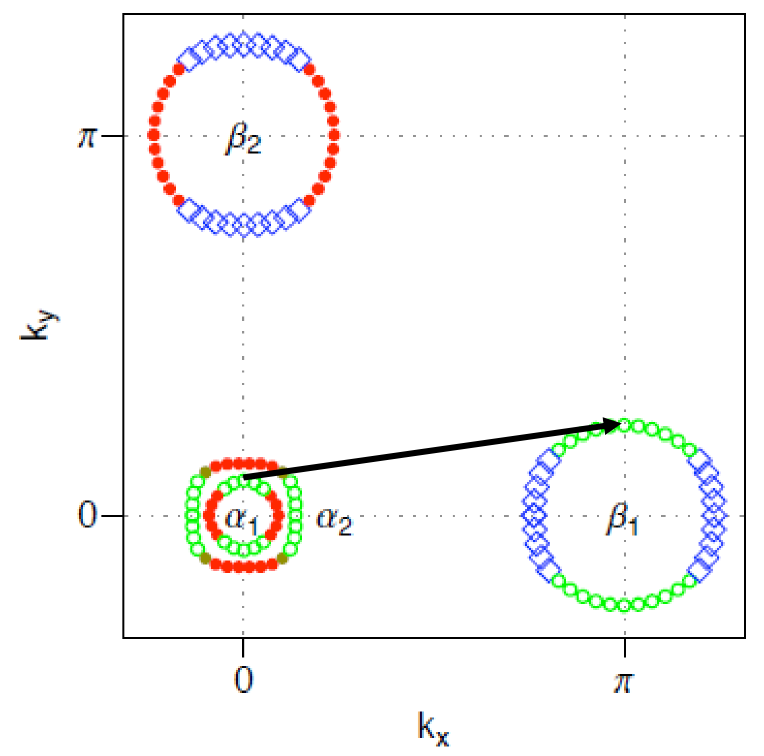
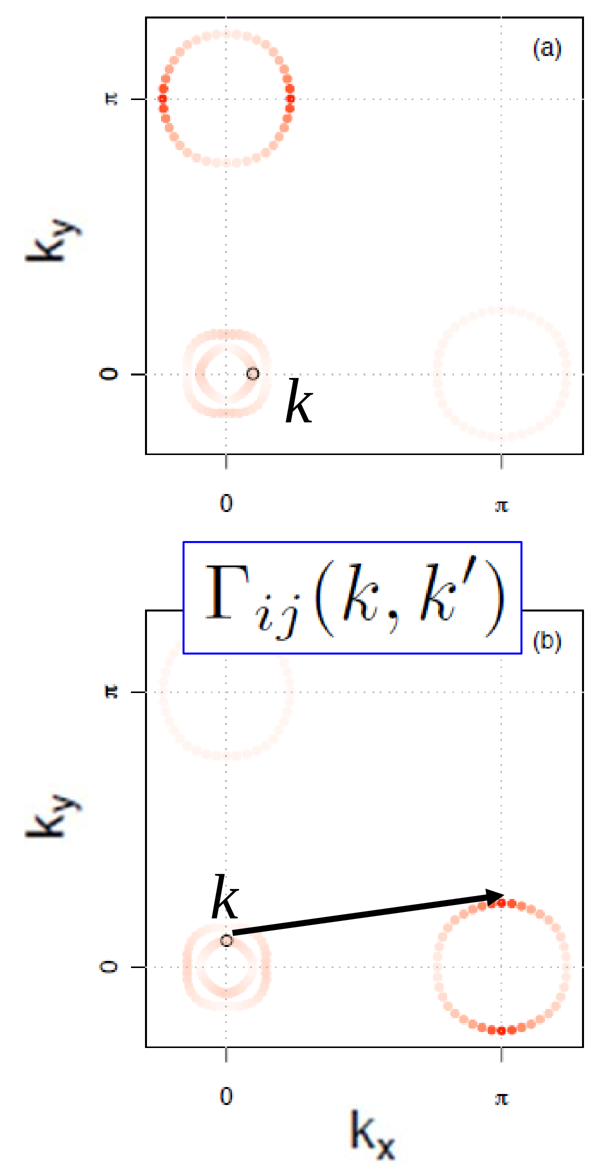
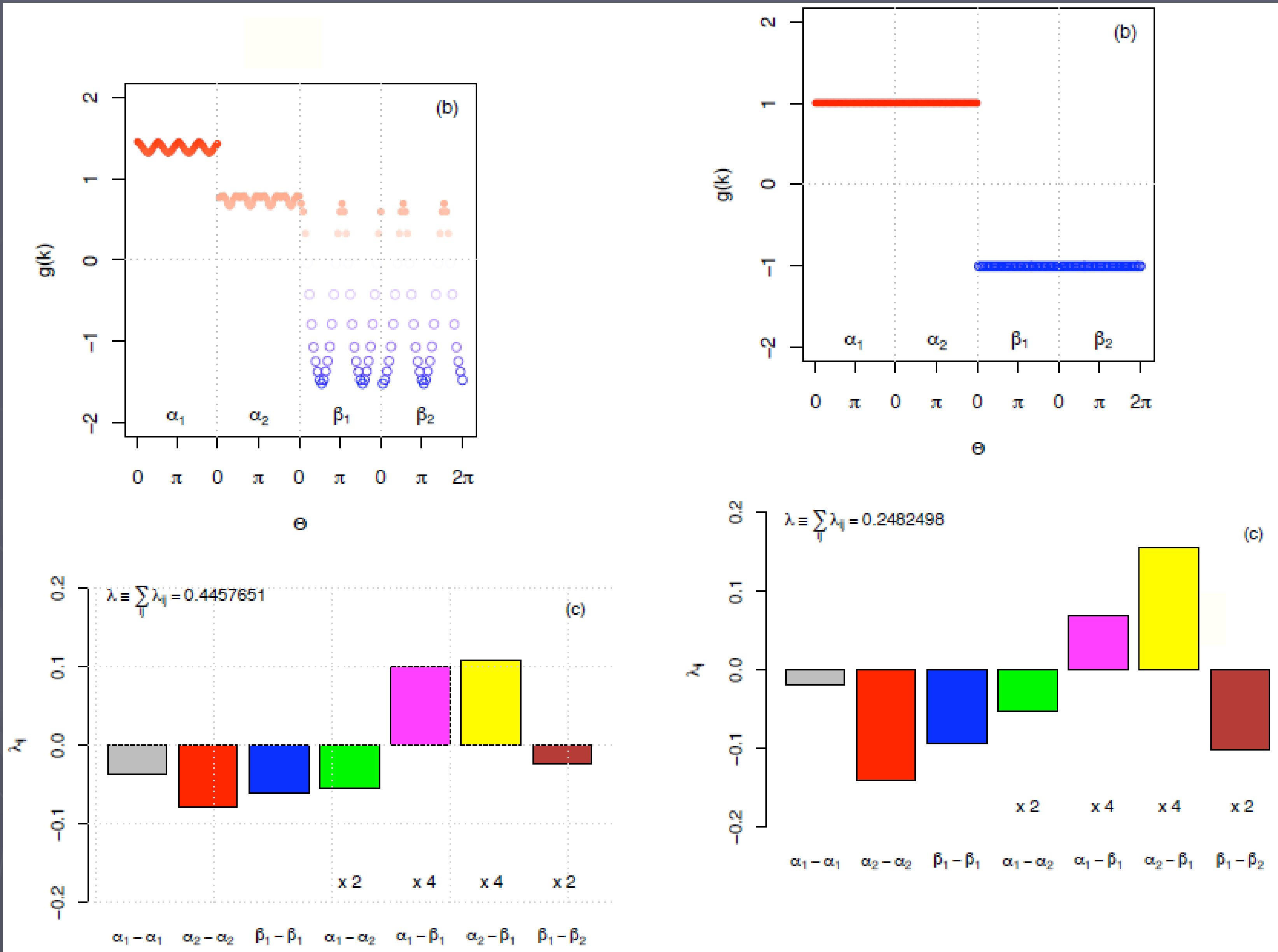


FIG. 1: (color online) The Fermi surface of the 5-orbital tight-binding model[15]. The main orbital contributions are shown by the following colors/symbols: d_{xz} (red/solid circles), d_{yz} (green/open circles), $d_{x^2-y^2}$ (blue/diamonds)

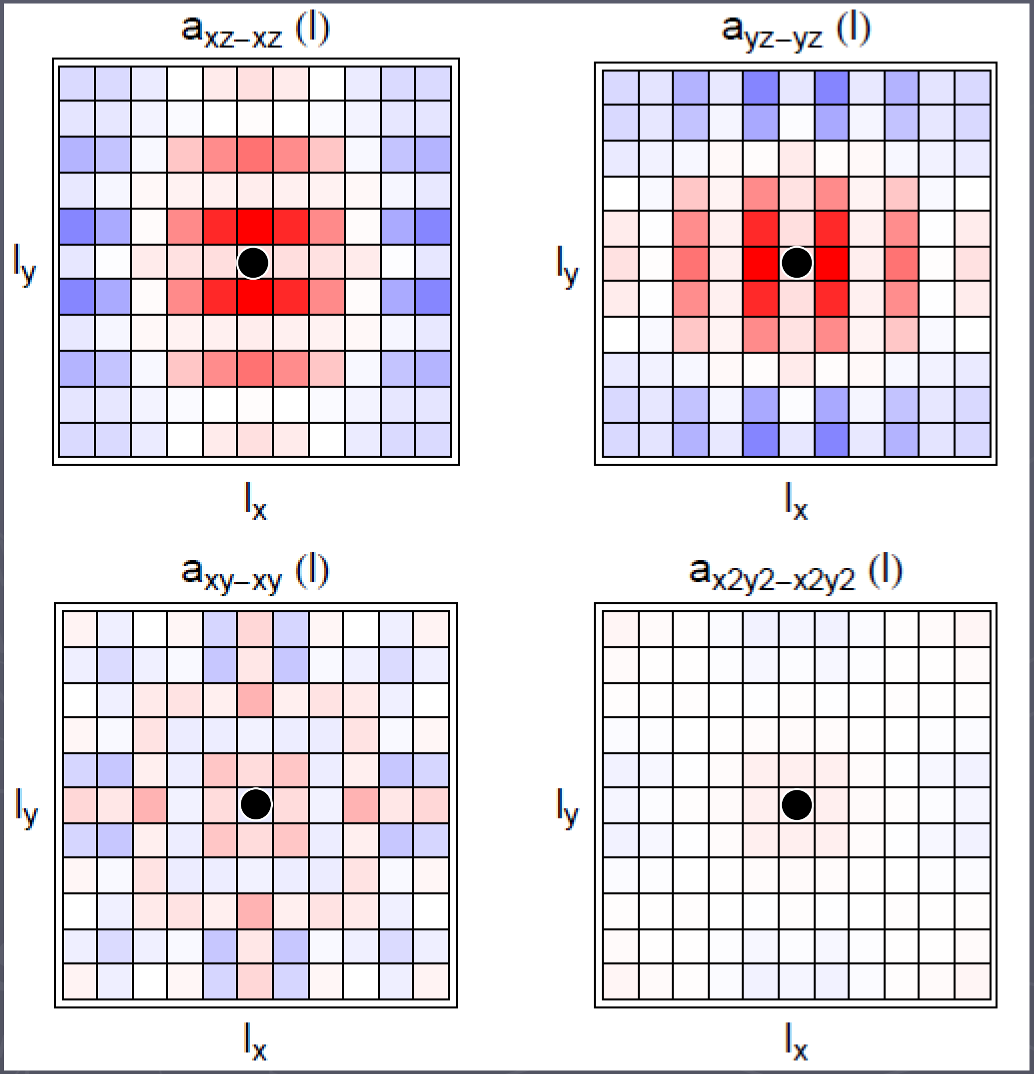


orbital weight factors favor scattering within given orbital

Contributions to pairing strength λ

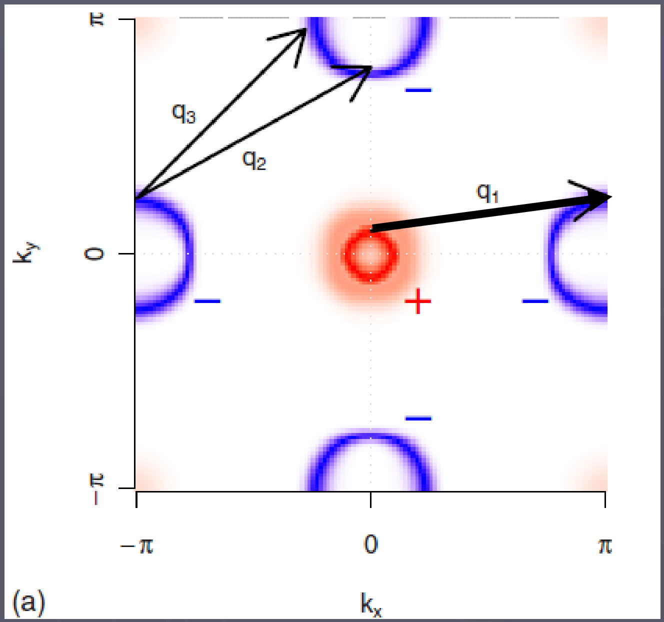


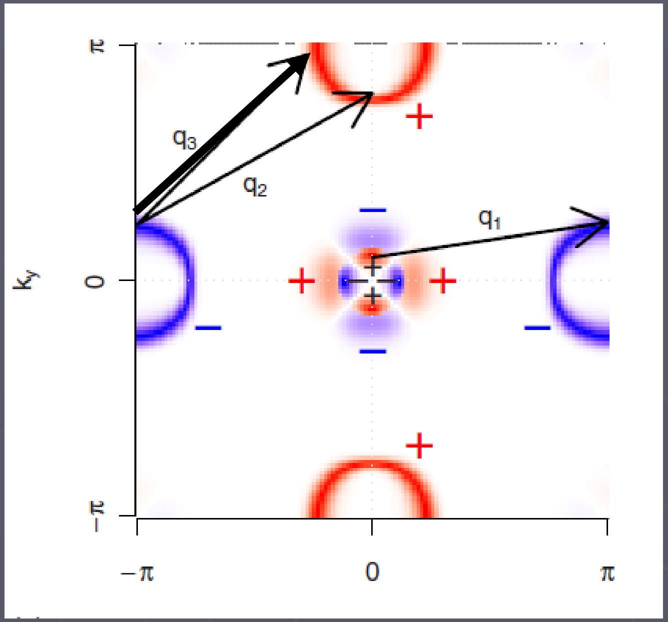
Real space structure of anisotropic A_{1g} states



consistent with cos k_x+cos k_y + higher harmonics

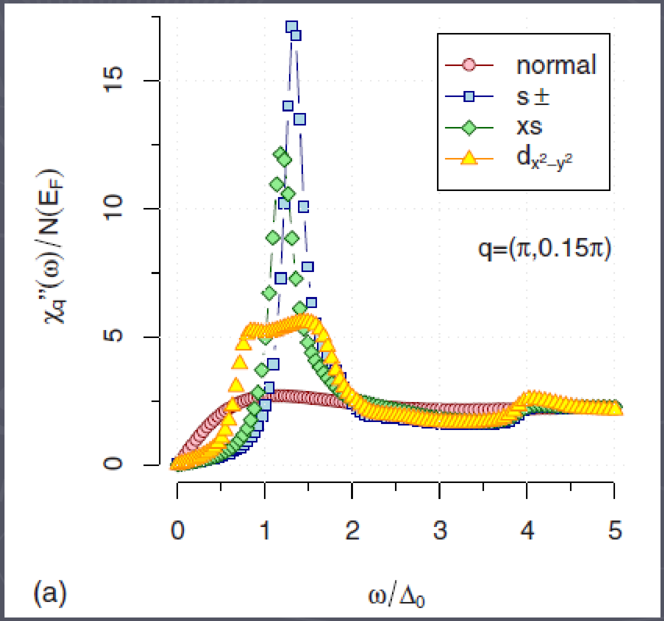
Distinguishing different sign-changing states by neutron resonance

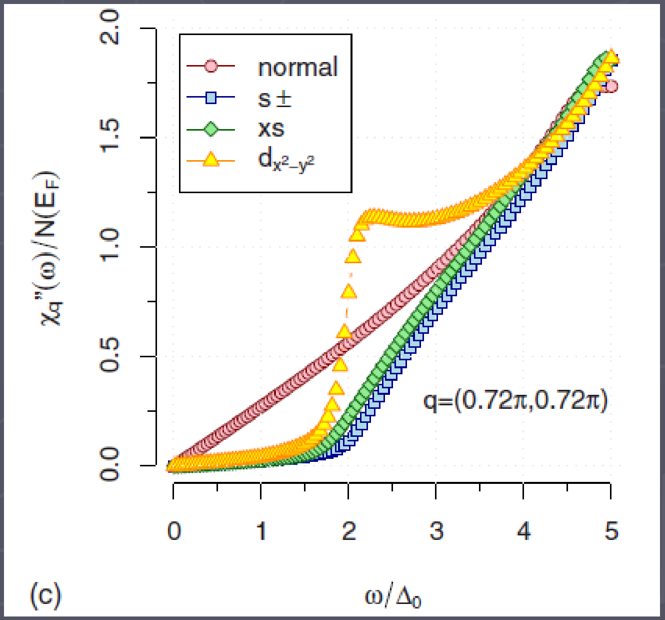




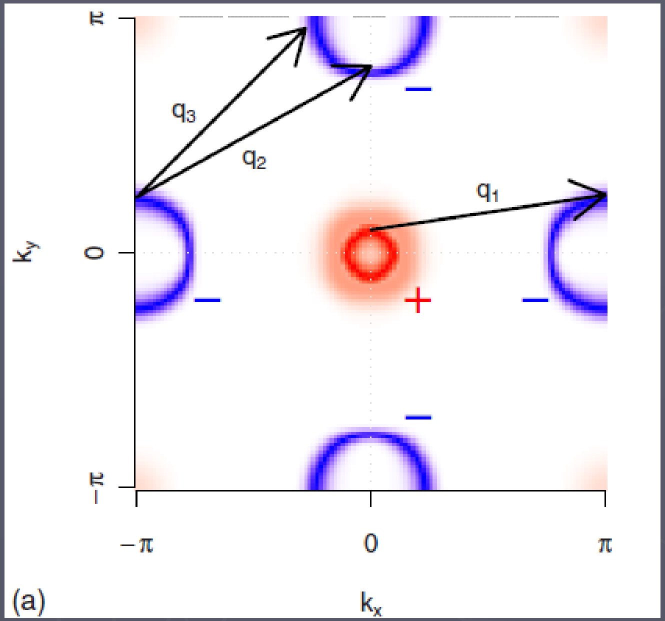
Maier et al
PRB 2009

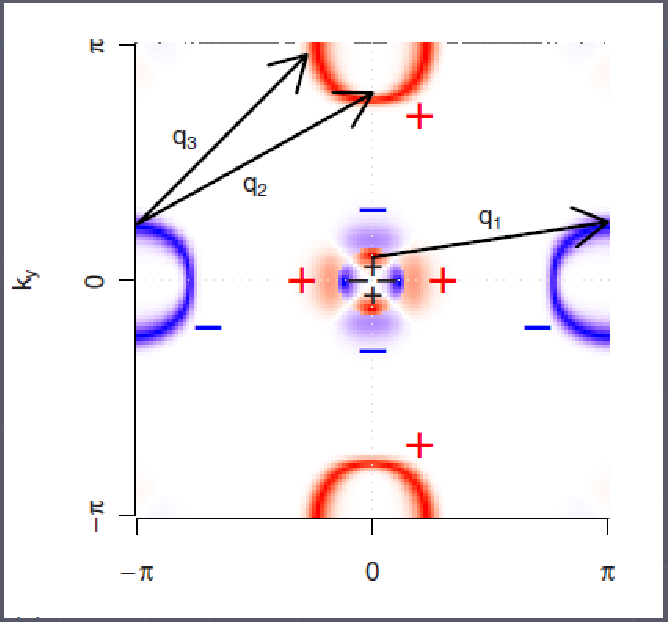
but



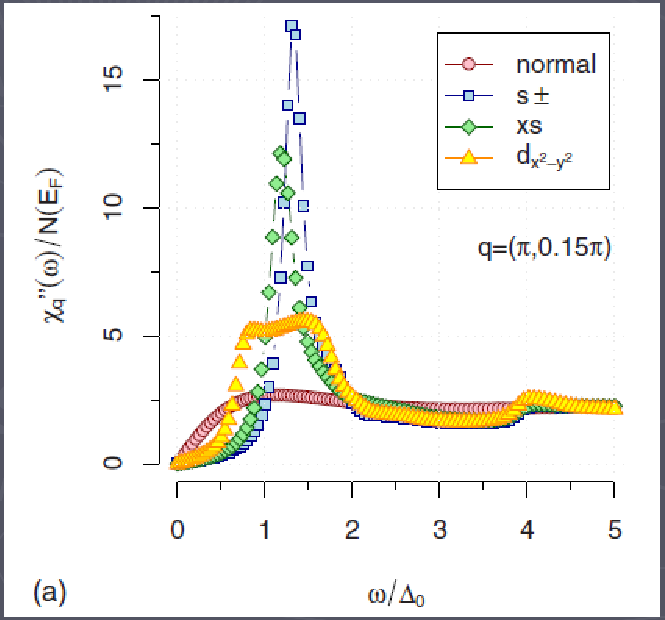


Distinguishing different sign-changing states by neutron resonance

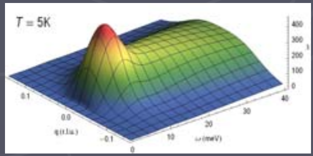




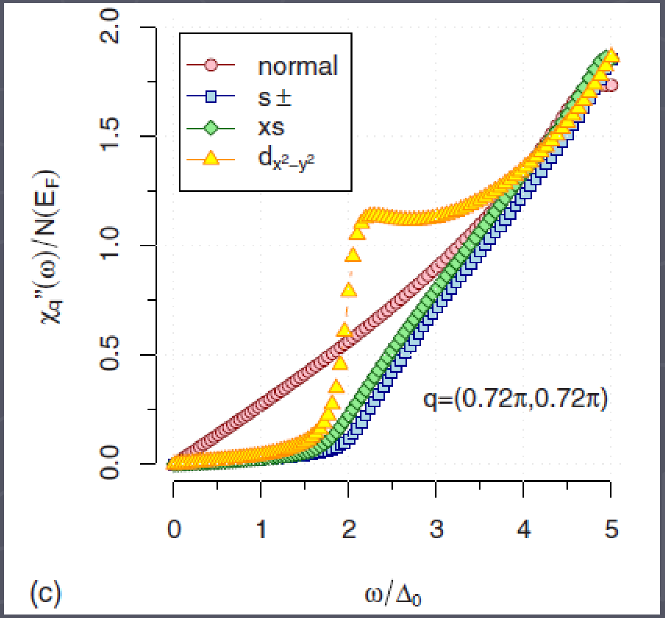
Maier et al
PRB 2009



but



no incomm.
response!



