The Abdus Salam
International Centre for Theoretical Physics

2157-5

Workshop on Principles and Design of Strongly Correlated Electronic Systems

2 - 13 August 2010

Accidental Order Parameter Nodes in Fe-pnictide Superconductors: Origins and Implications

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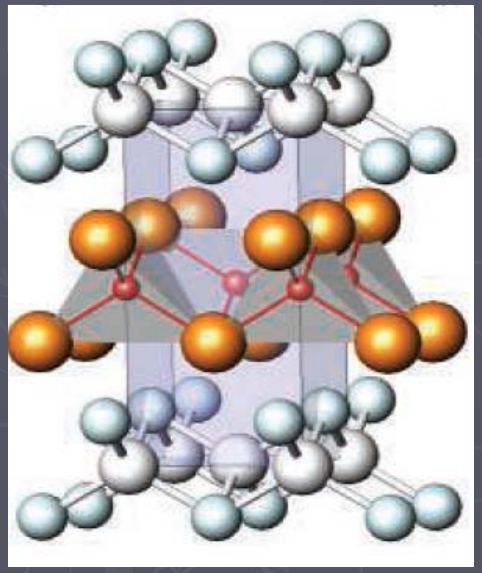
Accidental order parameter nodes in Fe-pnictide superconductors: origins and implications

P. Hirschfeld, U. Florida



S. Graser NJP 11, 025016 (2009)
V. Mishra et al PRB 79, 094512 (2009)
T. Maier et al PRB 79, 224510 (2009)
V. Mishra et al PRB 80, 224525 (2009)
S. Graser et al PRB 81, 214503 (2010)
A. Kemper et al NJP 12 073030 (2010)

Trieste August 2010

Collaborators

from U. Florida Dept. of Physics:

Vivek Mishra

Hai-Ping Cheng

from rest of world:

Doug Scalapino
UCSB

Thomas Maier
ORNL

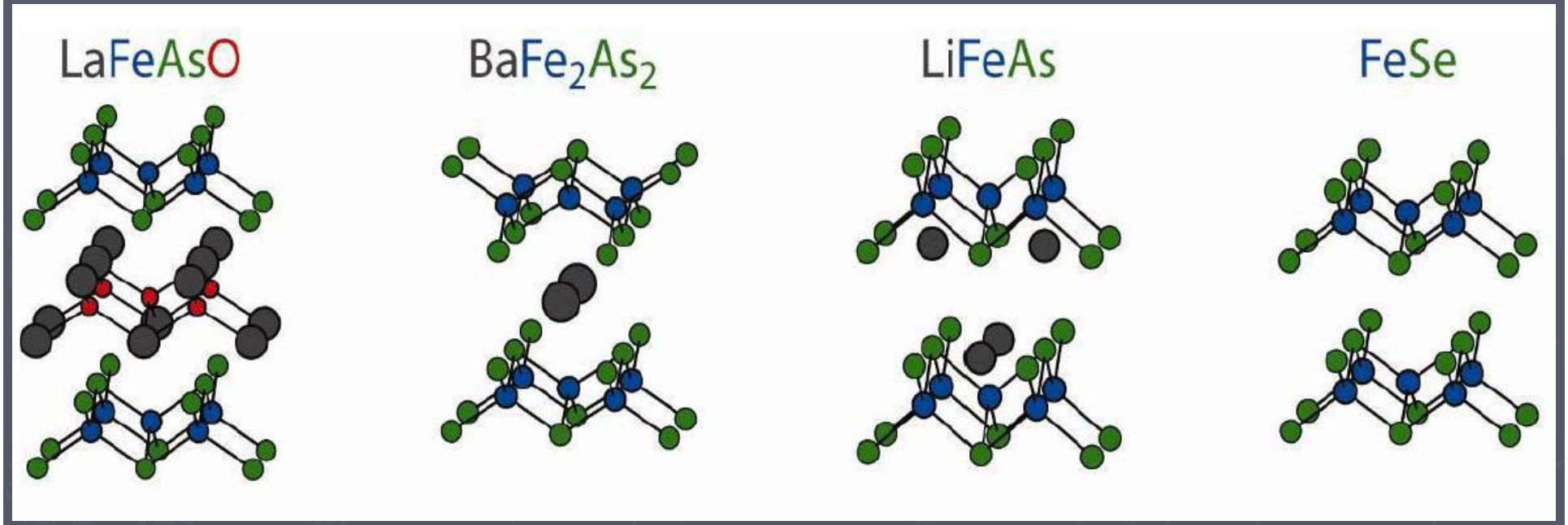
Siggi Graser
Augsburg

Lex Kemper
Stanford

Outline

- Fe-pnictide experiments on SC state: why is gap structure so sensitive?
- Spin fluctuation theory of Fe-pnictides
- Phenomenology: qp transport in 122 systems

Iron-based superconductors



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

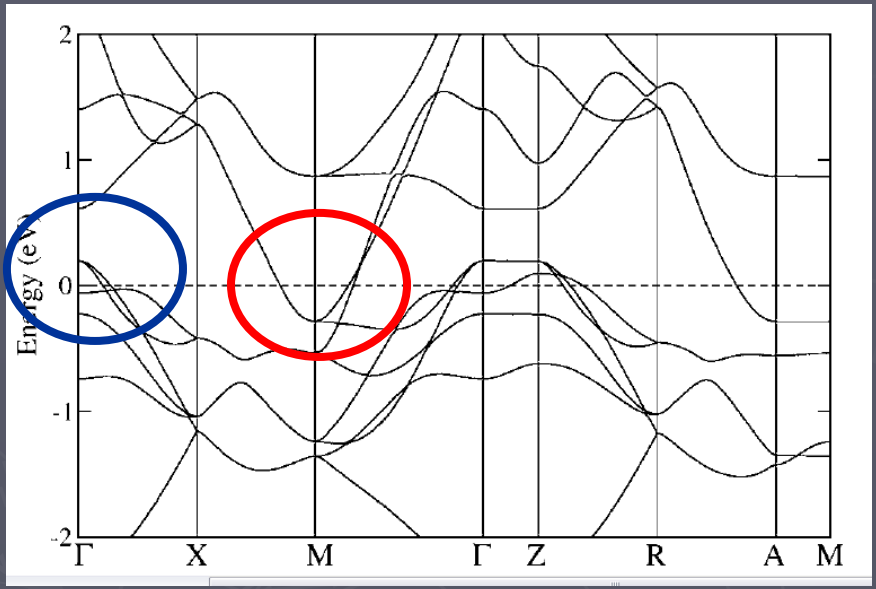
T_c=8K

Hsu et al
arXiv:0807.2369

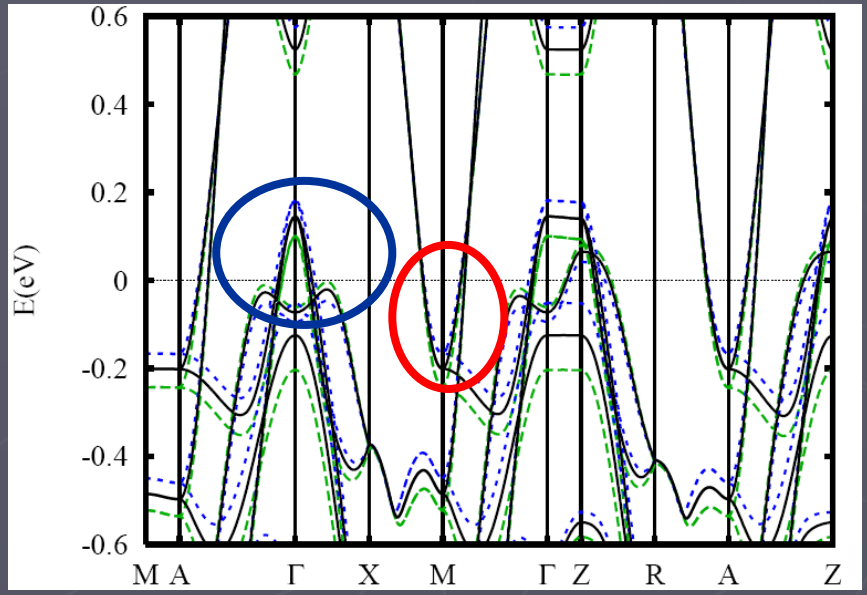
No arsenic ☺!

Electronic structure calculations

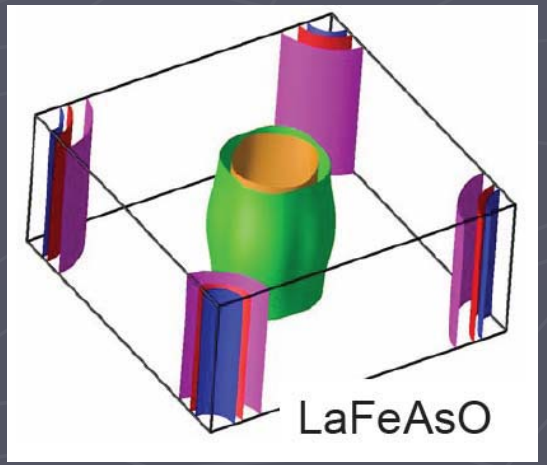
LOFP Lebegue 2007 (T_c=6K)



LOFA Singh & Du 2008 (T_c=26K)



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

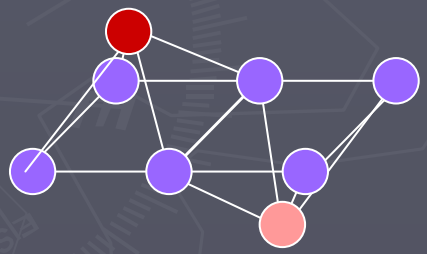


2D!

