Spin fluctuation pairing in Fe-based superconductors and its consequences

P. Hirschfeld, U Florida
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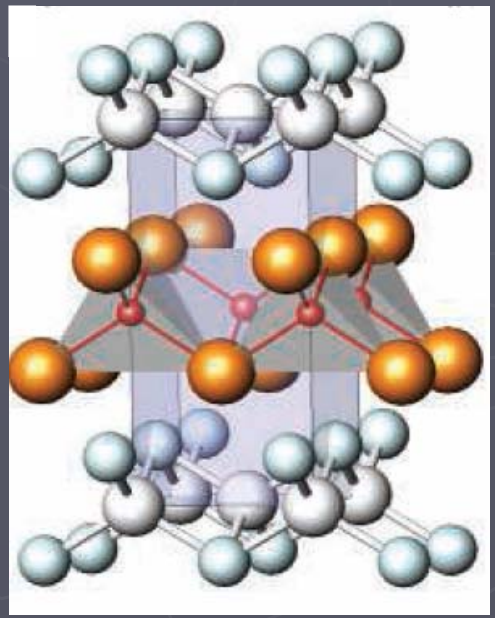
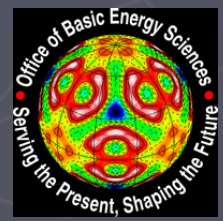


KITP, July 2009



Collaborators

from U. Florida Dept. of Physics:

Vivek Mishra

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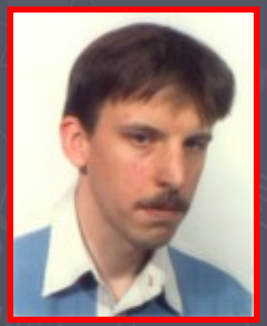

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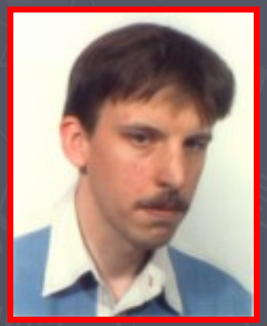
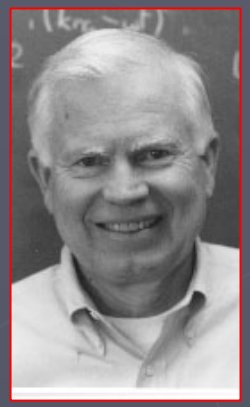


Siggi Graser

Chao Cao

from rest of world:



Doug Scalapino
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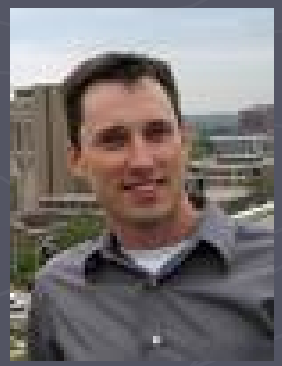
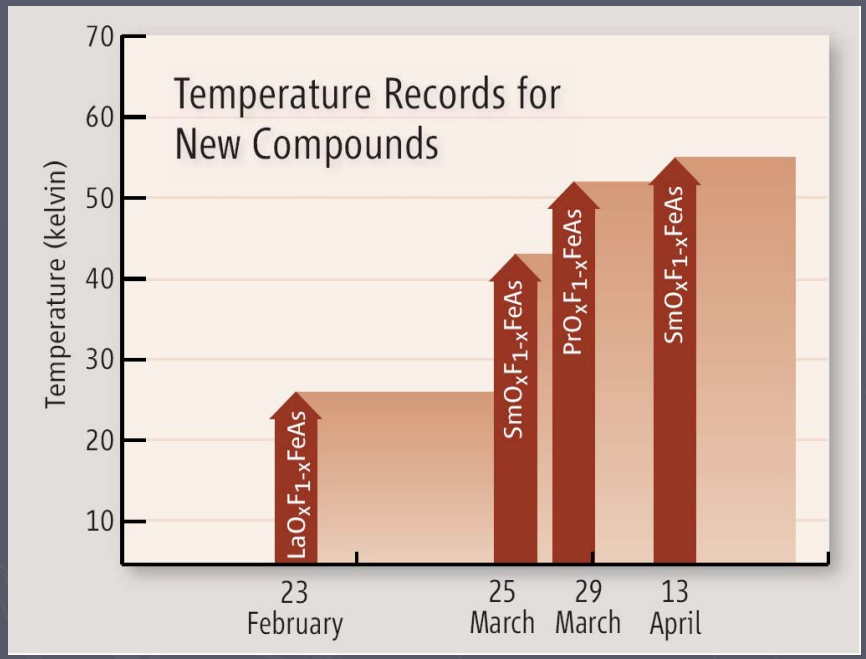


Anton Vorontsov
Montana State

Outline

- Review of Fe-based superconductivity
- Electronic structure/minimal band model
- “contradictory” experiments
- Theory: pair state/mechanism
- 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.

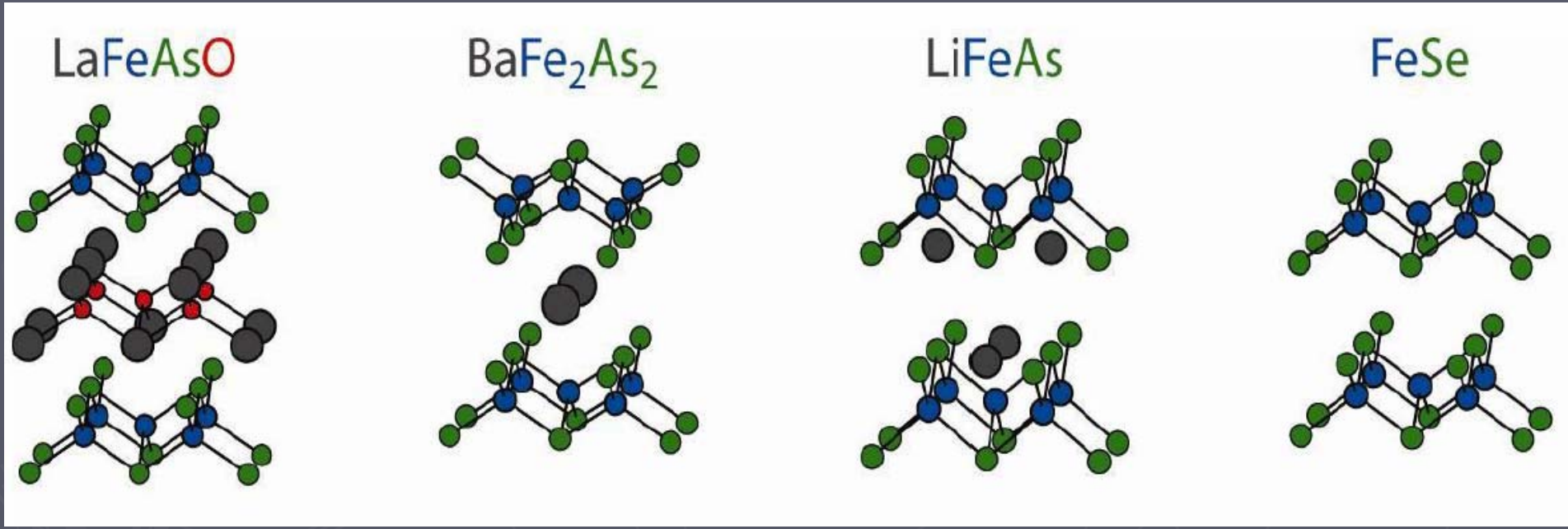
also:

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

Rare earths:

57	58	59	60	61	62	63
La	Ce	Pr	Nd	Pm	Sm	Eu
138.90	140.11	140.90	144.24	(145)	150.36	151.96

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

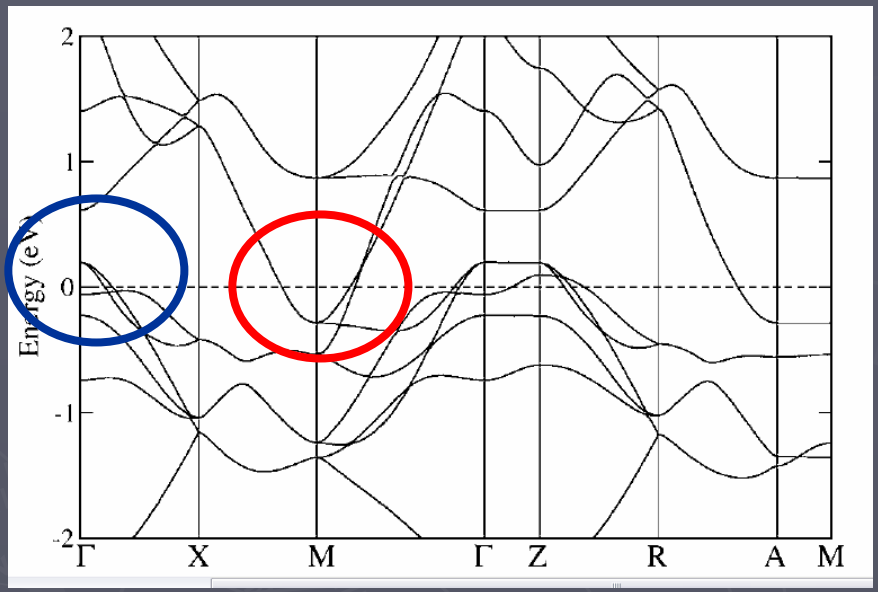
T_c=8K

Hsu et al
arXiv:0807.2369

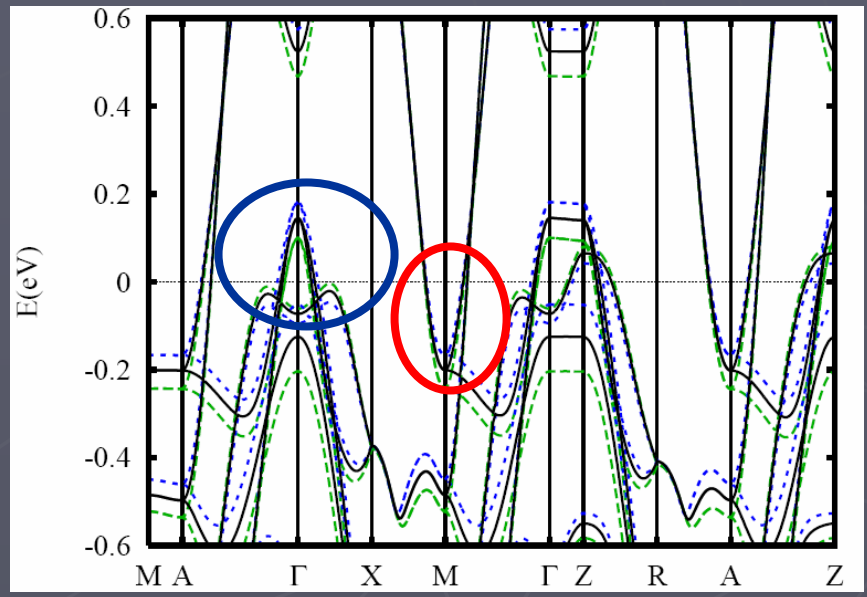
No arsenic ☺!

Electronic structure calculations

LOFP Lebegue 2007



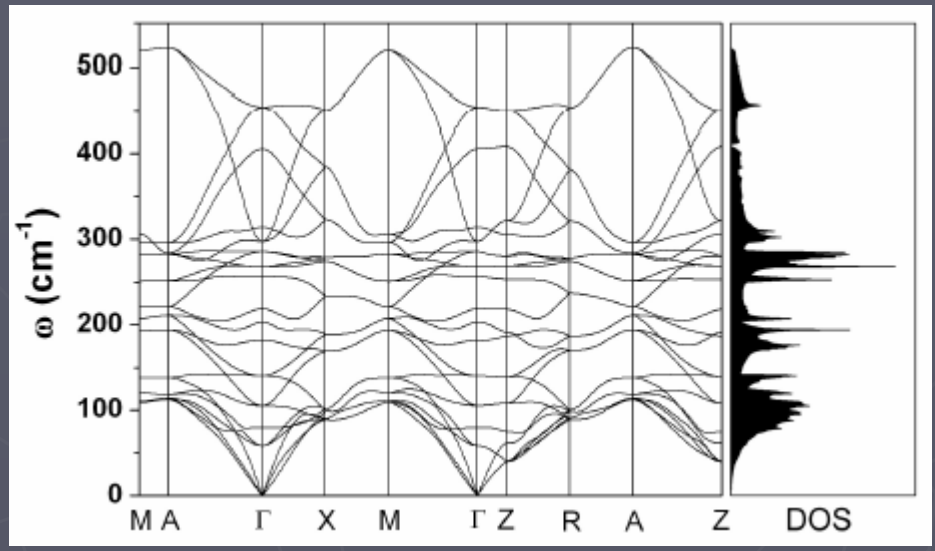
LOFA Singh & Du 2008



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

What accounts for factor 10 difference in T_c?

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



Singh & Du PRL 2008

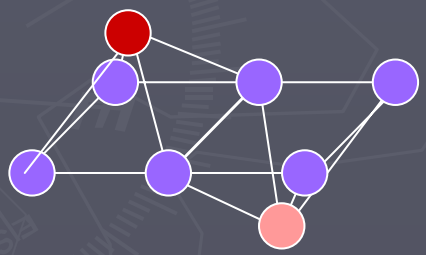
We have calculated *ab initio* the electron-phonon spectral function, $\alpha^2F(\omega)$, and coupling, λ, for the stoichiometric compound [9]. Some moderate coupling exists, mostly to As modes, but the total λ appears to be ~ 0.2, with $\omega_{log} \sim 250$ K, which can in no way explain $T_c \gtrsim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

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

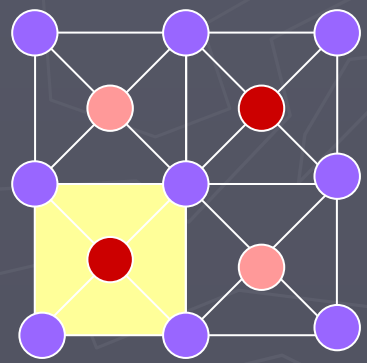
Understanding electronic structure

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

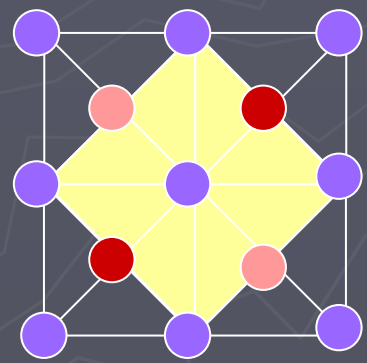
Real unit cell consists of 2 Fe and 2 As atoms, but due to the high degeneracy of the two As positions it is convenient to look at an effective unit cell with only 1 Fe and 1 As atom



Fe-Fe cell
„effective“ unit cell



Fe-As-Fe cell
„real“ unit cell

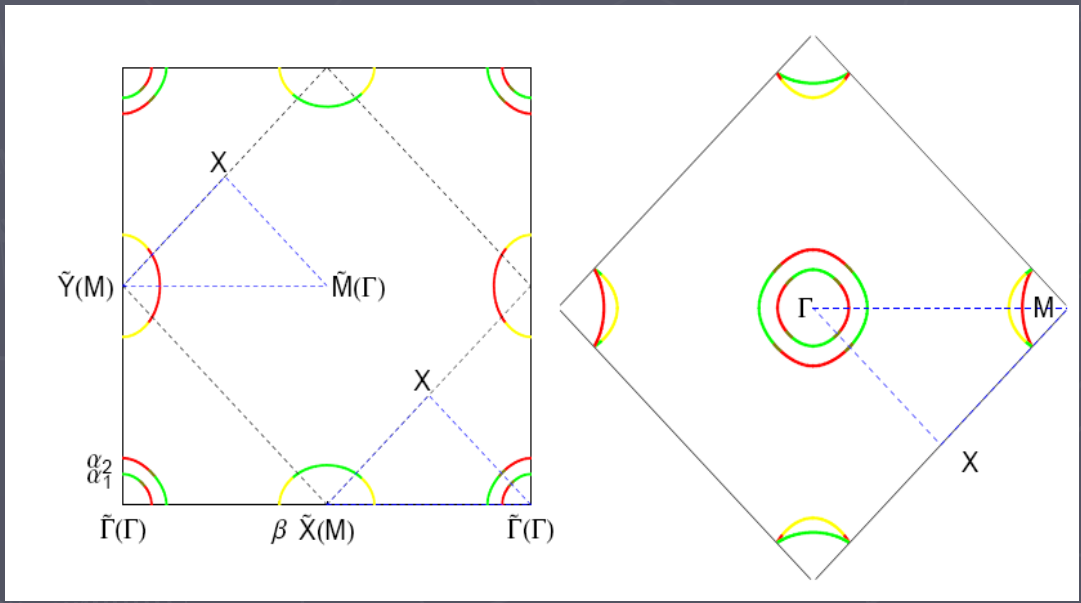


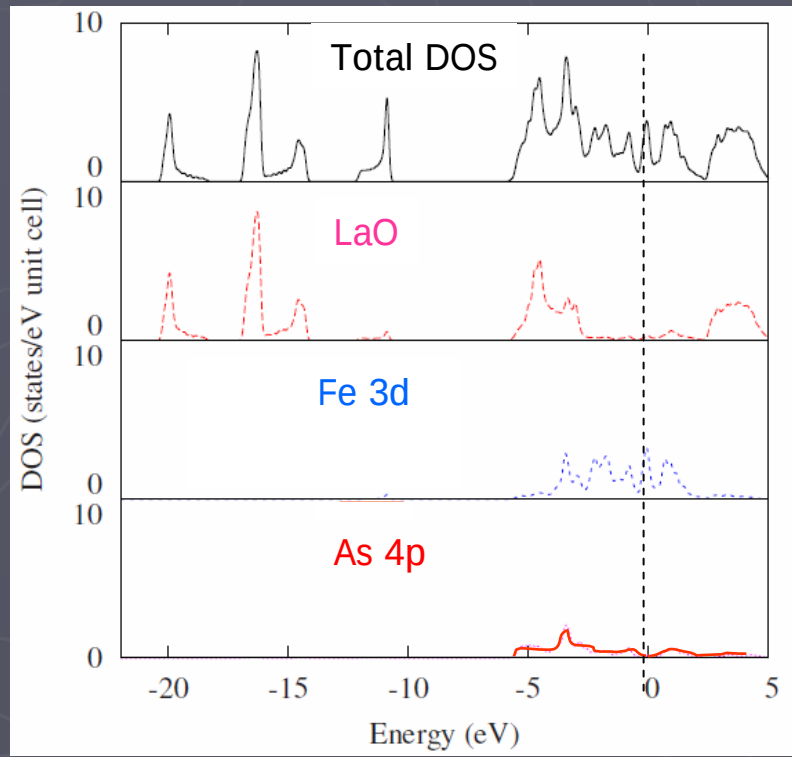
Understanding electronic structure

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

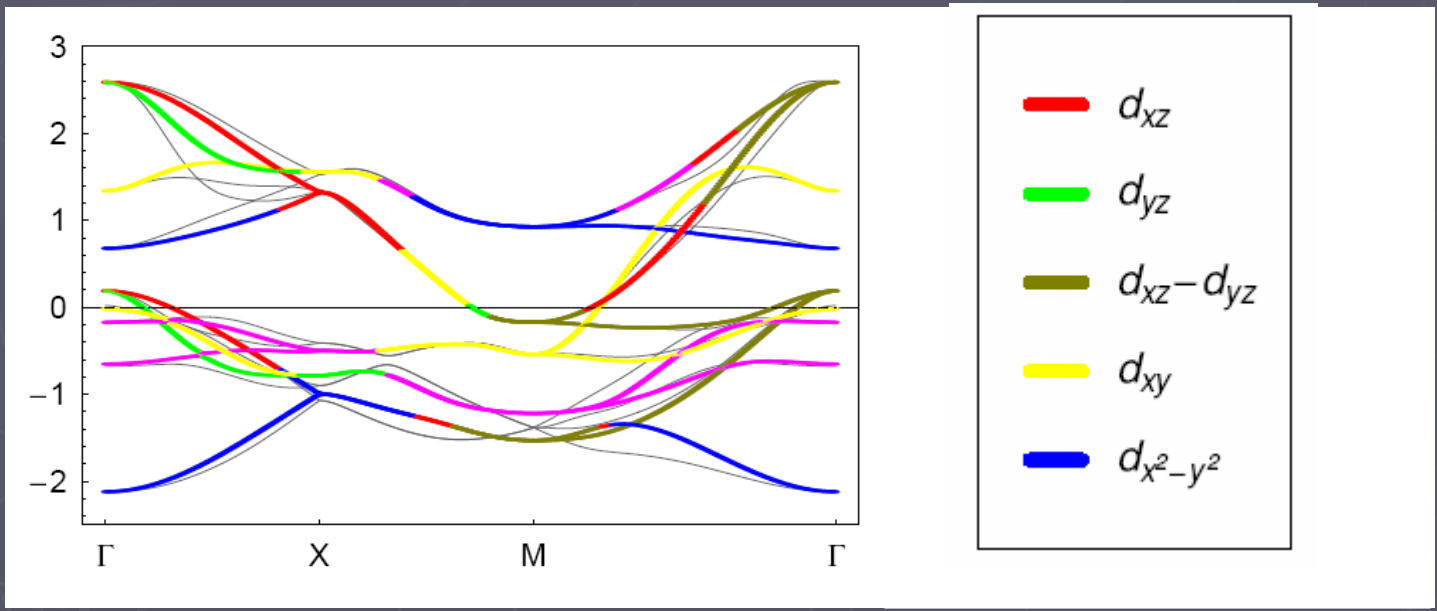




Band structure – Five band model

Graser et al. NJP 2009

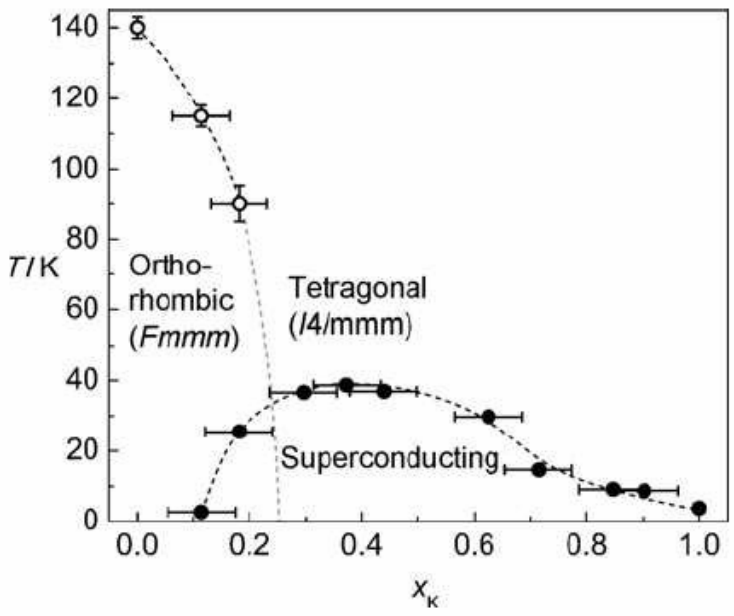
Fit to *Cao et al* PRB 77, 220506 (2008) see also *Kuroki et al* PRL **101**, 087004 (2008)