Summary of spin fluctuation theory results

- With apparently reasonable values of interaction parameters, realistic SF theories give high enough T_c
- s- and d- pairing channels are nearly degenerate
- States appear to be anisotropic and may have nodes

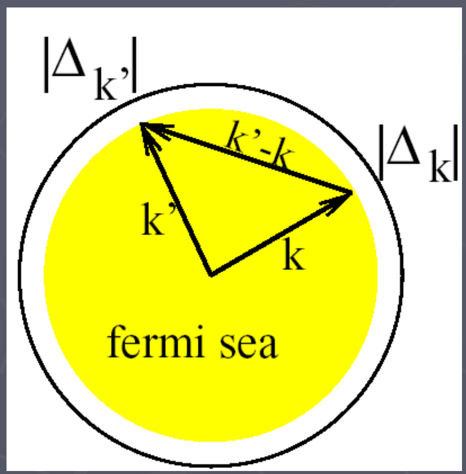
Some experiments show nodes, others not—why?

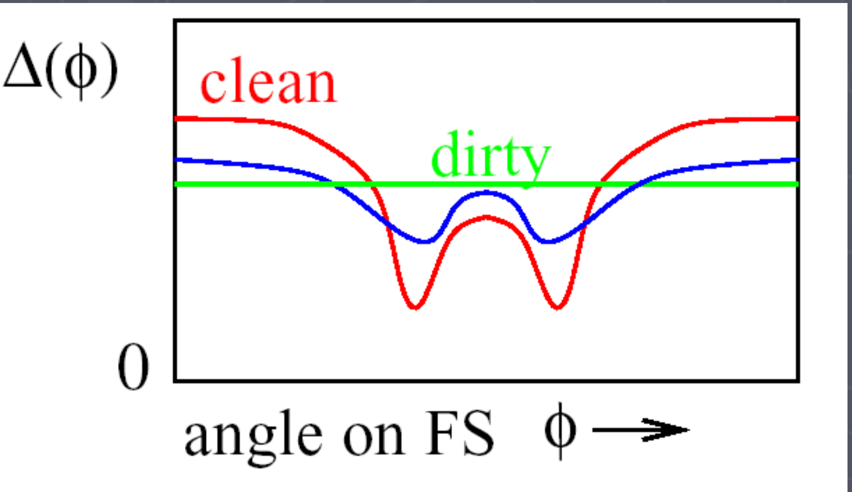
- varying parameter may give gapped—nodal transition in s-wave state
- " " s-wave -> d-wave state
- disorder may cause nodal-gapped transition

Disorder: Can we reconcile (some) experiments on SC state?

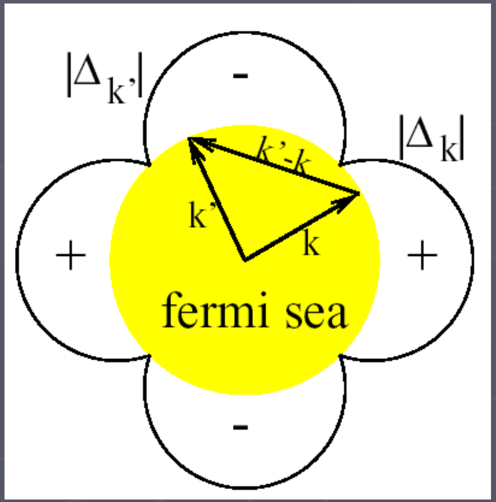
Reminder: how nonmagnetic disorder affects s- and d- wave SC

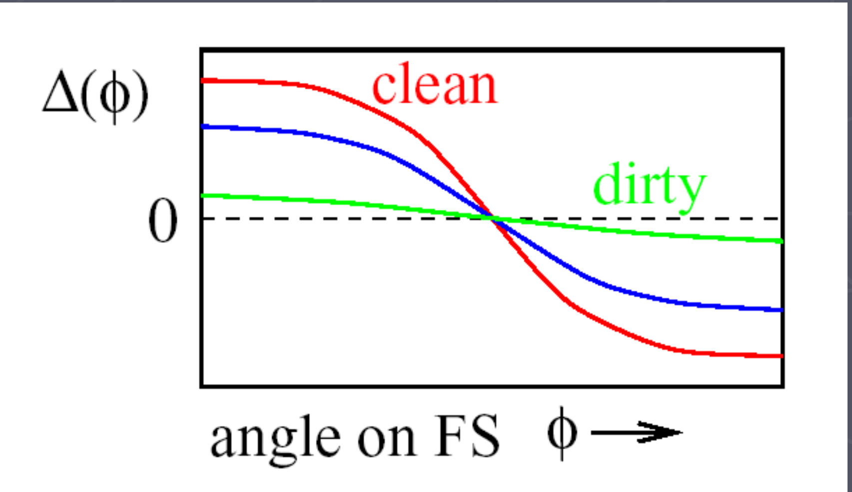
s-wave:
Impurities mix Δ_k with $\Delta_{k'}$:





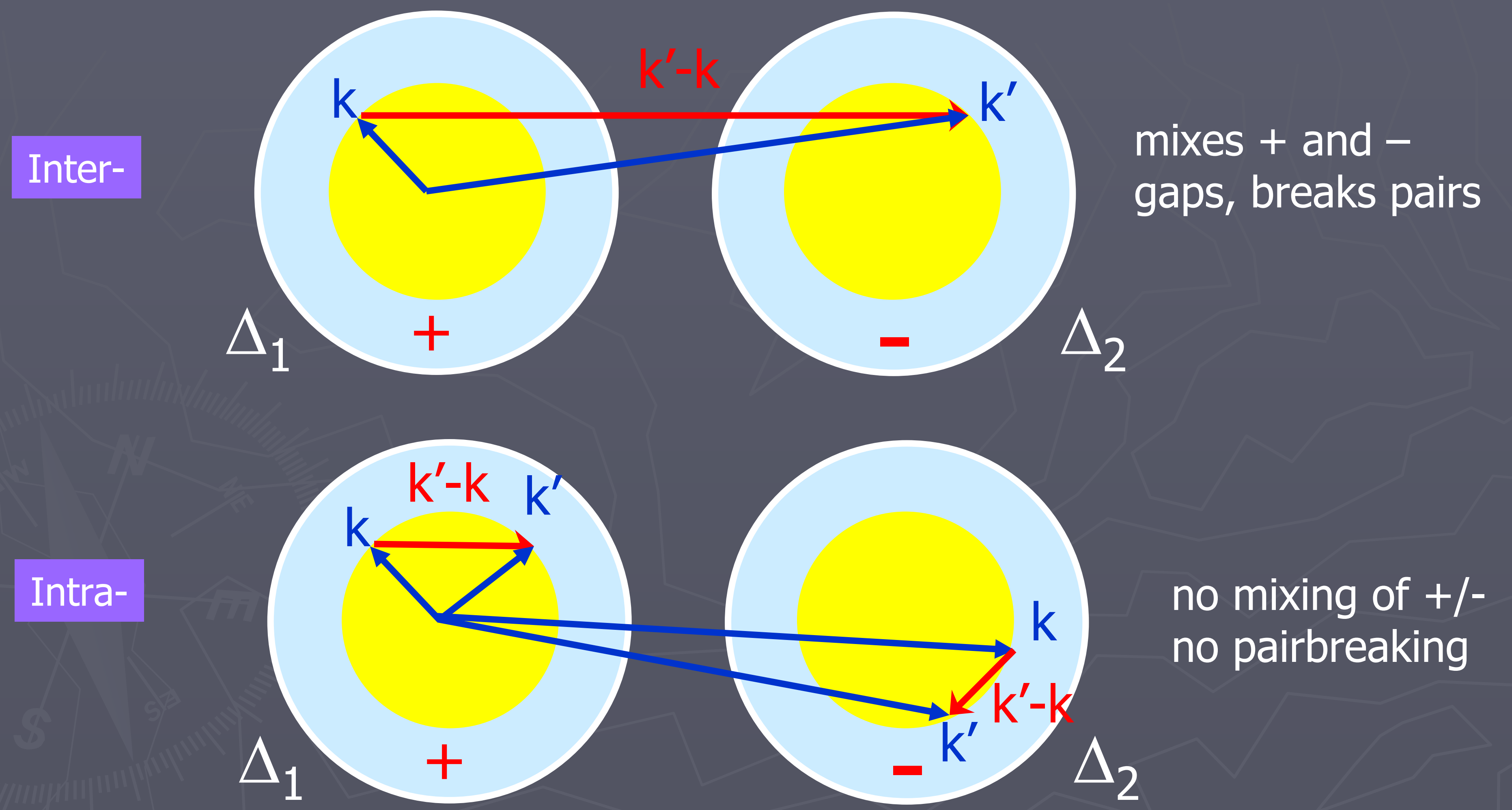
d-wave:
Mix Δ_k, $\Delta_{k'}$ with signs $\pm$:





Disorder: Can we reconcile (some) experiments on SC state?

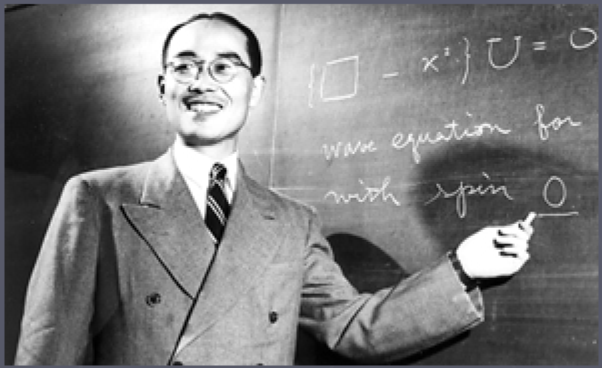
Inter- and intraband impurity scattering in 2-band $s_{+/-}$ system



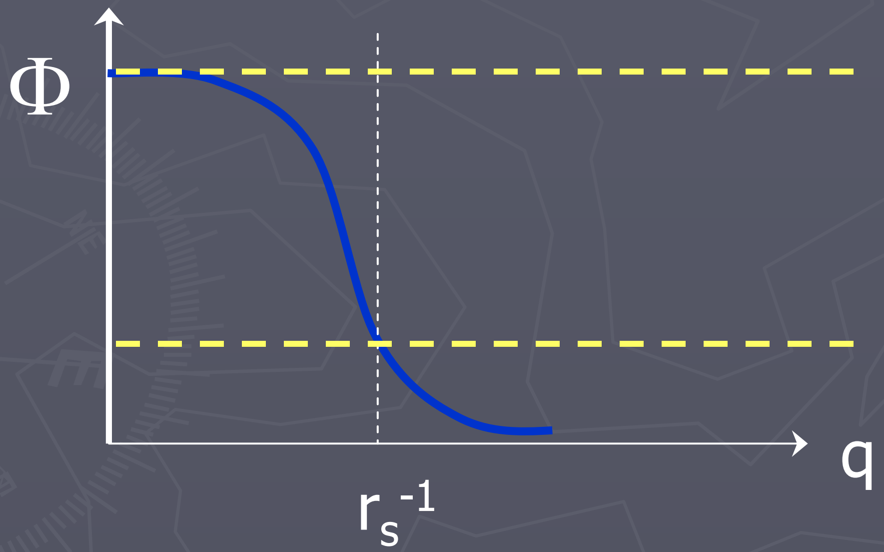
Disorder: Can we reconcile (some) experiments on SC state?

Screened Coulomb potential: intraband should be bigger!

$$\Phi = \frac{e}{4\pi\varepsilon_0\varepsilon \cdot r} e^{-r/r_s}$$



H. Yukawa



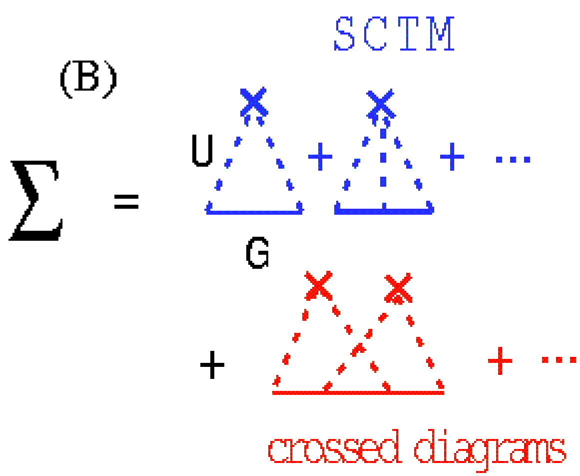
Normally expect $r_s \sim a$ for good metal, so $V_{inter} < V_{intra}$

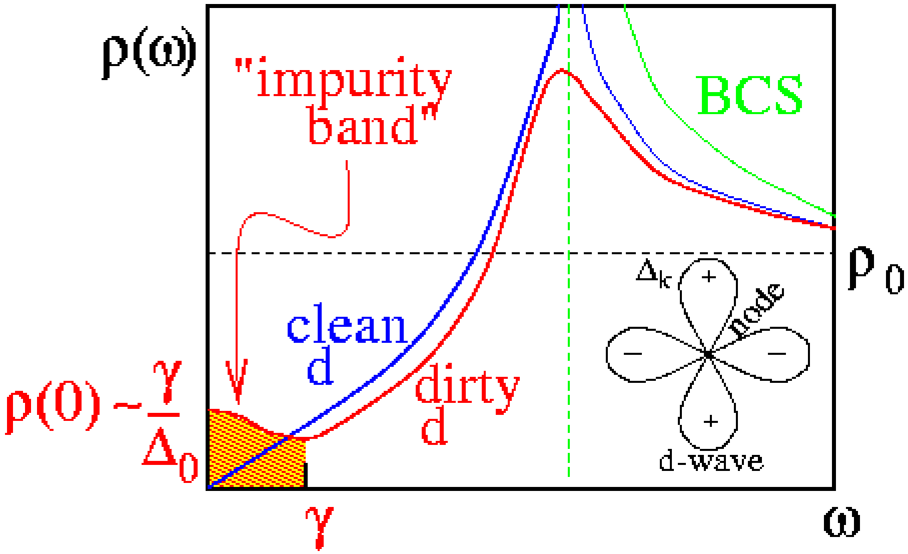
Disorder: self-consistent t-matrix approx. ("SCTMA","CPA"...)

Sum all multiple scattering diagrams from 1 impurity:

$$\underline{\Sigma} = n_i \underline{T}$$

$$\underline{T} = \underline{V} + \underline{V}\,\underline{G}\,\underline{T}$$

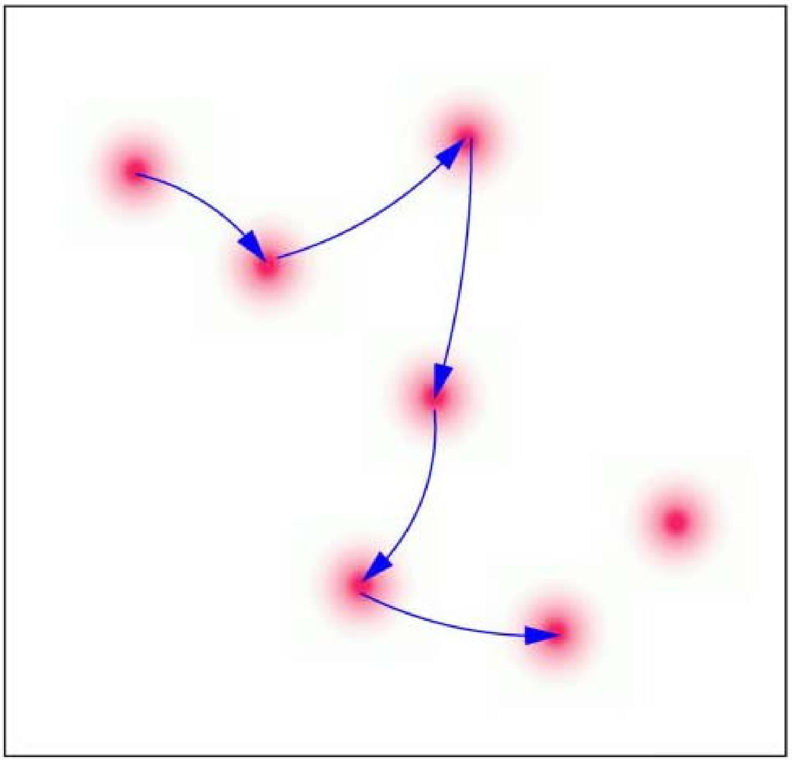




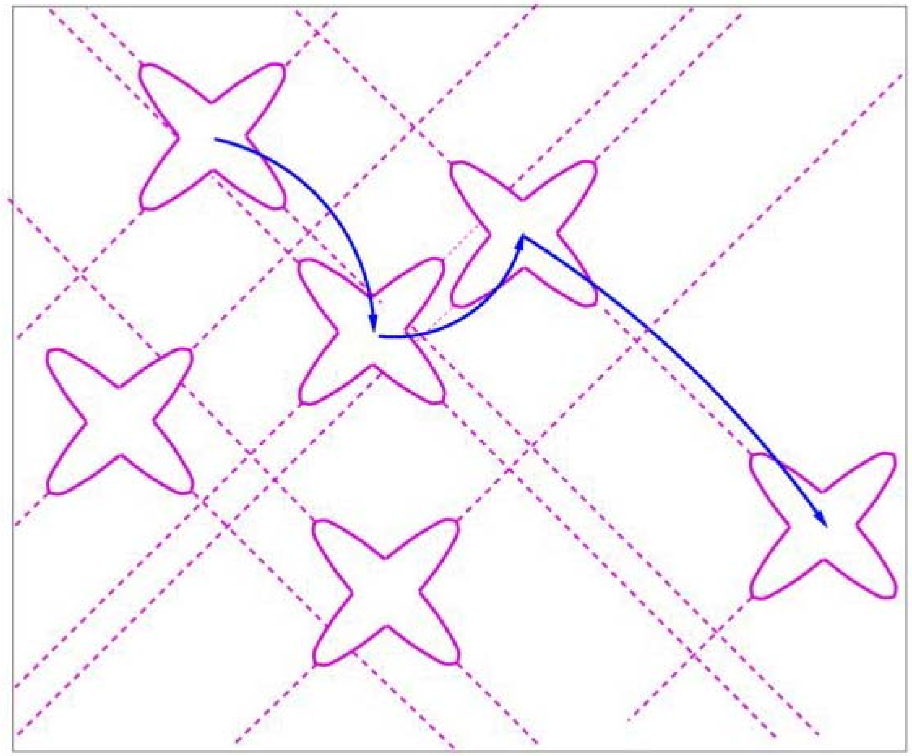
$$\rho(E \to 0) \simeq \rho_0 \left(\frac{\gamma}{\Delta_0}\right) \log\left(\frac{\Delta_0}{\gamma}\right)$$

where γ is residual scattering rate, Δ_0 gap max, ρ_0 normal state DOS.

Origin of "impurity band": hopping through tails of impurity states



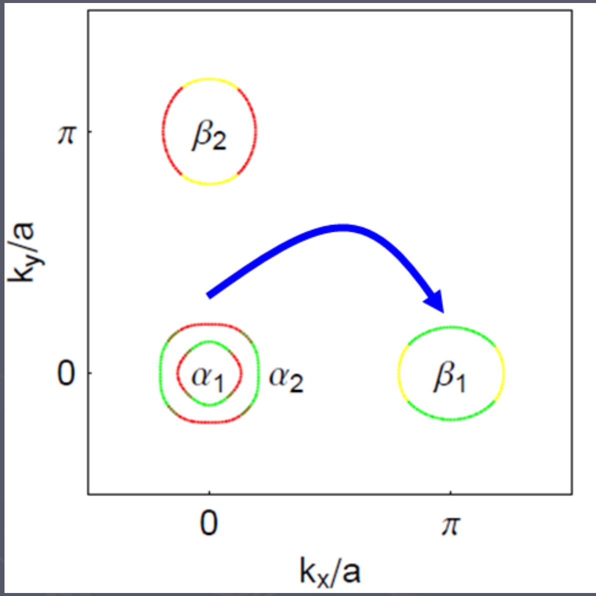
Semiconductor

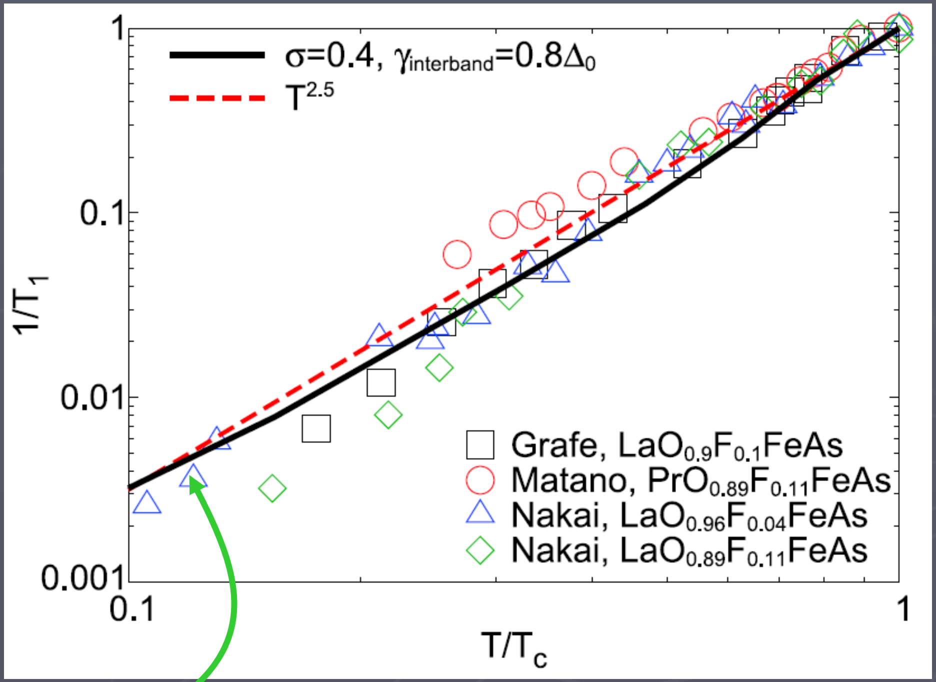


d-wave SC

Disorder: Can we reconcile (some) experiments on SC state?