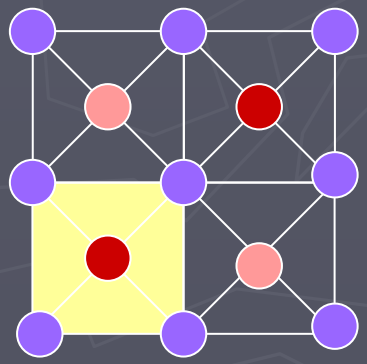
Understanding electronic structure

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

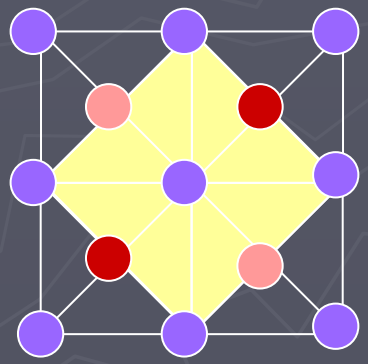
Real unit cell consists of 2 Fe and 2 As atoms, but due to the high degeneracy of the two As positions it is convenient to look at an effective unit cell with only 1 Fe and 1 As atom



Fe-Fe cell
„effective“ unit cell



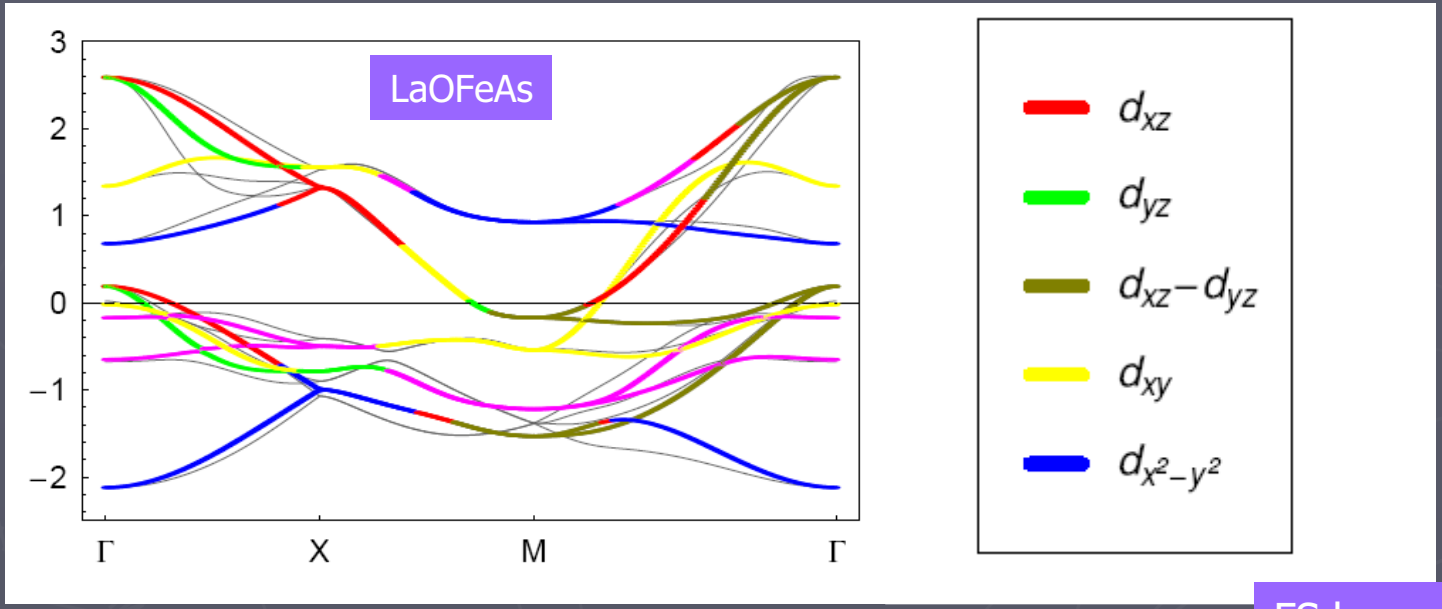
Fe-As-Fe cell
„real“ unit cell



Band structure – Five band model

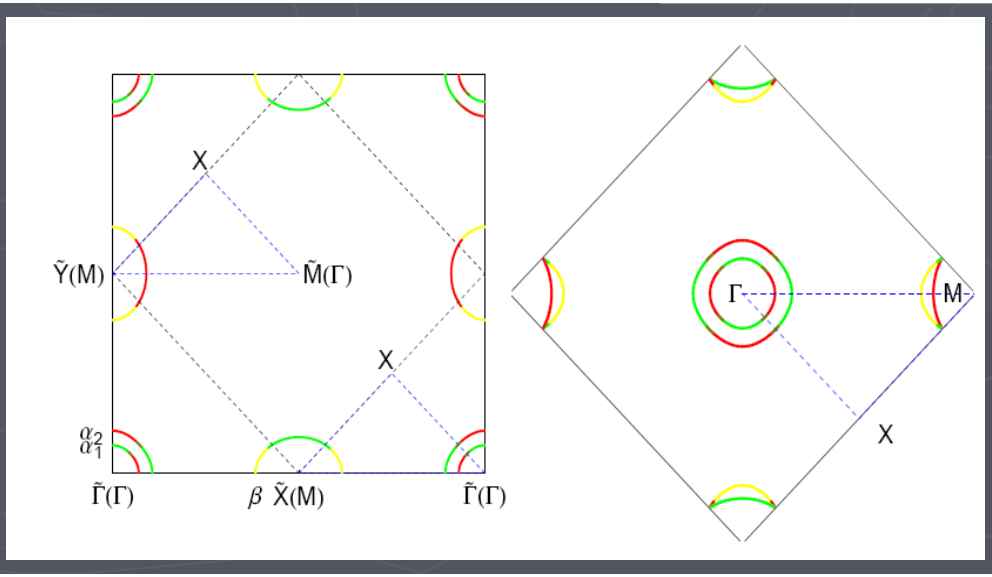
Graser et al. NJP 2009

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



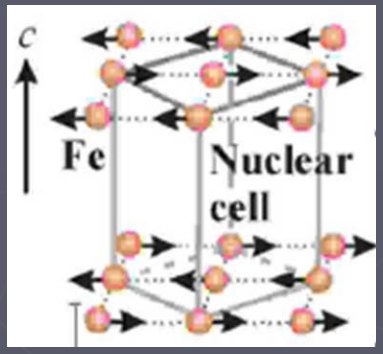
FS has multiple orbital character!

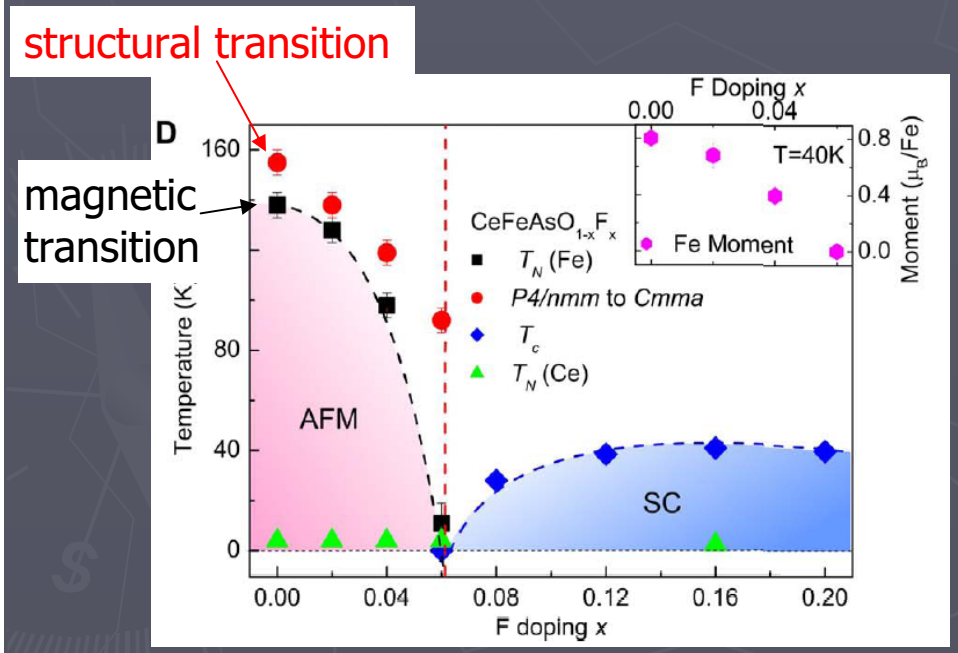
unfolded (1-Fe)



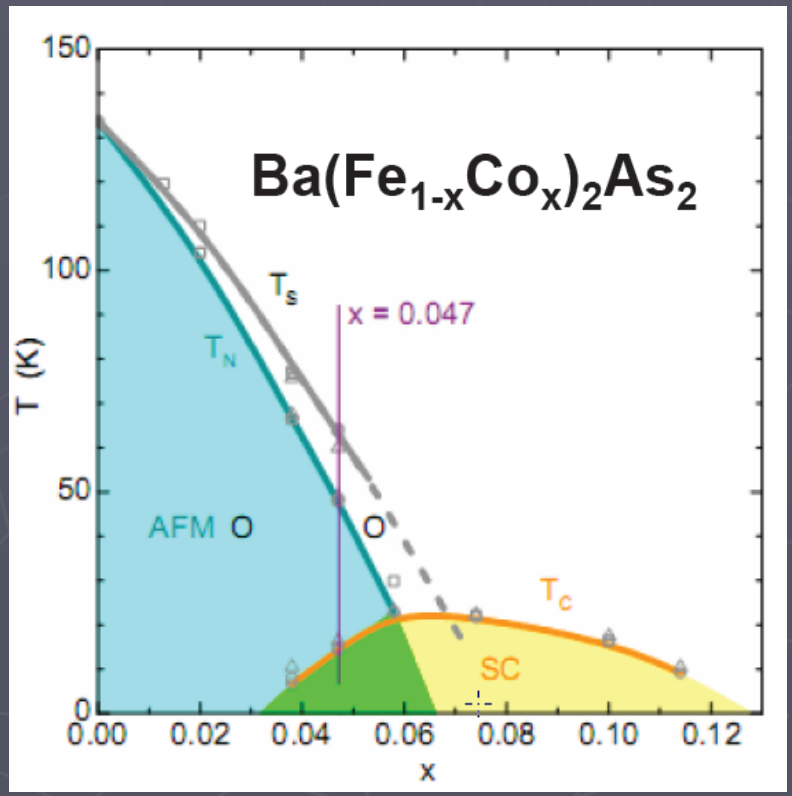
folded (2-Fe)