Notes on 122 materials

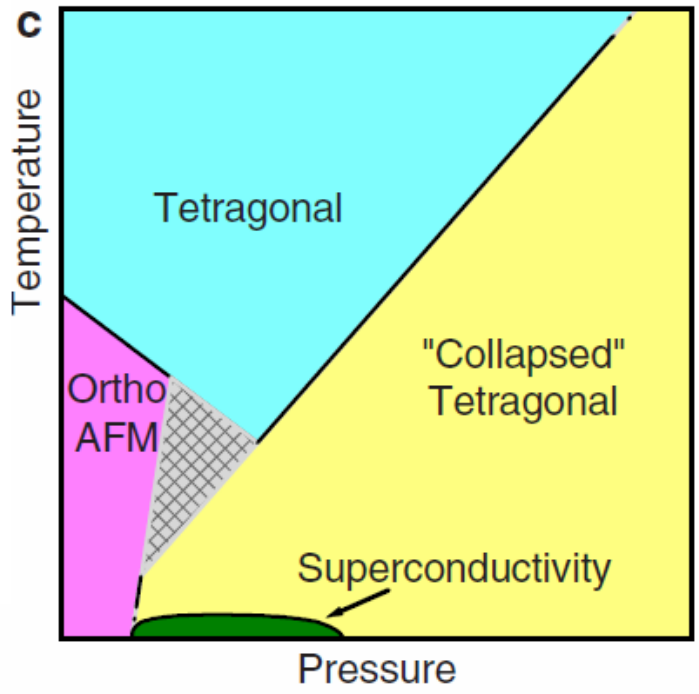
- T_c up to 38 K
- good crystals which cleave well—ARPES, STM
- dope with K or Co, or apply pressure to obtain superconductivity
- properties are more 3D than 1111 materials

$K_xBa_{1-x}Fe_2As_2$



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

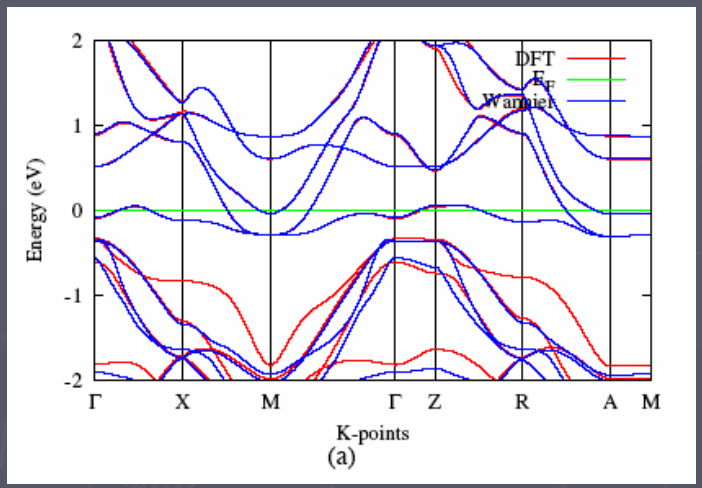
$CeFe_2As_2$ under pressure



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

Parent compounds are ordered antiferromagnets

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



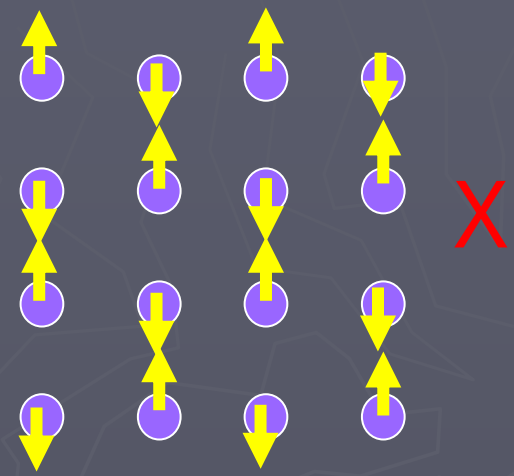
State with AF order is ~40meV lower in energy than paramagnetic state.

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

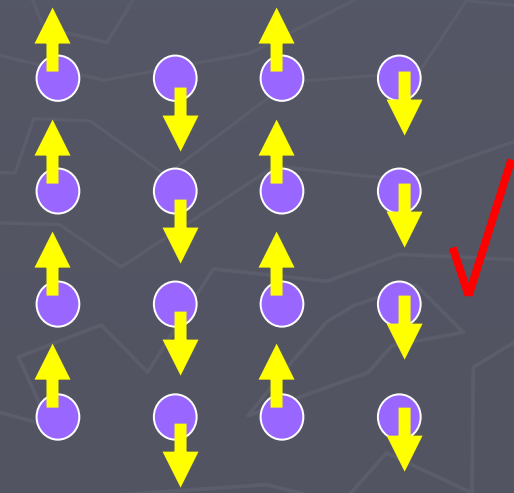
Both magnetic states found by LDA have ~$2\mu_B$ ordered staggered moment.
(exception: Yildrim PRL 2008)

Fe

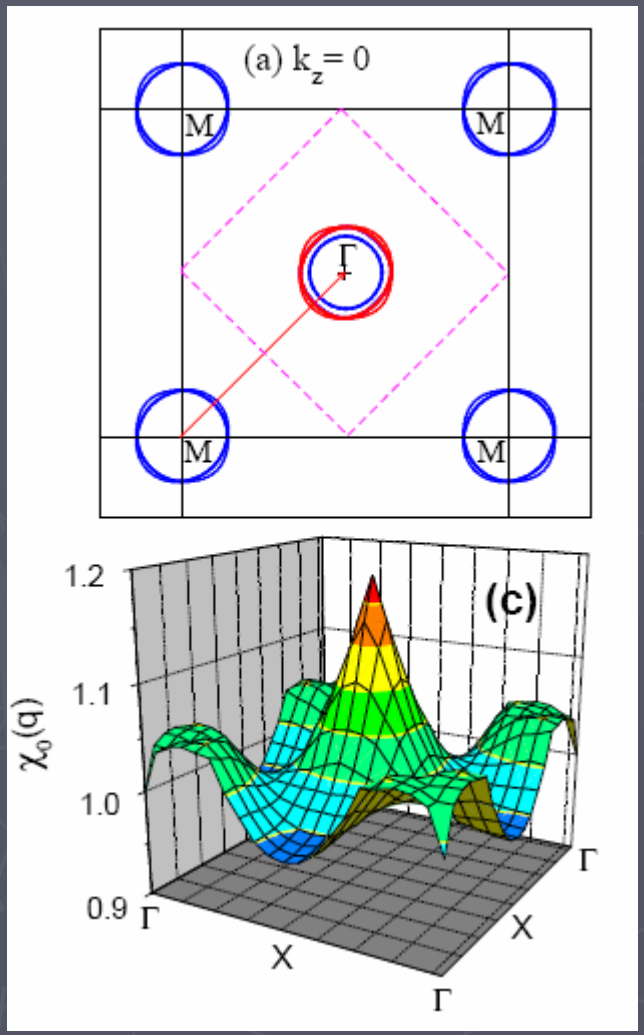
AF



"collinear SDW"



Weak coupling perspective: nesting of FS and susceptibility



Dong et al. EPL 2008

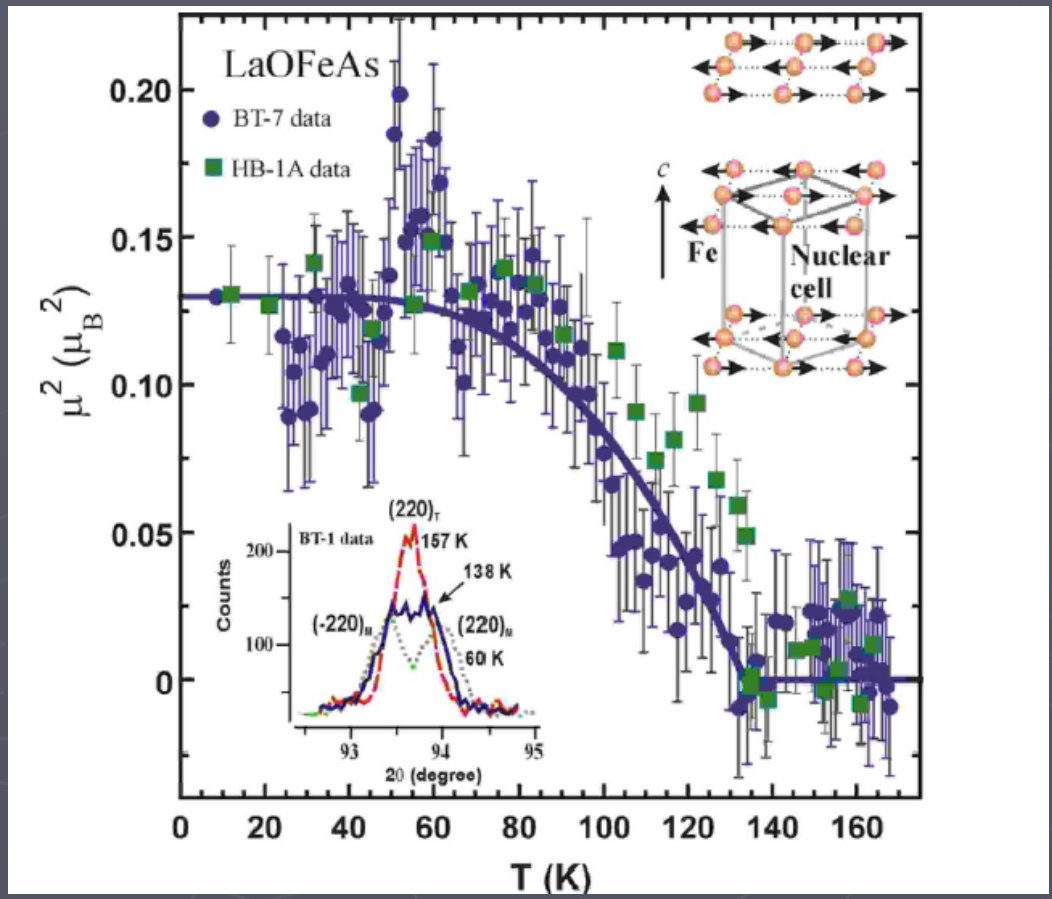
Simple picture put forward by Dong et al:

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)

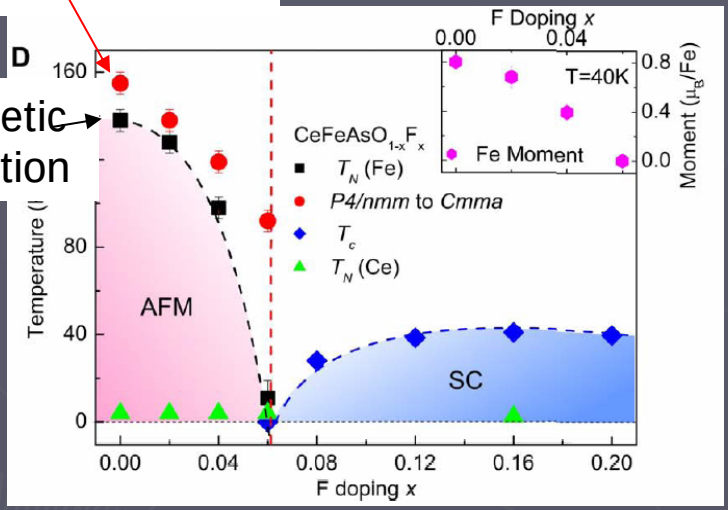


But size of ordered moment is only 0.36 μ_B!

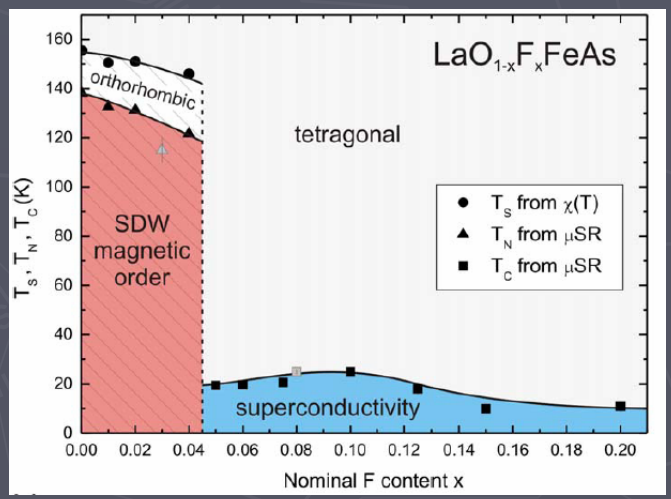
- Magnetic order tied to structural phase transition
- possible coexistence with superconductivity