Scenario 1: isotropic $s_{+/-}$ state + interband impurity scattering ⇒low-E power laws





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

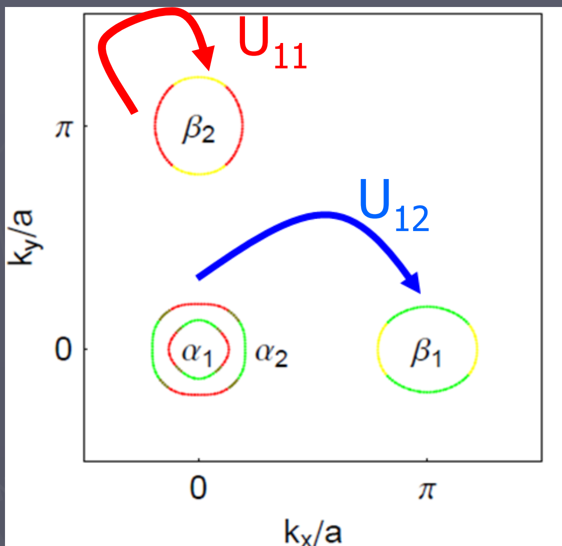
$$\sim T \text{ if } N(\omega=0) = const$$

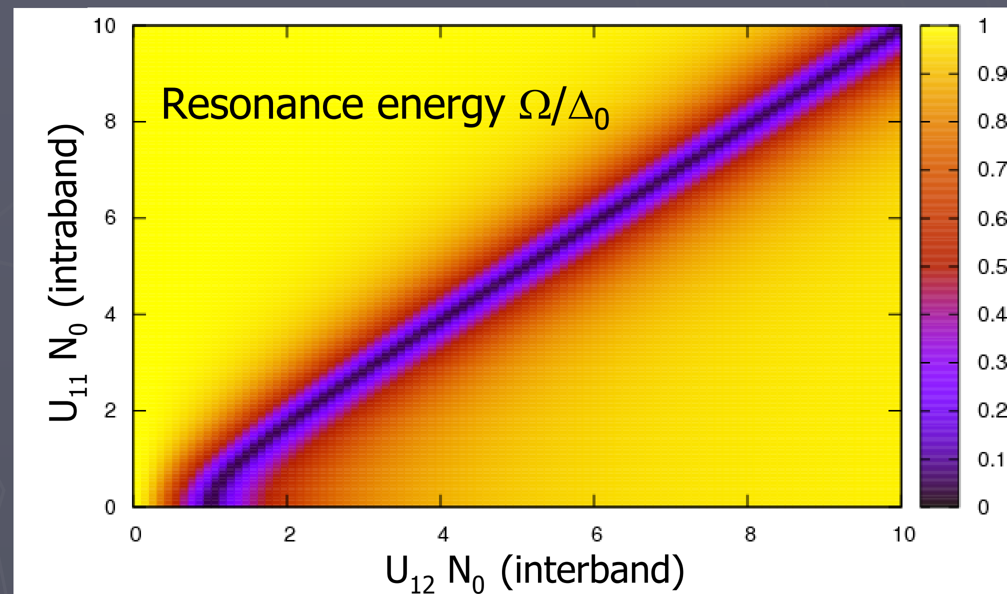
Parker et al PRB 2008
Chubukov et.al., PRB 2008
Vorontsov et al arXiv:0901.0719

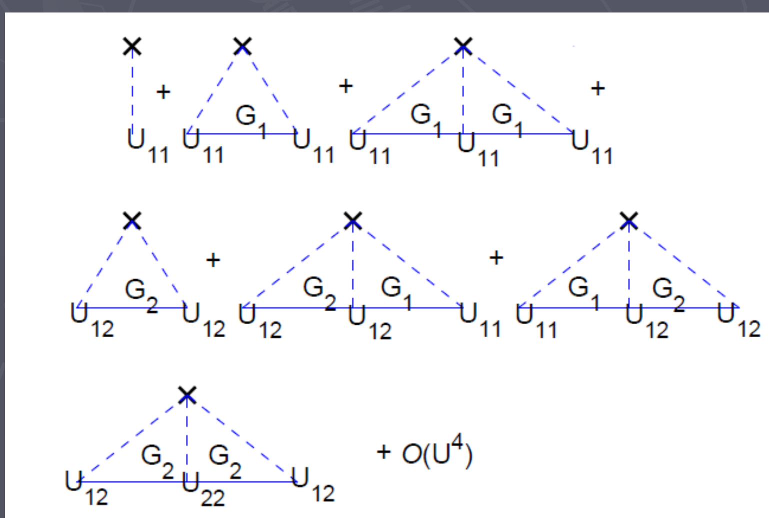
$s_{+/-}$ state has full spectral gap but interband scattering is pairbreaking (Muzikar 1990s)
Implication: samples showing full gap are clean; samples with low-E states are dirty

Some details: disorder in $s_{+/-}$ state

Muzikar 1996, Golubov & Mazin 1997, Kontani et al 2008, 2009, Parker et al 2008, Chubukov et al 2008, Mishra et al 2009







In isotropic $s_{+/-}$ picture, scattering must be carefully tuned to create qp states near Fermi level.

If intraband >> interband as expected, no such states are created

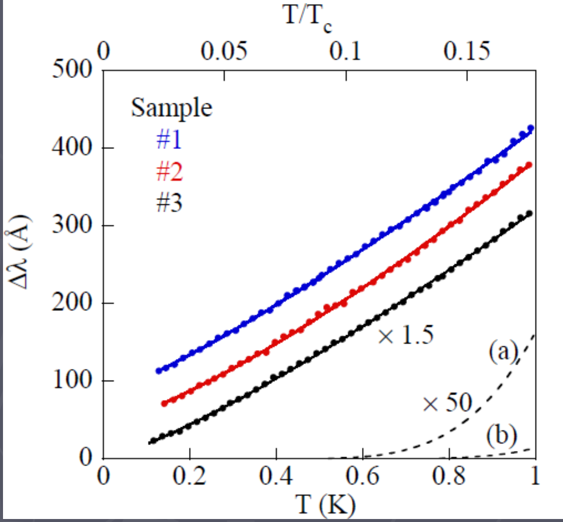
Reconciling contradictory experiments cont'd.

Scenario 2: anisotropic states with intraband scattering

recall

Fletcher et al 2008 LaFePO T_c=6K

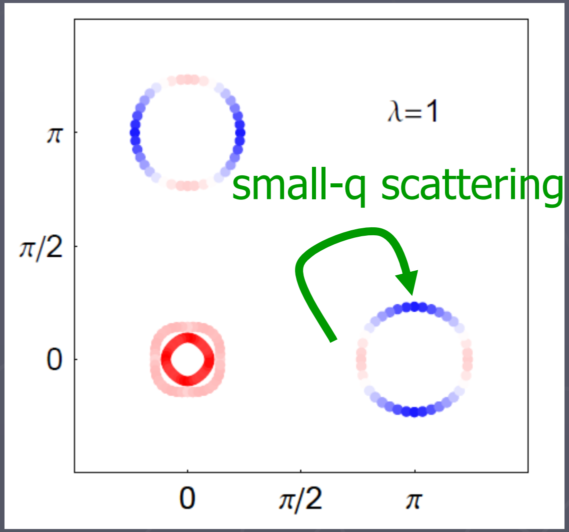
$\lambda \sim T \Rightarrow$ nodes!

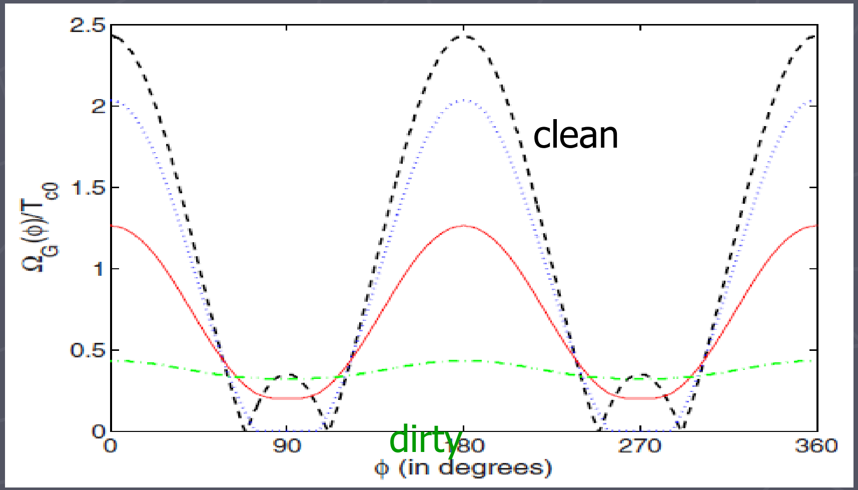


intraband scattering averages gap anisotropy, removes nodes!

$\Rightarrow$ clean systems have nodes, dirty ones full gaps!

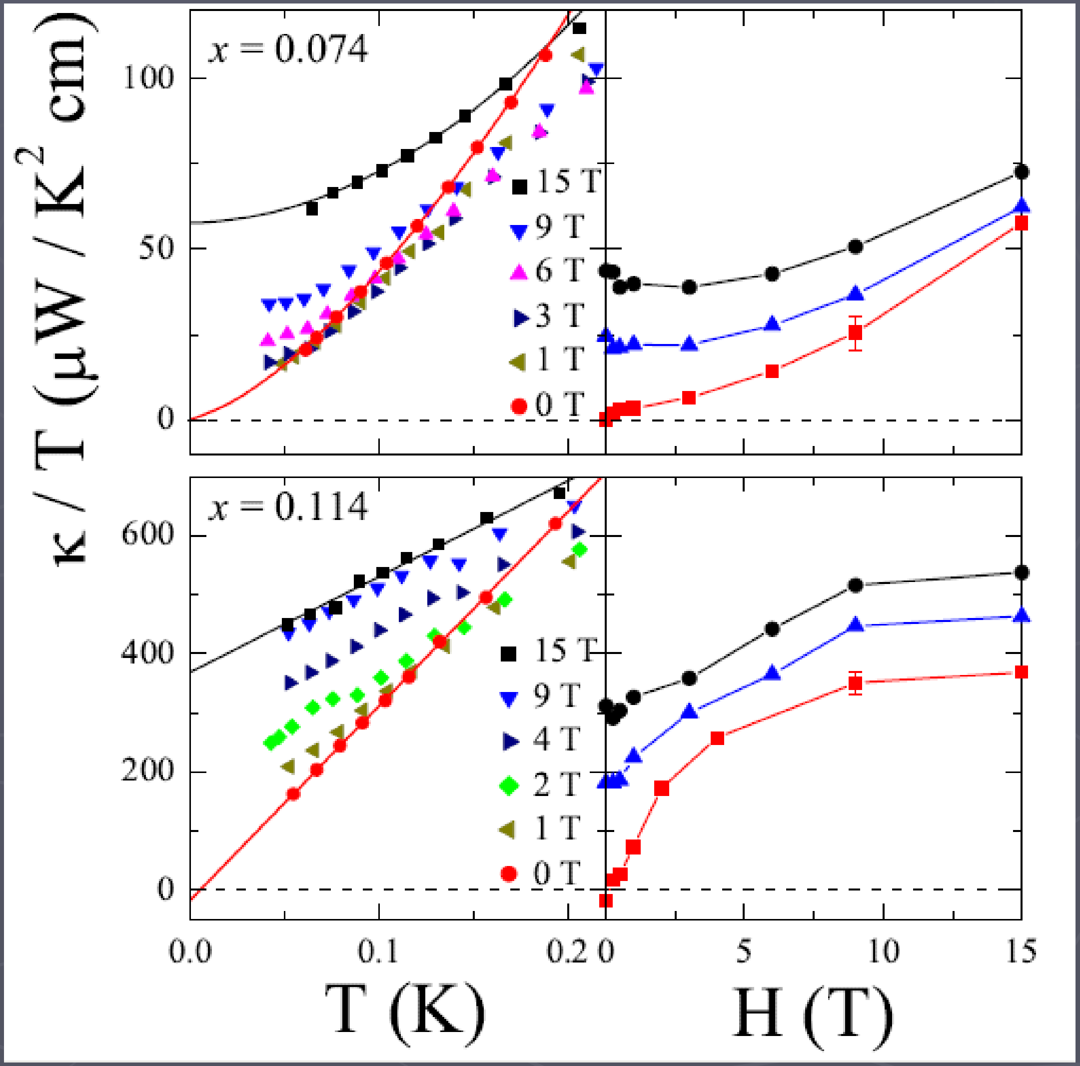
Mishra et al PRB 2009





Reminder: thermal conductivity in Co-122

Co-doped Ba-122: Tanatar et al aXv:0904.4049

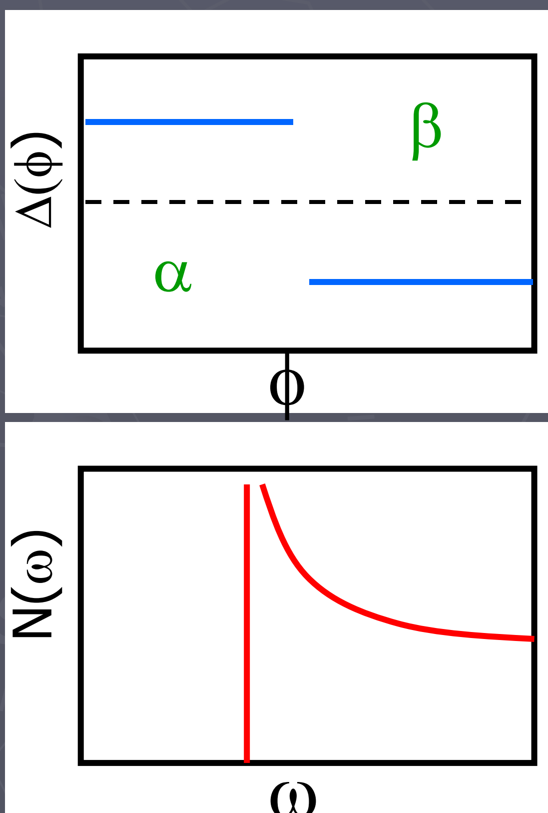


Theory of thermal conductivity

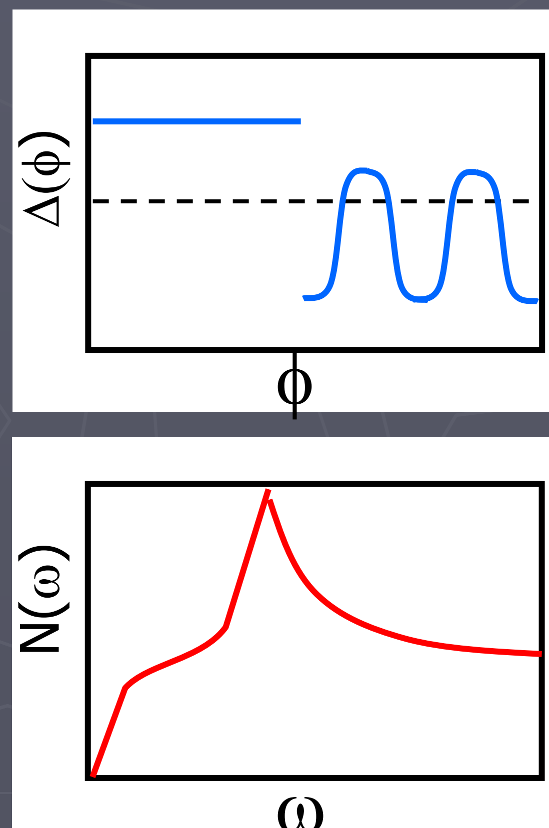
Mishra, Vorontsov, Vekther and PH 2009

2-band phenomenological calculation:

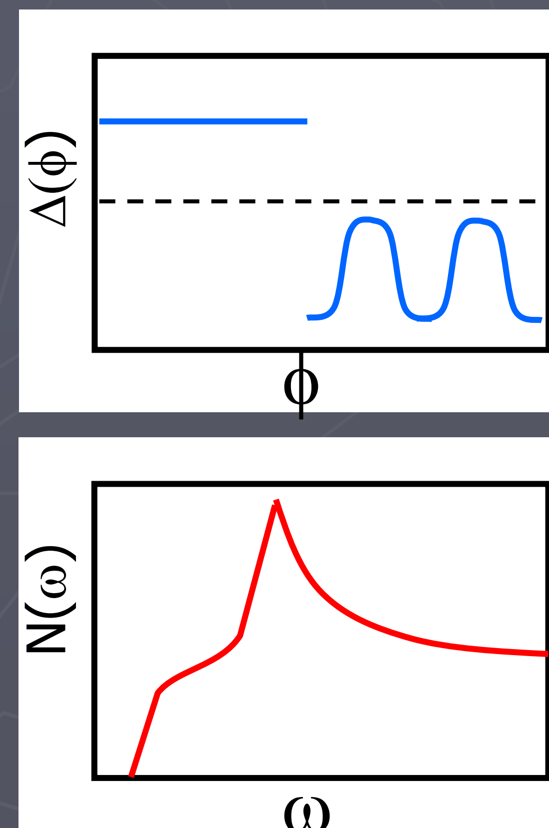
a) isotropic $s_{+/-}$



b) nodes



c) deep minima



Theory of thermal conductivity cont'd

$$\kappa = \sum_i \frac{N_i v_{Fi}^2}{8} \int_0^\infty d\omega \frac{\omega^2}{T^2} \text{sech}^2(\frac{\omega}{2T}) \times \left\langle \frac{1}{\text{Re}\sqrt{\tilde{\Delta}_i^2 - \tilde{\omega_i}^2}} \left[1 + \frac{|\tilde{\omega_i}|^2 - |\tilde{\Delta}_i|^2}{|\tilde{\Delta}_i^2 - \tilde{\omega_i}^2|} \right] \right\rangle_\phi$$

Both ω and Δ are renormalized by disorder

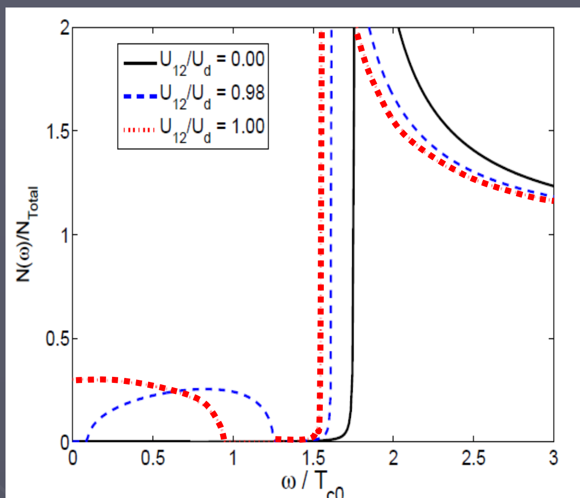
In d-wave case as T→0, $\tilde{\Delta}=\Delta$ and $\kappa \sim N_0 v_F^2 / v_\Delta$ (universal)

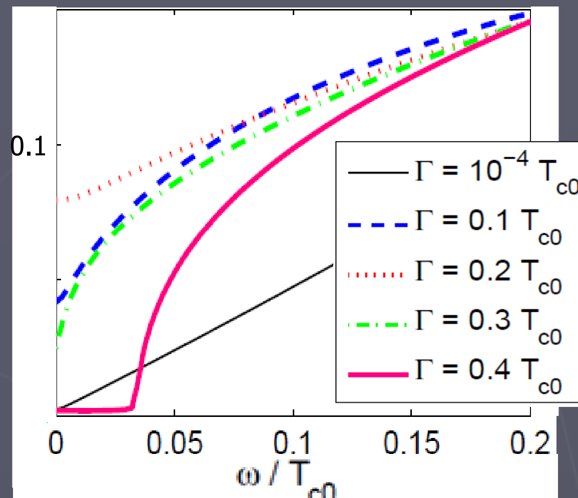
Q: what happens in 2-band A1g cases as T→0?