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





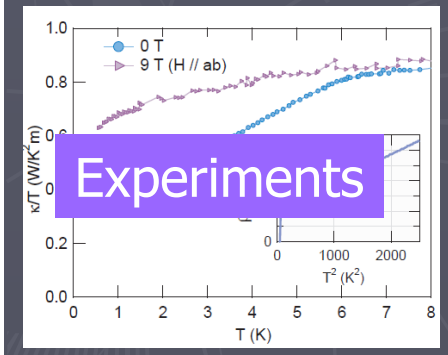
Zhao et al Nat. Mat. 2008

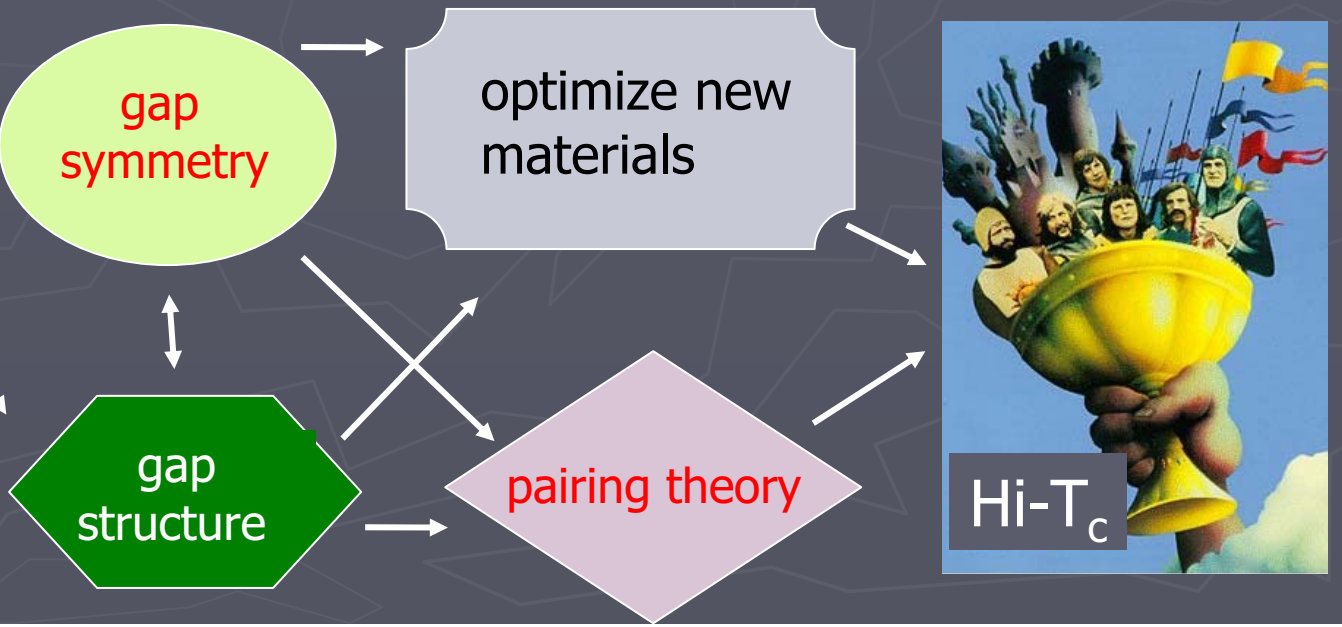


D.K. Pratt et al, aXv 0903.2833

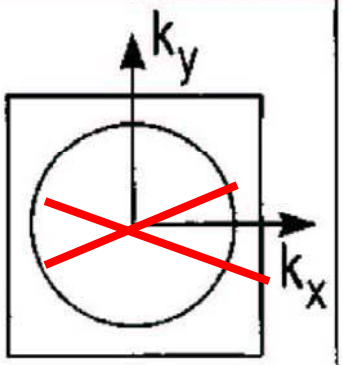
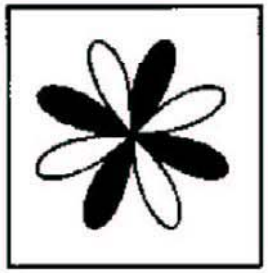
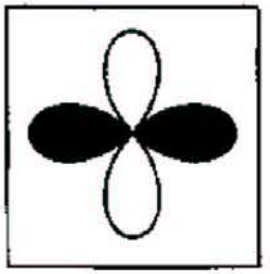
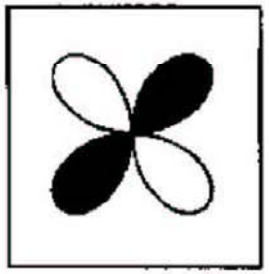
Controversy: symmetry of order parameter?

- 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, thermal conductivity on some samples $\Rightarrow$ nodeless or 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
- Hope:



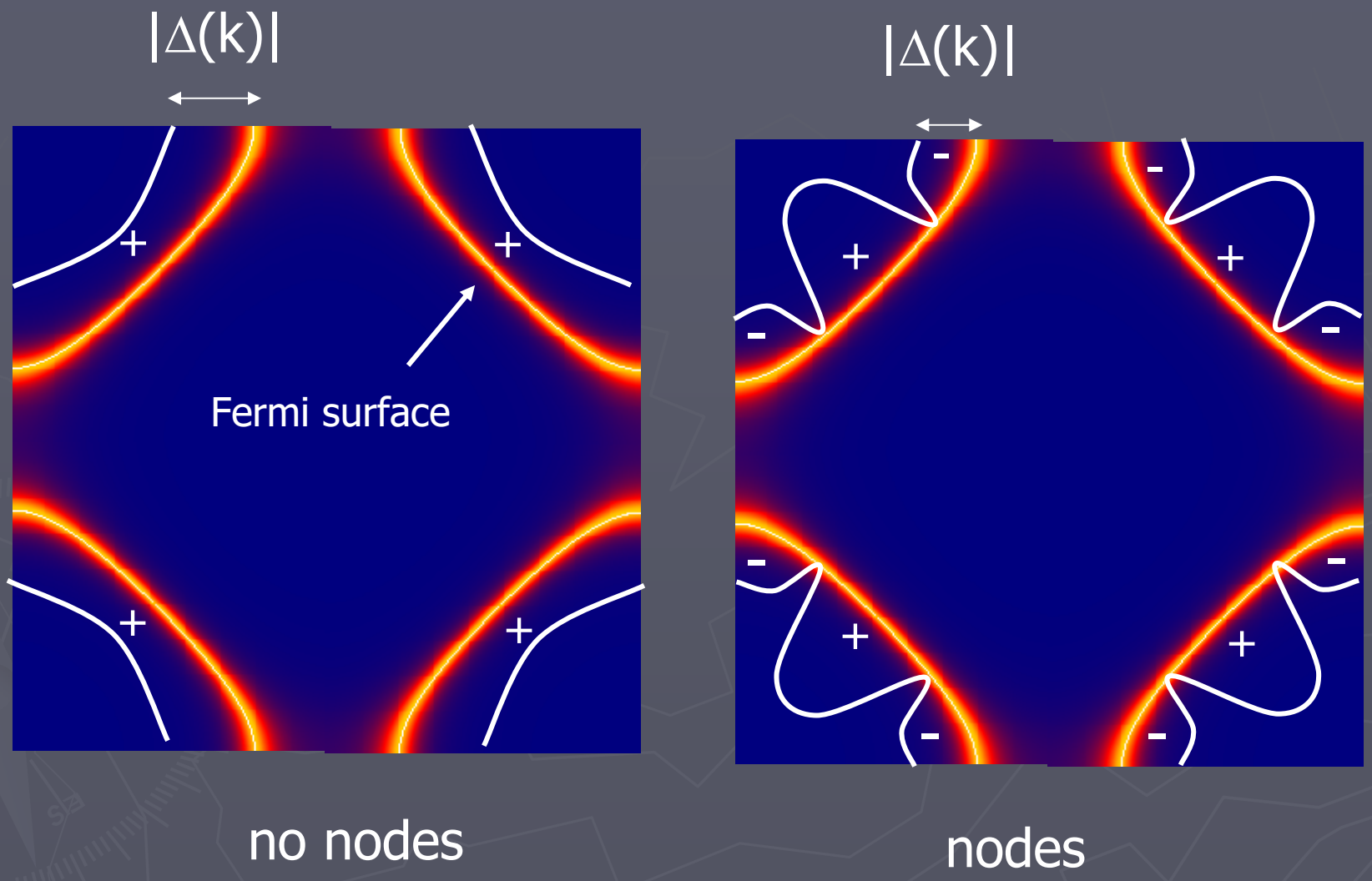


Unconventional superconductors (1-band)

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??