structural transition

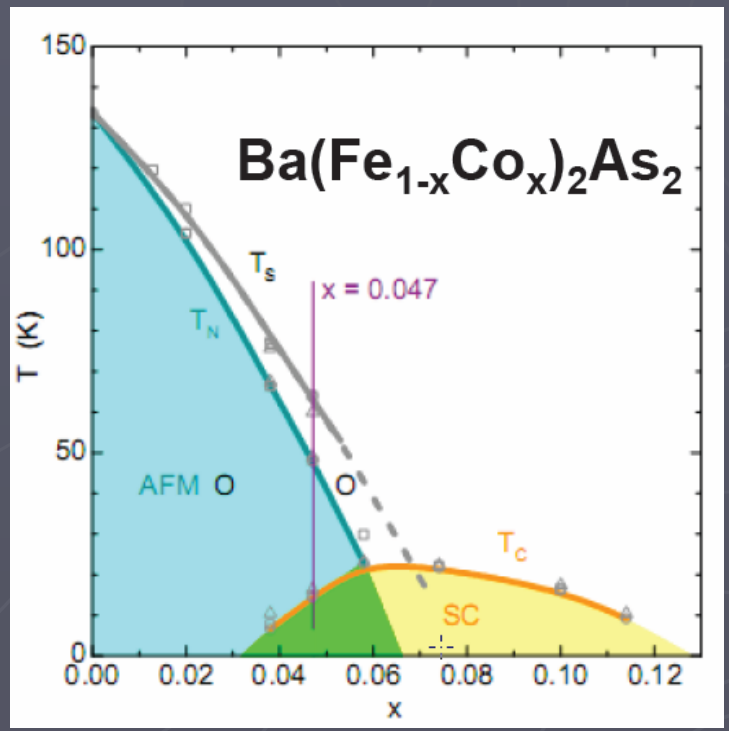
magnetic transition



Zhao et al arXiv:0806.2528



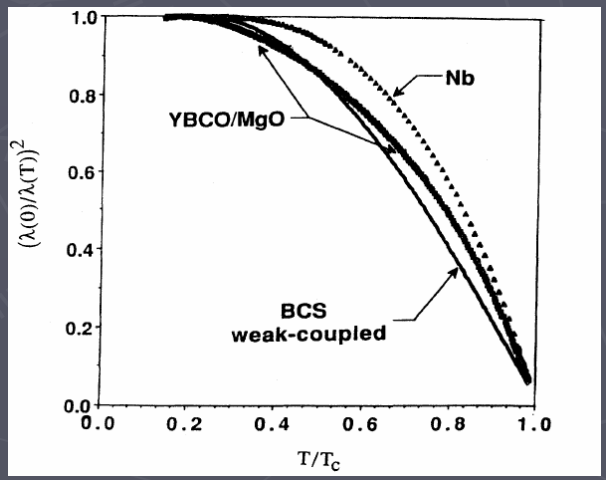
Luetkens et al arXiv:0806.3533

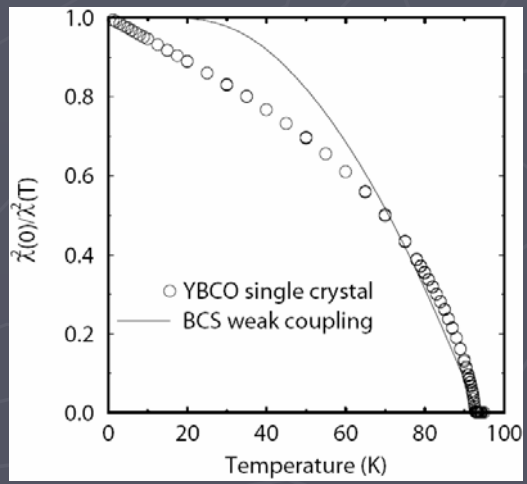


D.K. Pratt et al, aXv 0903.2833

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

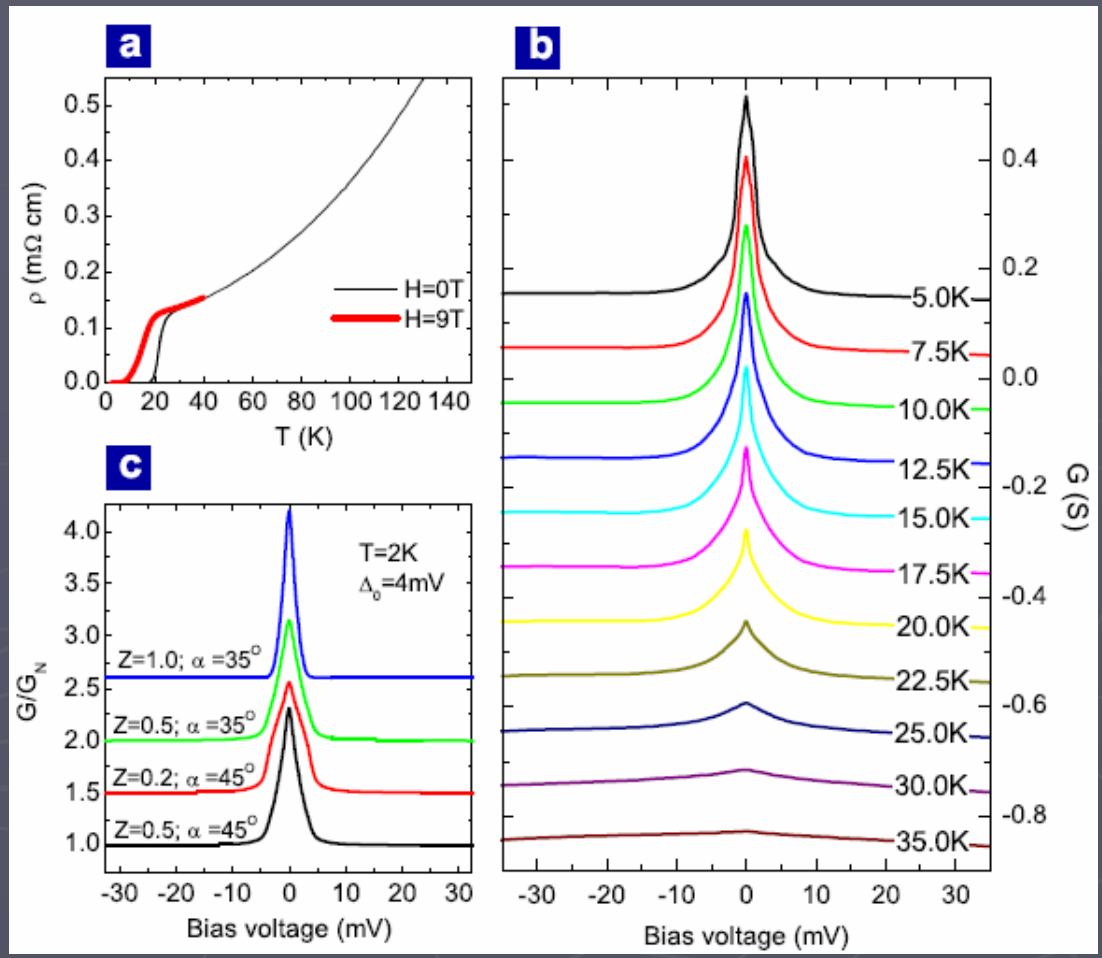




Early evidence for nodes 1: Andreev pt contact spectroscopy

Shan et al EPL 2008

LOFFA



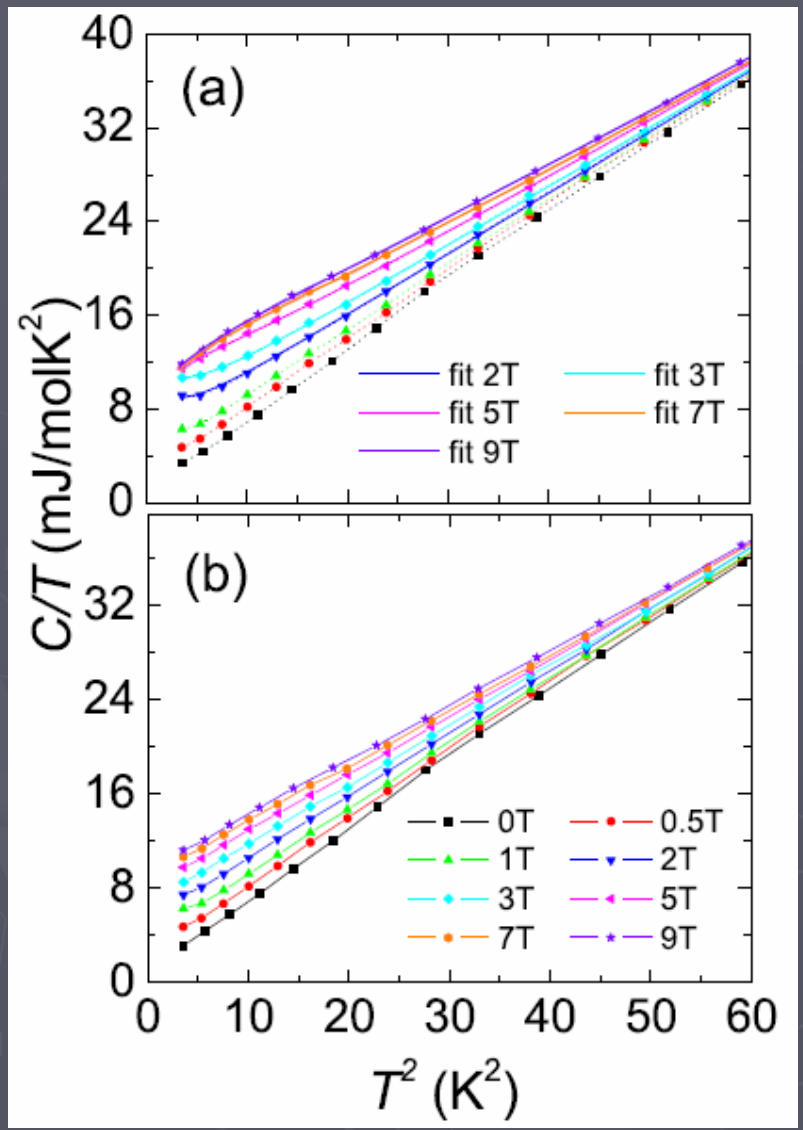
expt

BTK theory

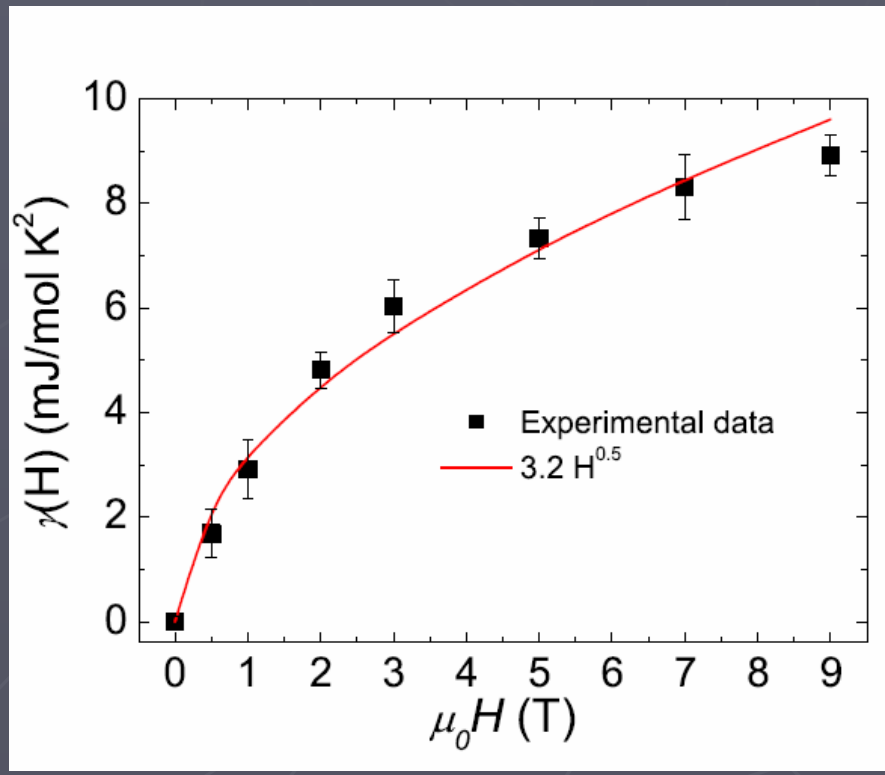
(similar to d-wave)

Early evidence for nodes II: Volovik effect

Mu et al aXv March/Chin.Phys.Lett. (2008)

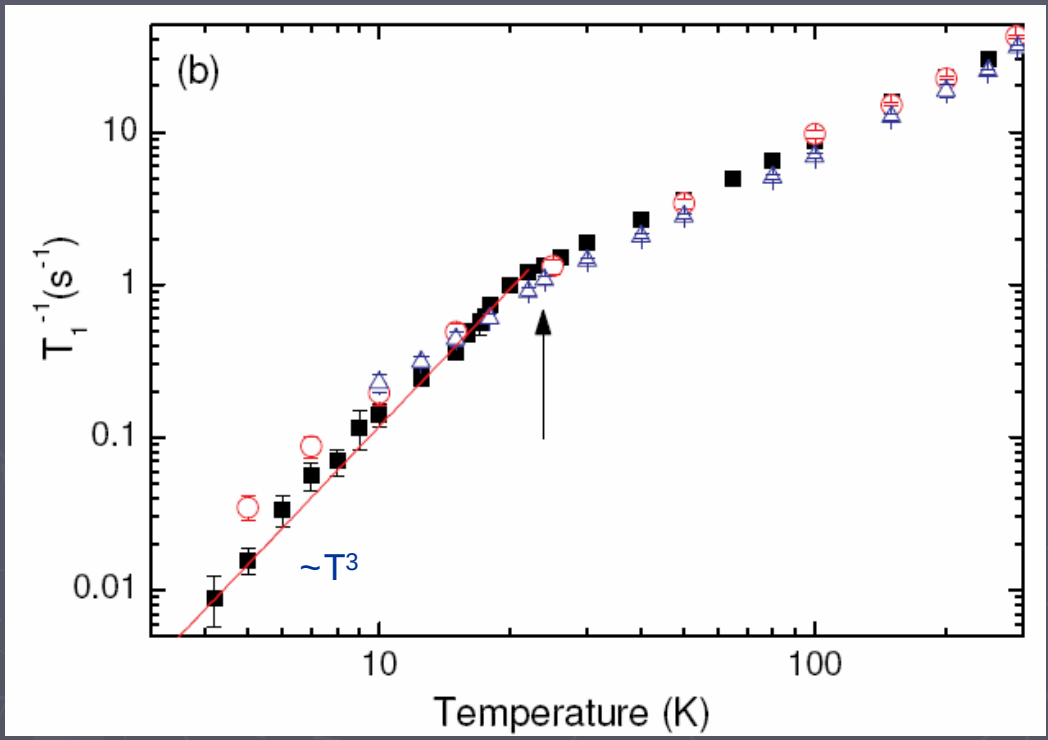


LOFFA

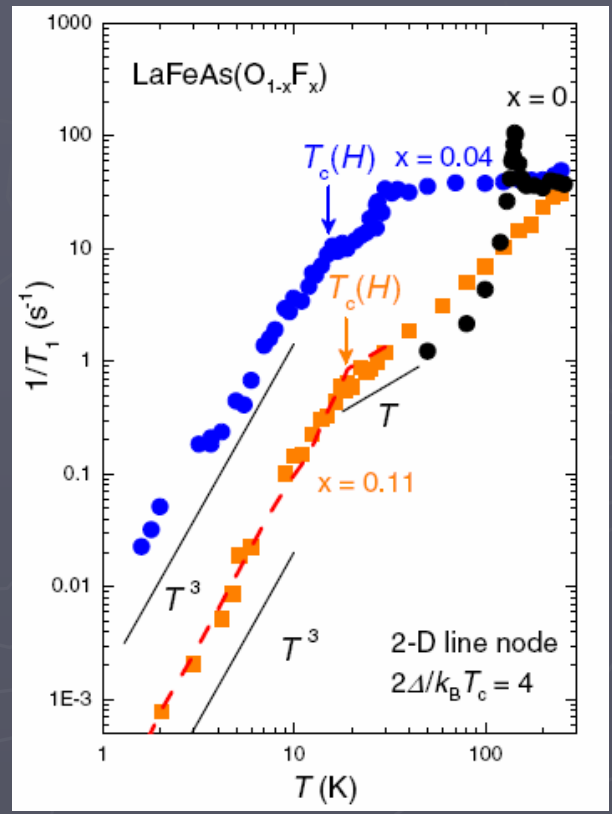


Early evidence for nodes III: NMR

LOFFA



Grafe et al Phys. Rev. Lett. (2008)



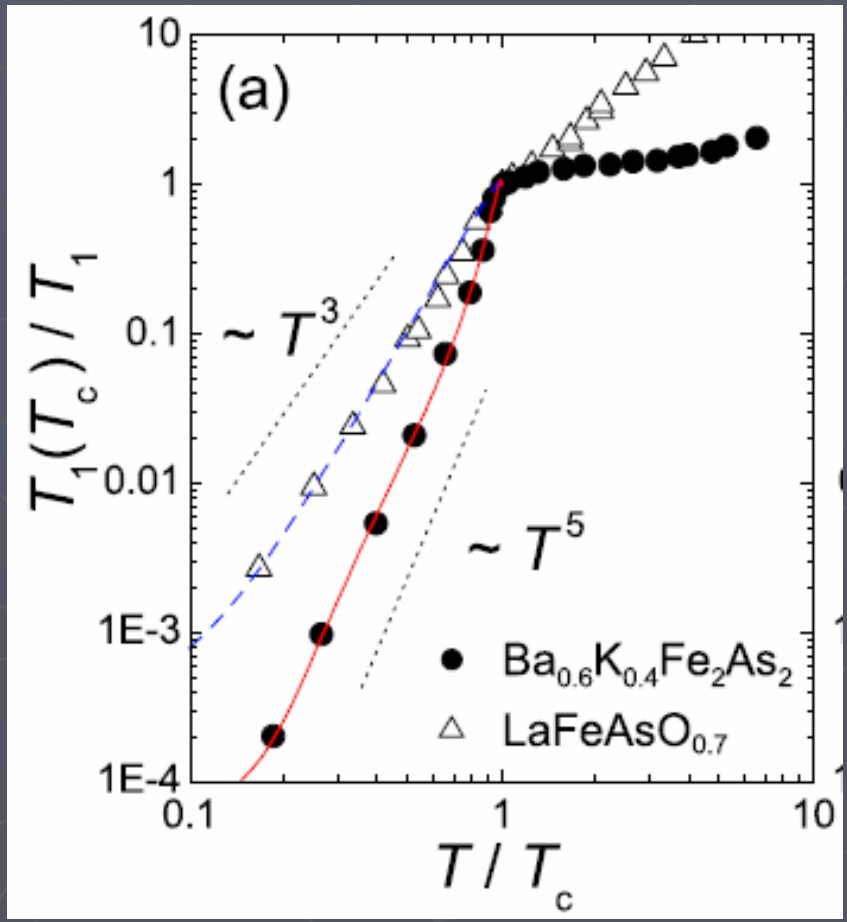
Nakai et al. JPSJ (2008)

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

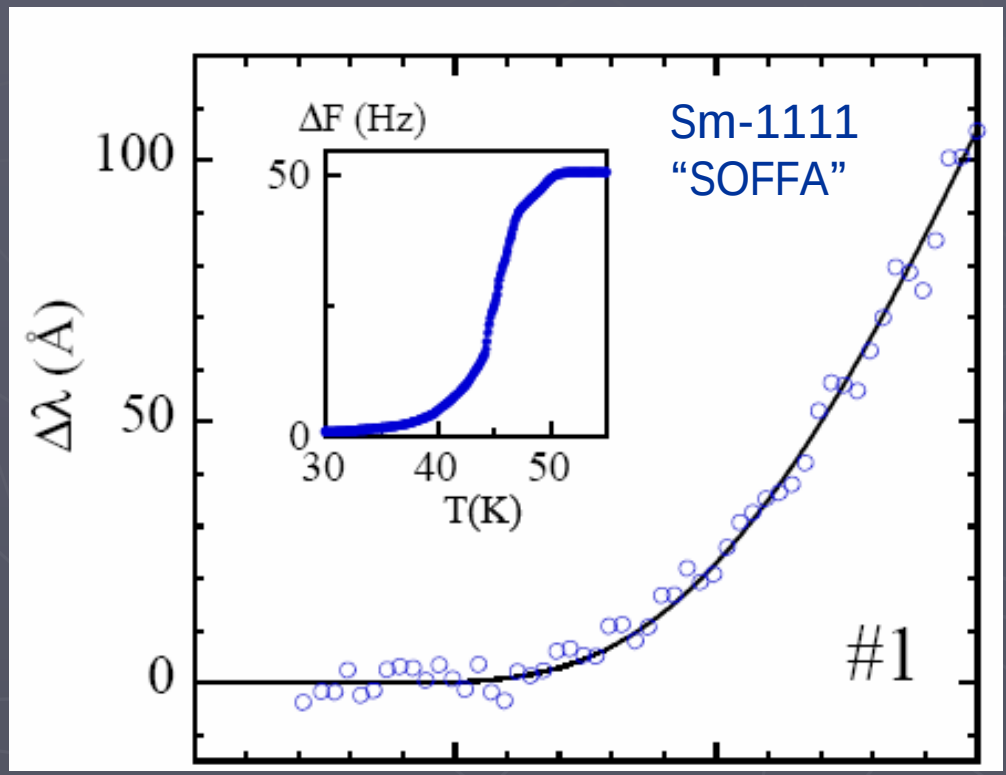
PH et al 1988 ⟷ line nodes $\Rightarrow N(\omega) \sim \omega \Rightarrow T^3$!

NMR on K-doped Ba-122

Yashima et al arXiv:0905.1896



Early penetration depth experiments reported *exponential* $\lambda(T)$ ($\Rightarrow$ full gap)