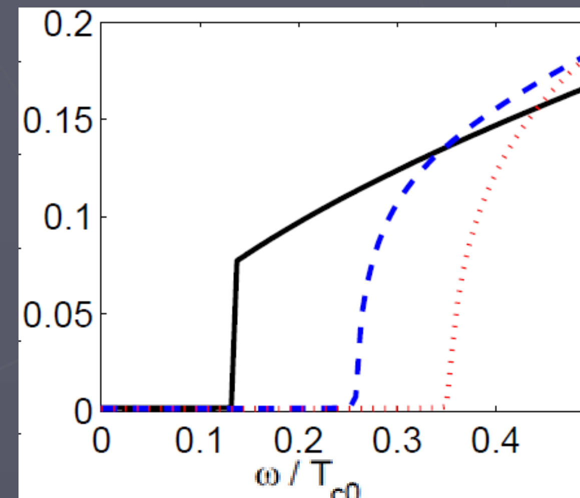
Theory of thermal conductivity cont'd

isotropic Γ=0.3T_{c0} | nodes c=0.07 | deep minima c=0.07

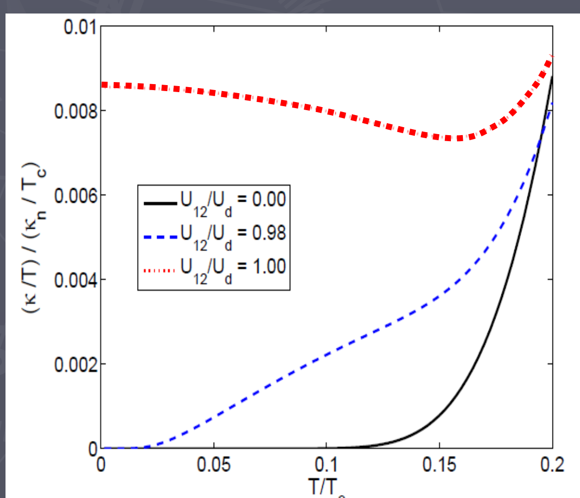
DOS

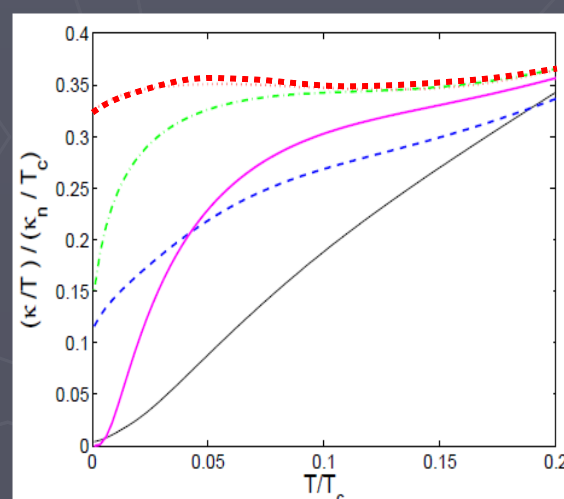


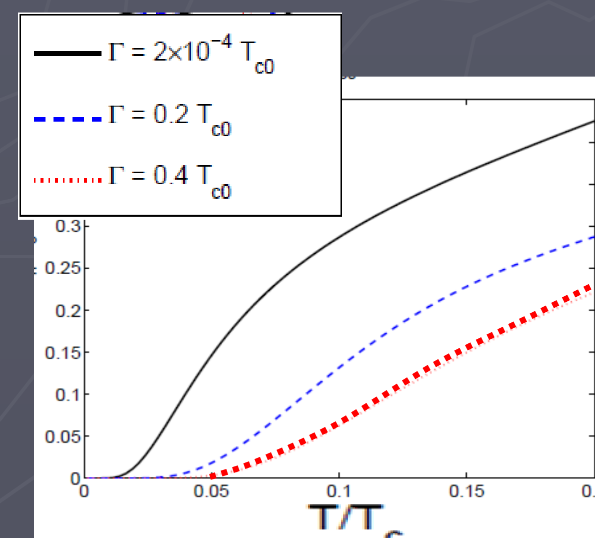




Thermal cond/T

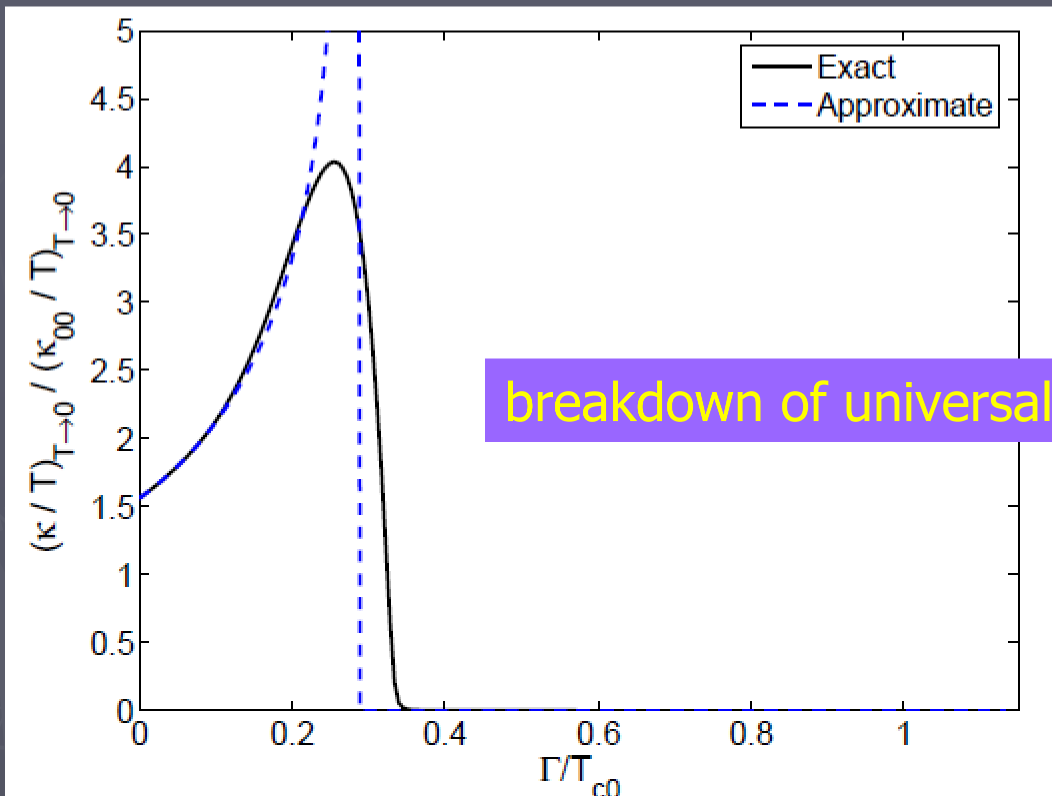




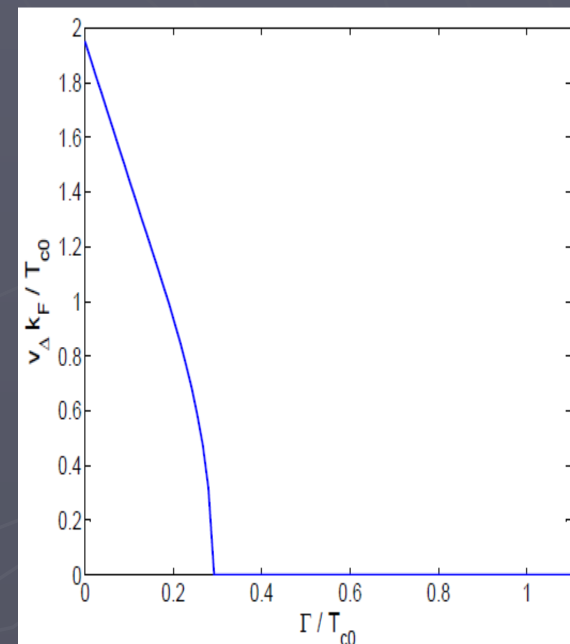


Theory of thermal conductivity cont'd

b) Nodes



breakdown of universality



Same form as in d-wave case,
but v_Δ is strongly disorder-dependent

$$\kappa \sim N_0 v_F^{\ 2} / v_\Delta$$

Field dependence of thermal conductivity: BPT method

$$\left[-2i\tilde{\varepsilon}+\mathbf{v_F}\left(\nabla_R-\frac{2ie}{c}\mathbf{A}(\mathbf{R})\right)\right]f=2ig\tilde{\Delta}(\mathbf{R},\phi)$$

Input: vortex lattice

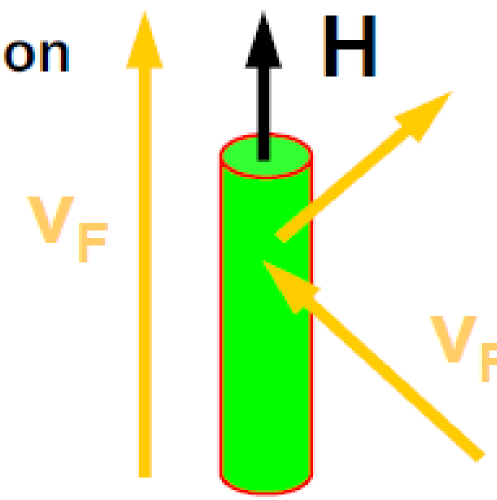
- Brandt-Pesch-Tewordt approximation: g → spatial average
- Nearly exact near H_{c2}, good down to low fields
- Closed form expression for the Green's function

$$g(\hat{\mathbf{p}},\varepsilon)=-i\pi\left[1-i\sqrt{\pi}\left(\frac{2\Lambda\Delta_0}{|\mathbf{v}_F^{\perp}|}\right)^2 Y^2(\hat{\mathbf{p}})W'\left(\frac{2\tilde{\varepsilon}\Lambda}{|\mathbf{v}_F^{\perp}|}\right)\right]^{-1/2}$$

– self-consistency in T,H, impurities

– DOS, specific heat, thermal conductivity

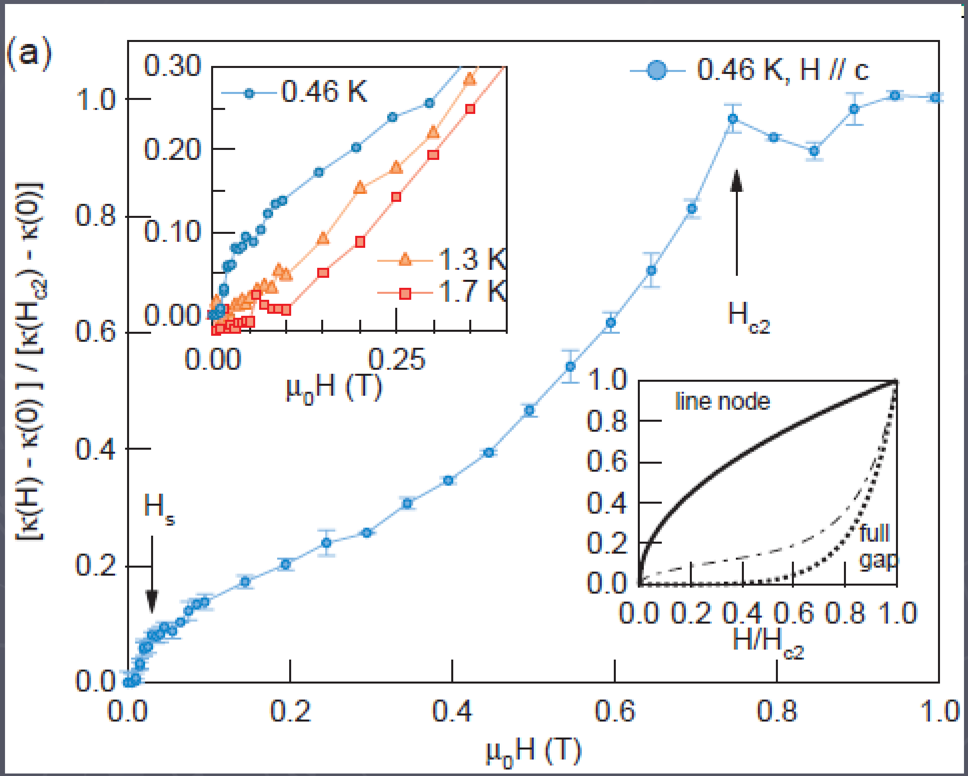
– angle-dependent scattering on the vortices



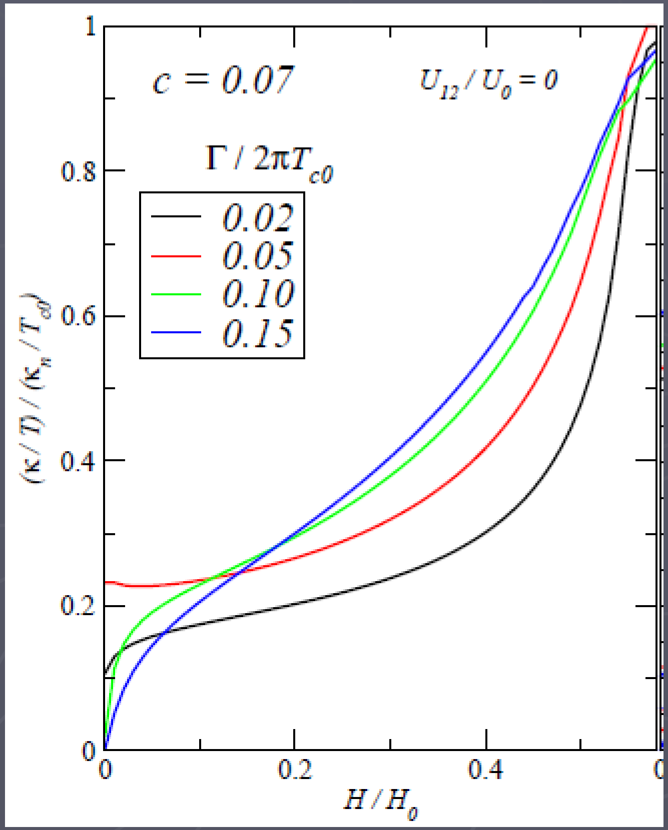
A. Houghton and I. Vekhter '98, H. Kusunose '04, A. Vorontsov and I.Vekhter, '06

Field dependence of thermal conductivity: results

Expt: LaFePO Yamashita et al



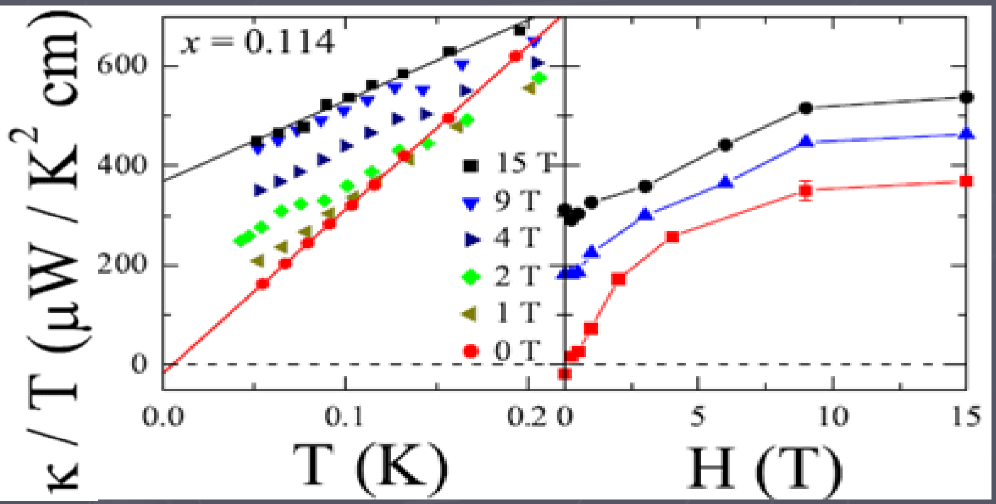
Theory: nodes, pure intraband scatt only

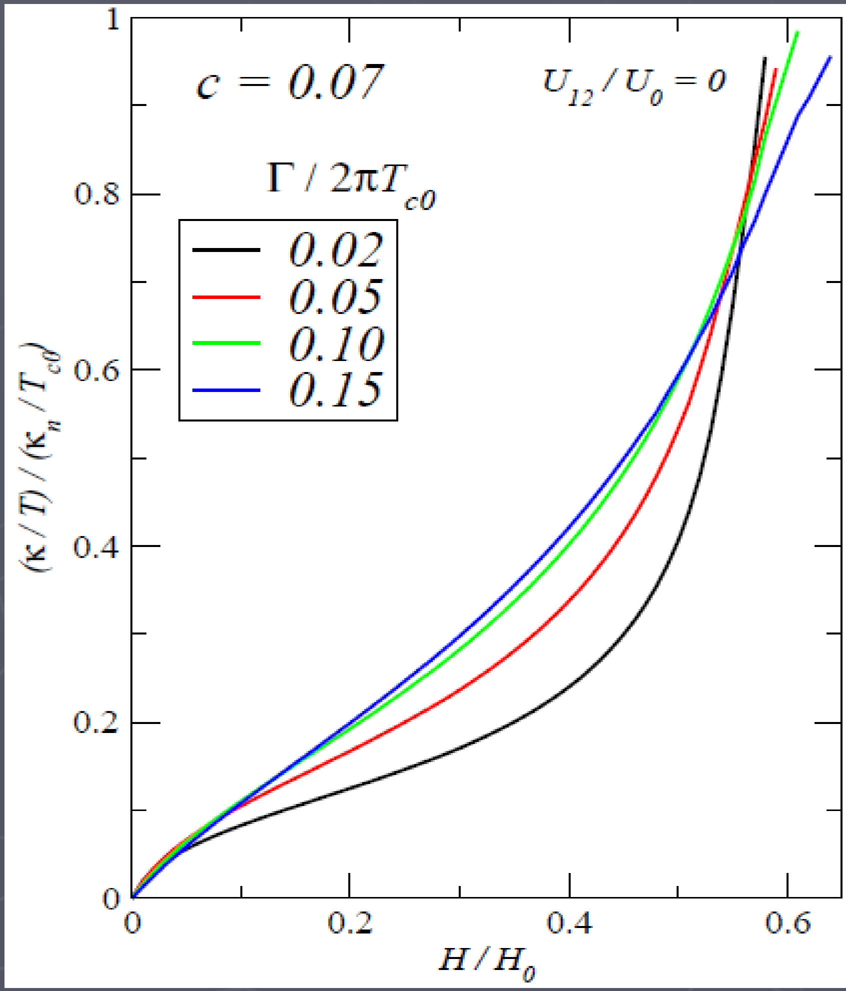


Field dependence of thermal conductivity: results cont'd

Theory: deep gap minima

Expt: Co-doped Ba-122 Tanatar et al



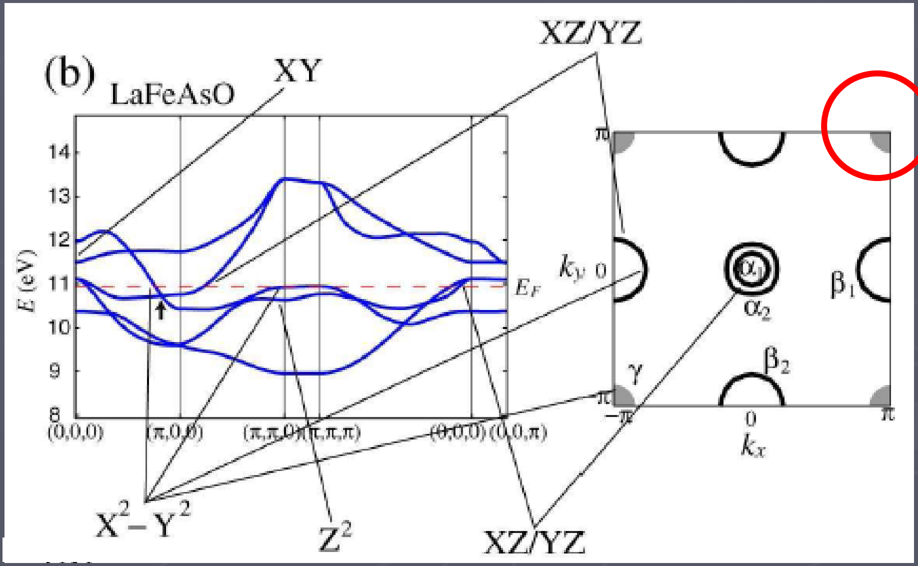


Field dependence with deep gap minima not qualitatively different from nodes!

Higher Tc? Systematics of T_c's and pair state in 1111's

H. Kuroki et al., Phys. Rev. B 79, 224511 (2009)

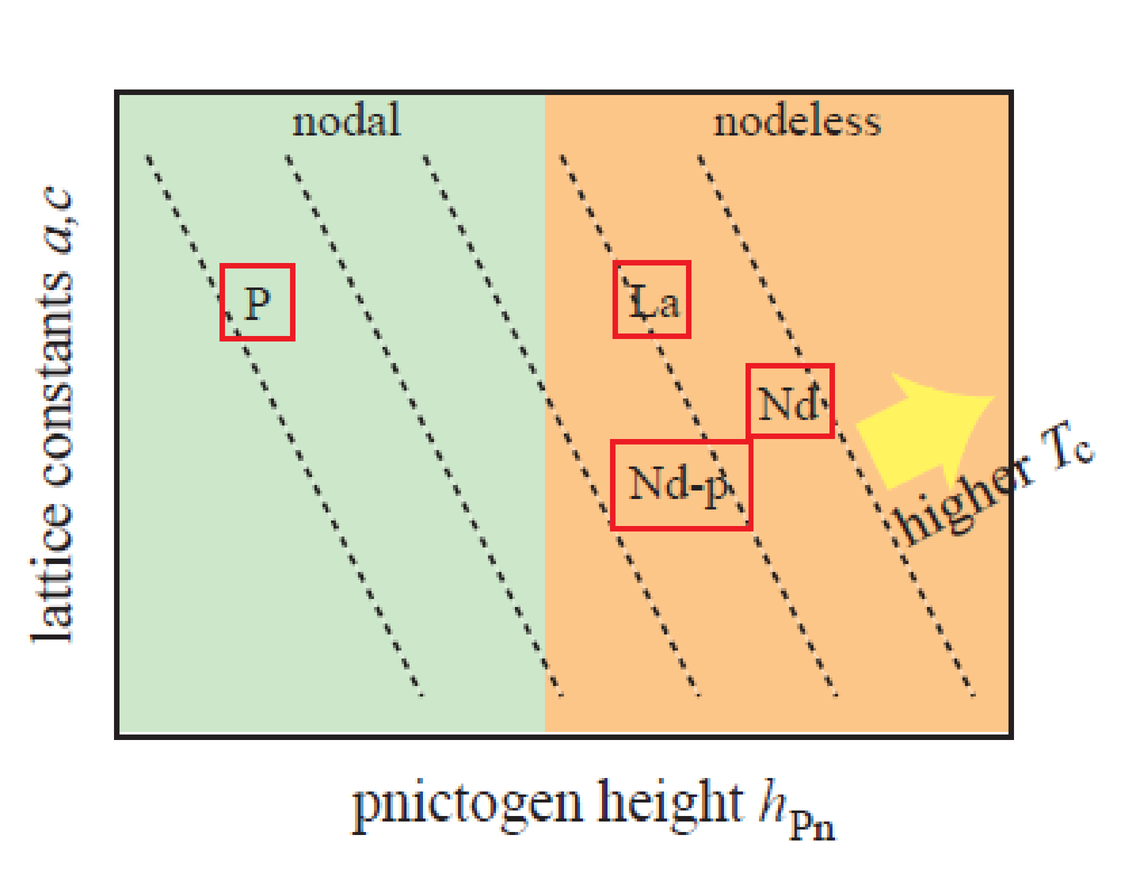
Look at effective tight-binding spin fluctuation models for various 1111 materials



	a(Å)	c(Å)	z_{Pn}	h_{Pn} (Å)	α	$t_{X^2-Y^2}$	$t'_{X^2-Y^2}$	t_{XZ}	t'_{XZ}
La[1]	4.04	8.74	0.6512	1.32	113.6	0.163	0.124	−0.210	0.329
$h_{\mathrm{As}} = 1.38$Å	4.04	8.74	0.6580	1.38	111.2	0.132	0.113	−0.191	0.309
$h_{\mathrm{As}} = 1.14$Å	4.04	8.74	0.6304	1.14	121.1	0.261	0.153	−0.240	0.364
$a = 3.95$Å	3.95	8.74	0.6512	1.32	112.4	0.148	0.123	−0.210	0.346
$c = 8.40$Å	4.04	8.40	0.6573	1.32	113.6	0.174	0.132	−0.209	0.327
Nd[50]	3.94	8.51	0.6624	1.38	109.9	0.135	0.123	−0.202	0.332
Nd-p[81]	3.92	8.37	0.6584	1.33	111.9	0.172	0.138	−0.217	0.350
Nd-ud[50]	3.97	8.57	0.6571	1.35	111.7	0.156	0.129	−0.213	0.341
P[49]	3.96	8.51	0.6339	1.14	120.2	0.253	0.156	−0.234	0.377

Higher Tc?