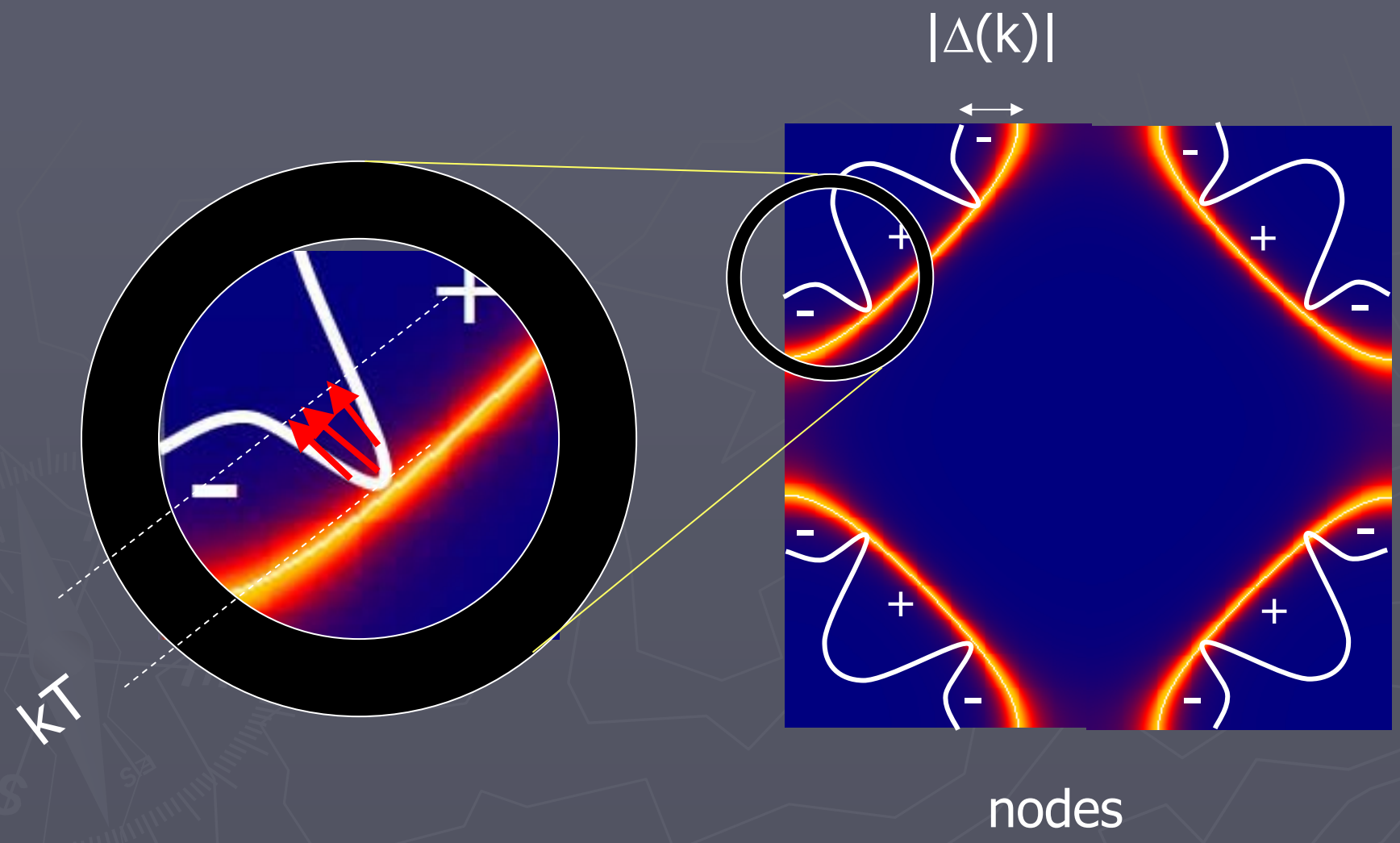
Order parameter $\Delta(k)$ shape in A_{1g} representations—1 band



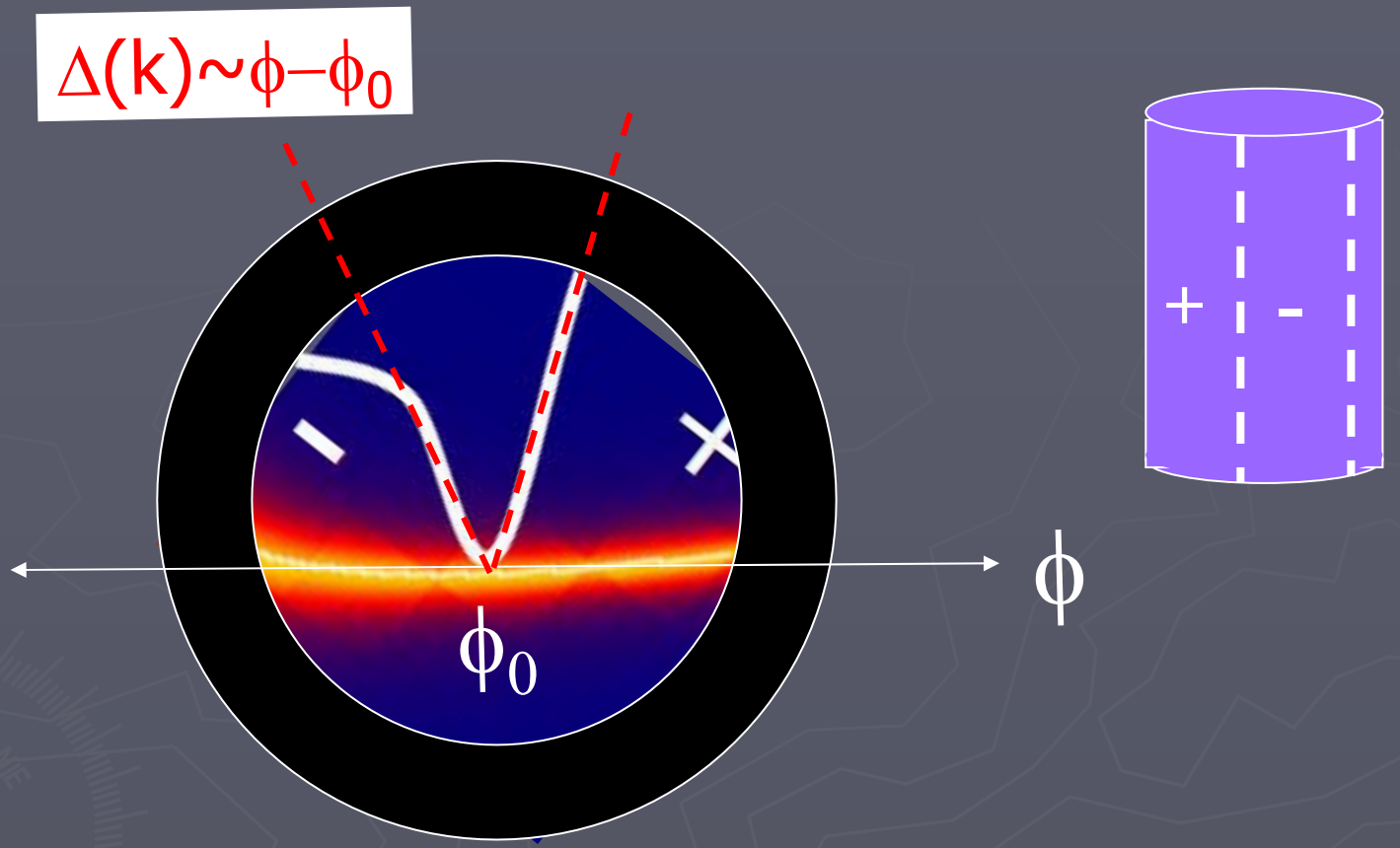
no nodes

nodes

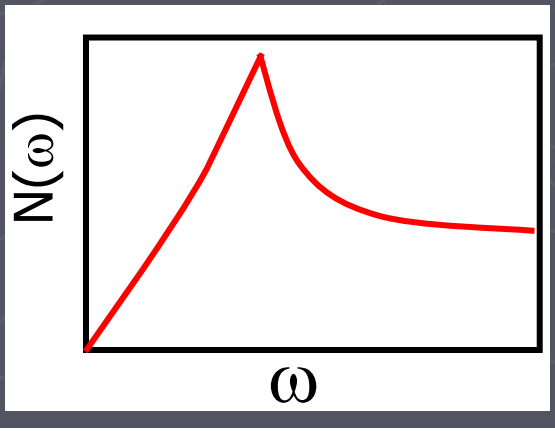
Nodal excitations dominate low T properties



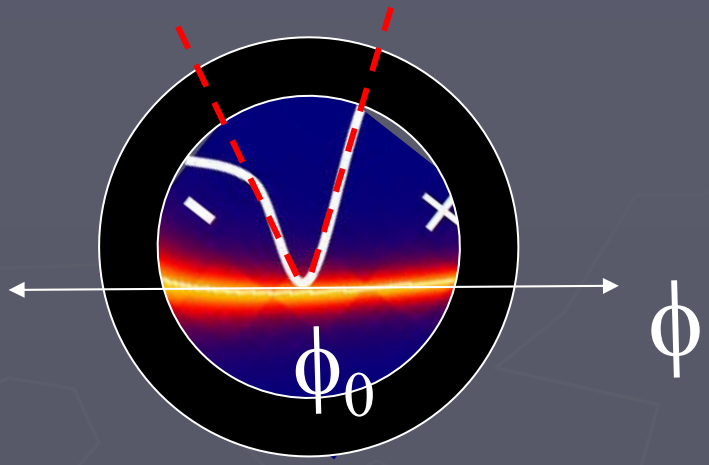
Linear DOS from *line* nodes



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



Example: T^2 specific heat from line nodes



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

excitations

energy/ excitation

Estimate for energy of free Fermi gas:

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

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

Estimate for energy of d-wave SC:

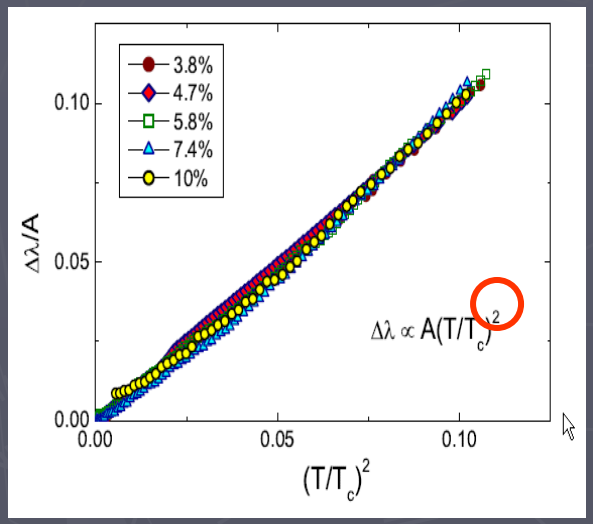
$$E = \int d\omega\, \omega N(\omega) f(\omega) \simeq N_0 \int d\omega \left(\frac{\omega}{\Delta_0}\right) \omega f(\omega) \sim \left(\frac{T^2}{\Delta_0 E_F}\right) \cdot T \sim \frac{T^2}{E_F}$$