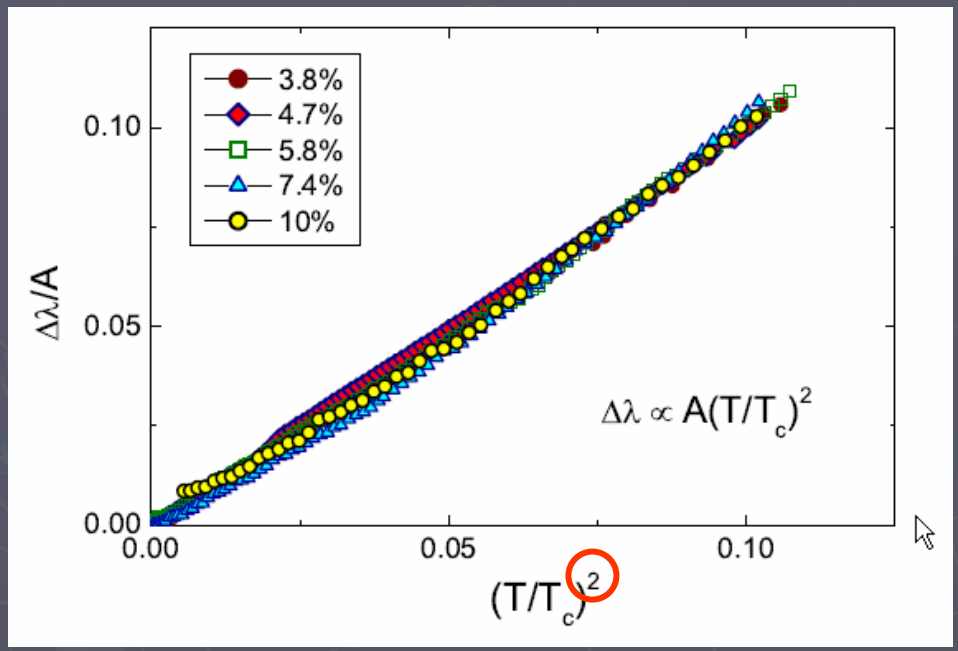


Malone et al Phys. Rev. B 2009

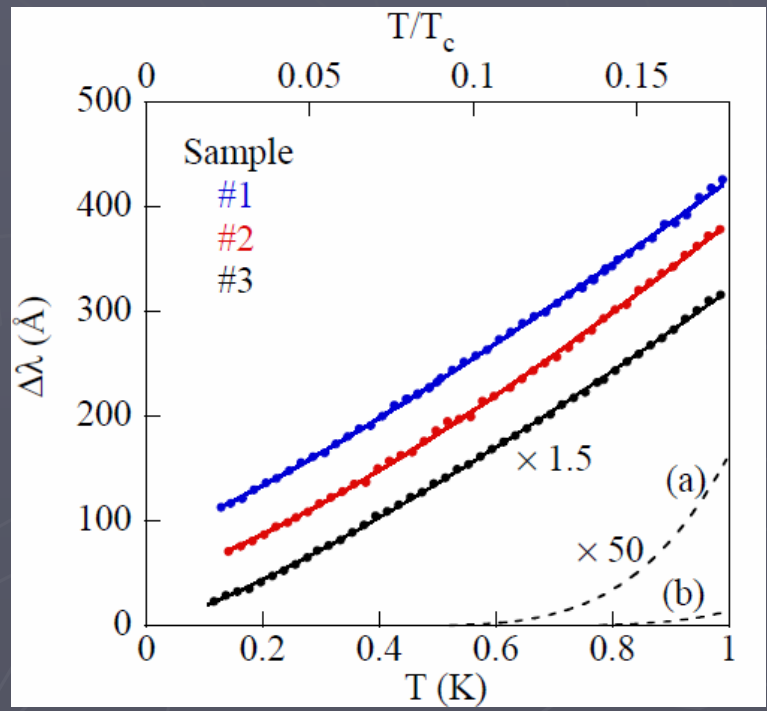
Caution: magnetism of rare earth ions

Other pen. depth experiments

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



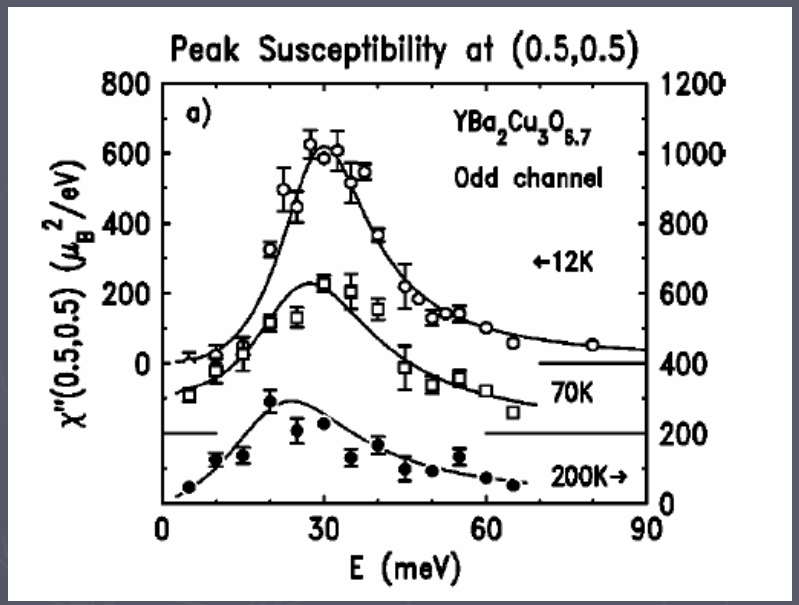
Fletcher et al 2008 LaFePO T_c=6K



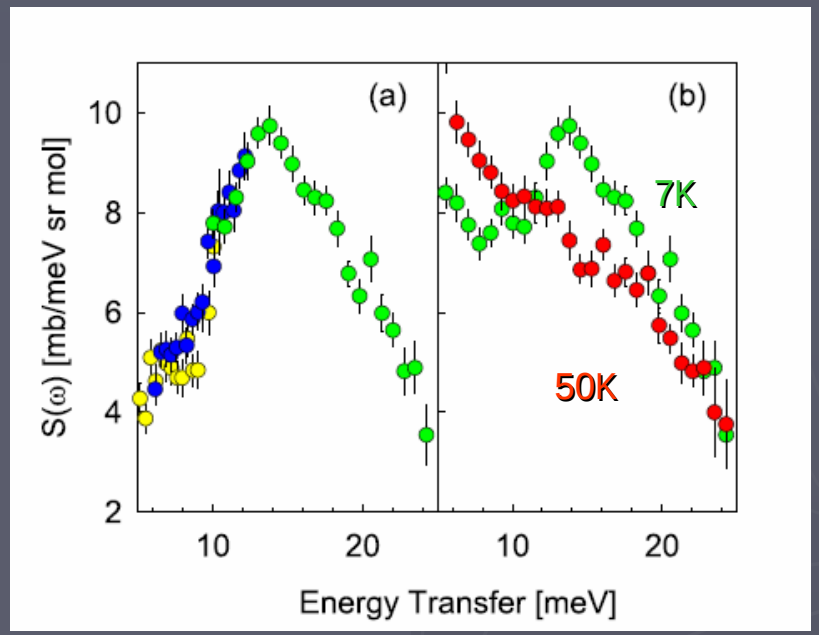
Recall $\Delta\lambda \simeq \int d\omega \left(-\frac{\partial f}{\partial \omega}\right) N(\omega)$ and for dirty $N(\omega) \simeq N_0 + a\omega^2$ clean $N(\omega) \simeq \omega$ nodal SC so $\Delta\lambda \simeq \begin{cases} T^2 & dirty \\ T & clean \end{cases}$

Resonant mode in inelastic neutron scattering

Reminder: cuprates: Fong et al PRB 2000



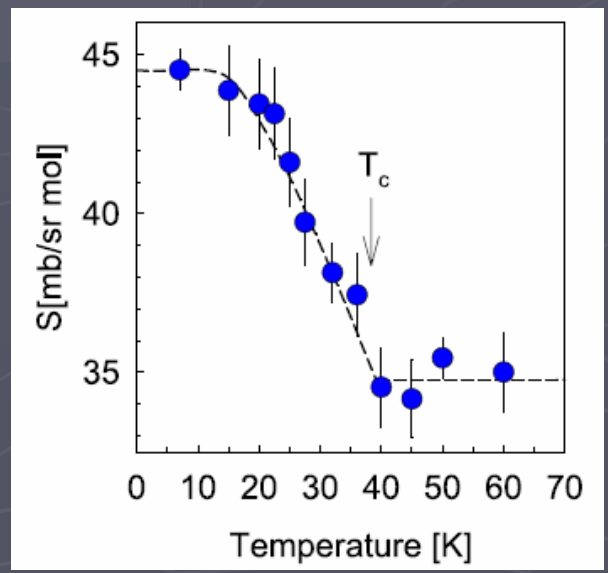
$Ba_{0.6}K_{0.4}Fe_2As_2$: Christianson et al aXv:0807.3932



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

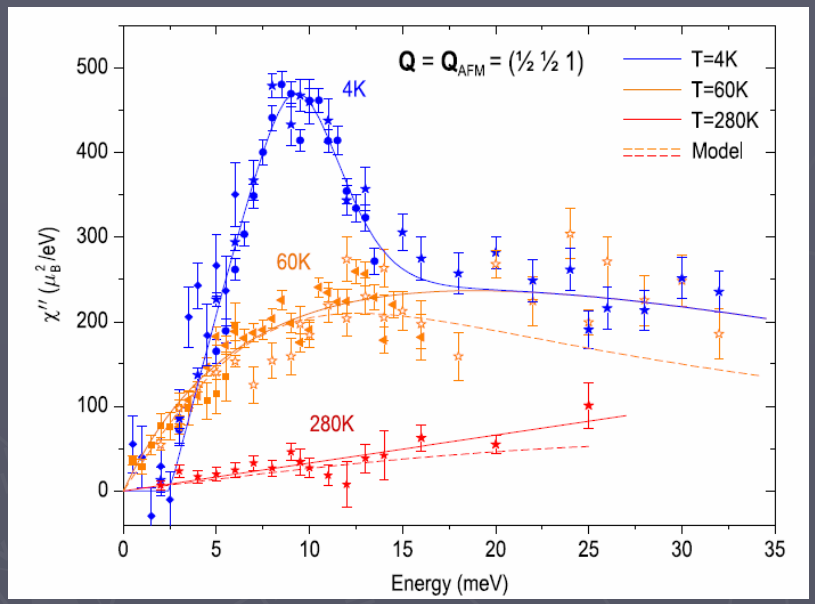
Appears only in SC state (like opt. doped cuprates)

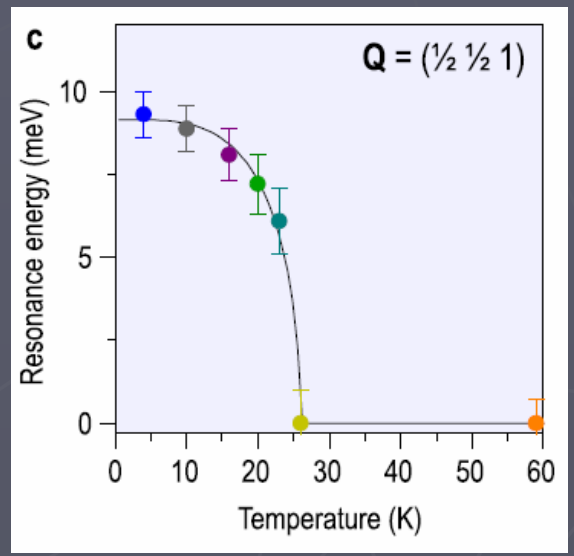
In 1-band models $\Rightarrow \Delta_{k+Q} = -\Delta_k \Rightarrow$"unconventional"

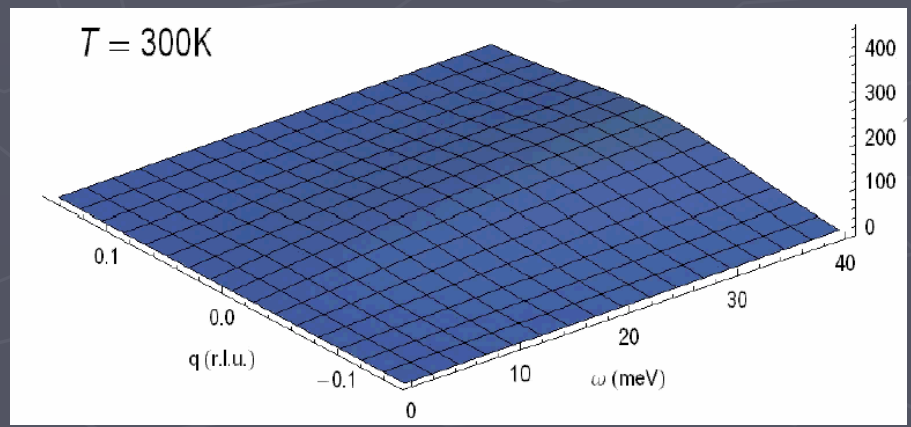


Neutron response/resonant mode II

Inosov et al arXiv:0907.3632



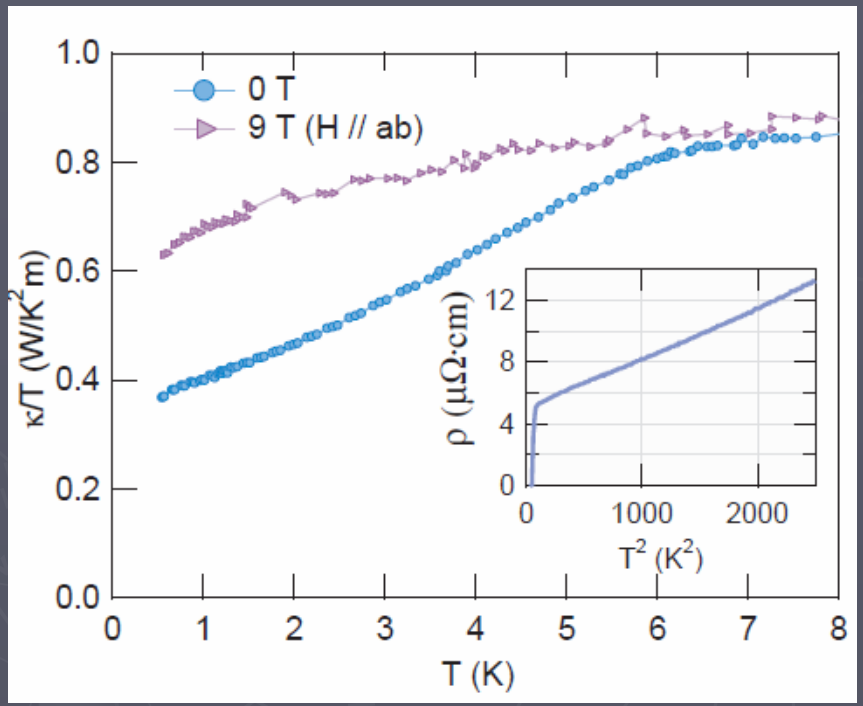




Thermal conductivity (H=0)

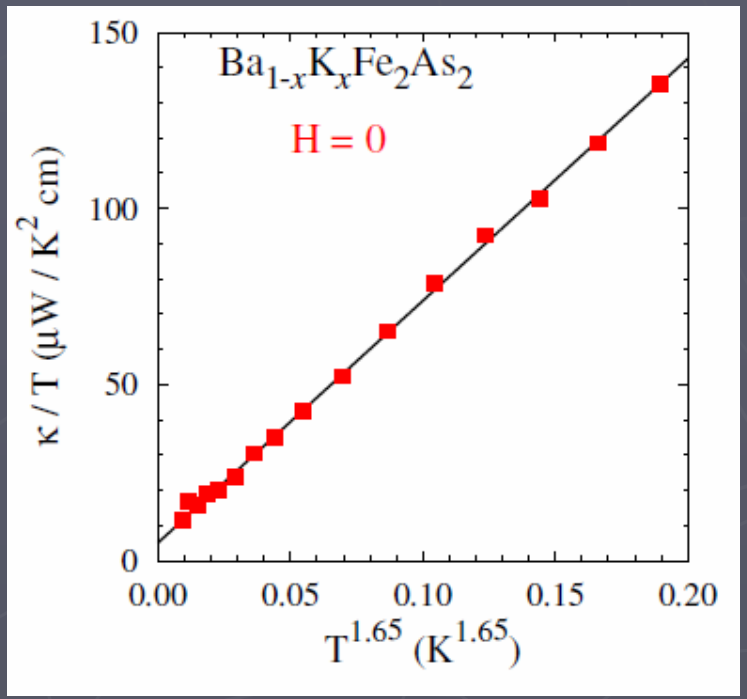
(bulk probe, lowest temperatures thus far)

LaFePO: Yamashita et al aXv:0906.0622



Big linear T term

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

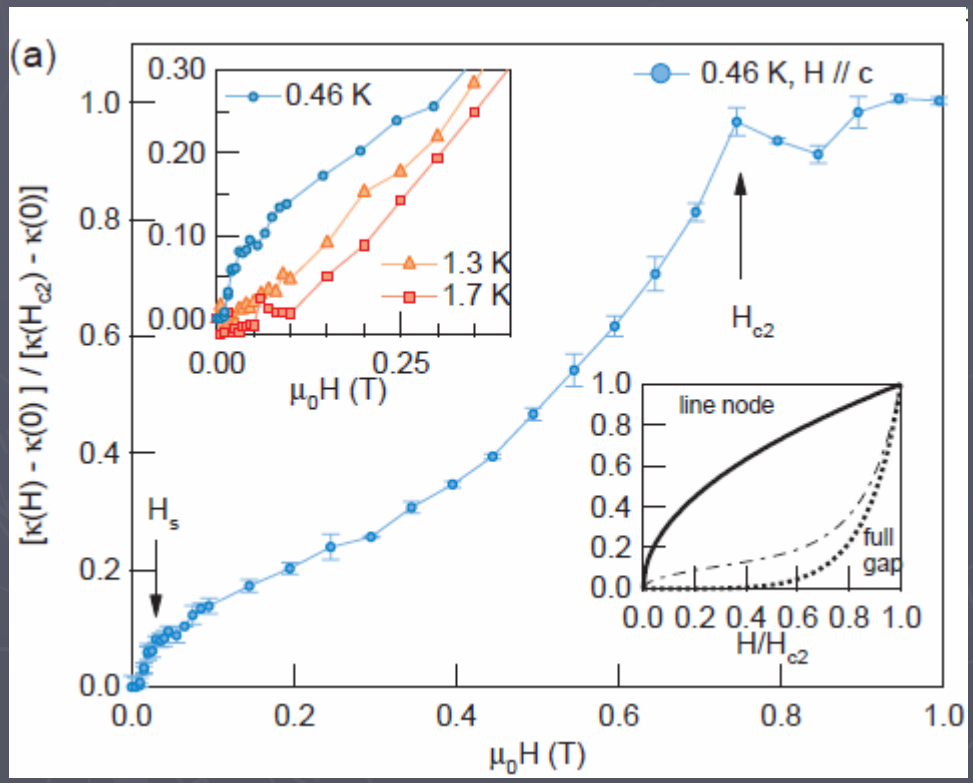


Tiny or zero linear T term

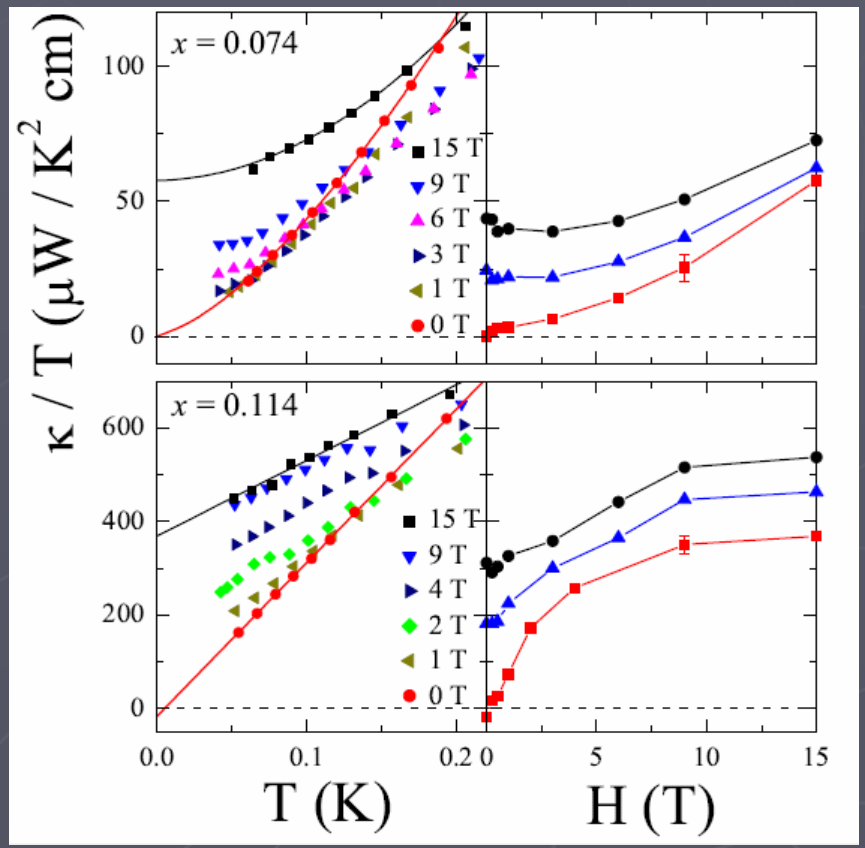
Recall in theory of nodal SC linear T term ⇒ residual qp excitations (metallic-like)
for d-wave superconductor this term is "universal" $\kappa \sim N_0 v_F^2/\Delta_0$

Thermal conductivity (H>0)

LaFePO: Yamashita et al aXv:0906.0622

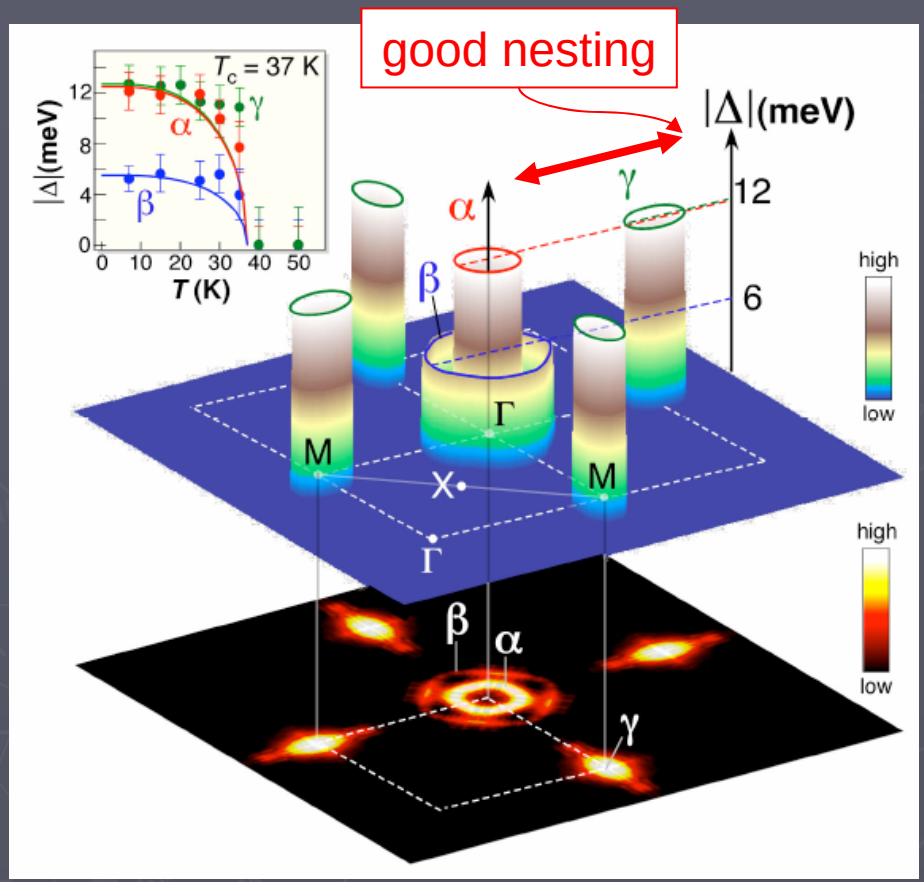


Co-doped Ba-122: Tanatar et al aXv:0904.4049

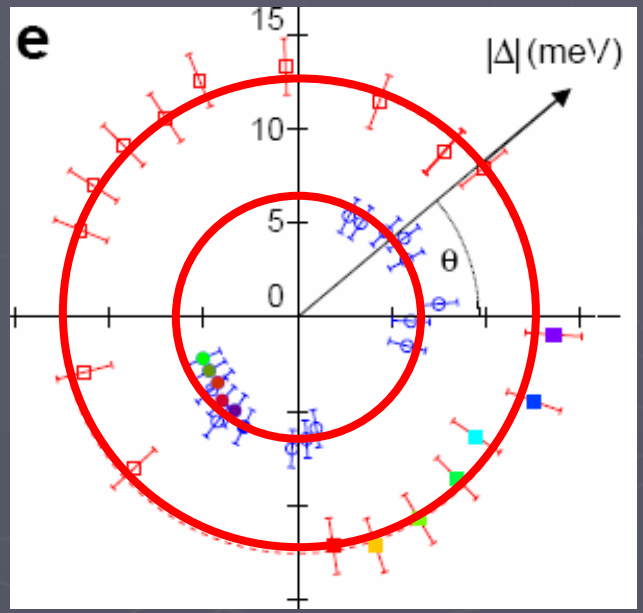


ARPES

$Ba_{0.6}K_{0.4}Fe_2As_2$



Gap size



Many ARPES measurements, none find highly anisotropic gap

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

Spin fluctuation theories of pairing

S. Graser, T. Maier, PH & D.J. Scalapino NJP 2009

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

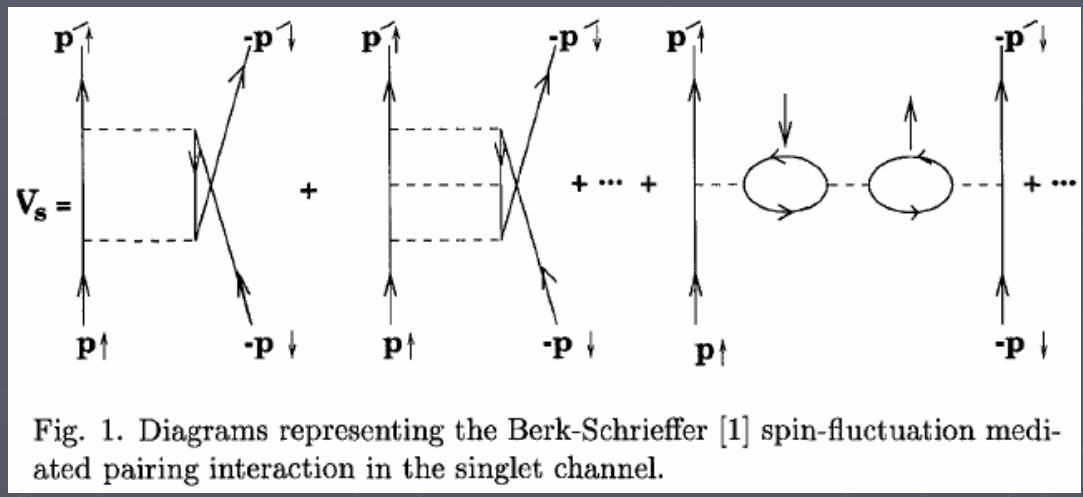


Fig. 1. Diagrams representing the Berk-Schrieffer [1] spin-fluctuation mediated pairing interaction in the singlet channel.