Kuroki et al. PRB '09



Tc, pair structure trends from band structure changes alone

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

Conclusions

- Spin fluctuation calculations predict reasonable Tc, find dominant A1g sign-changing (s-wave) but nearby d-wave. Can systems display SC symmetry transitions as function of external parameter?

- challenge: explain apparently commensurate magnetic response

- s-wave is always highly anisotropic on electron sheets in theory

- Hope: use such theories to predict *systematics* of Tc within family (Kuroki)

- Order parameter symmetry controversial, expts. disagree.

A1g (nodes vs. no nodes?) vs. B1g?

2 different scenarios which attempt to reconcile by accounting for disorder: distinguish by systematic disorder experiments

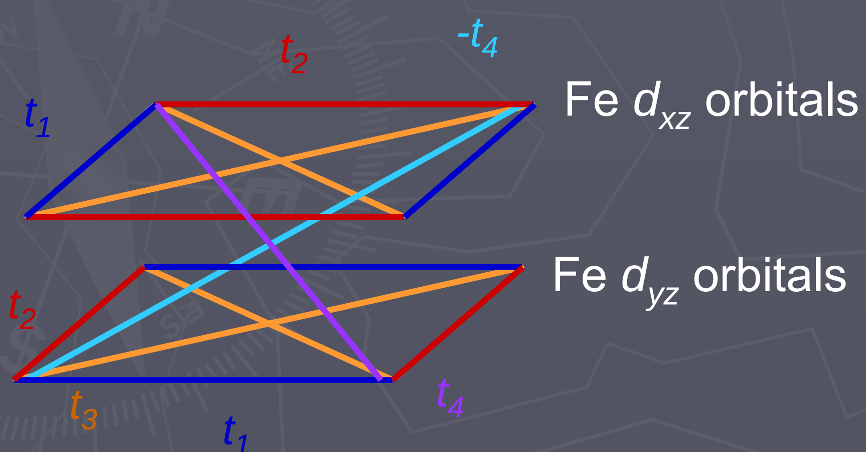
Belief: LFPO have nodes, some 122's have deep gap minima, which decrease with overdoping ($BaFe_2(As,P)_2$) $\Rightarrow$more low-E qp's. Spoiler: ARPES?

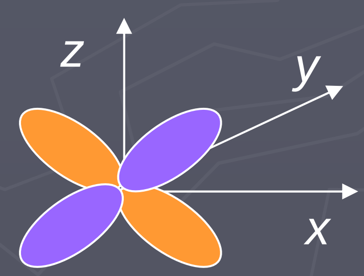
Band structure – Two-band approximation

Assumption: Most important inter- and intra-orbital hopping between the Fe d_{xz} and d_{yz} orbitals mediated by As p_x and p_y orbitals

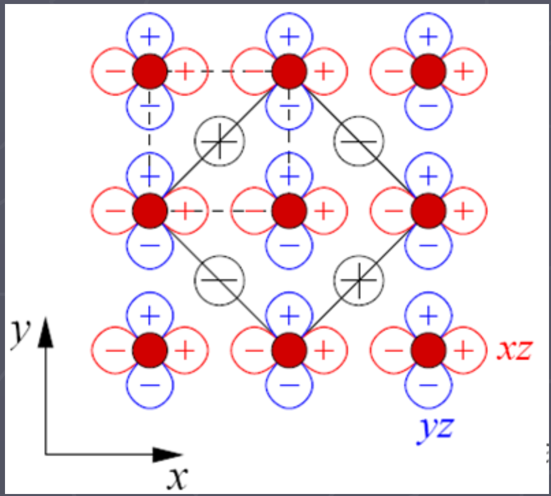
Derivation of effective Fe-Fe hopping terms e.g. from the Slater-Koster table of directional dependent matrix elements:

- Give the correct symmetry
- Must be adjusted in size to give the correct FS sheets





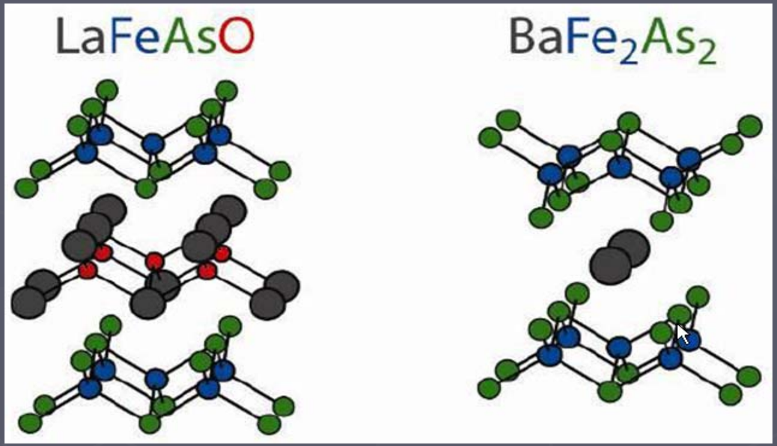
d_{xz} orbital



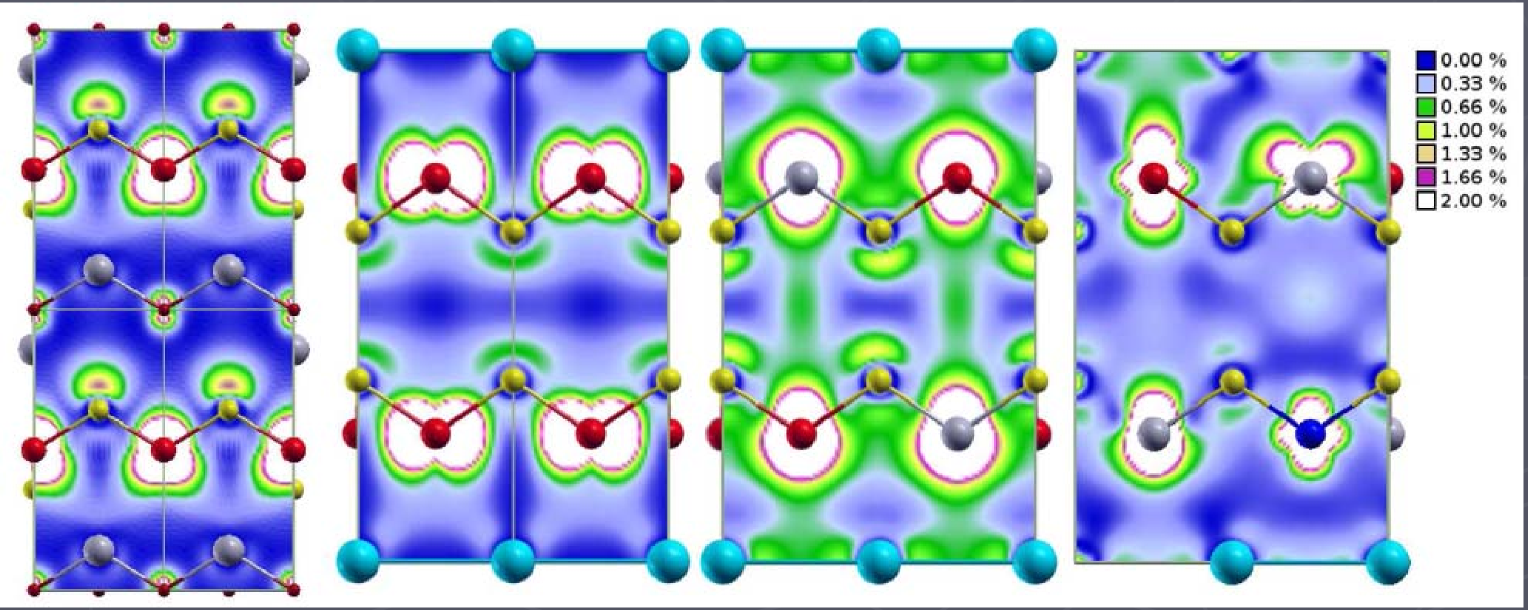
Electronic structure of 122 materials more 3D

Kemper et al arXiv:0904.1257

As in phase



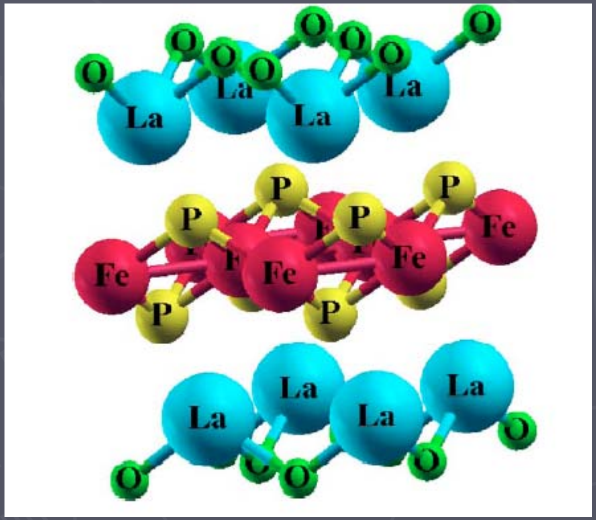
As out of phase

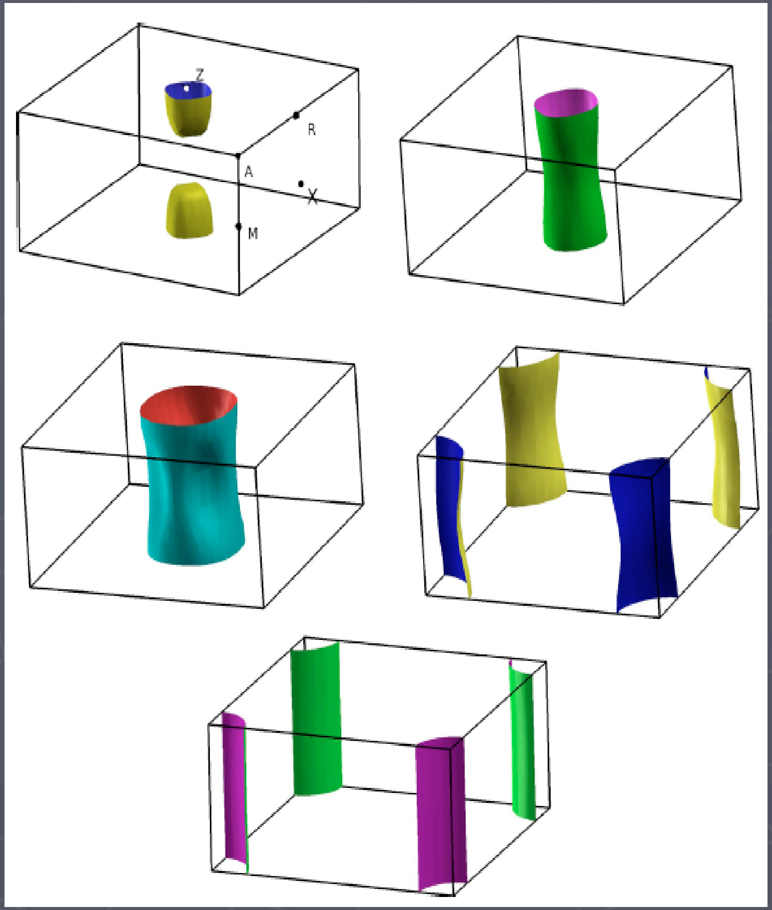


LaFeAsO $BaFe_2As_2$(PM) $BaFe_2As_2$(SDW) $BaFe_{2-x}Co_xAs_2$(SDW)

Prehistory

- Discovery of LaOFeP superconductor T_c=3-6K (Kamihara et al 2006)
- Material is layered
- Fermi surf.: 4 2D sheets



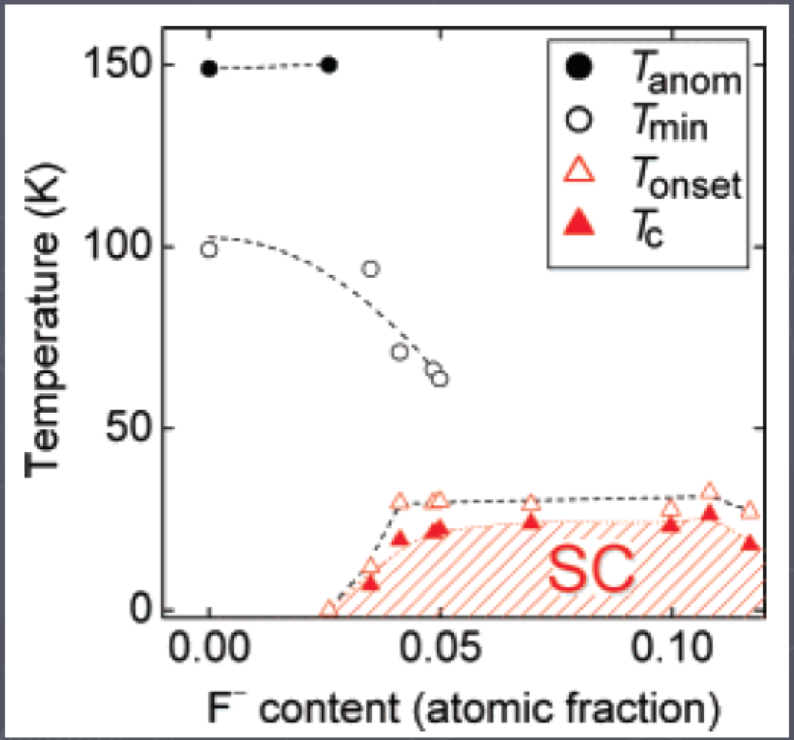


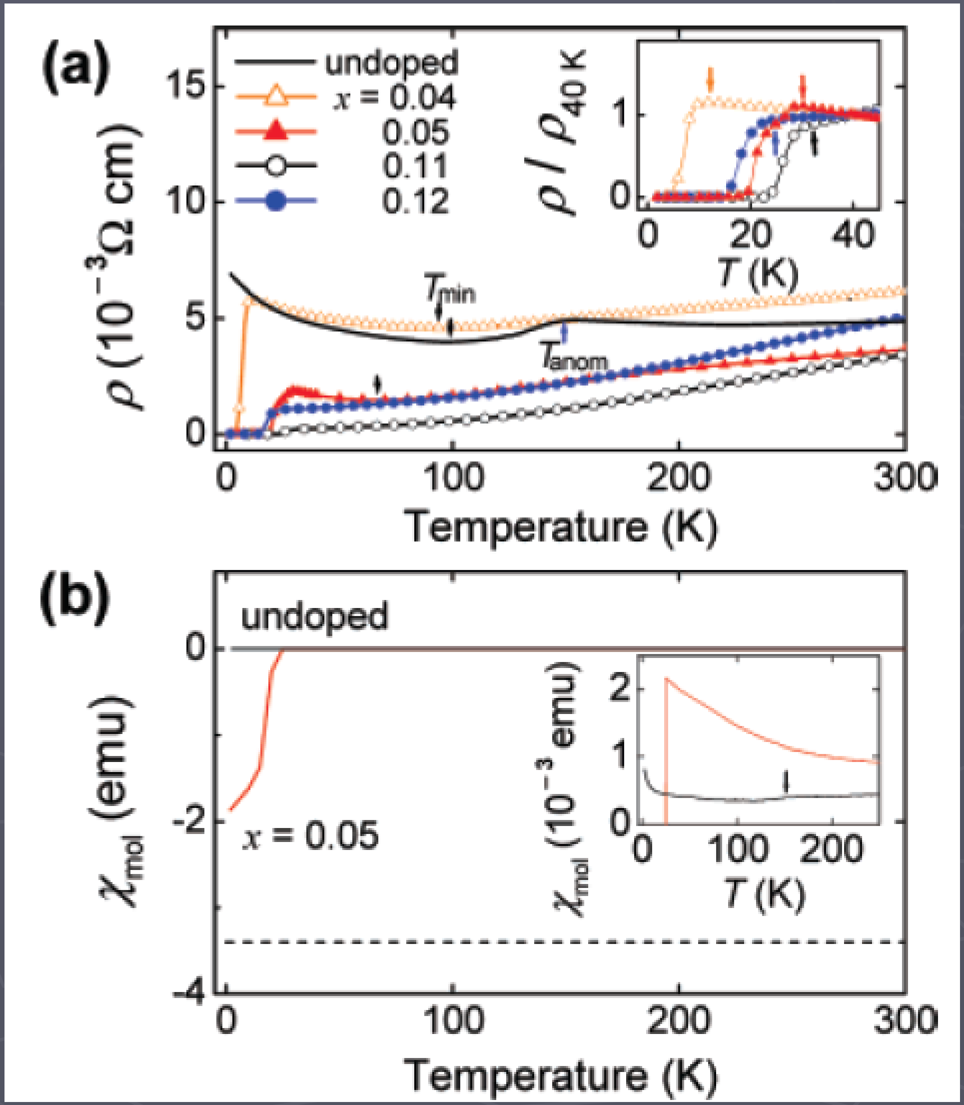
Lesbegue 2006

Discovery of LOFFA ($LaO_{1-x}F_xFeAs$)

Kamihara et al JACS 2008

$T_{c,max}$=26 K

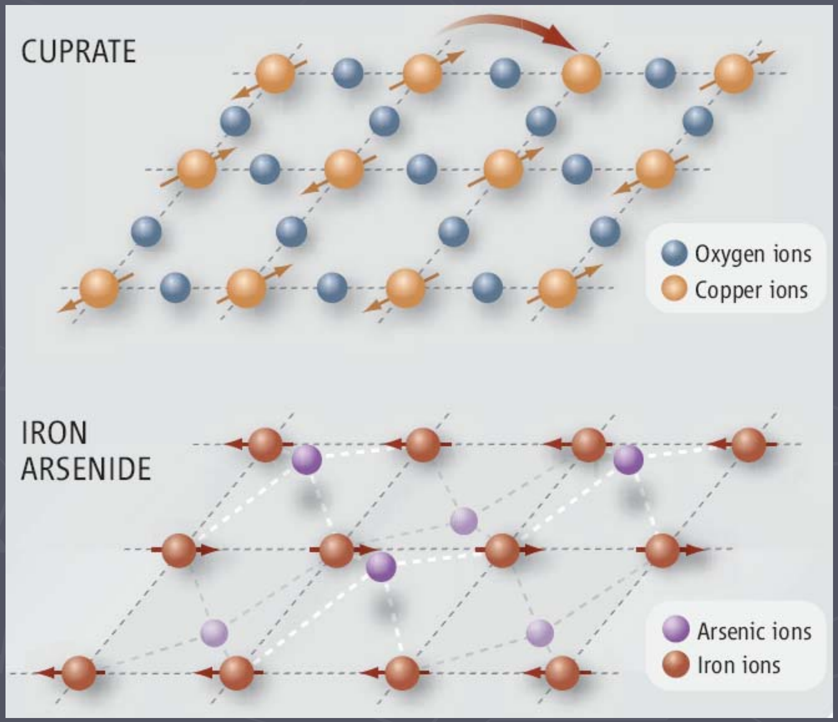


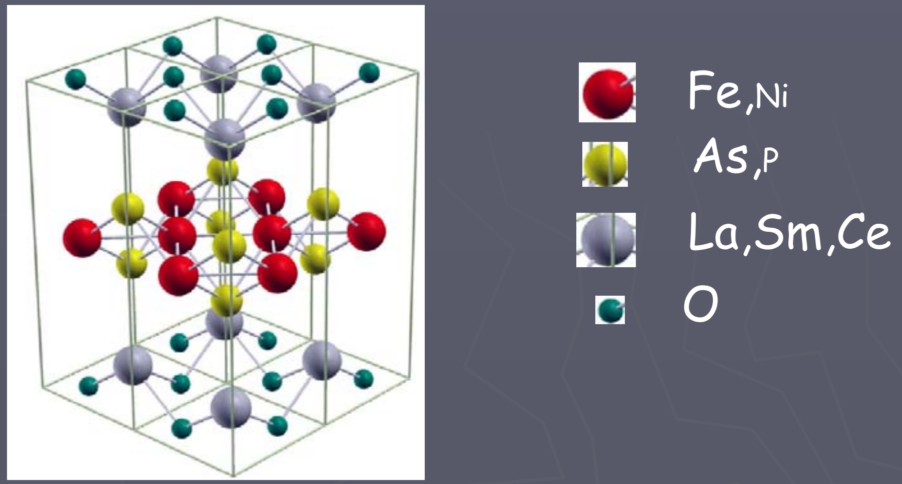


Crystal Structure:Tetragonal I4/mmm (high T)

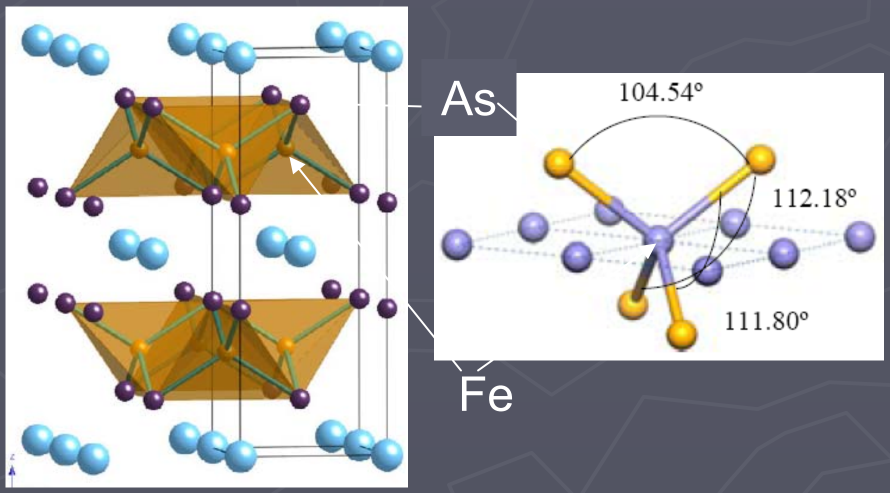
R $O_{1-x}F_x$ FeAs
R O_{1-x} FeAs

- 2D square lattice of Fe
- Fe - magnetic moment
- As-similar then O in cuprates





But As is not in the plane!