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

Penetration depth experiments

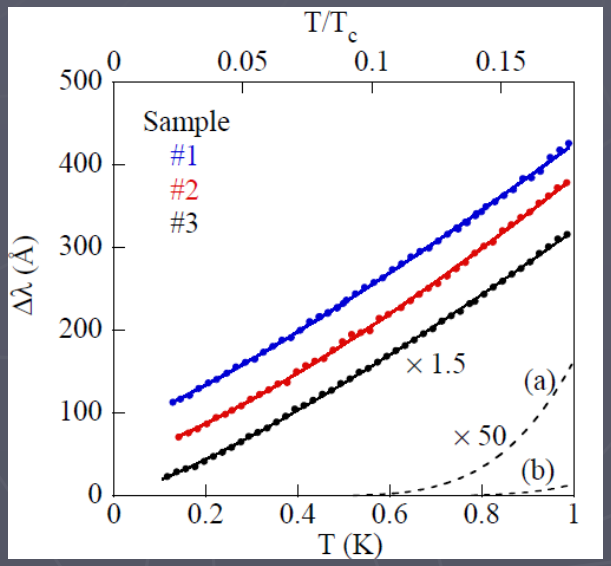
Gordon et al 2008

$Ba_{1-x}Co_xFe_2As_2$ $T_{c,max}$=38K



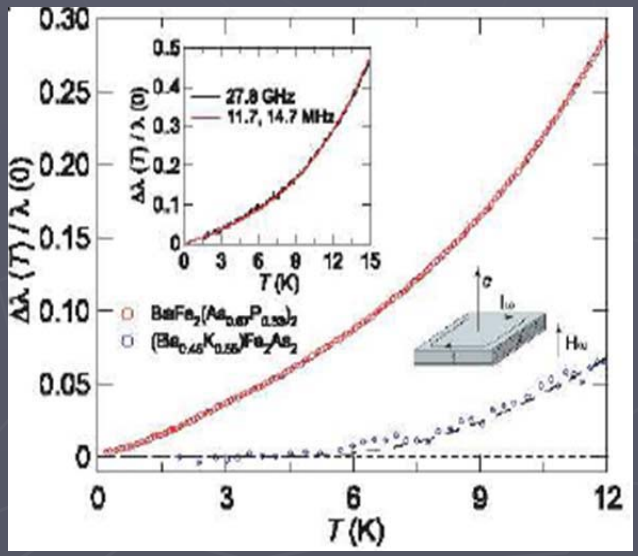
Fletcher et al 2008

LaFePO T_c=6K



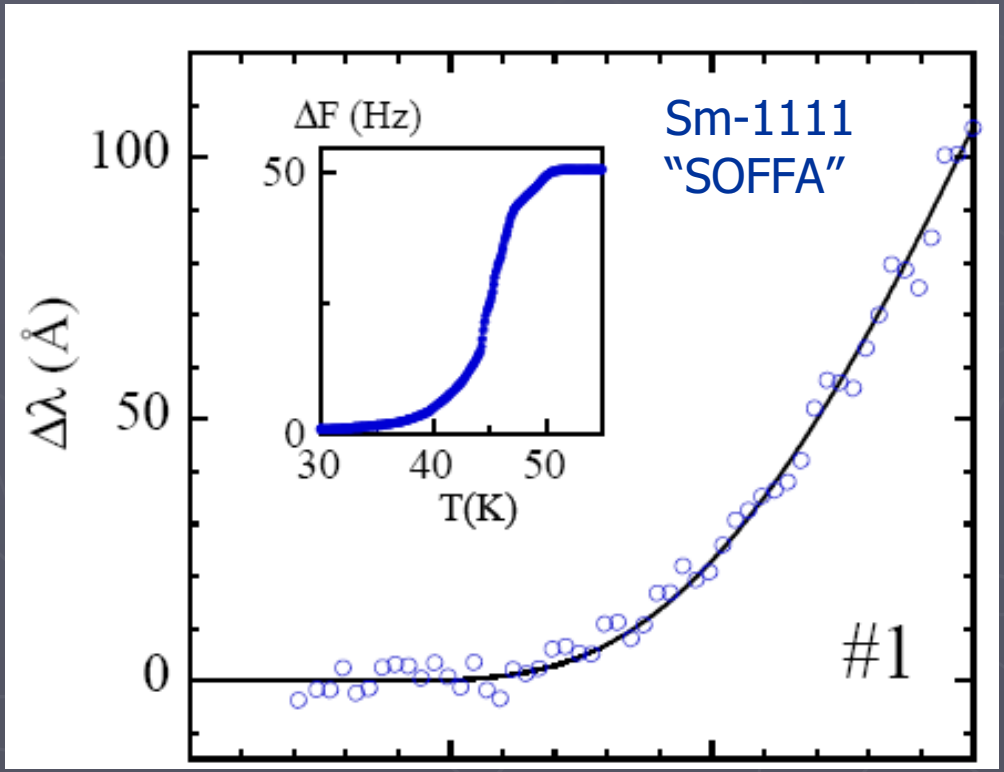
Hashimoto et al 2009

$BaFe_2(As_{1-x}P_x)_2$ $T_{c,max}$=30K



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

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



Malone et al Phys. Rev. B 2009

Caution: magnetism of rare earth ions

Literature on pnictides penetration depth measurement (single cystals)

	Sample (single crystal)	1 full gap	$\lambda_{ab}^2(T)/\lambda_{ab}^2(0)$	$\Delta\lambda_{ab}$		method	group	reference
			2 full gaps	T: nodal	T^2			
1111	$SmFeAsO_{0.8}F_{0.2}$	✖	✔	✖	-	RF oscillator	Bristol	PRB 79, 140501
	$PrFeAsO_{1-y}$	✖	✔	✖	-	microwave	Kyoto	PRL 102, 017002
	$LaFeAsO_{0.9}F_{0.1}$ $NdFeAsO_{0.9}F_{0.1}$	✖	?	✖	✔	RF oscillator	Ames	PRL 102, 247002
P-based	LaFePO	✖	✖	✔	✖	RF oscillator	Bristol	PRL 102, 147001
	LaFePO	✖	✖	✔	✖	scanning SQUID	Stanford	PRL 103, 127003
122	$BaFe_2(As_{1-x}P_x)_2$	✖	✖	✔	✖	microwave	Kyoto	arXiv 0907.4399
	$(Ba_{1-x}K_x)Fe_2As_2$	✖	✔	✖	-	microwave	Kyoto	PRL 102, 207001
	$(Ba_{1-x}K_x)Fe_2As_2$	✖	?	✖	✔	RF oscillator	Ames	PRB 80, 020501
	$Ba(Fe_{1-x}Co_x)_2As_2$	✖	?	✖	✔	RF oscillator	Ames	PRL 102, 127004 PRB 79, 100506

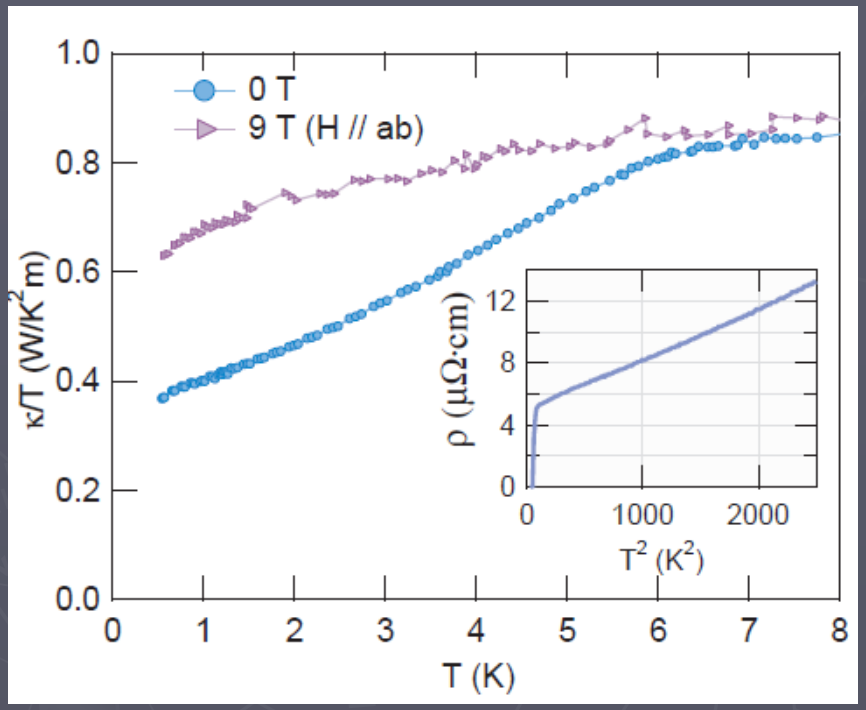
✖ : ruled out
✔: preferred explanation by authors
? : not ruled out
- : no comment

Thanks: KA Moler

Thermal conductivity (H=0)

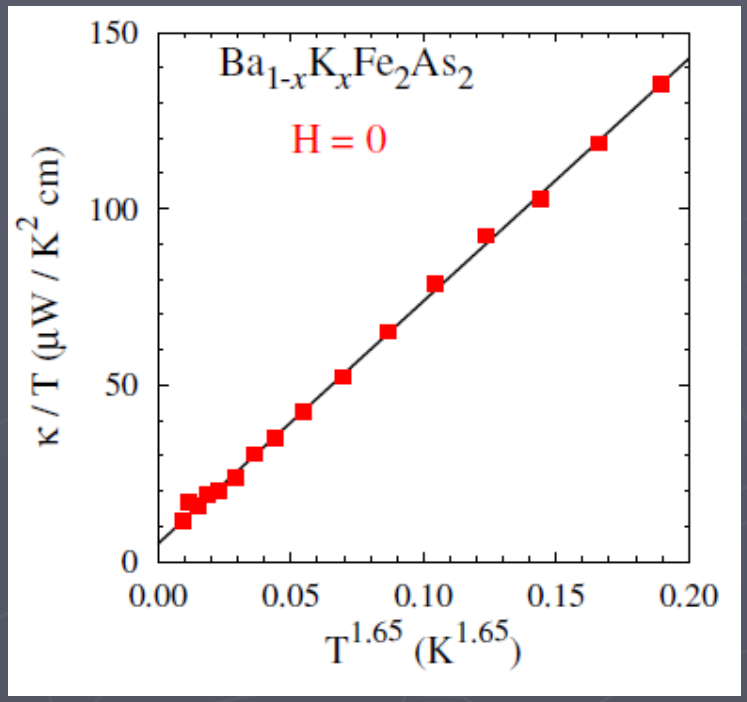
(bulk probe, lowest temperatures thus far)

LaFePO: Yamashita et al aXv:0906.0622



Big linear T term

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



Tiny or zero linear T term

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

questions

- What controls whether Fe-based material is nodal or gapped superconductor?
- Role of disorder?
- Can we identify order parameter structure in a given material?
- What is role of 3D Fermi surfaces in some pnictides?
- How can we make a theory with predictive power to guide search for higher T_c, more isotropic 3D superconductors?

Spin fluctutation pairing theories in Fe-pnictides

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

Early calculations of spin-fluctuation pairing :

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

Recent studies of nodal-gapped transition:

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

Graser et al 2008, 2009; Kemper et al 2010 calculation starting point:

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

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

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

most general 2-body Hamiltonian with intrasite interactions only!