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

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

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

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

$$\Gamma 0^{pq}_{st}(\mathbf{k},\mathbf{k}',i\Omega) = -\frac{1}{2}\left(U_0 - 3U_1\right)^{tq}_{ps}(\mathbf{k}-\mathbf{k}',i\Omega)$$

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

$$U0^{tq}_{ps} = \left[\tfrac{1}{2}\gamma_0 + \gamma_0\chi_0^{\mathrm{RPA}}\gamma_0\right]^{tq}_{ps}$$

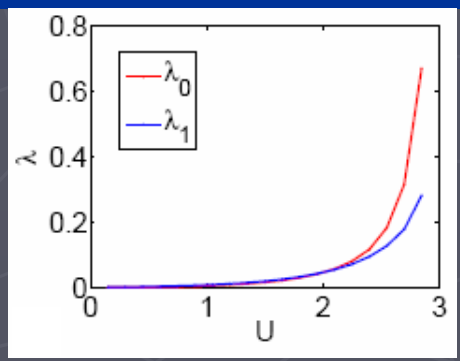
$$U1^{tq}_{ps} = \left[\tfrac{1}{2}\gamma_1 + \gamma_1\chi_1^{\mathrm{RPA}}\gamma_1\right]^{tq}_{ps}$$

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:

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

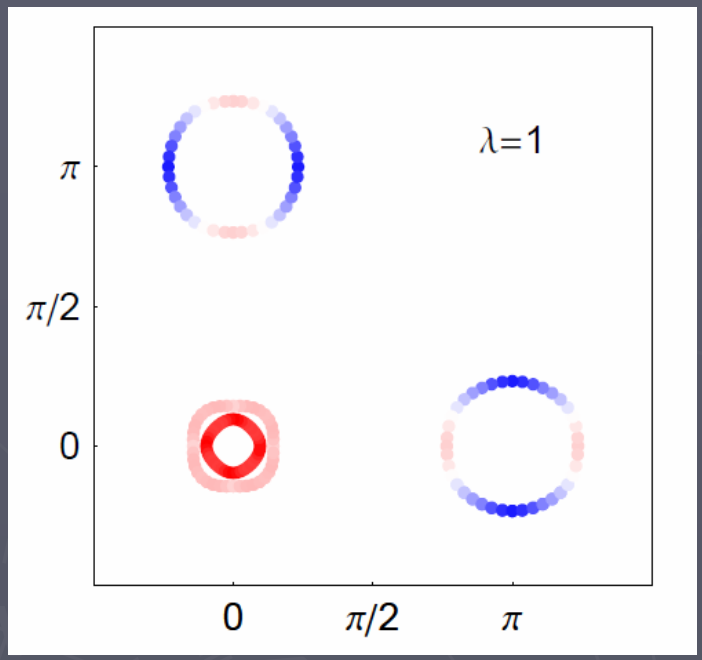


Qi et al (2-band)
Lee-Wen (3-band)
Mazin et al (2-band)
Kuroki et al (nodes)
Zhang et al (aniso)
Graser et al (nodes)

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

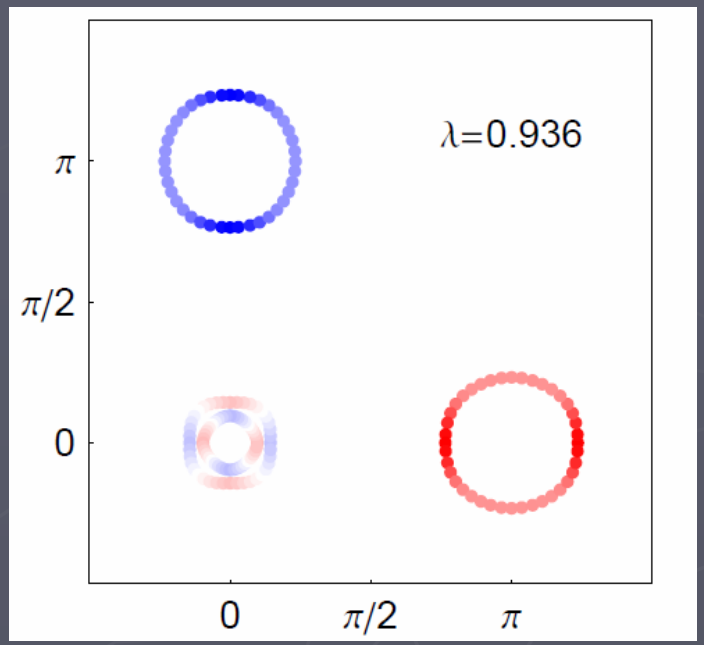
Graser et al: The "winning" pairing functions for $U \to U_c$ display gap nodes!

"anisotropic extended-s"-wave



U=1.73 J=0

nearby: dx2=y2



U=1.78 J=U/2

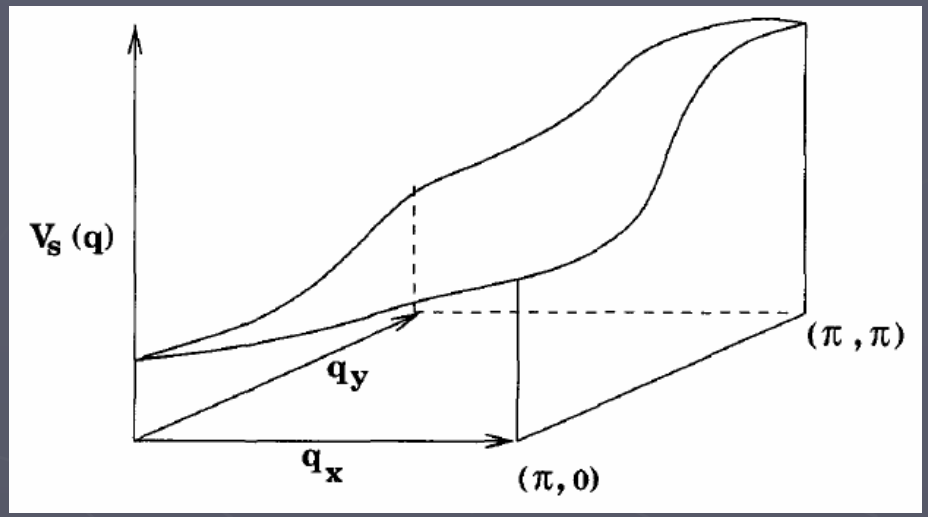
(x=0.125 e-doped)

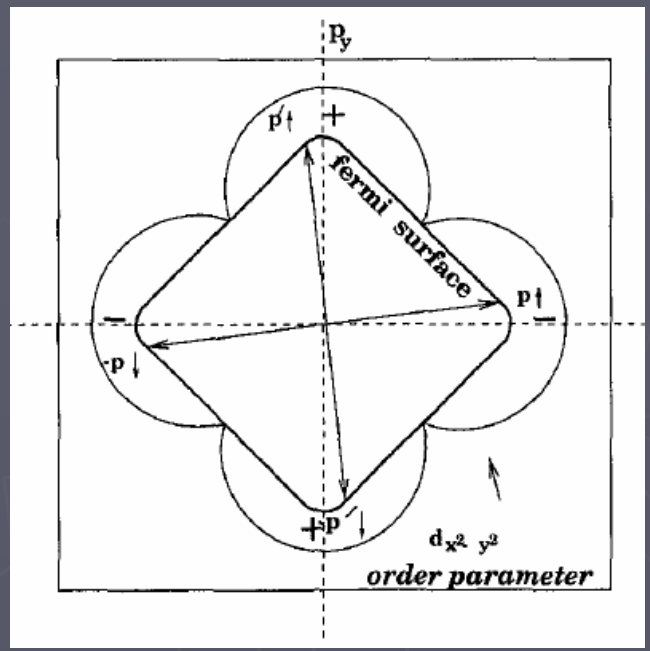
Two pairing channels appear to be nearly degenerate within this scheme:

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



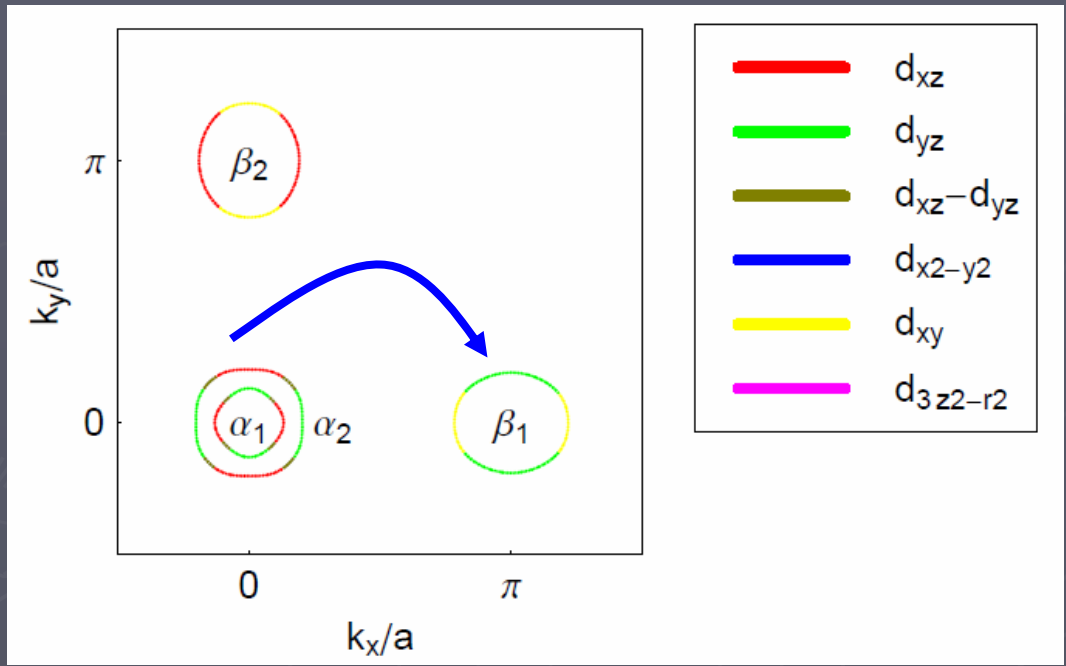


$$\Delta_p = -\sum_{p'} \frac{V(p-p')\Delta_{p'}}{2E_{p'}}$$

d-wave 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 α–β pair scattering

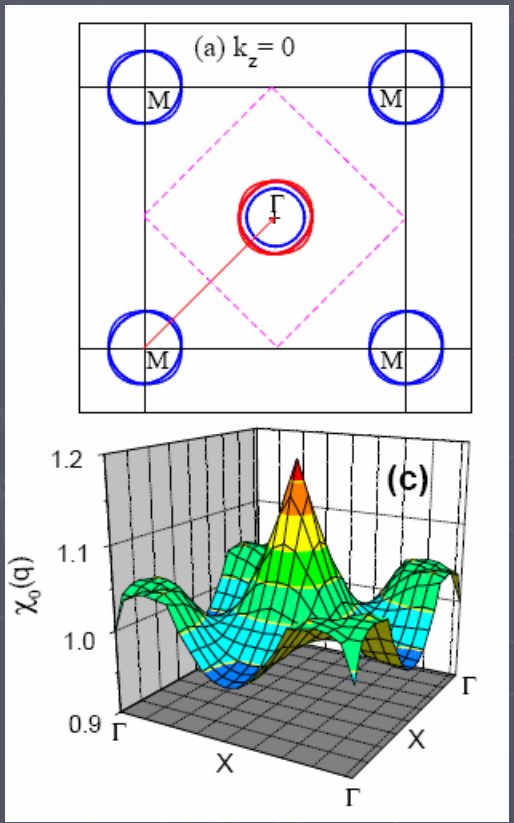


- nesting peaks interaction V_s at π,0 in 1-Fe zone.
- interaction is constant over sheet since they are small.
- therefore *isotropic* sign-changing $s_{+/-}$ state solves gap eqn

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

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

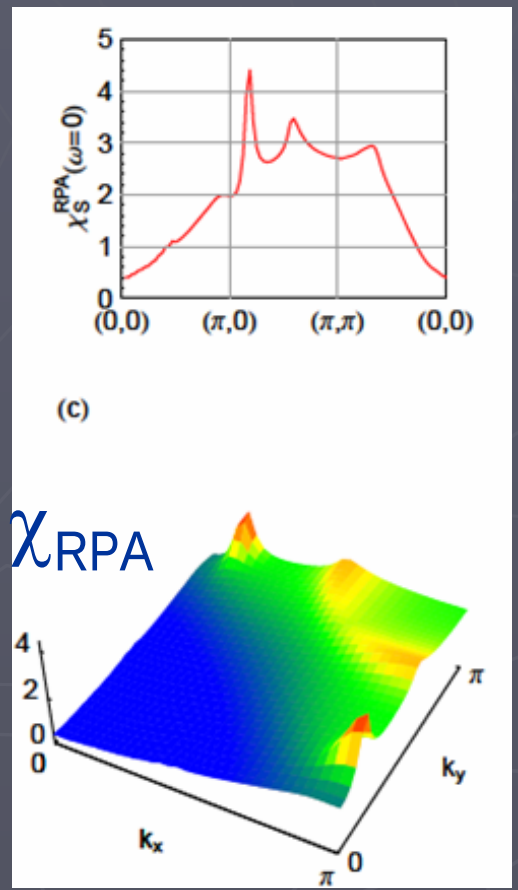


Dong et al, Mazin et al 2008:
orbital character neglected

$$\chi_{st}^{pq}(q,\omega) =$$

$$-\frac{1}{N}\sum_{k,\mu\nu}\frac{a_\mu^s(k)a_\mu^{p*}(k)a_\nu^q(k+q)a_\nu^{t*}(k+q)}{\omega+E_\nu(k+q)-E_\mu(k)+i0^+}$$

$$\times\left[f(E_\nu(k+q))-f(E_\mu(k))\right]$$



Graser et al 2009

Importance of orbital character on Fermi sheets

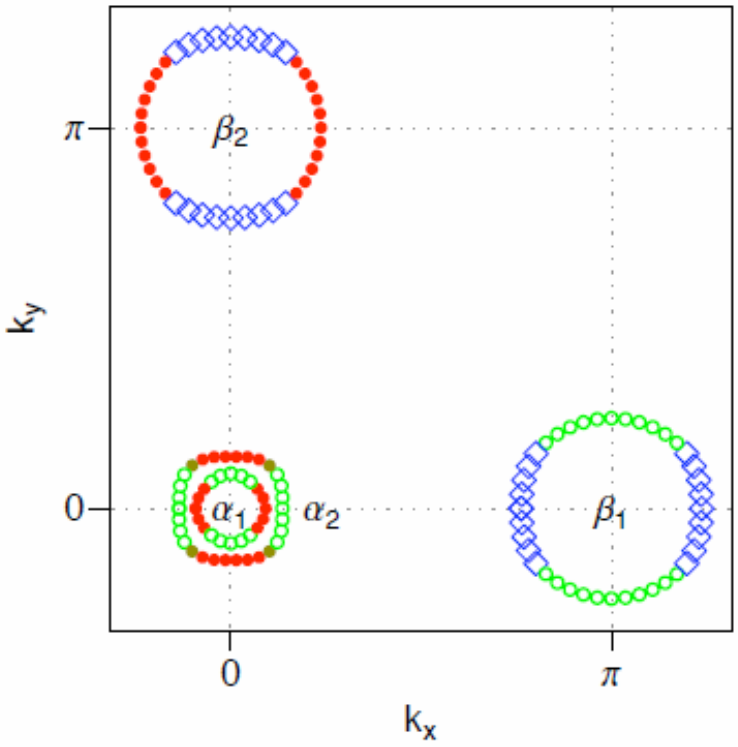
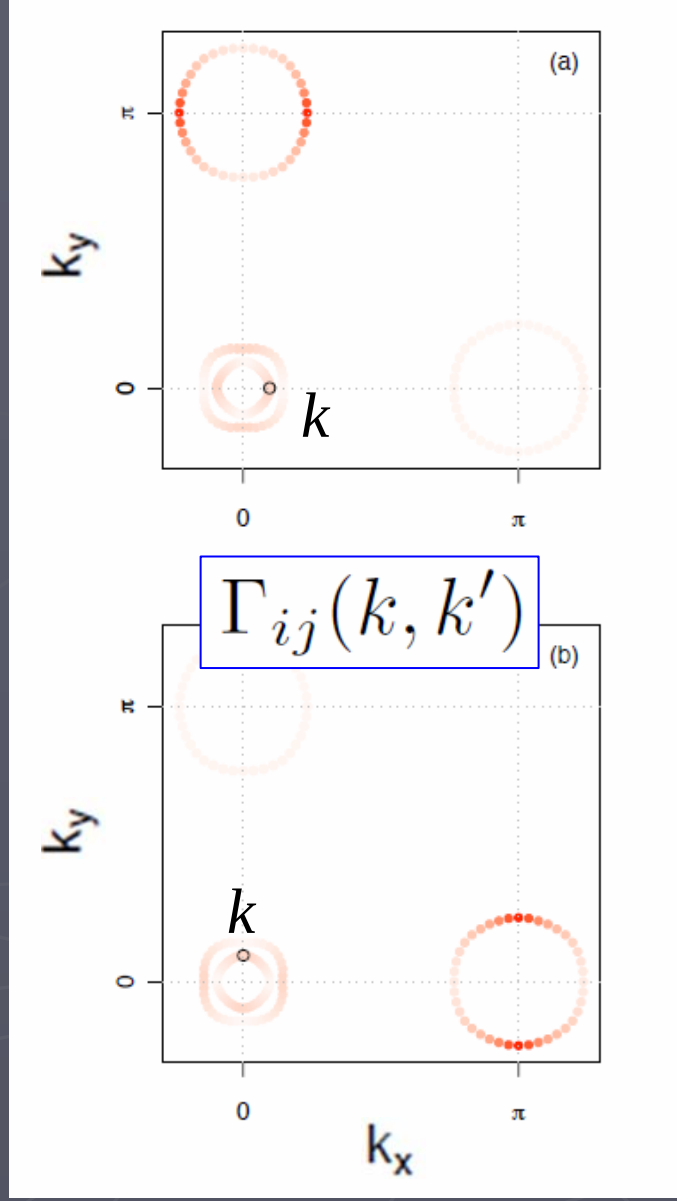
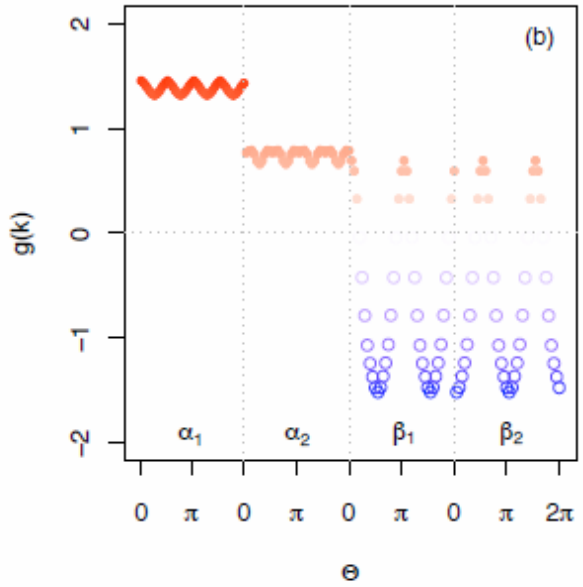