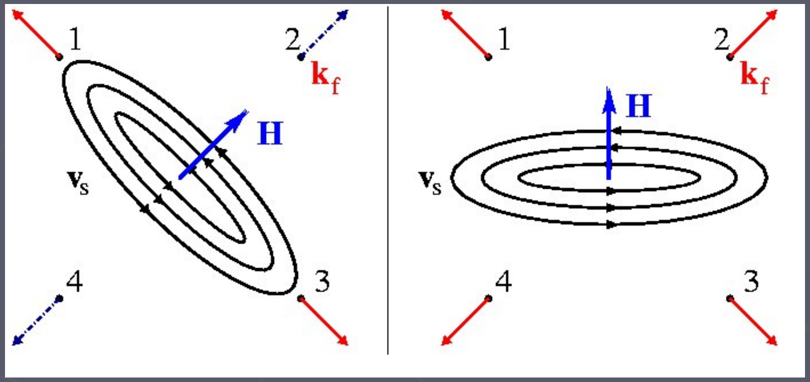


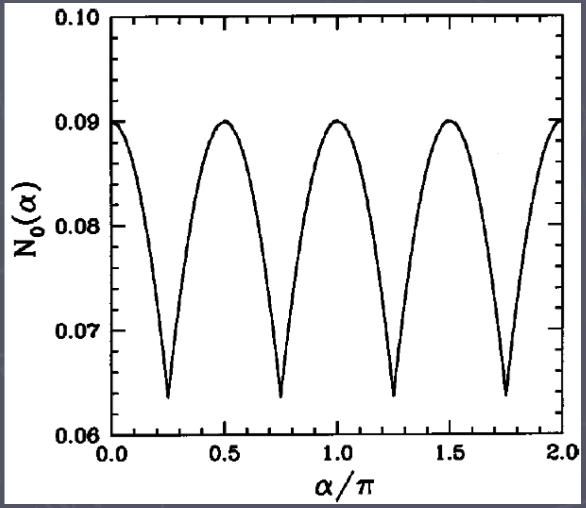
Perfect tetrahedra 109.47°

Bulk probe of order parameter symmetry: specific heat oscillations

Vekhter et al PRB 1999

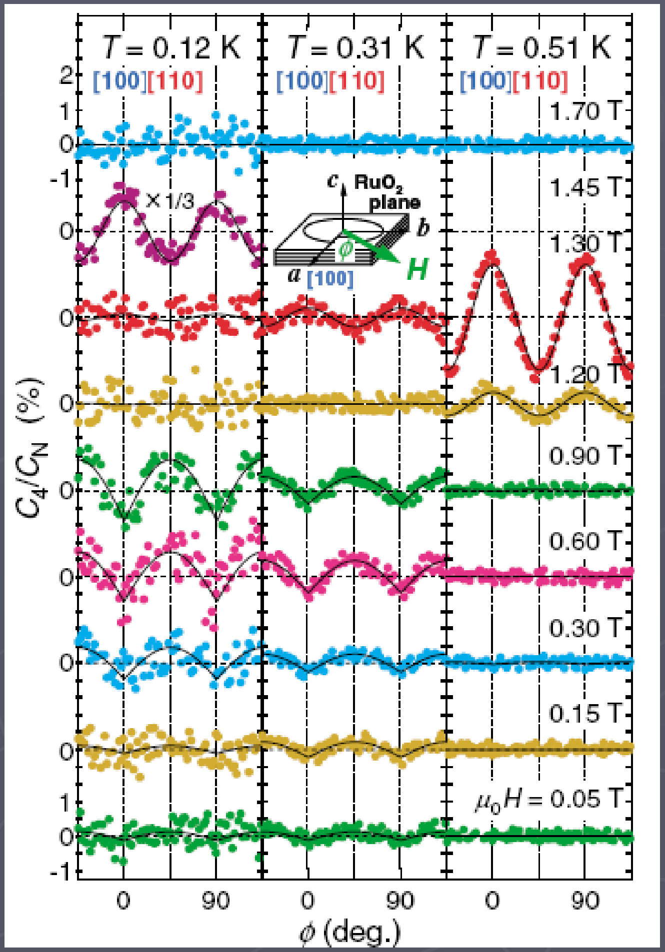
e.g. Sr_2RuO_4

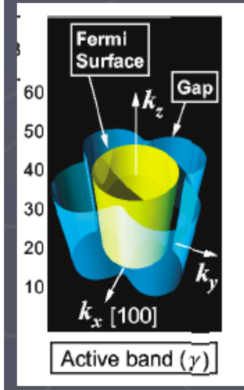




$$N_0(\alpha) = \frac{2\sqrt{2}E_H}{\Delta_0 \pi} \max(|\sin\alpha|, |\cos\alpha|)$$

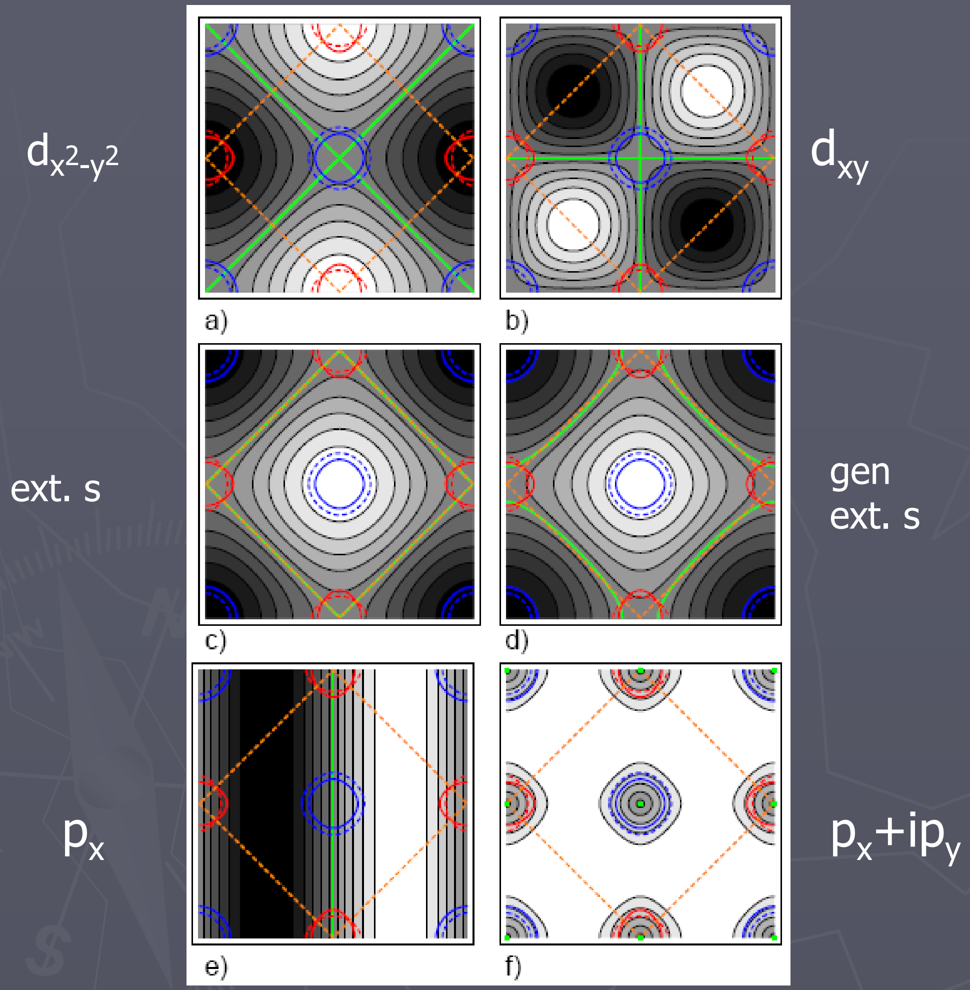
(d-wave)



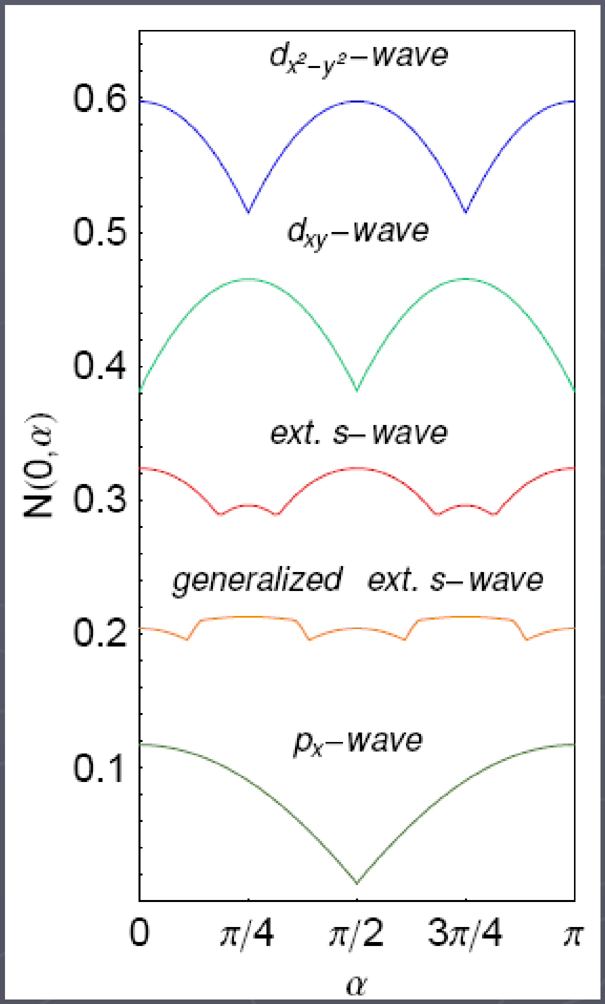


Deguchi et al PRL 2004

Spec. Heat Oscillations cont'd



Anisotropic states proposed in early FeAs papers

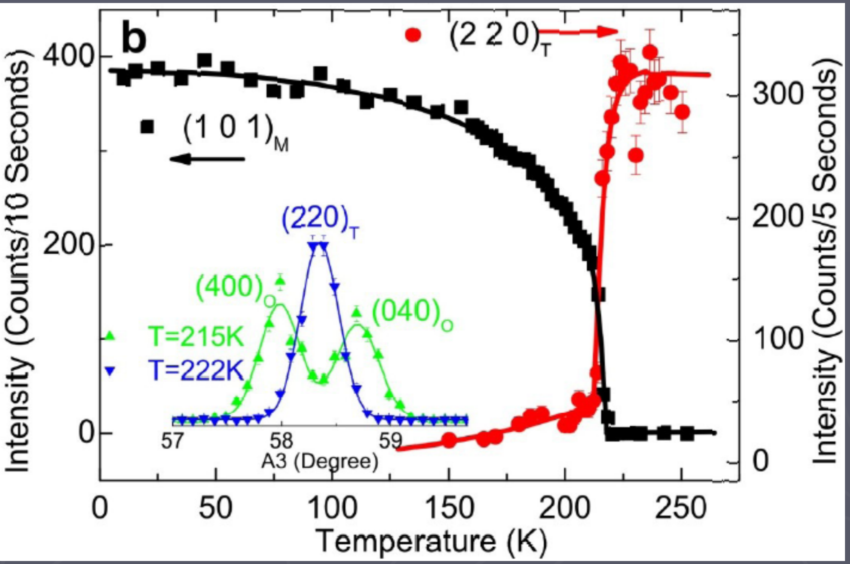


Graser et al PRB **77**, 180514 (2008)

Neutron measurements on 122 single xtals

Zhao et al: 0807.1077

- transitions at 200K in Sr-112
- structure 1st order (few degrees hysteresis, magn. 2nd order
- alignment of spins along long (b) axis tells us something:



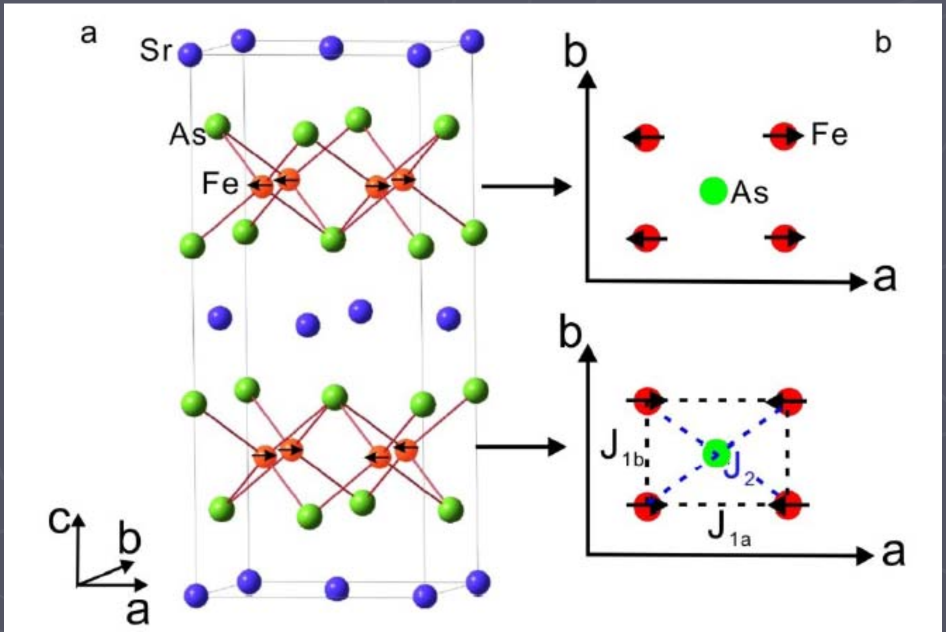
- J_1=nearest neighbor exchange
- $J_1 = J_1^s - J_1^d$

  s=superexchange (As)
  d=direct exchange

- Lattice distortion $\delta \Rightarrow$

  $\Delta J_1^s \sim \delta^2 \qquad \Delta J_{1a}^d \sim -\delta, \ \Delta J_{1b}^d \sim \delta$

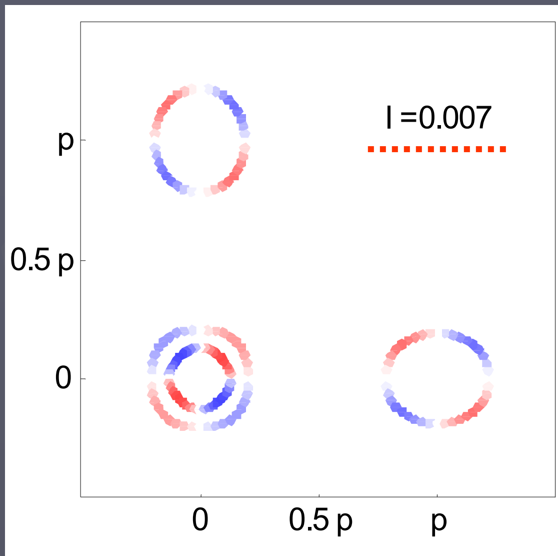
- So direct exchange tuned by structural change, locks spins to point along a.



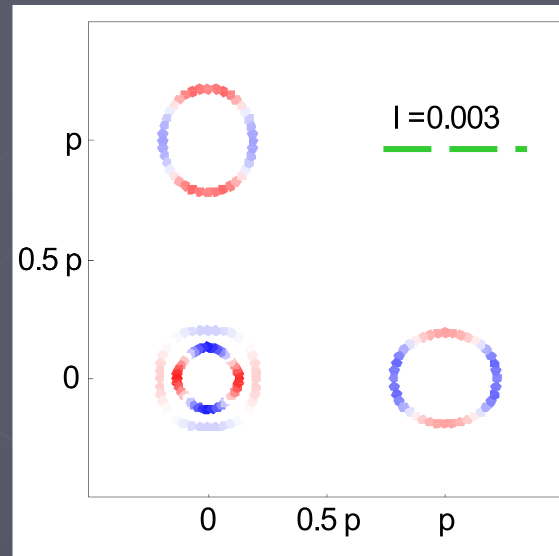
5-band spin fluctuation pairing analysis

S. Graser, T. Maier, PH, D.J. Scalapino NJP 2008

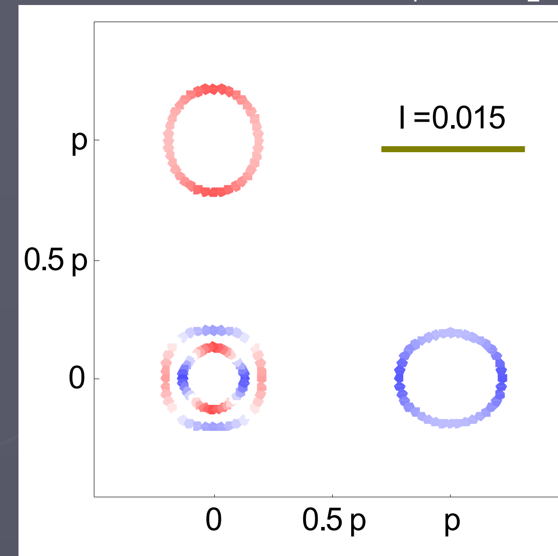
d_{xy} symmetry without sign change between α_1 and α_2



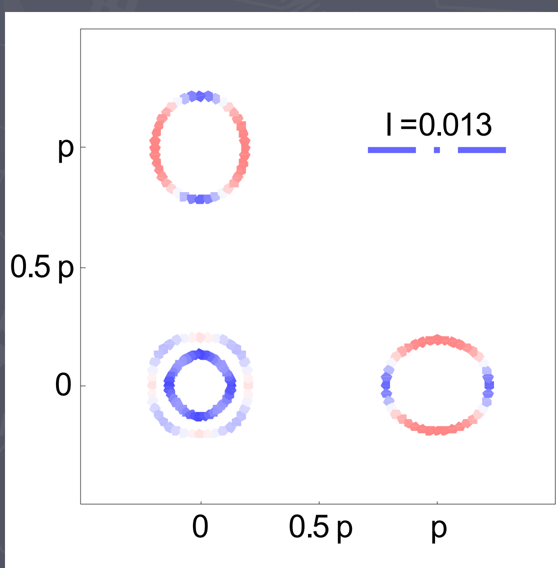
d_{x2-y2} symmetry without sign change between α_1 and α_2



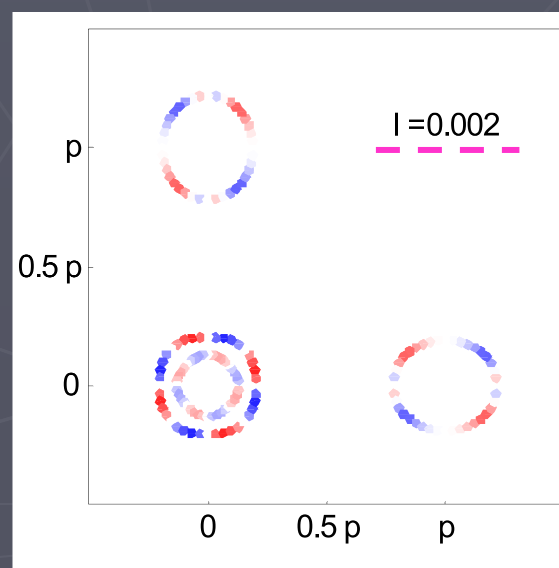
d_{x2-y2} symmetry with sign change between α_1 and α_2



extended *s*-wave



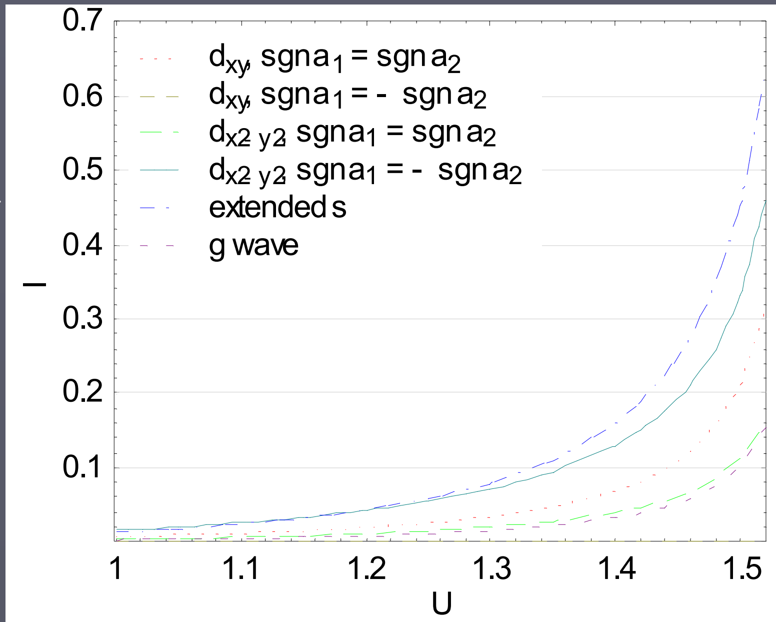
g-wave



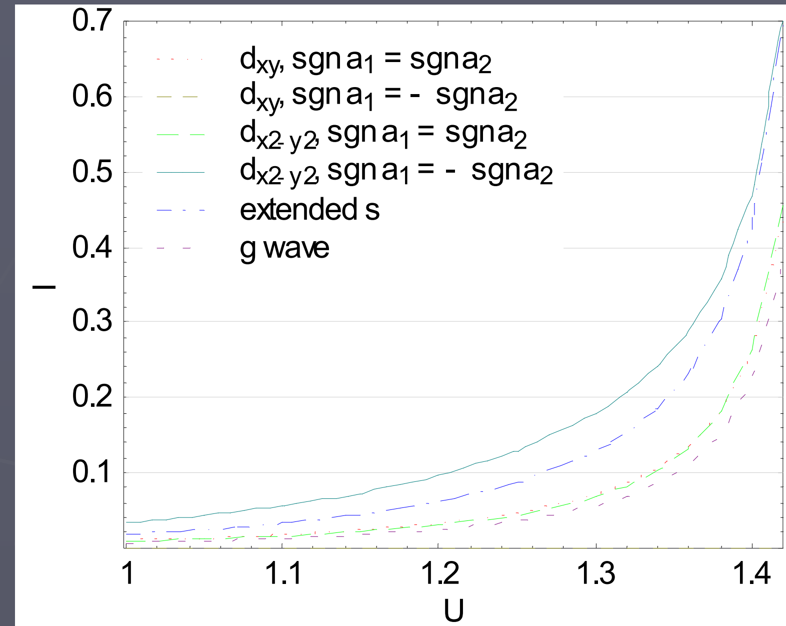
e.g., fit of C. Cao et al bandstructure with x=0 for U=1