Spin fluctuation theories of pairing

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

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

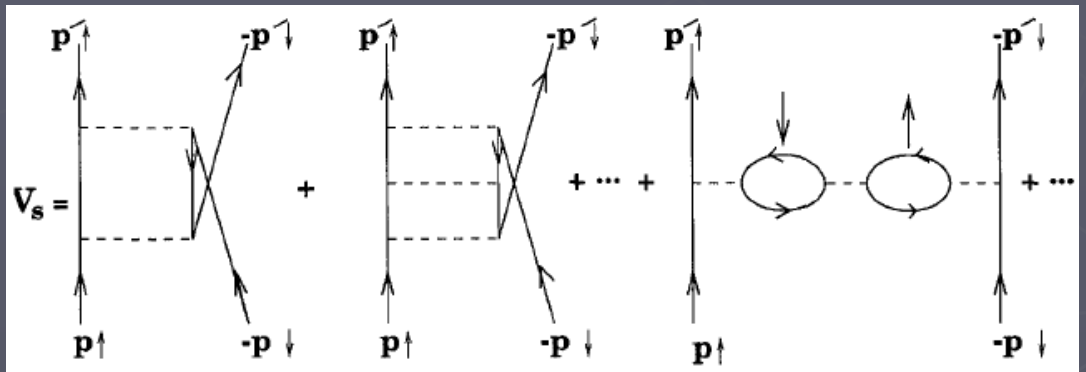


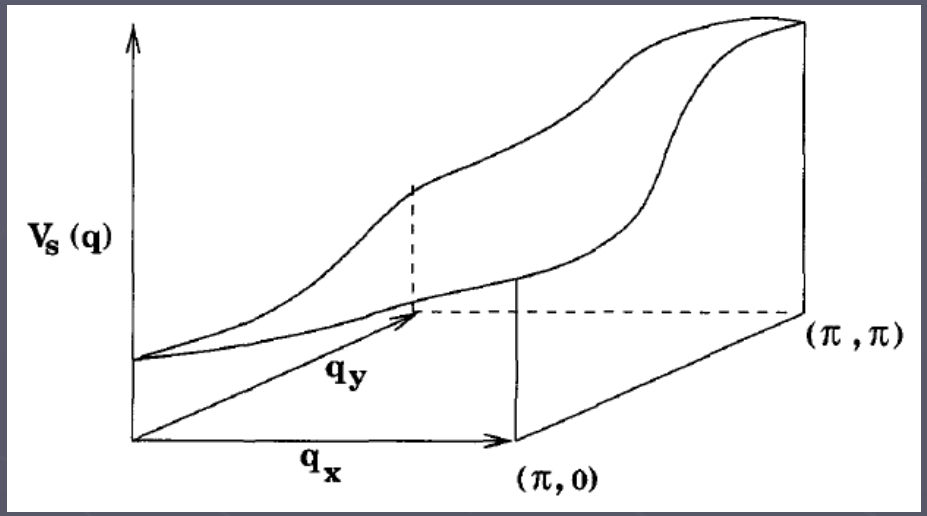
Fig. 1. Diagrams representing the Berk-Schrieffer [1] spin-fluctuation mediated pairing interaction in the singlet channel.

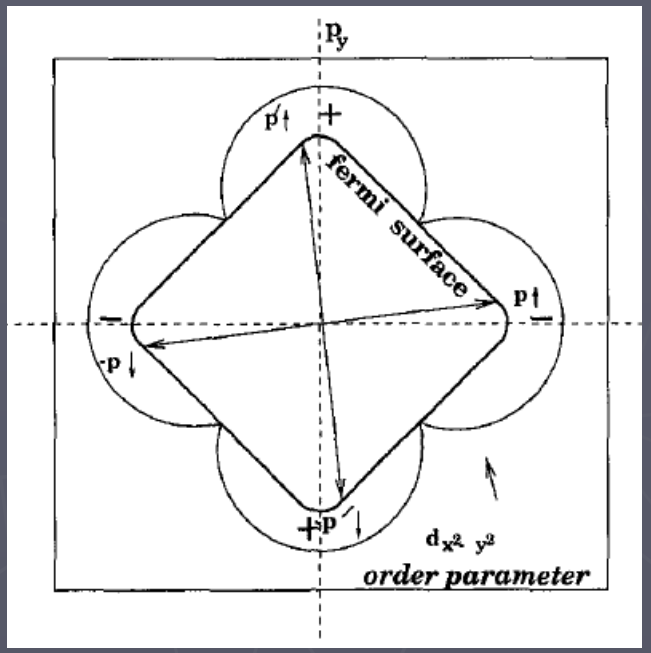
$$V_s(q,\omega) \cong \frac{3}{2}\,\frac{\bar{U}^2\chi_0(q,\omega)}{1-\bar{U}\chi_0(q,\omega)}$$

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

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

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



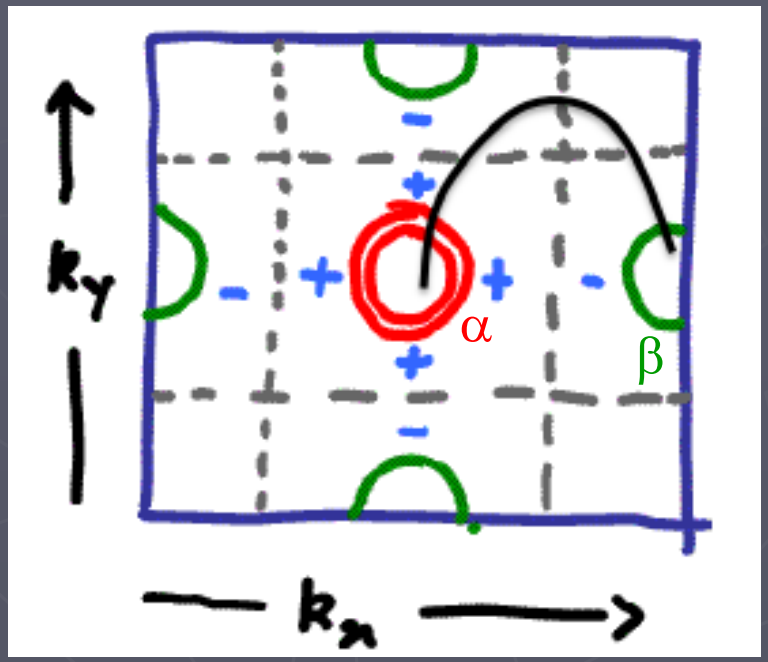


$$\Delta_p = -\sum_{p'} \frac{V(p-p')\Delta_{p'}}{2E_{p'}}$$

d-wave takes advantage of peak in spin fluct. 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



also:

Seo et al. 2008

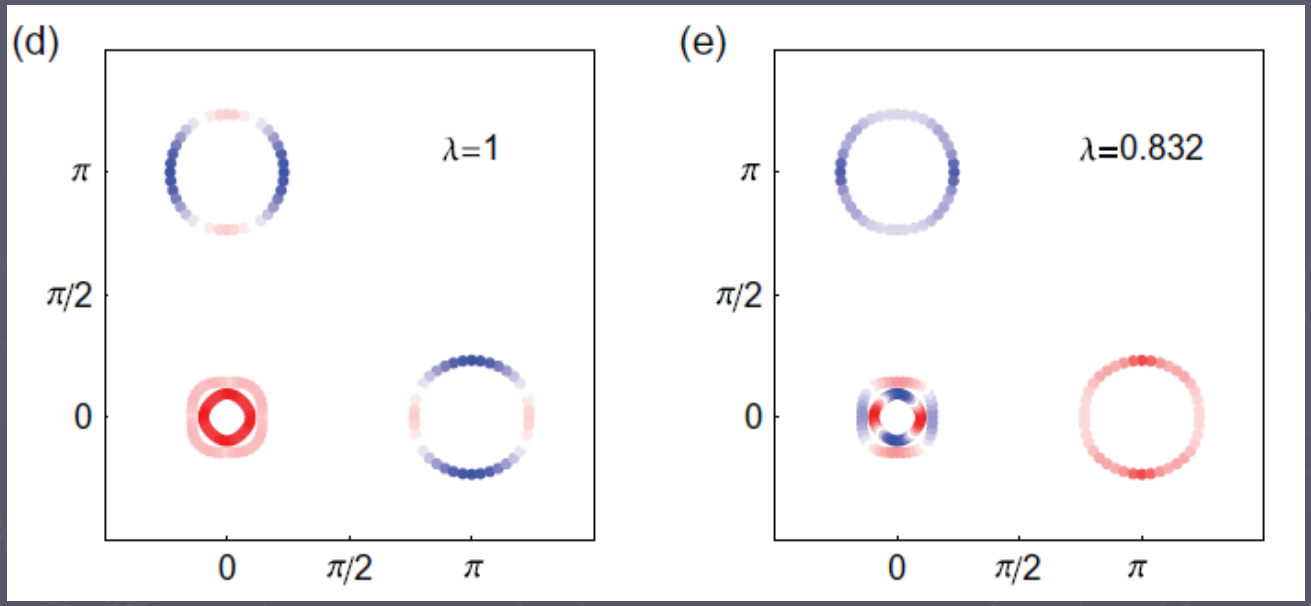
$$\Delta_p = -\sum_{p'} \frac{V(p-p')\Delta_{p'}}{2E_{p'}}$$

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

Graser et al 2009: pairing functions for $U \rightarrow U_c$ display gap nodes

Also: Kuroki et al '08, '09, Ikeda et al '09, '10, …

"anisotropic extended-s"-wave nearby: $d_{x^2-y^2}$

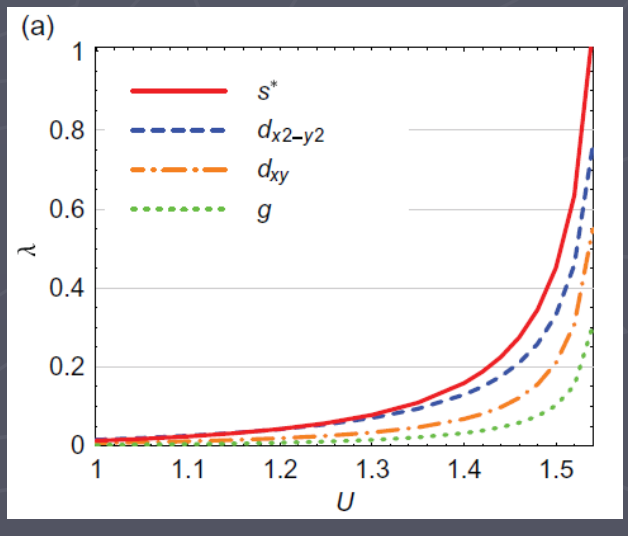


(x=0.125 e-doped) U=1.54 J=0

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

a) Can different FeAs materials have different symmetries?