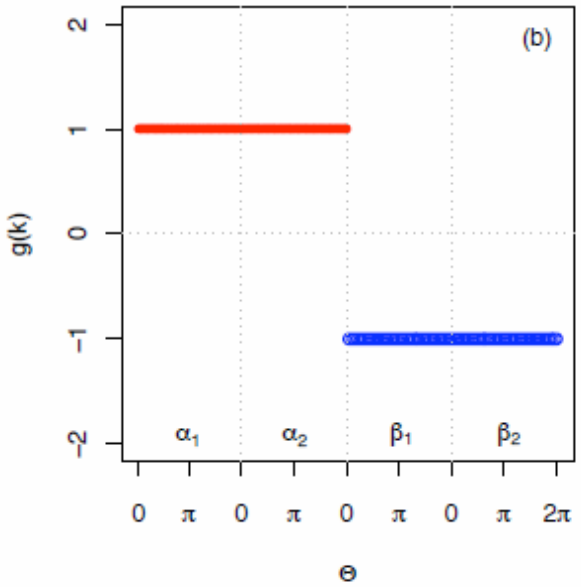
FIG. 1: (color online) The Fermi surface of the 5-orbital tight-binding model[15]. The main orbital contributions are shown by the following colors/symbols: d_{xz} (red/solid circles), d_{yz} (green/open circles), $d_{x^2-y^2}$ (blue/diamonds)

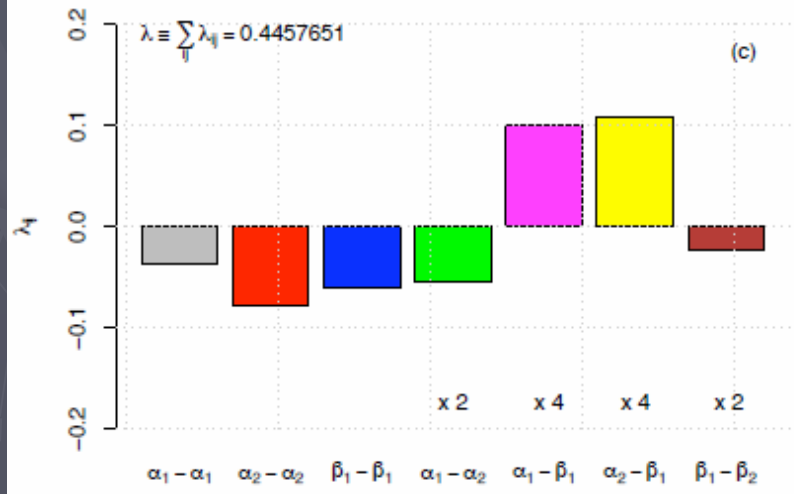


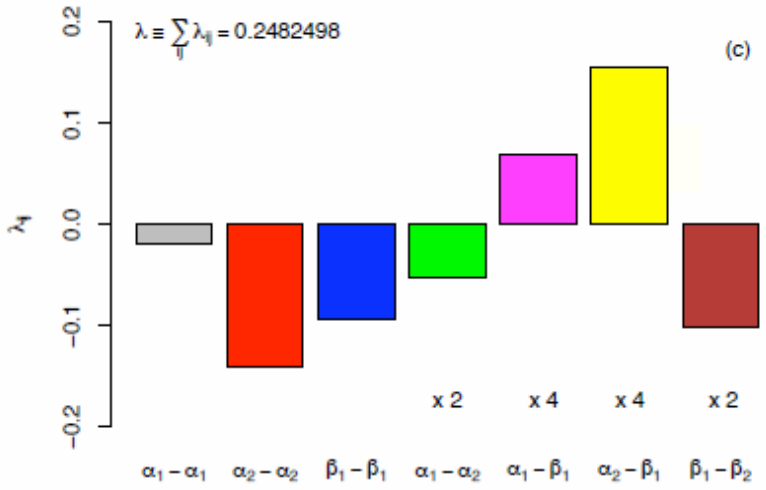
orbital weight factors favor scattering within given orbital

Contributions to pairing strength λ

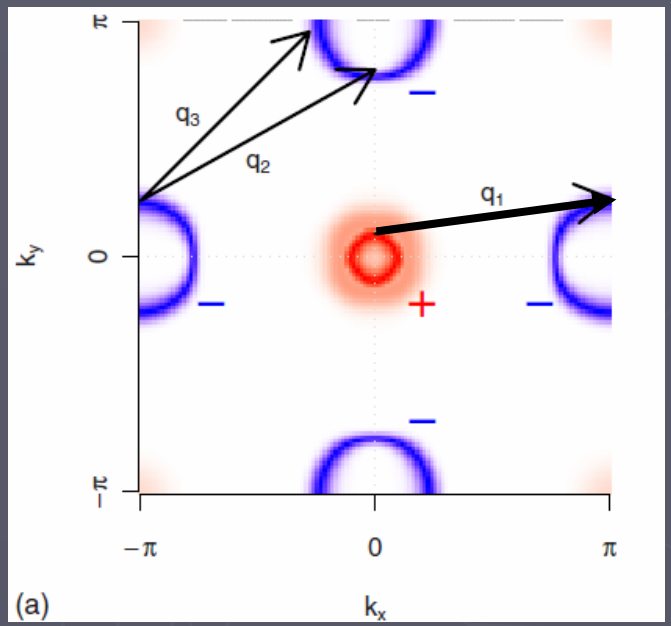


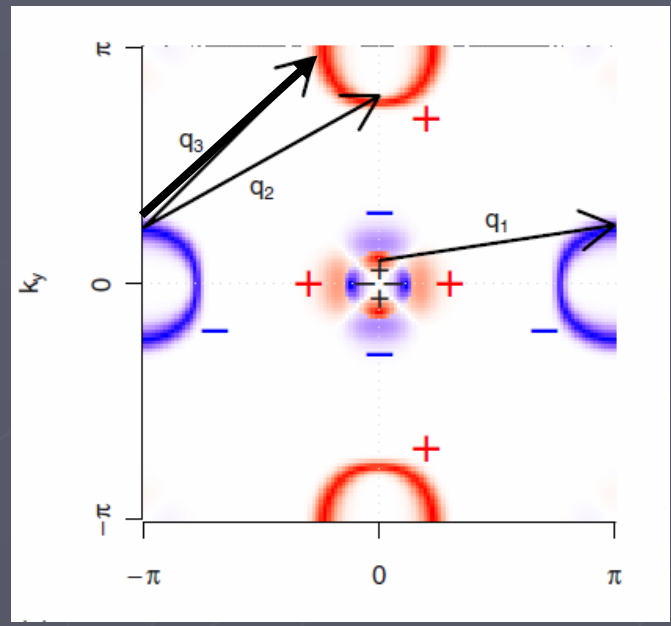






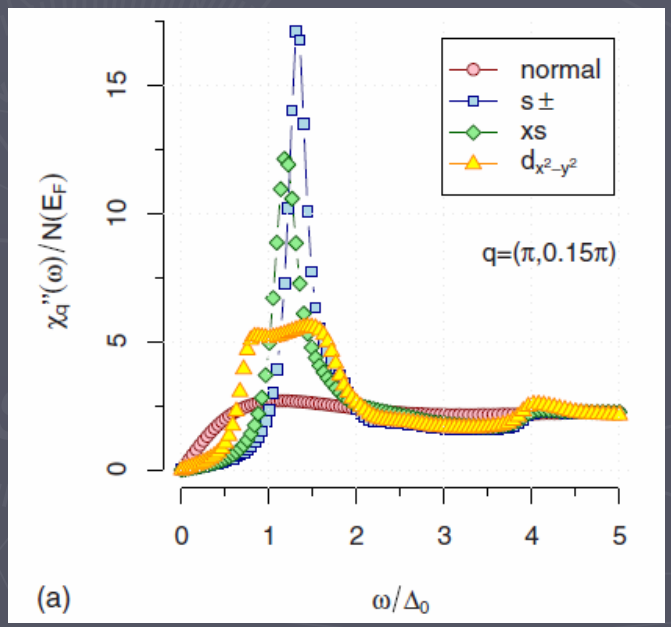
Distinguishing different sign-changing states by neutron resonance

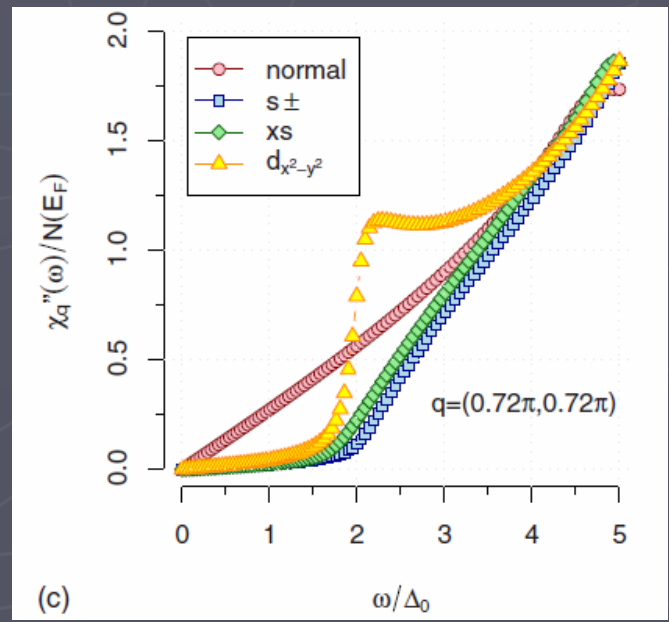




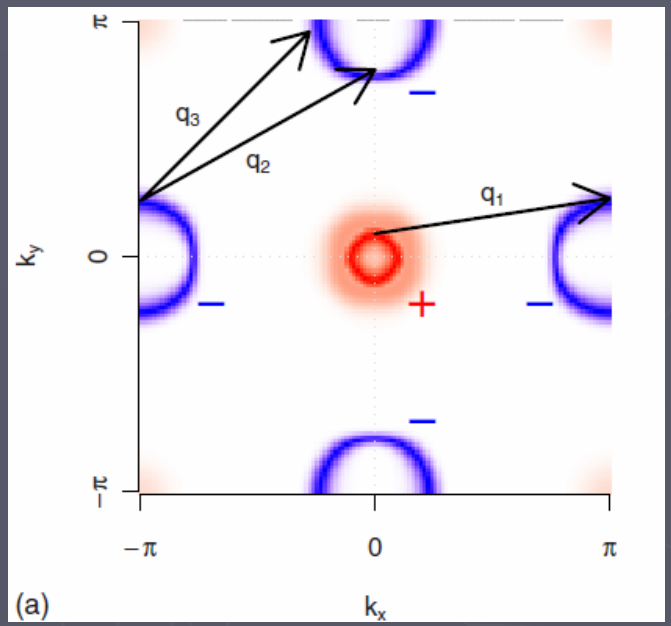
Maier et al
PRB 2009

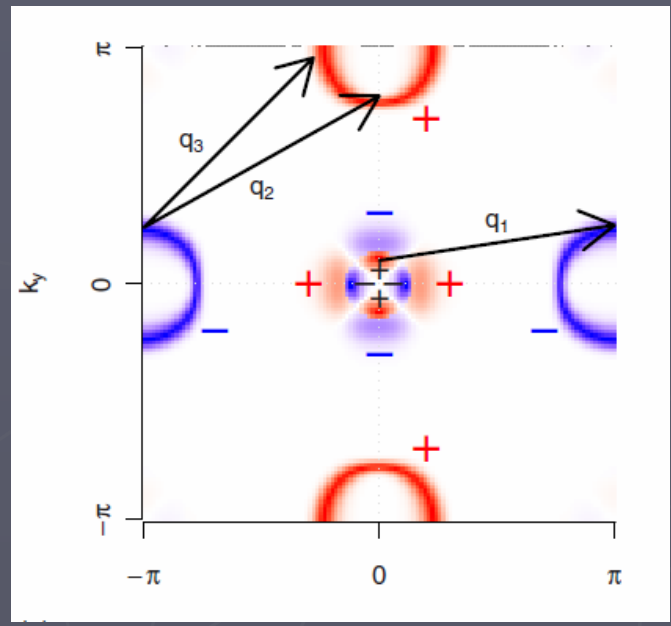
but





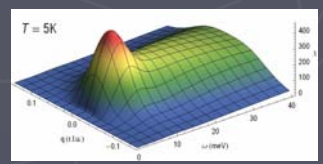
Distinguishing different sign-changing states by neutron resonance



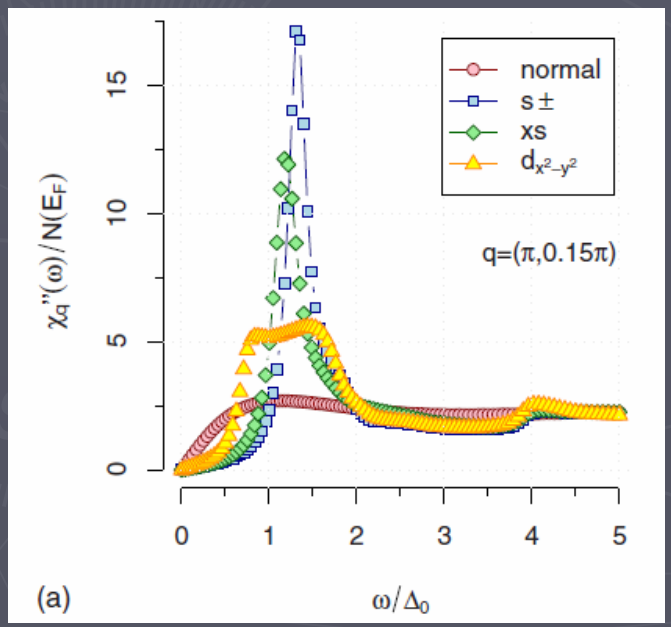


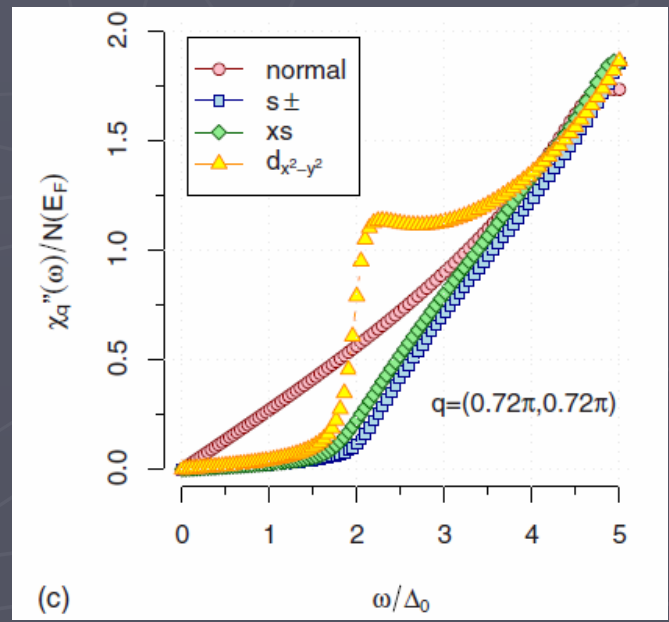
Maier et al
PRB 2009

but



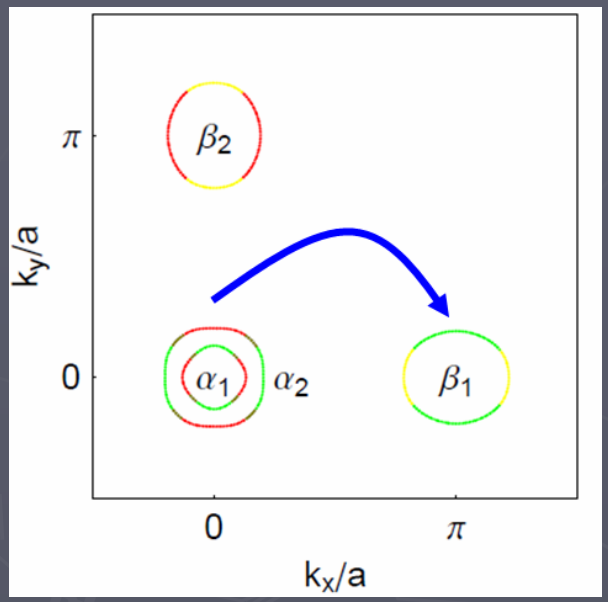
no incomm. response!

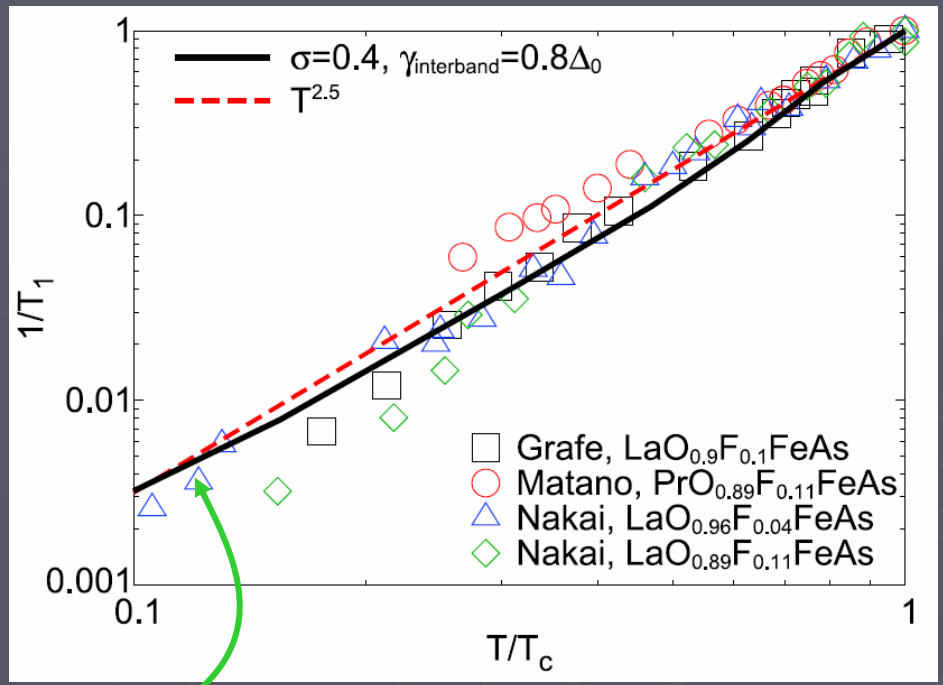




Disorder: Can we reconcile (some) experiments on SC state?