Changes in λ_i as a function of *U*

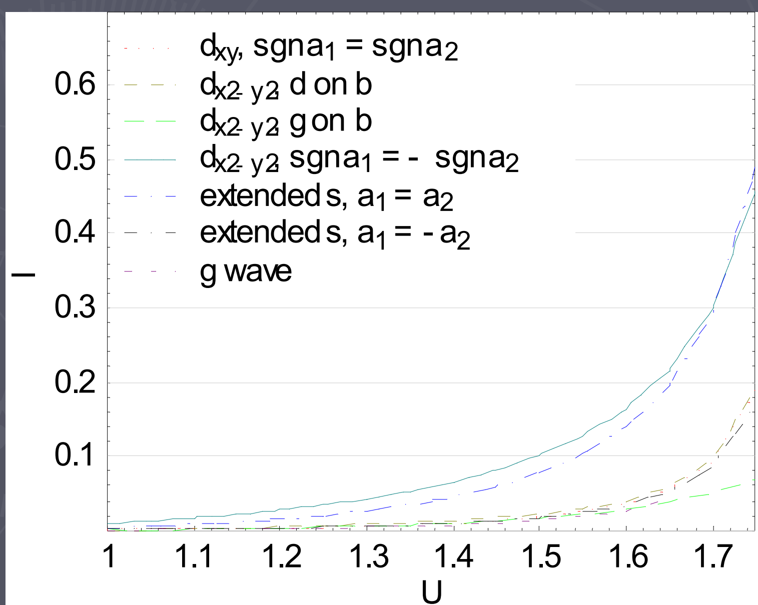
5 band Cao fit, $x = 0$



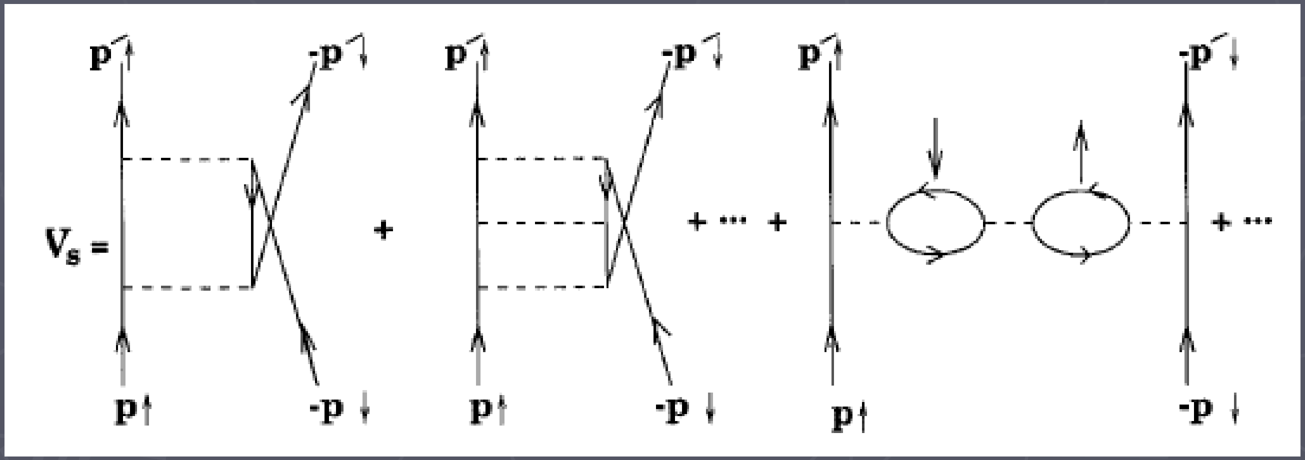
Kuroki's parameters



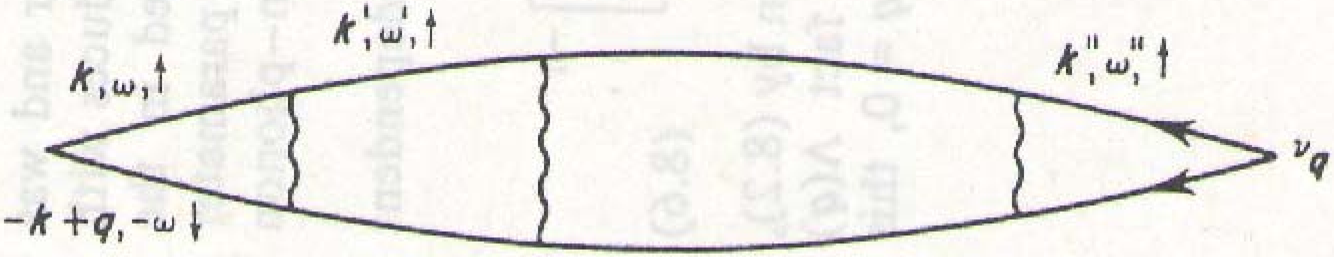
5 band Cao fit, $x = 0.125$



Origin of order parameter anisotropy in spin-fluctuation theories of ferropnictides



Superconductivity as instability of normal state to pairing field



Ladder diagrams representing the response of a metal to a pairing field ν.

$$\sum_{k,q} \left(\nu_q c^{+}_{k\uparrow} c^{+}_{-k+q\downarrow} \; \nu^{*}_q c_{-k+q\downarrow} c_{k\uparrow}\right)$$

$$\left\langle \sum_{k} c_{-k+q\downarrow} c_{k\uparrow} \right\rangle = \beta^{-1} \sum_{k,\omega} G(k, i\omega) G(-k+q, i\omega) \Lambda(k, q, i\omega) \nu_q$$

where

$$\Lambda(k, q, i\omega) = 1 + \beta^{-1} \sum_{k',\omega'} |g_{kk'}|^2 D(k-k', i\omega - i\omega') \times G(k', i\omega) G(-k'+q, -i\omega') \Lambda(k', q', i\omega').$$

$$|g^2_{kk'}|\,D(k-k', i\omega - i\omega') = \begin{cases} V, & \text{a constant, for } |\omega|, |\omega'| < \omega_D \\ 0, & \text{for } |\omega| \text{ or } |\omega'| > \omega_D . \end{cases}$$

$$\Lambda(q) = \left[1 - \beta^{-1} \sum_{k,\,|\omega| < \omega_D} G(k, i\omega) G(-k+q, -i\omega)\right]^{-1}$$

$$\begin{aligned} 1 &= V\beta^{-1} \sum_{\omega} \int d^3k\, G(k, i\omega) G(-k, -i\omega) \\ &= V\beta^{-1} \sum_{|\omega| < \omega_D} N(0) \int_{-\infty}^{\infty} d\epsilon/(\omega^2 + \epsilon^2)^{-} \\ &= N(0)V(2\pi/\beta) \sum_{\omega=0}^{\omega_D} (|\omega|)^{-1} \\ &= N(0)V \sum_{n=0}^{\beta\omega_D/2\pi} (n + \tfrac{1}{2})^{-1}. \end{aligned}$$

At very low temperatures $\beta\omega_D$ is large and the sum is

$$\gamma + \ln(2\beta\omega_D/\pi)$$

$$T_c = 1.13(\omega_D/k_B) \exp[-1/N(0)V]$$

But multiorbital spin fluct. calculations [Graser et al. NJP 11, 025016 (2009)]. find *anisotropic* A_{1g} states

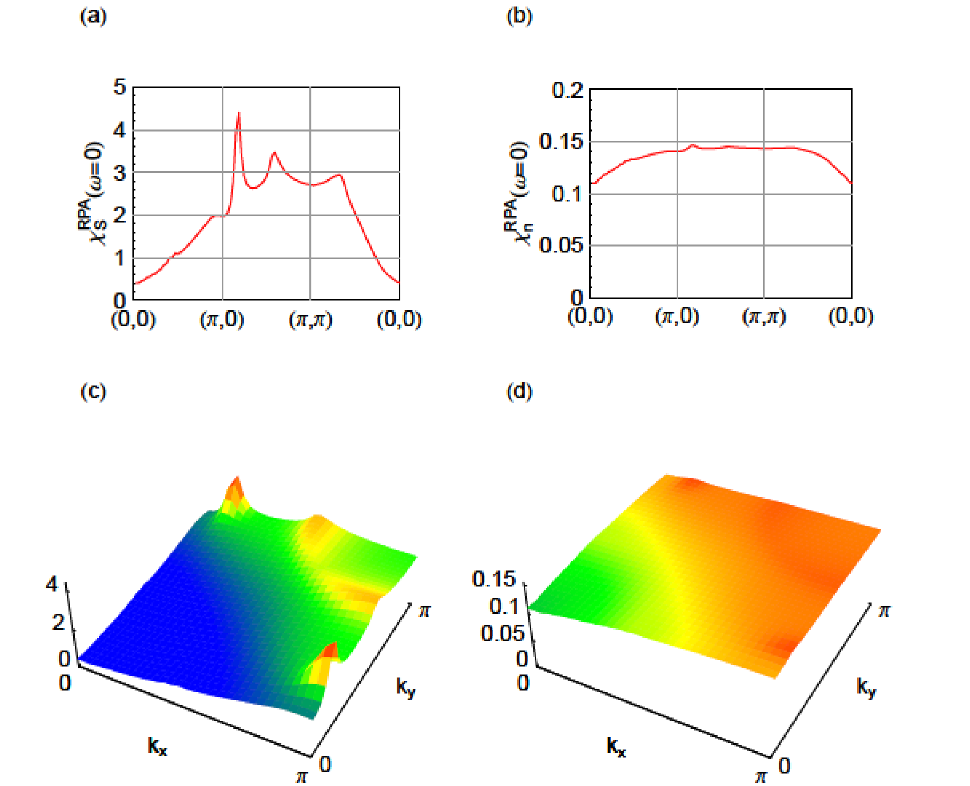


FIG. 8: (Color online) The RPA enhanced susceptibilities calculated for the electron doped compound ($x = 0.125$). The interaction parameters have been chosen as $U = V = 1.65$ and $J = 0$. (a) and (c) are plots of the spin susceptibility, (b) and (d) are plots of the charge susceptibility.

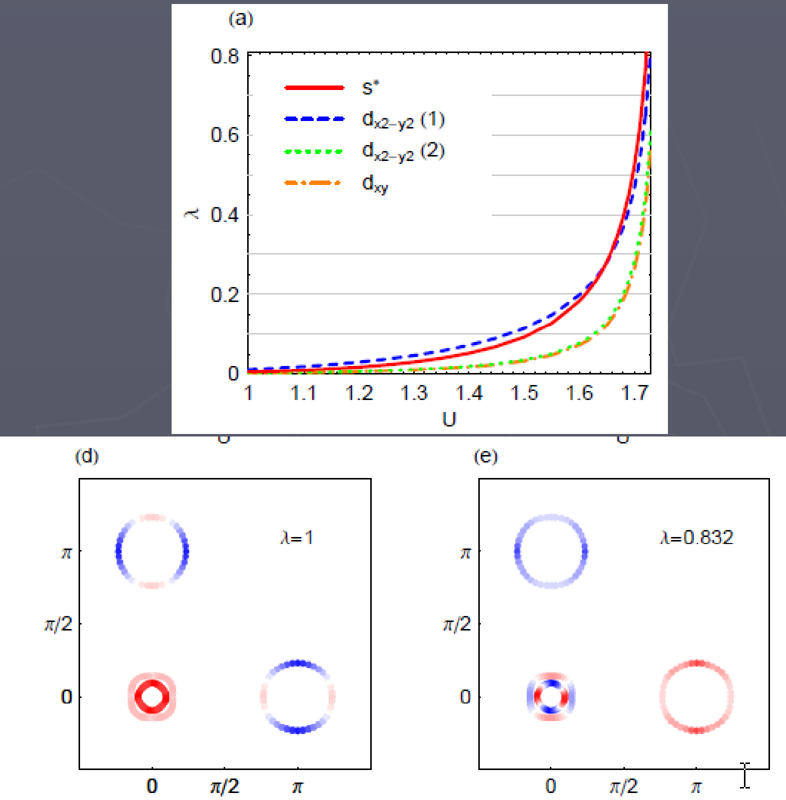
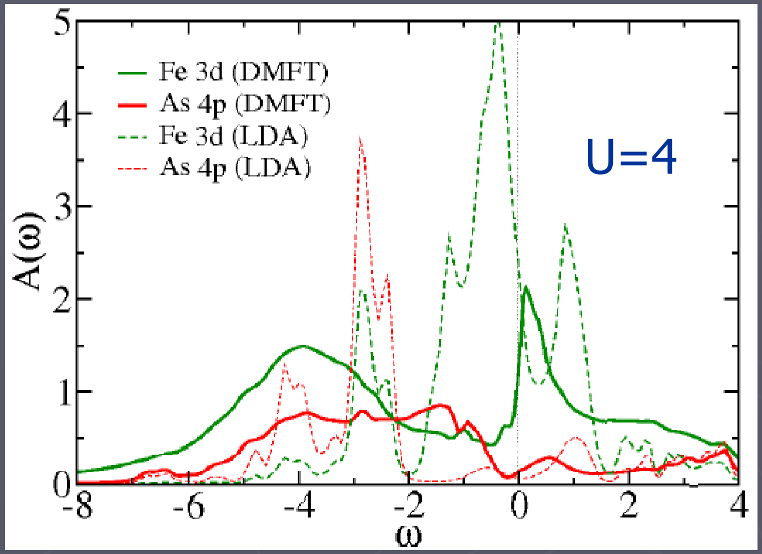
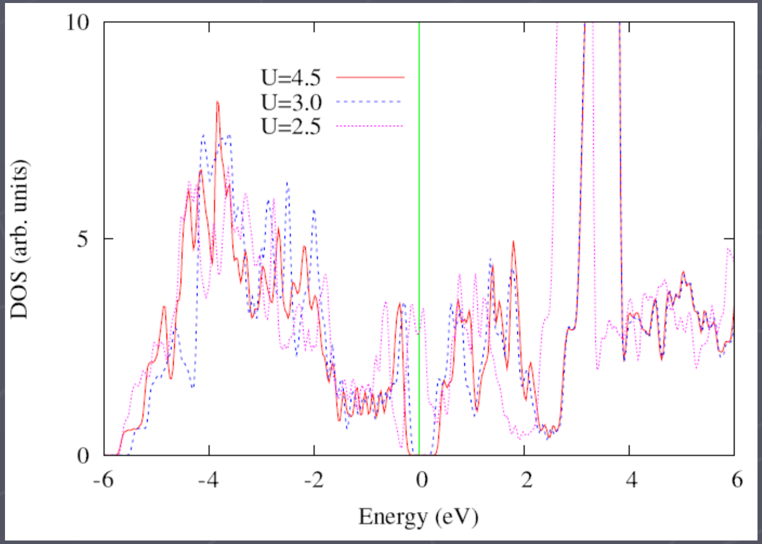


FIG. 13: (Color online) The eigenvalues and eigenfunctions for the electron doped compound ($x = 0.125$) for $U = V$ and $J = J' = 0$. The four largest eigenvalues as a function of U (a) and the different inter- and intraband contributions to the eigenvalues λ for the two symmetries with largest eigenvalues, extended s (b) and $d_{x^2-y^2}$ (c) wave. Color coded plot of the extended s wave (d) and the $d_{x^2-y^2}$ wave (e) pairing functions along the different Fermi surface sheets, calculated close to the instability ($U = V = 1.73$).

Proximity to Mott insulator?



Haule et al, PRL **100**, 226402 (2008)
LDA+DMFT: LOFA is at verge of M-I transition system opens gap between U=4 – 4.5 eV for Fe

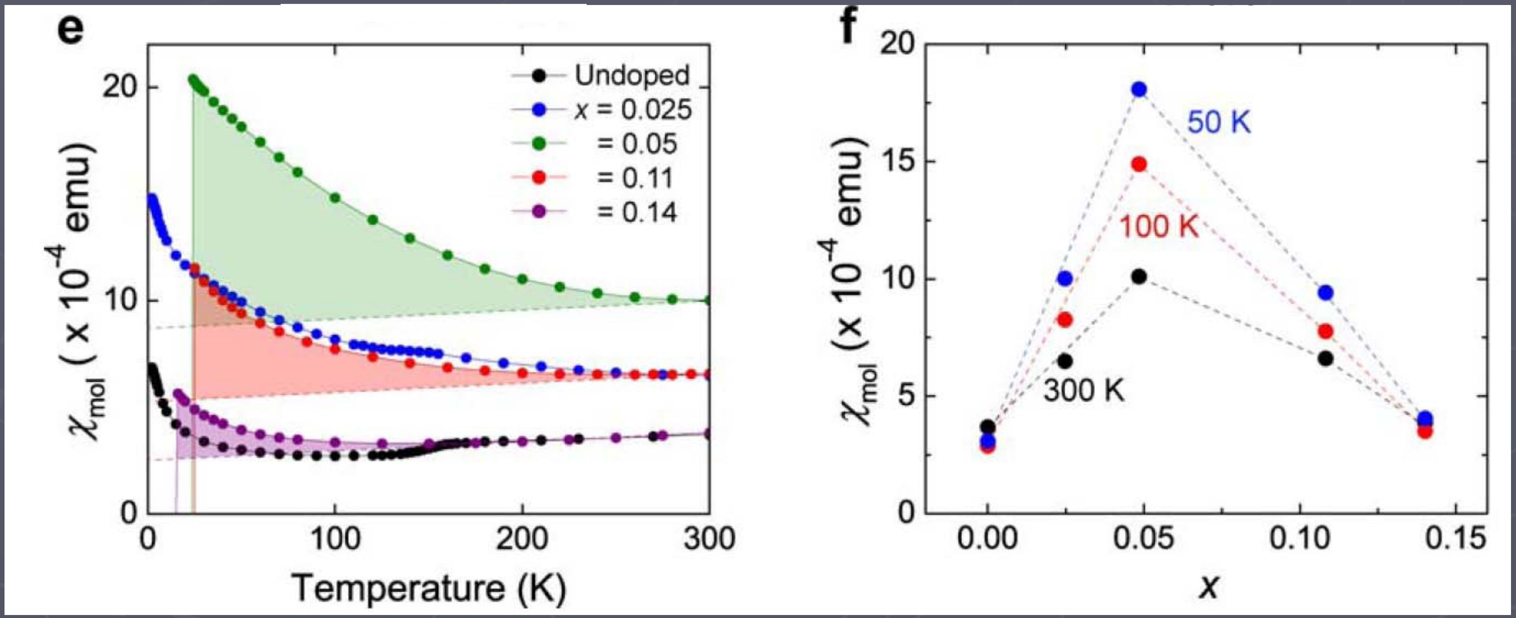


Cao et al. PRB 77, 220506 (2008)
Similar result for LDA+U, smaller U_c~3eV

Anisimov et al. aXiv: 0807.0547
microscopic calc of U~3-4, J~0.5eV -- many Fe orbitals -- correlations relatively *weak*

Evidence for importance of correlations

Doped LaOFeAs



Susceptibility 50x larger than LDA Pauli

T. Nomura et.al., aXv:0804.3569

LOFFA=$LaO_{1-x}F_xFeAs$
LOFA=LaOFeAs

Literature (Mar. 27)