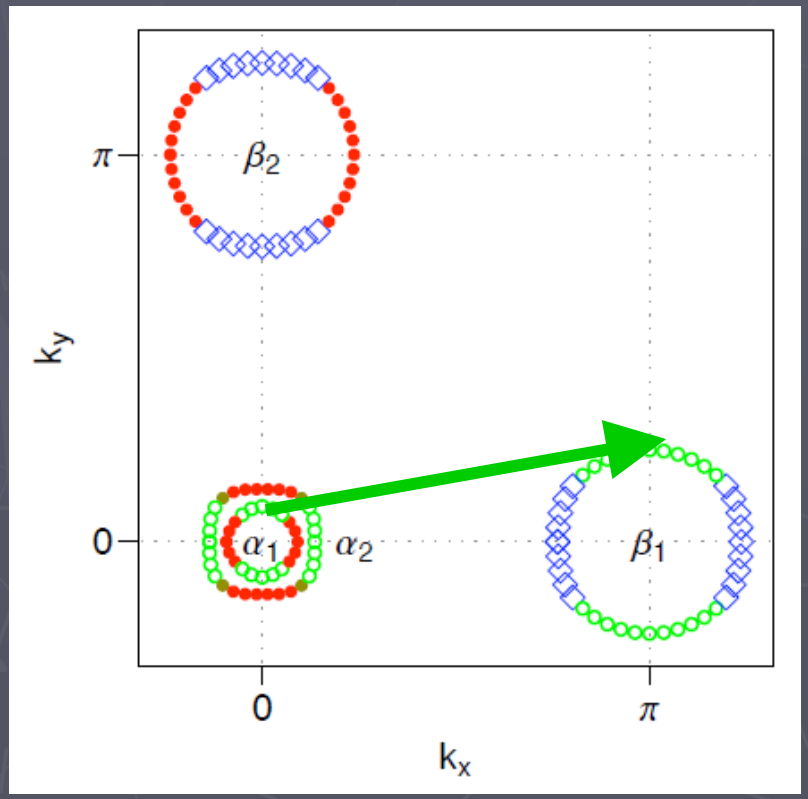
b) More likely: s-wave *symmetry*, differing gap *structures* for different materials

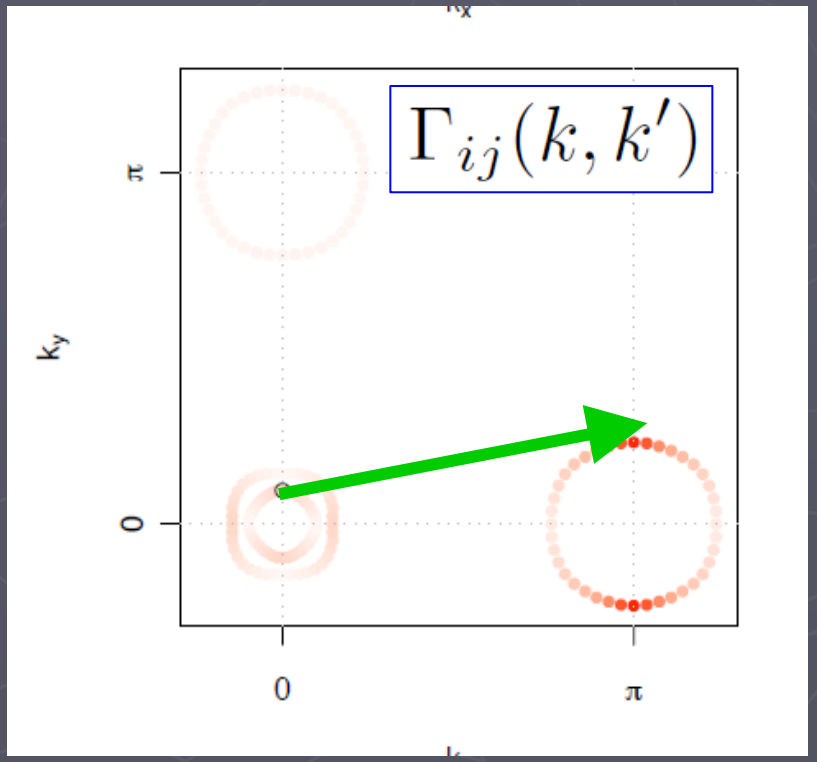


What is the origin of the gap anisotropy [Maier et al PRB 09]?

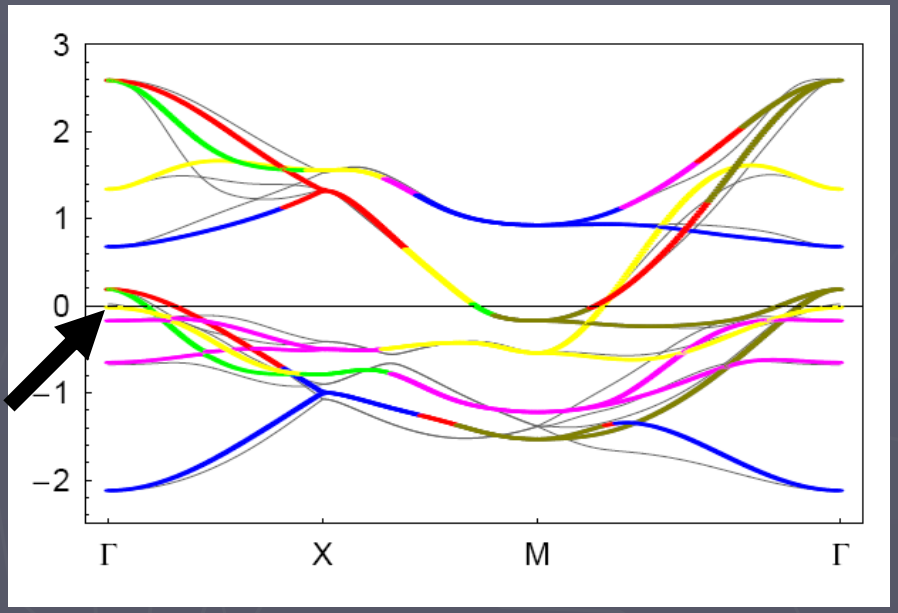
1. **importance of orbital character on Fermi sheets**
2. scattering between β_1 and β_2 sheets
3. intraband coulomb repulsion

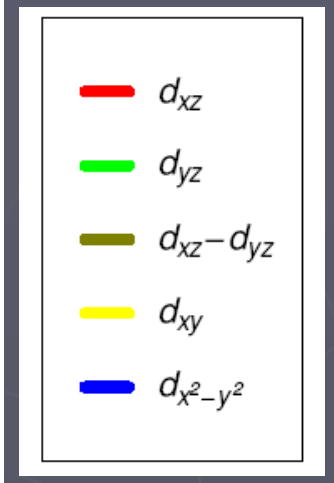
See also: Chubukov et al 2009, Thomale et al 2009 (band picture), Thomale et al 2010, Kemper et al 2010

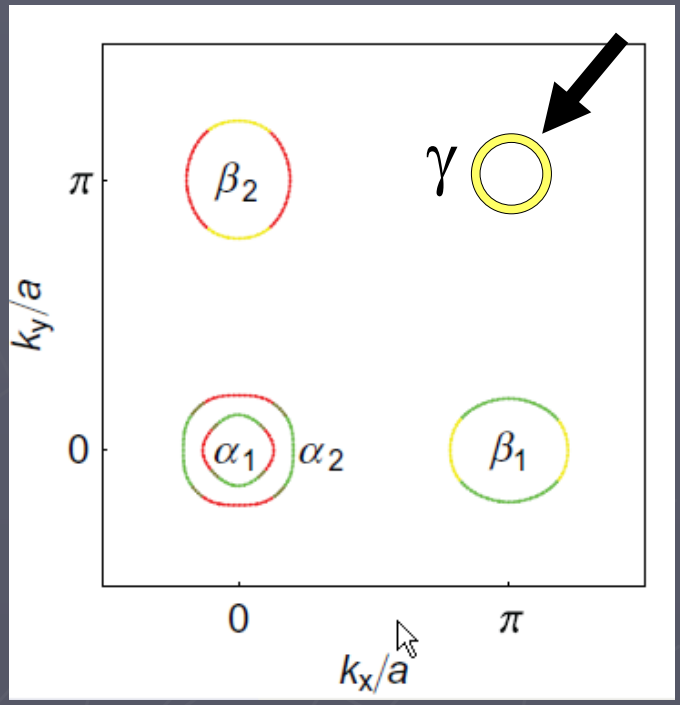




Importance of γ (π,π) pocket







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

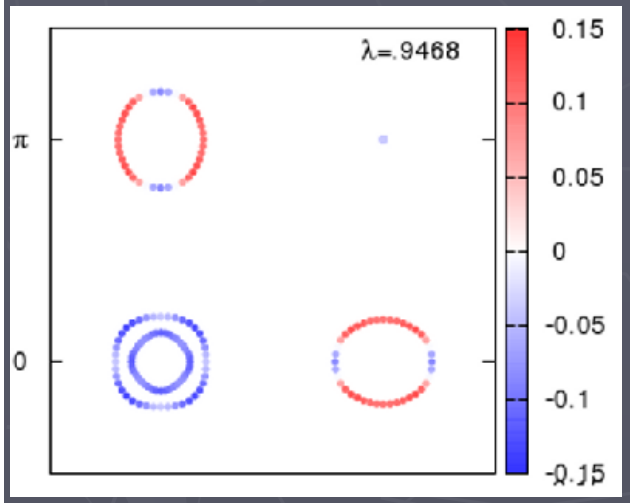
Presence of pocket can be controlled by doping AND by tuning the height of As above the Fe plane