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





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

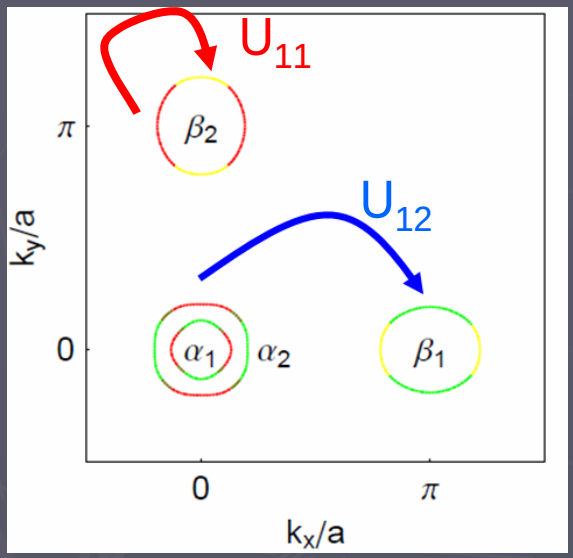
$$\sim T \text{ if } N(\omega = 0) = const$$

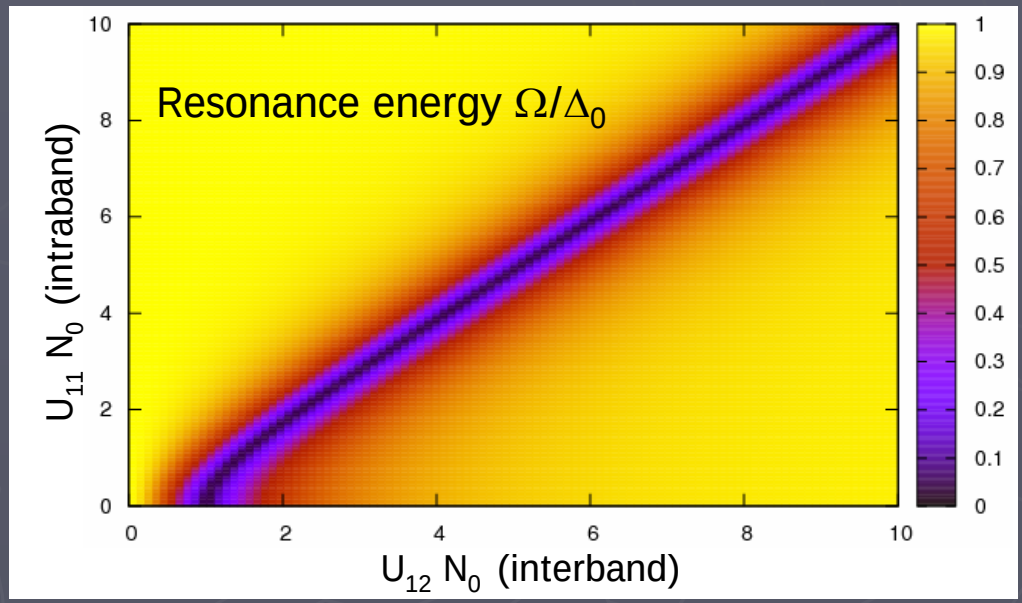
Parker et al PRB 2008
Chubukov et.al., PRB 2008
Vorontsov et al arXiv:0901.0719

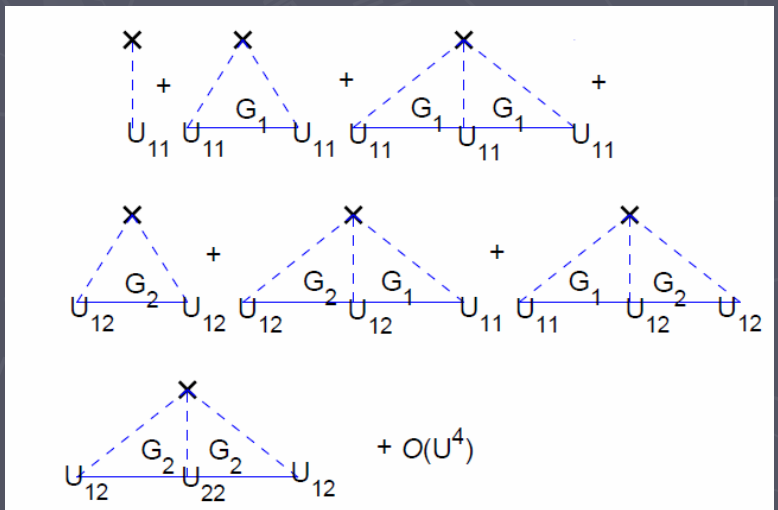
$s_{+/-}$ state has full spectral gap but interband scattering is pairbreaking (Muzikar 1990s)
Implication: samples showing full gap are clean; samples with low-E states are dirty

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

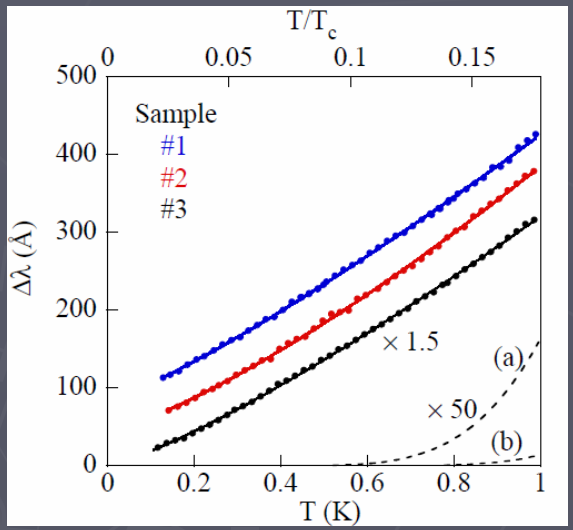
Reconciling contradictory experiments cont'd.

Scenario 2: anisotropic states with intraband scattering

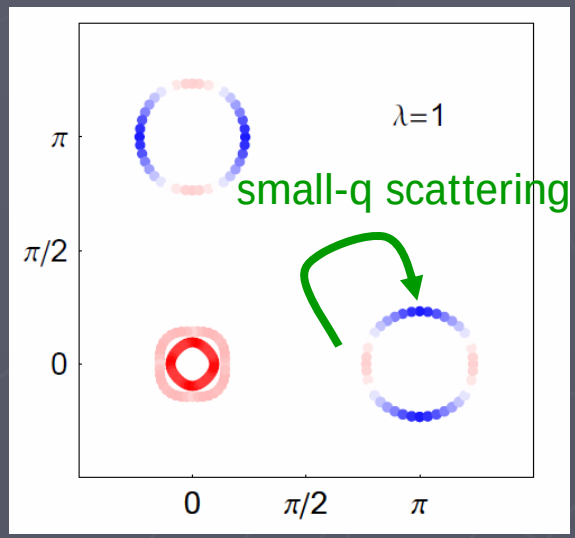
recall

Fletcher et al 2008 LaFePO T_c=6K

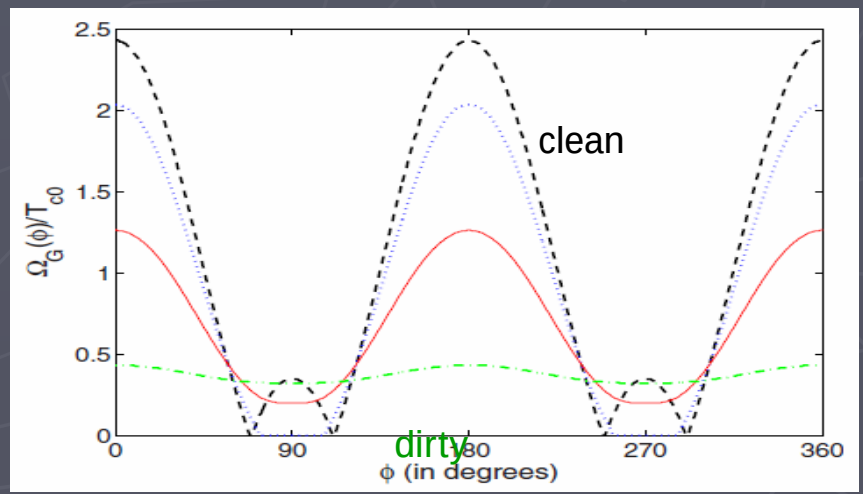
$\lambda \sim T \Rightarrow$ nodes!



Mishra et al PRB 2009



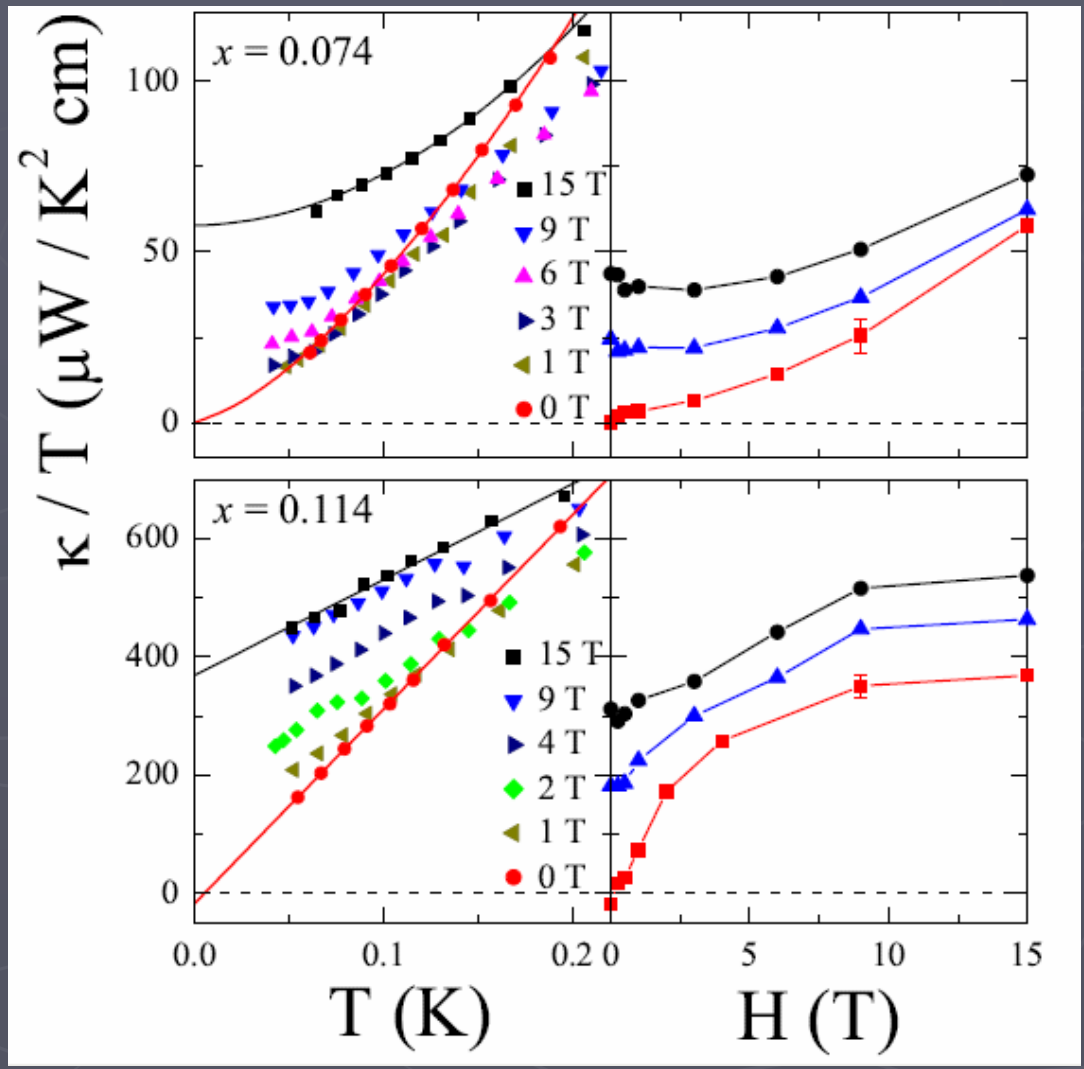
intraband scattering averages gap anisotropy, removes nodes!



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

Reminder: thermal conductivity in Co-122

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

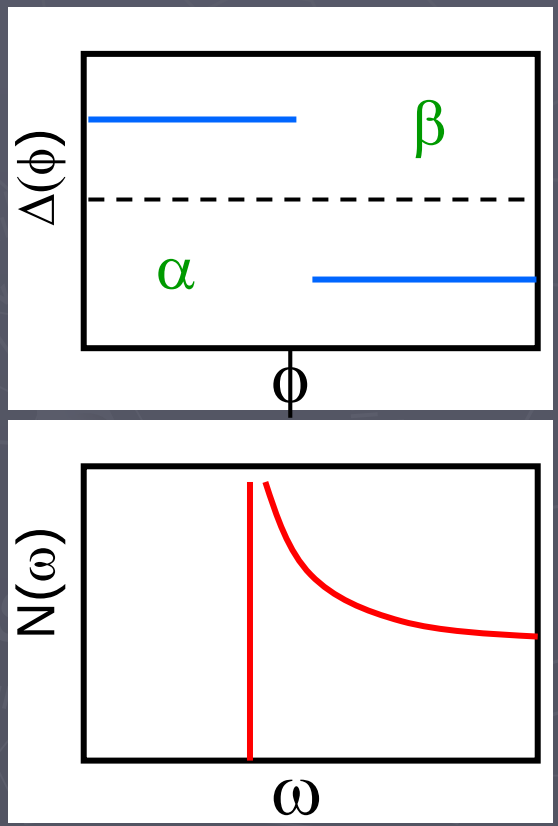


Theory of thermal conductivity

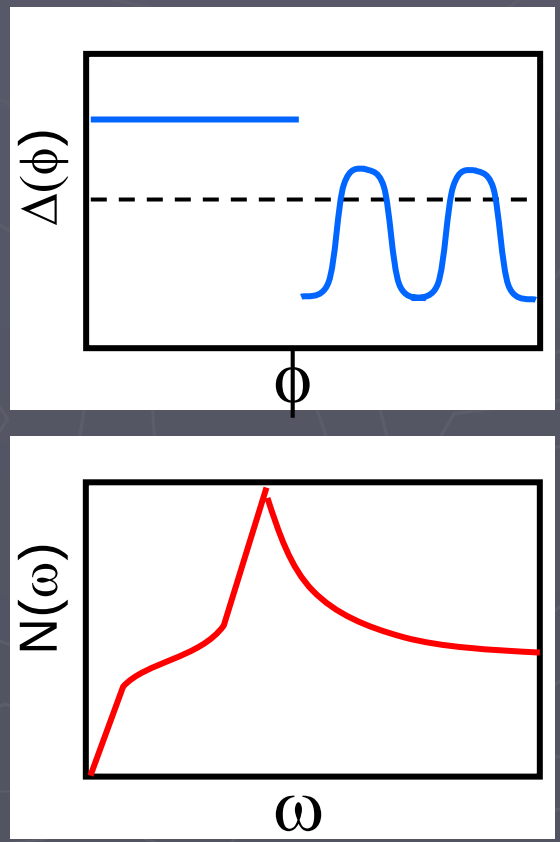
Mishra, Vorontsov, Vekther and PH 2009

2-band phenomenological calculation:

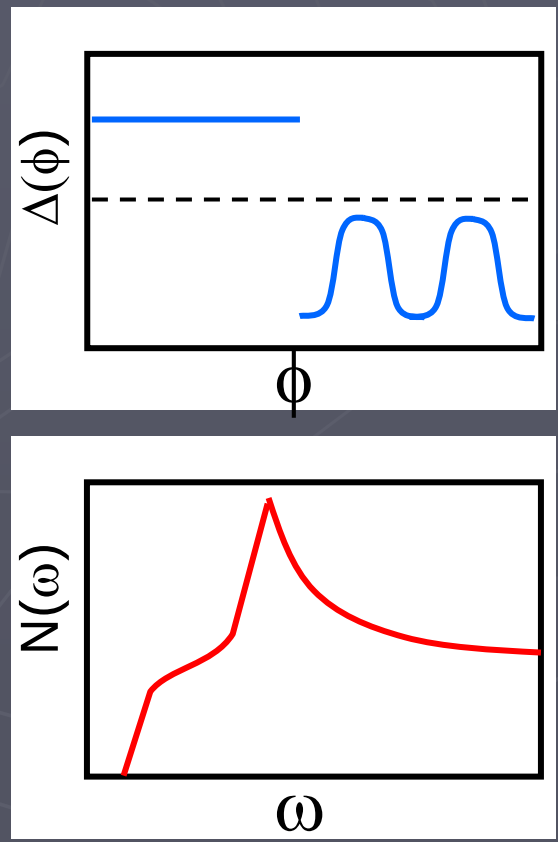
a) isotropic $s_{+/-}$



b) nodes



c) deep minima



Theory of thermal conductivity cont'd

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

Both ω and Δ are renormalized by disorder

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

Q: what happens in 2-band A1g cases as $T \to 0$?