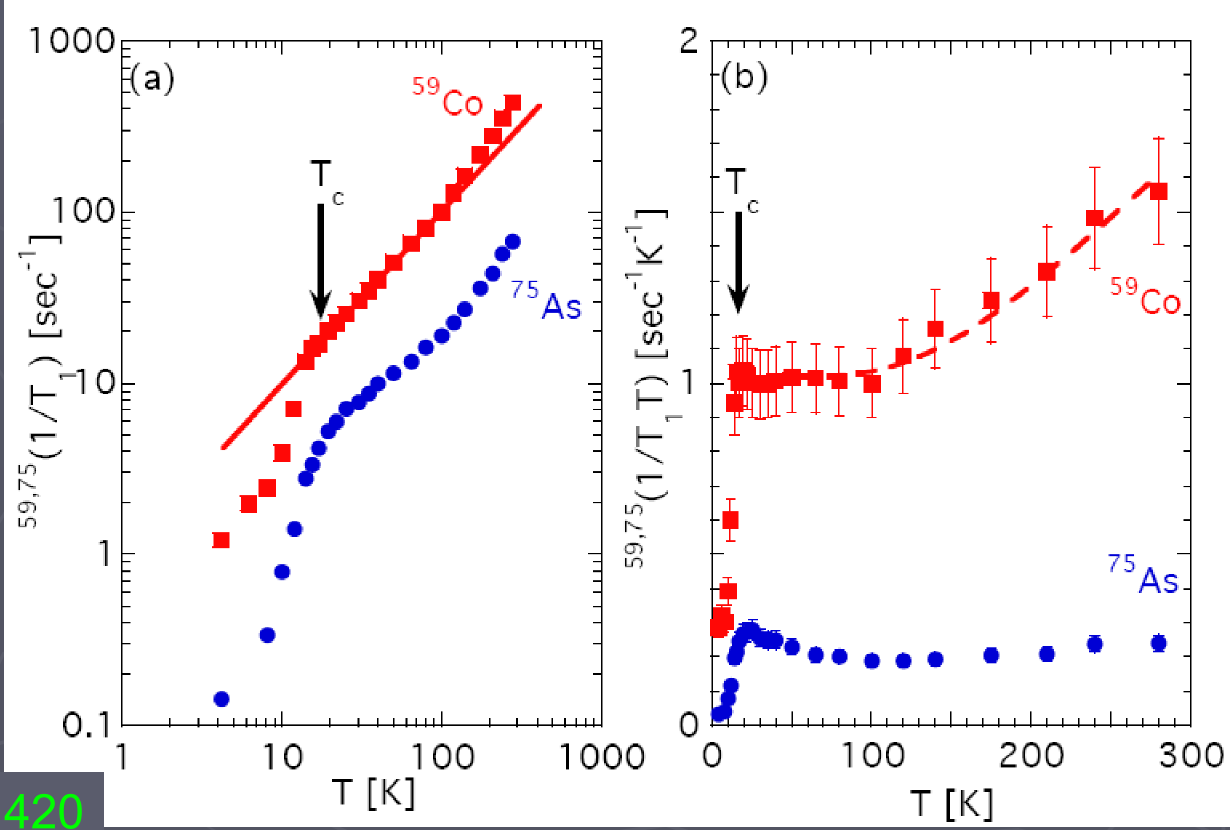
SOFFA=$SmO_{1-x}F_xFeAs$

- Y. Kamihara et al., J. Am. Chem. Soc. **128**, 10012 (2006).
- S. Lebegue, "Electronic structure and properties of the Fermi surface of the superconductor LaOFeP", Phys. Rev. B **75**, 035110 2007.
- Y. Kamihara et al., "Iron-based layered superconductor LOFFA", J. Am. Chem. Soc. 130, 3296 (2008)
- D. Singh and M. Du, "LOFFA: A low carrier density superconductor near itinerant magnetism", aXv:0803.0429.
- L. Boeri et al., "Is LOFFA an electron-phonon superconductor?", aXv:0803.2703
- I. Mazin et al, "Unconventional sign-reversing supercond. in LOFFA, aXv:0803.2740
- C. Cao et al, "Coexistence of antiferromagnetism with superconductivity in LOFFA: effective Hamiltonian from ab initio studies", aXv:0803.3236.
- K. Haule et al., "Correlated electronic structure of LOFFA", aXv:803.1279
- K. Kuroki et al, "Unconventional superconductivity originating from disconnected Fermi surfaces in LOFFA", aXv:0803.3325
- F. Ma and Z.-Y. Lu, "Iron-based layered superconductor LOFFA: an antiferromagnetic semimetal", aXv:0803.3286.
- J. Dong et al, "Competing Orders and SDW Instability in LOFFA, aXv:0803.3426
- L. Shan et al, "Non-conventional pairing symmetry in Fe-based layered superconductor revealed by pt-contact spectroscopy measurements", aXv:0803.2405
- A. Sefat et al, "Electron Correlations in the Low Carrier Density LOFFA Superconductor", aXv:0803.2528
- "Superconductivity at 43 K in Samarium-arsenide Oxides SOFFA", Chen et al, aXv:0803.3603

Nonmagnetic impurities possibly not detrimental to SC

- Fe replaced by Co
- Impurities do not destroy SC (like Zn doping in cuprates)
- No signature of Curie-Weiss susc.

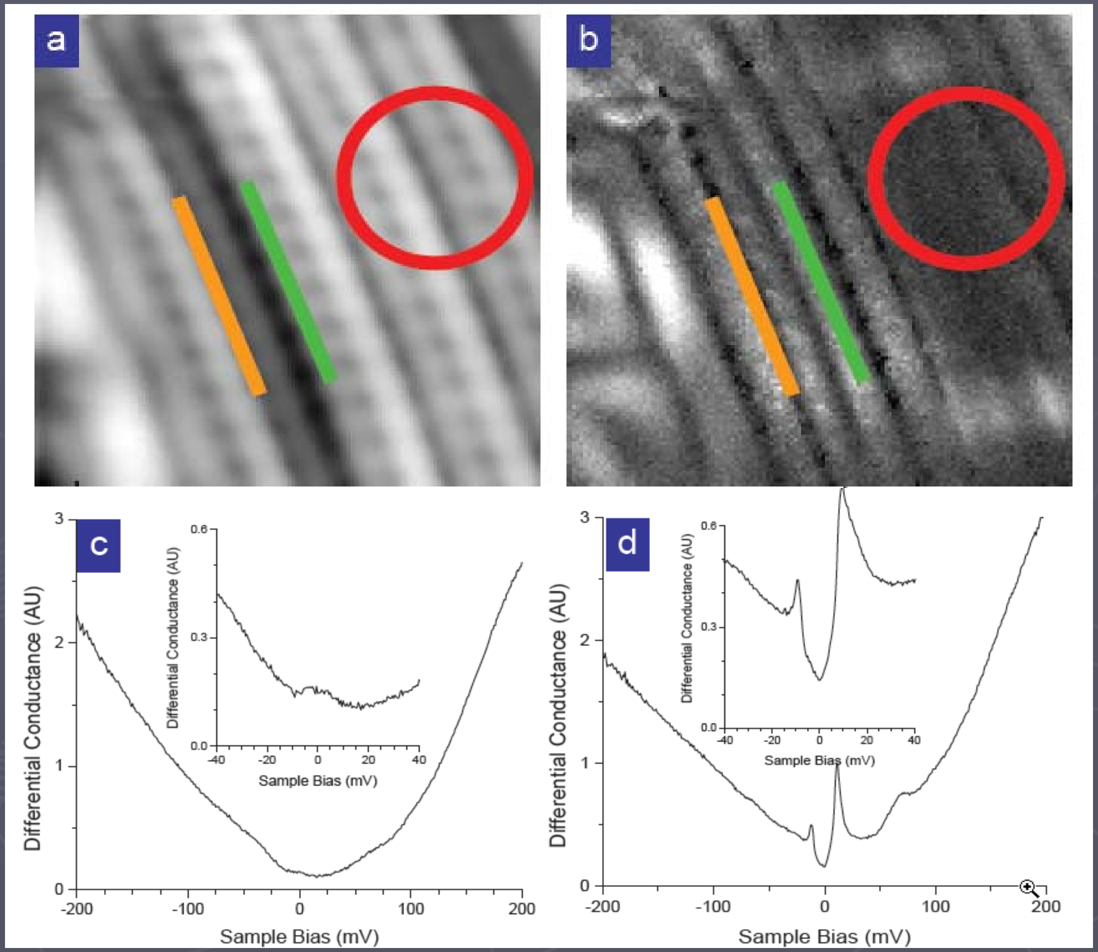
$BaFe_{1.8}Co_{0.2}As_2$: Tc~22K



F.L. Ning et.al, arXiv:0808.1420

STM on 122 crystals

Boyer et al aXv:0806.4400 $SrKAs_2Fe_2$



- 2 different types of surfaces revealed by cleave
- one shows "non-s-wave" gap

Comparison of different ARPES results

Evtishinsky et al.
PRB 2009

Ref. num.	[2]	[3]	[4]	[5]	[6]	This paper
T_c	53 K	37 K	35 K	53 K	37 K	32 K
Inner Γ-barrel	20	12.5	12	15	12	9.2 ± 1
Outer Γ-barrel	—	5.5	8	—	6	<4
X-pocket	—	12.5	10	—	11	9 ± 2
Blades	—	—	(11)	—	—	~ 9
Gap anisotropy	—	<3	2	<5	<3	<1.5

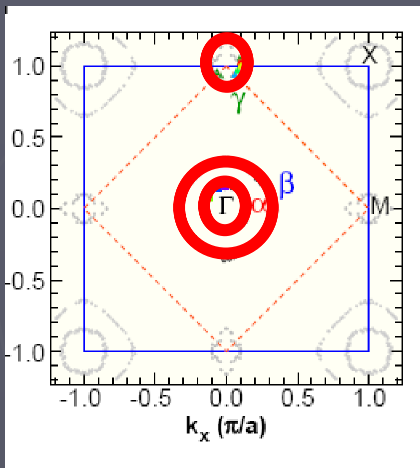
Table I: Momentum dependence of the superconducting gap in iron-arsenic superconductors, as revealed by ARPES studies from five independent groups, sorted by the time of appearance on the arXiv.org. Values of the gap and estimates of the gap anisotropy on the inner Γ-barrel are given in millielectron-volts.

Ref. num.	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	This paper
Large gap	9	8.1	8.2	6.8	7.5	3.7	9.6	4	6.8
Small gap	—	3.6	5.5	—	3.9	—	3.4	—	<3

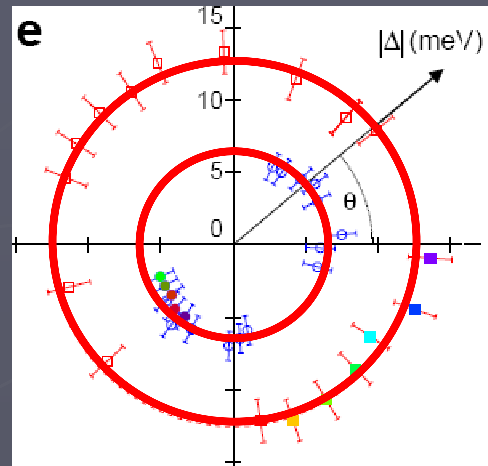
Table II: Coupling strength, $2\Delta/k_B T_c$, in iron-arsenic superconductors, as revealed by different experimental techniques — compare to the BSC universal value 3.53. Most of the available studies reveal two superconducting gaps of different magnitudes, which are represented in the table as "large" and "small". Refs. [2], [3], [4], [5], [6] are ARPES studies, Refs. [7], [8] are Andreev spectroscopy studies, Ref. [9] is a specific heat study.

Gap anisotropy (ARPES)

Fermi surface

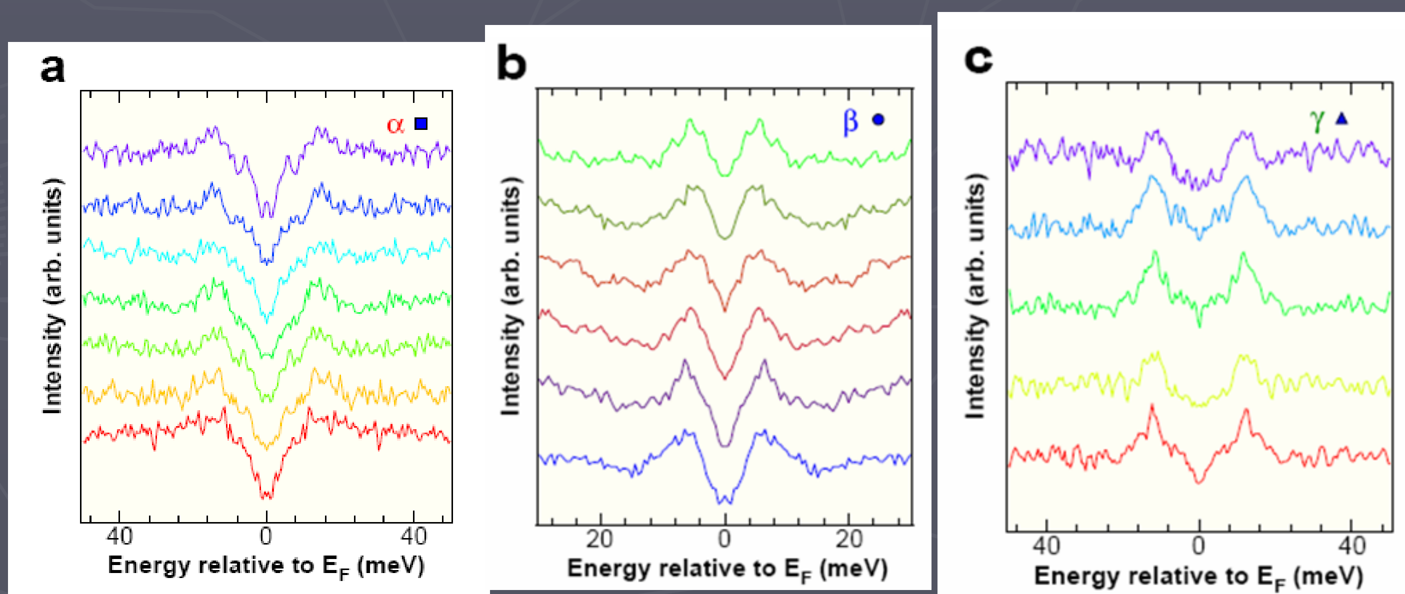


Gap size



H. Ding et.al.,
Europhys. Lett. 83, 47001 (2008).

Negligible anisotropy.
D-wave gap excluded!

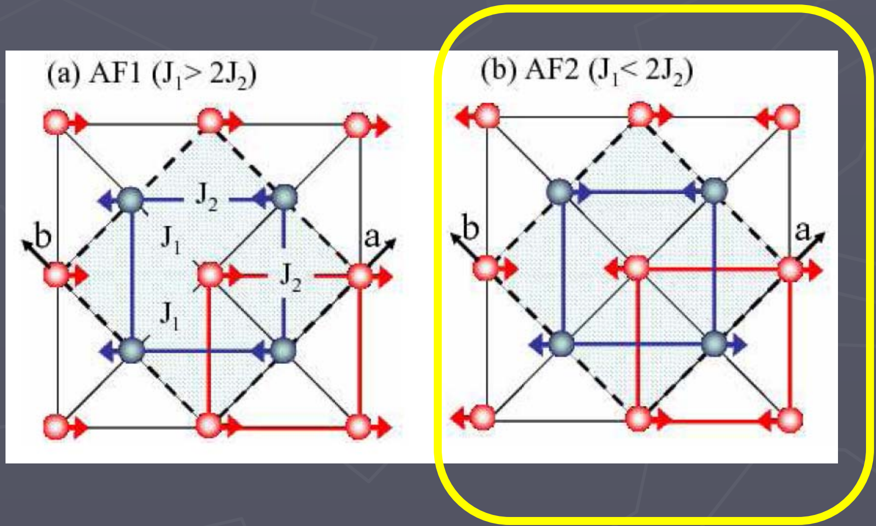


Scenarios for low AF Fe moment: 1. strong coupling + frustration

competing superexchange interactions J1 and J2
(Yildrim arXiv:0804.2252)

linear SDW implies $J_2 > J_1/2 \Rightarrow$ large nnn exchange!

system lowers frustration by structural distortion



see also Fang et al, arXiv:0804.3843
Cvectovic & Tesanovic arXiv:0804.4678
Abrahams & Si, arXiv:0804.2480

2. Weak coupling: proximity to SDW transition gives sensitivity to internal pressure

SDW temperature and magnetic moment vary strongly between compounds:

LaFeAsO: T_{SDW}~140K μ~0.3-0.4μ_B de la Cruz et.al, Nature 453, 899 (2008).

NdFeAsO: T_{SDW}~1.96K μ~0.9μ_B/Fe G. Bo, et.al., arXiv:0806.1450

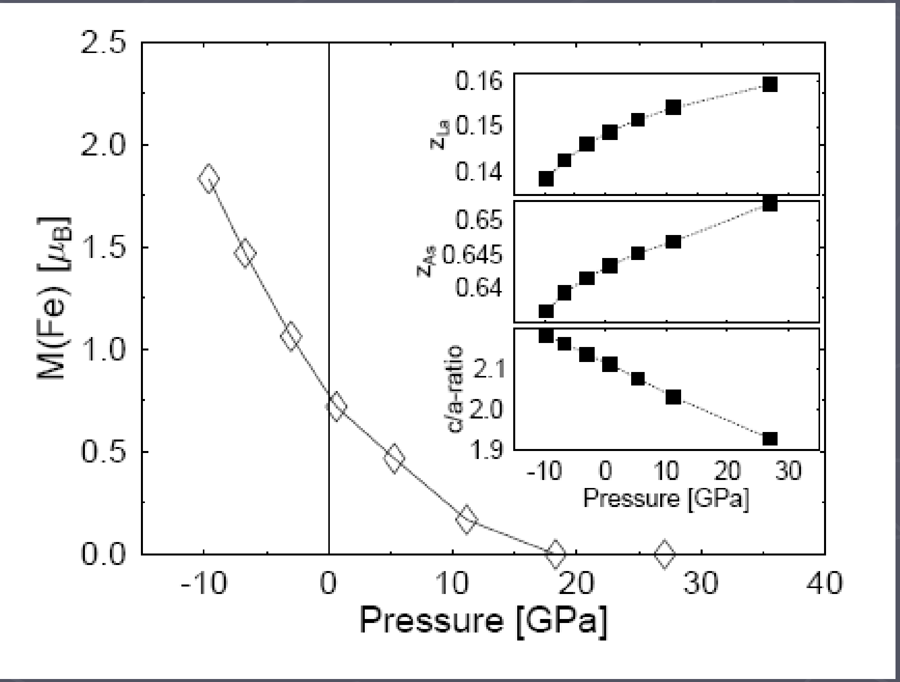
$BaFe_2As_2$: T_0~T_{SDW}~100K μ~0.9μ_B/Fe Huang, Q. *et al.*, arXiv:0806.2776

$SrFe_2As_2$: T_0~T_{SDW}~205K μ~1.01μ_B/Fe K. Kaneko et.al., arXiv: 0807.2608

…and may depend sensitively on pressure:

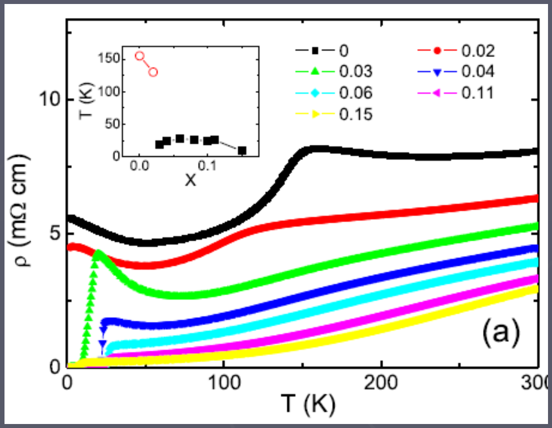
Opahle et al PRB 2009:

predict strong variation of As z-coordinate and moment size on pressure of few GPa

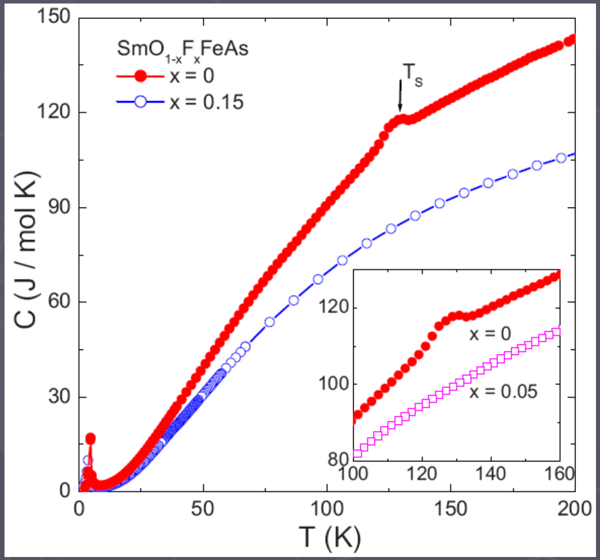


Relation between magnetic & structural phase transitions

Recall: 150K anomaly in ρ, C

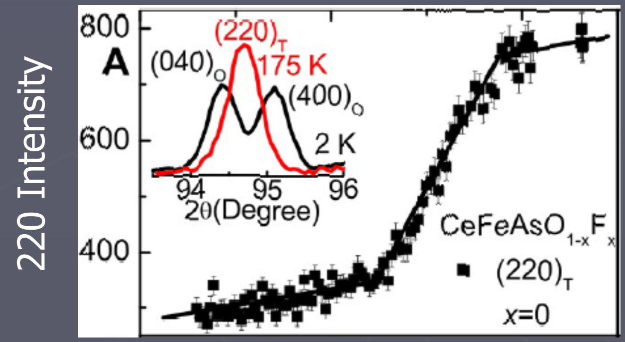


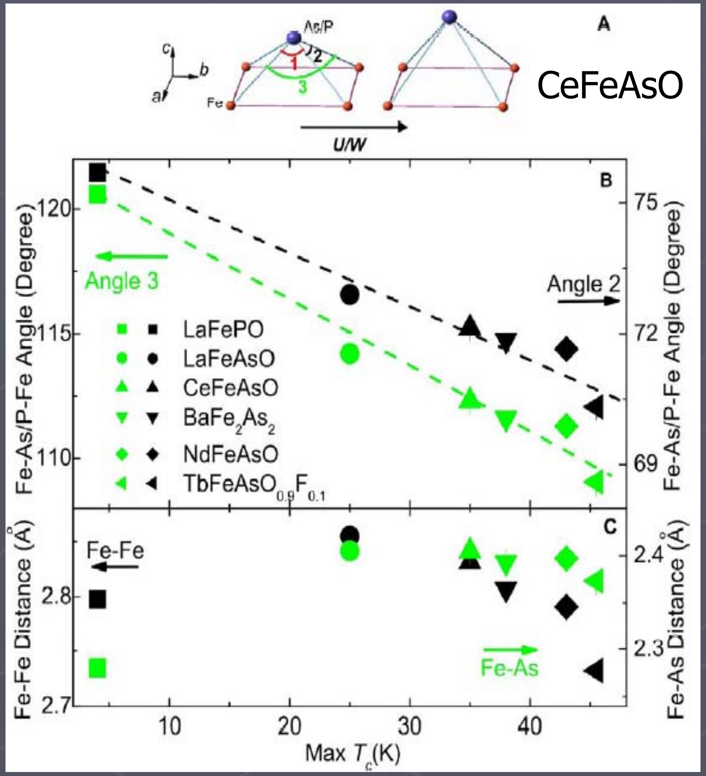
Kamihara JACS 08, Dong EPL 08



Ding et al. PRB **77**, 180510 (2008)

ORNL group: anomaly is structural transition





Zhao et al arXiv:0806.2528