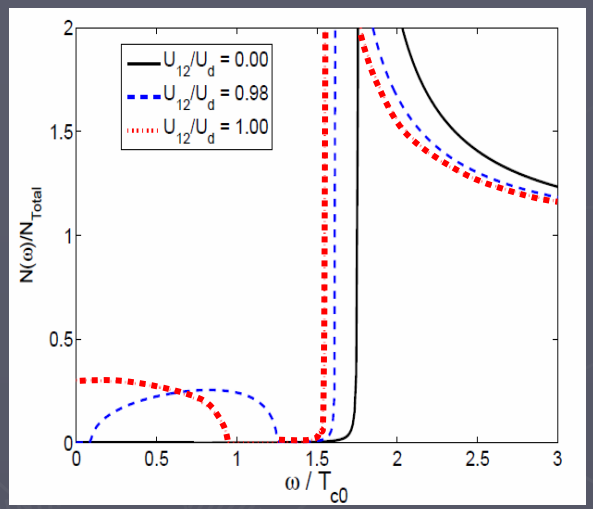
Theory of thermal conductivity cont'd

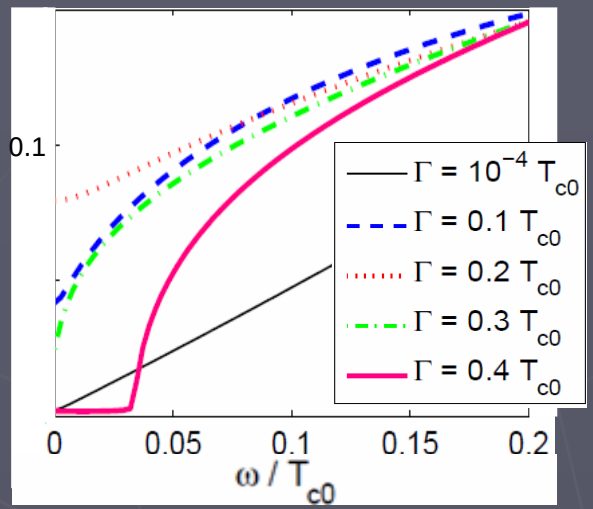
isotropic $\Gamma=0.3T_{c0}$

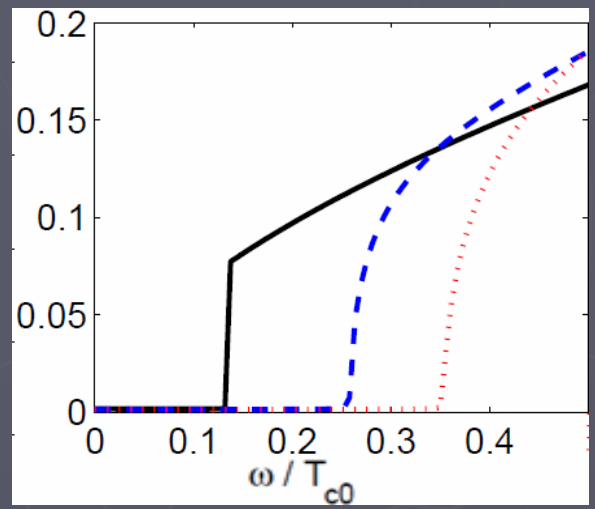
nodes c=0.07

deep minima c=0.07

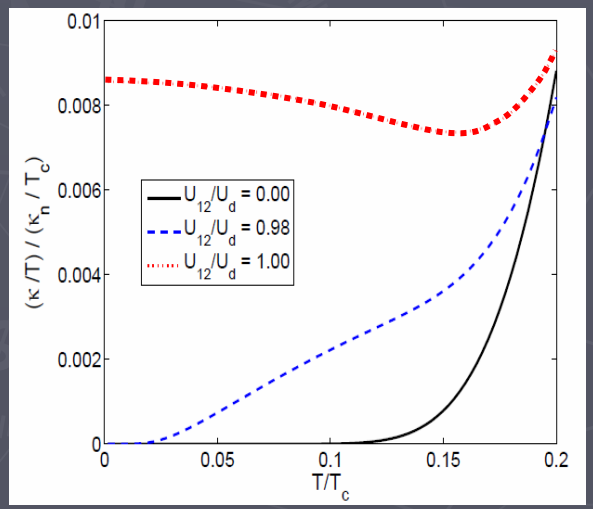
DOS

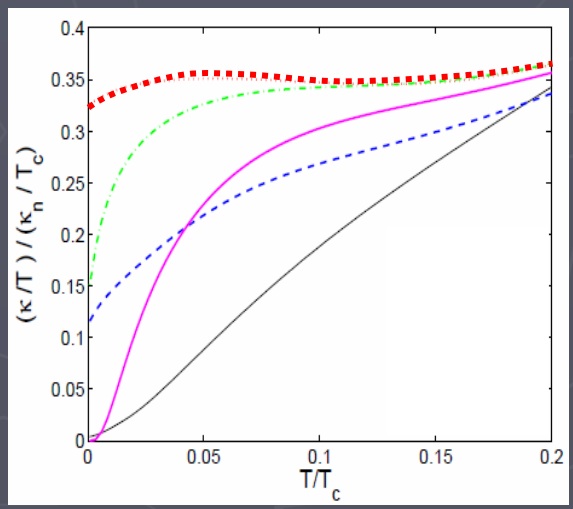


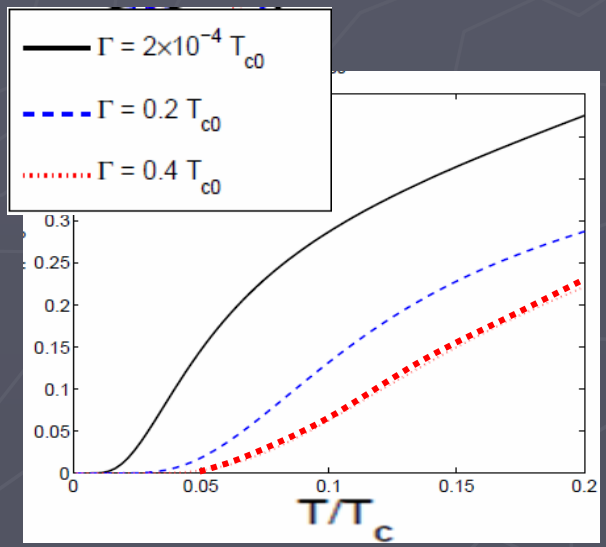




Thermal cond/T

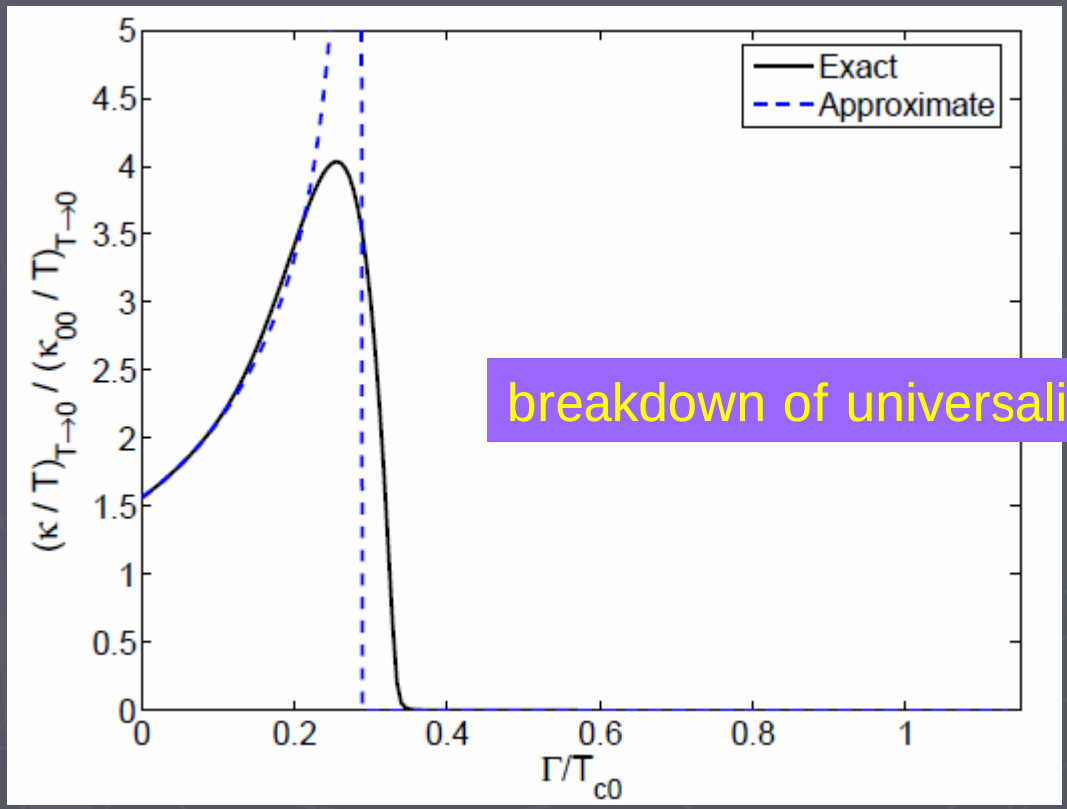




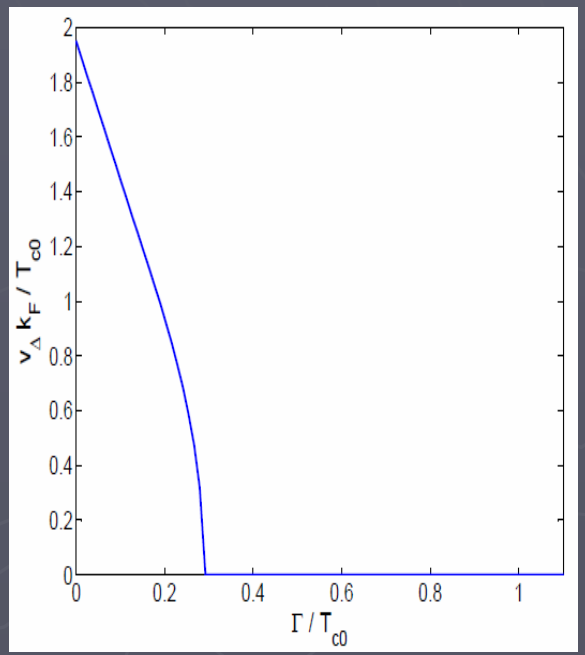


Theory of thermal conductivity cont'd

b) Nodes



breakdown of universality



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

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

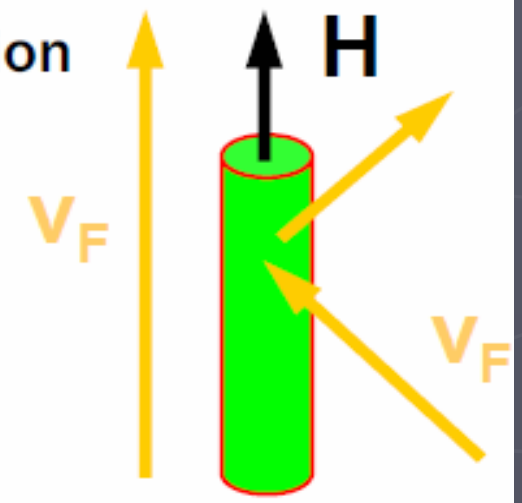
Field dependence of thermal conductivity: BPT method

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

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

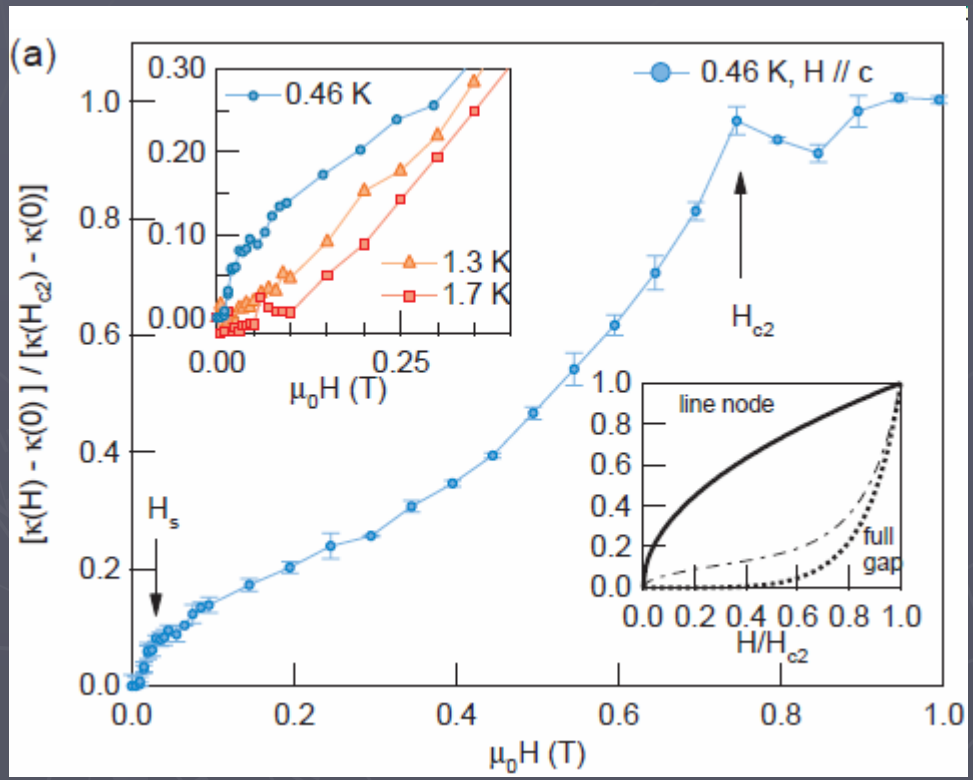
– DOS, specific heat, thermal conductivity

– angle-dependent scattering on the vortices

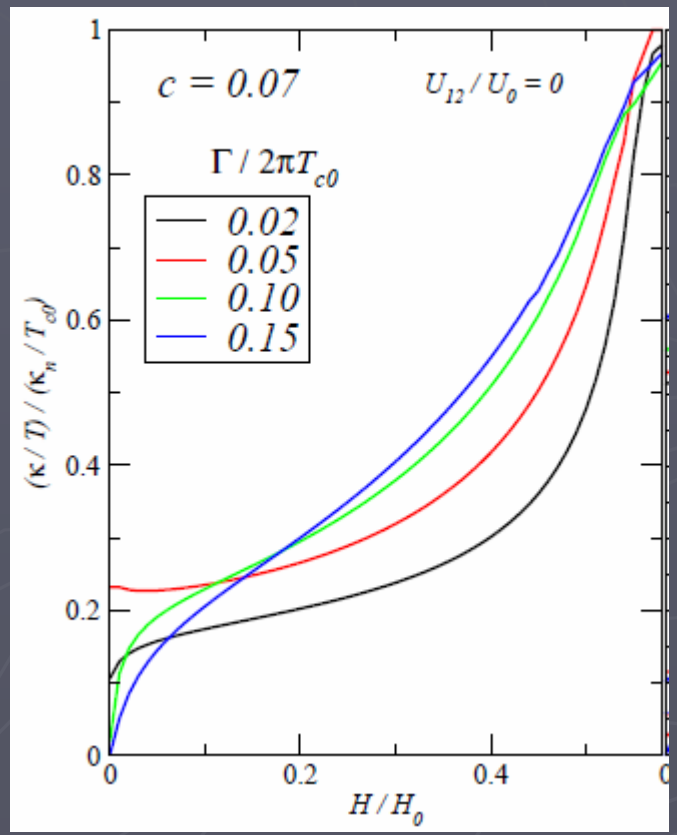
A. Houghton and I. Vekhter '98, H. Kusunose '04, A. Vorontsov and I.Vekhter, '06

Field dependence of thermal conductivity: results

Expt: LaFePO Yamashita et al



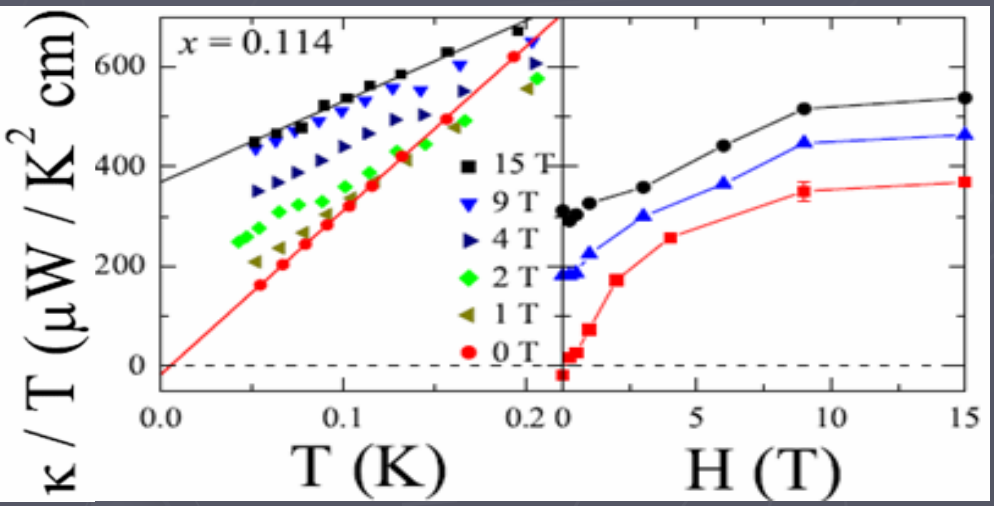
Theory: nodes, pure intraband scatt only

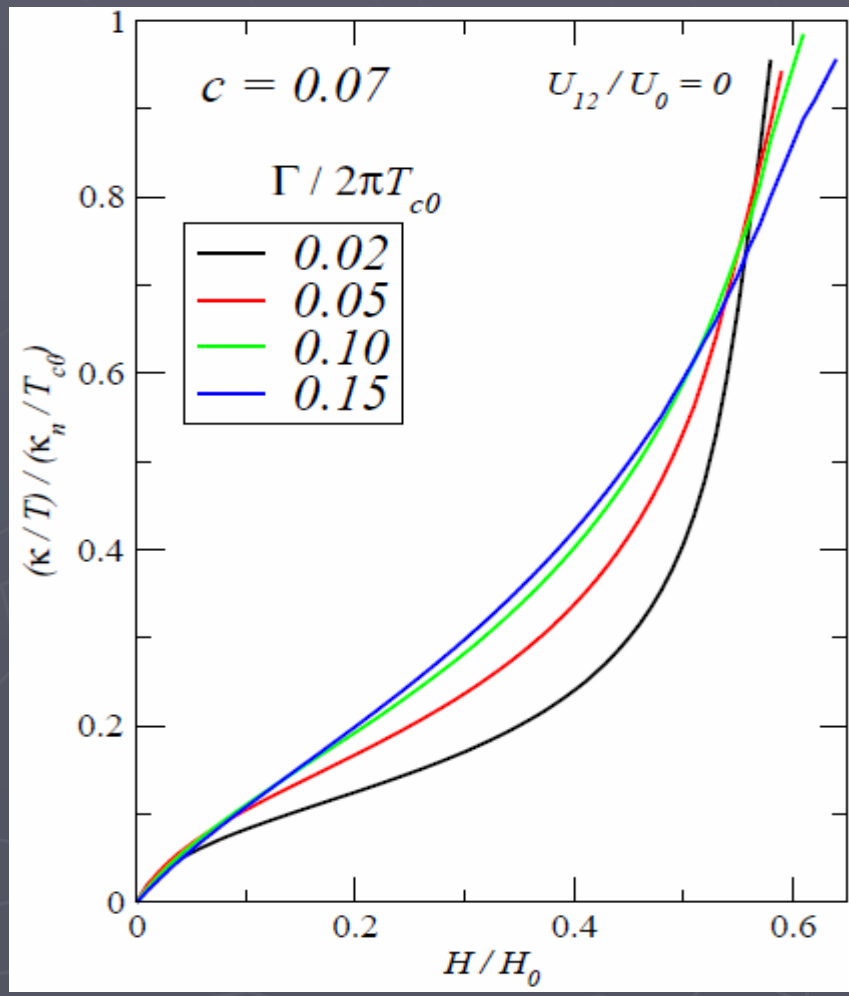


Field dependence of thermal conductivity: results cont'd

Theory: deep gap minima

Expt: Co-doped Ba-122 Tanatar et al



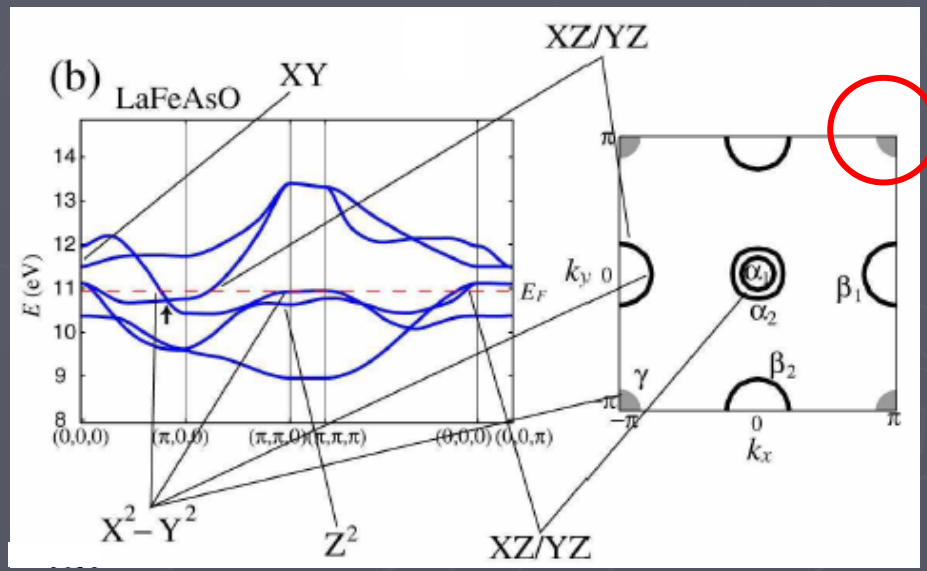


Field dependence with deep gap minima not qualitatively different from nodes!

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

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

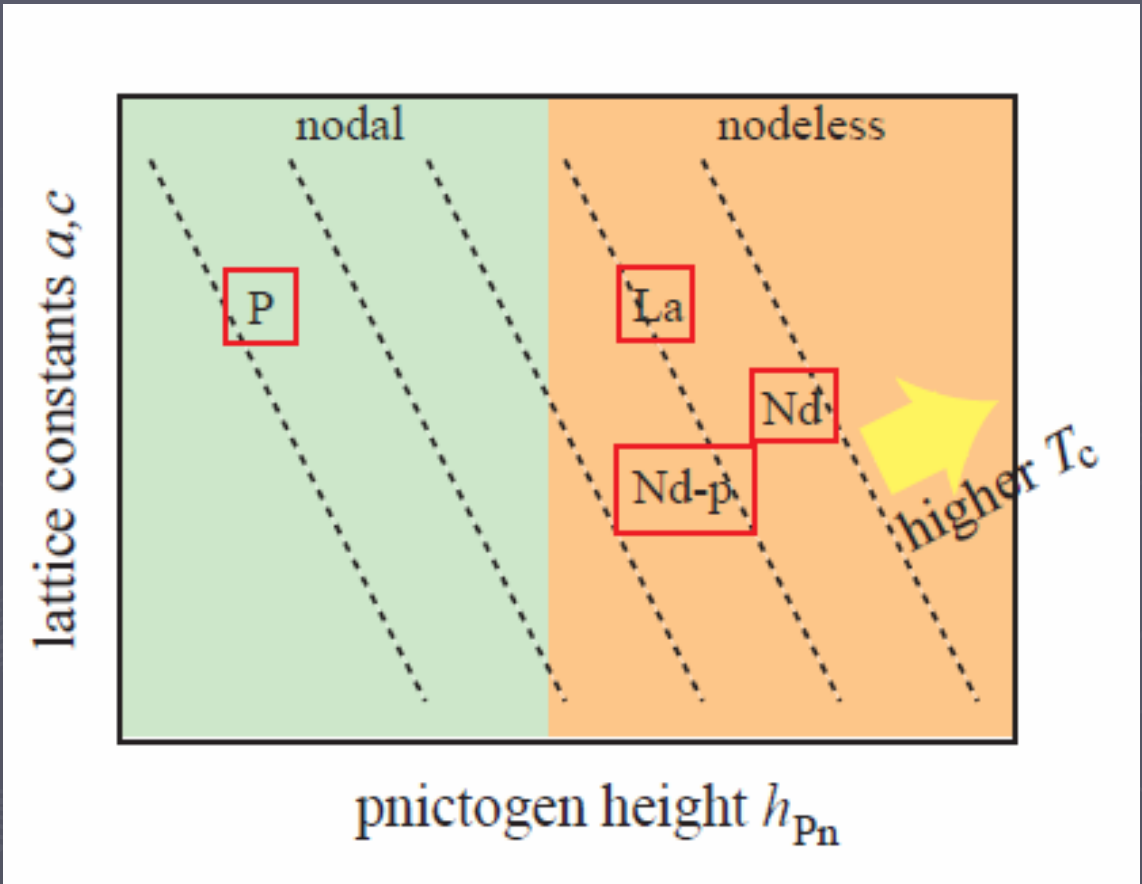
Look at effective tight-binding spin fluctuation models for various 1111 materials



	a(Å)	c(Å)	$z_{\rm Pn}$	$h_{\rm Pn}$ (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
$h_{\rm As} = 1.38$Å	4.04	8.74	0.6580	1.38	111.2	0.132	0.113	−0.191	0.309
$h_{\rm As} = 1.14$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 has nodes, 122's have deep gap minima, which decrease with overdoping $\Rightarrow$more low-E qp's. Spoiler: ARPES?