Nodal-gapped transition as function of hole doping

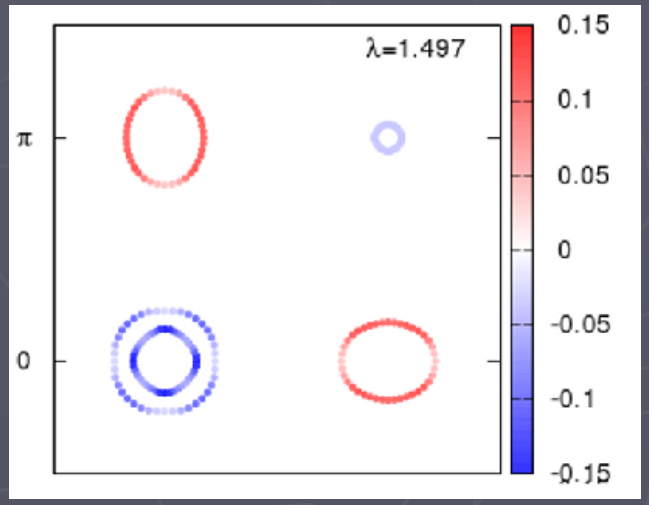
RPA: Kemper et al. NJP 2010

LaOFeAs Fermi surface

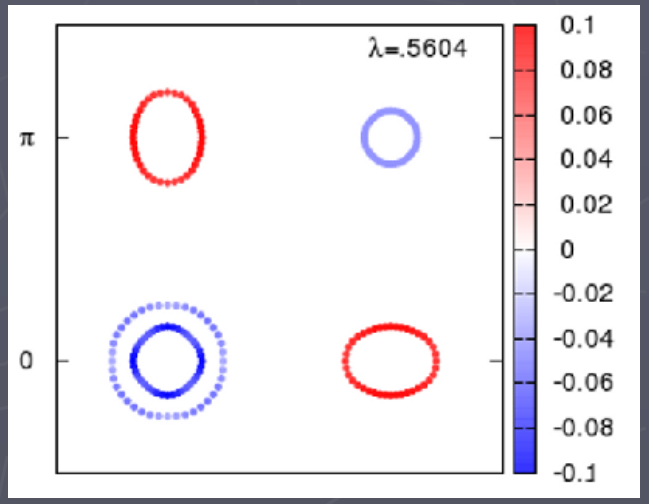
$\bar{U}$=1.2 $\bar{J}$=0.3



n=6.030

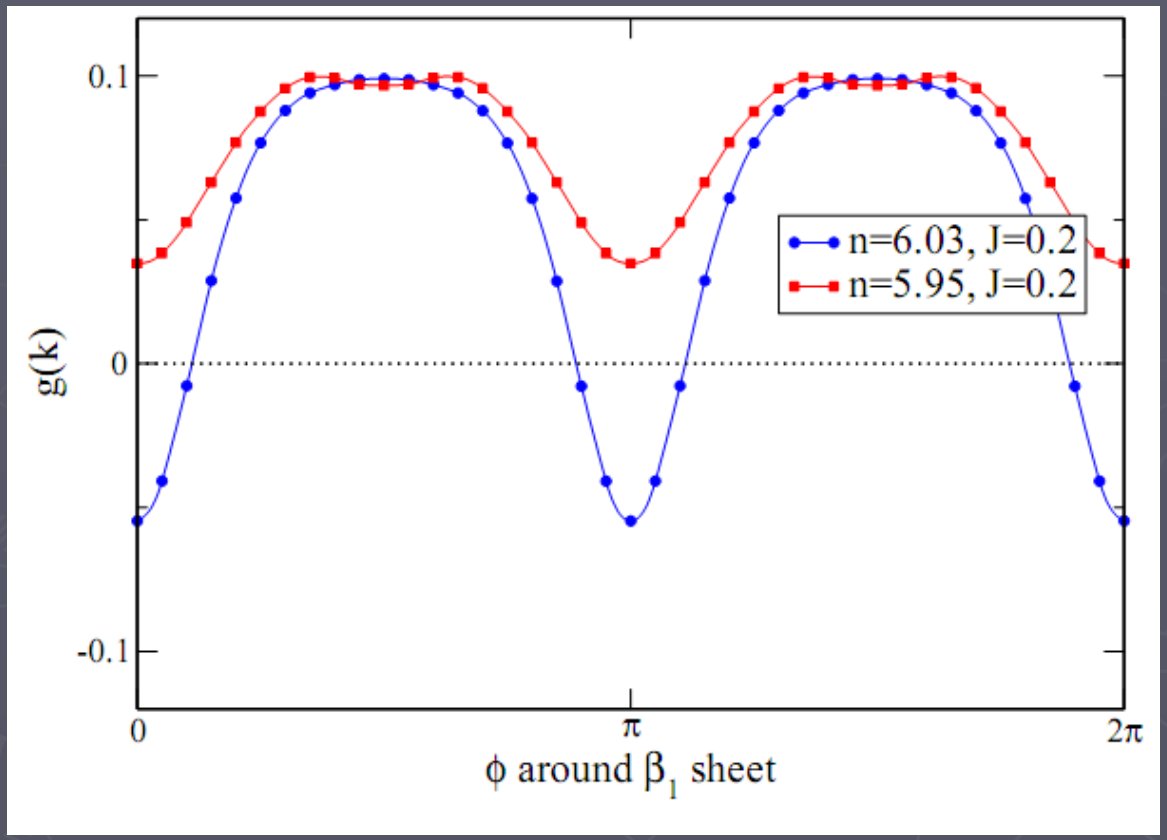


n=5.987



n=5.935

Close-up on electron sheet



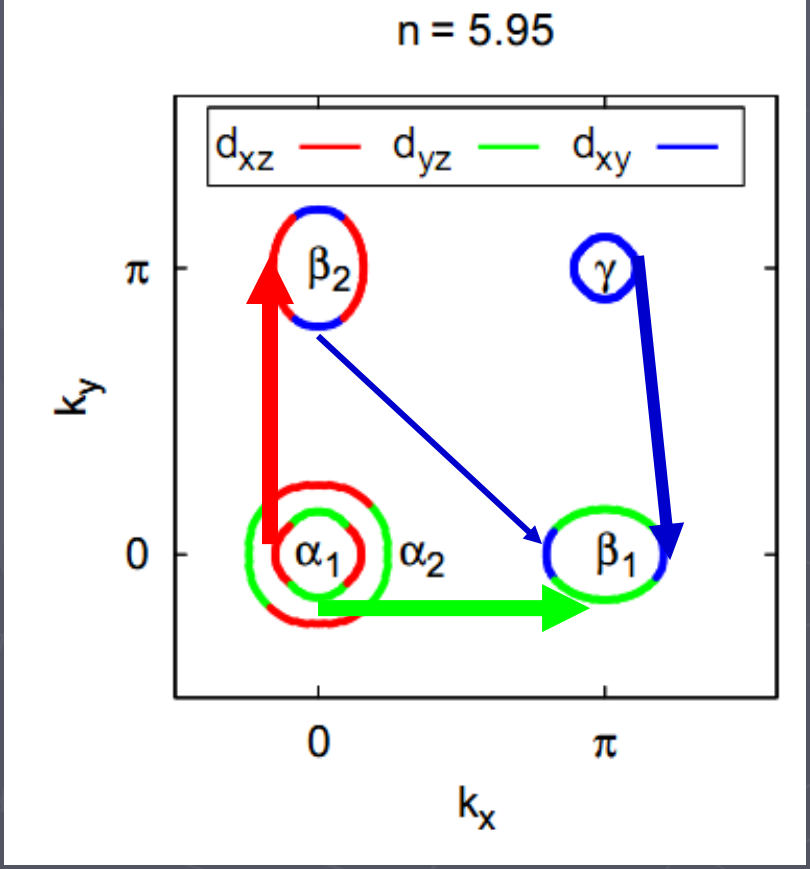
N.B. Need sizeable Hund's rule coupling J to get isotropic $s_{+/-}$ state

This sensitivity to interaction parameters not seen in Wang et al 2010

Orbital decomposition of $\Gamma_{ij}(k,k')$

Kemper et al. NJP 2010

$$\Gamma^{pq}_{st}(k,k',\omega) = \left[\frac{3}{2}U^s\chi_1^{RPA}(k-k',\omega)U^s + \frac{1}{2}U^s - \frac{1}{2}U^c\chi_0^{RPA}(k-k',\omega)U^c + \frac{1}{2}U^c\right]^{tq}_{ps}$$

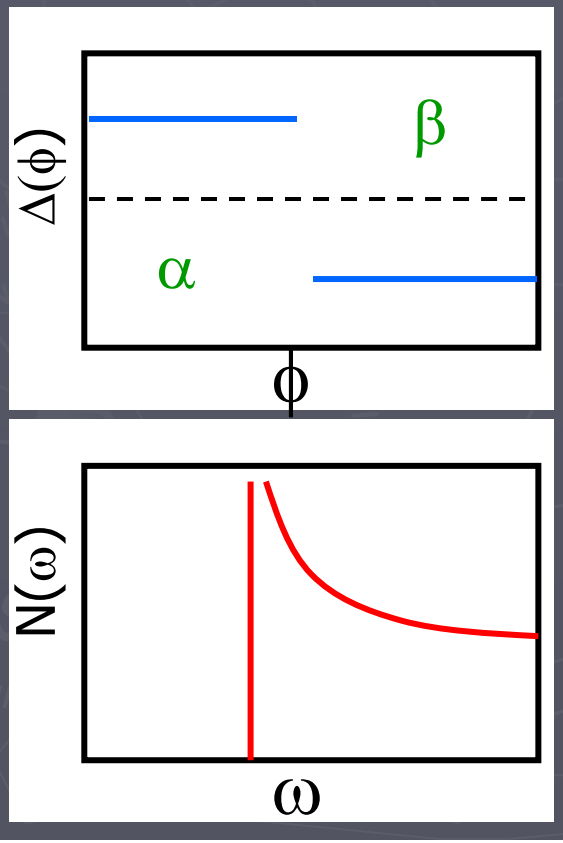


- Large intra-orbital pairing stabilizes $s^{\pm}$ state on xz,yz portions of Fermi surface
- xy parts determined by subdominant intra- and inter-orbital scattering
- γ pocket helps overcome frustration by intraband Coulomb repulsion, β–β scattering

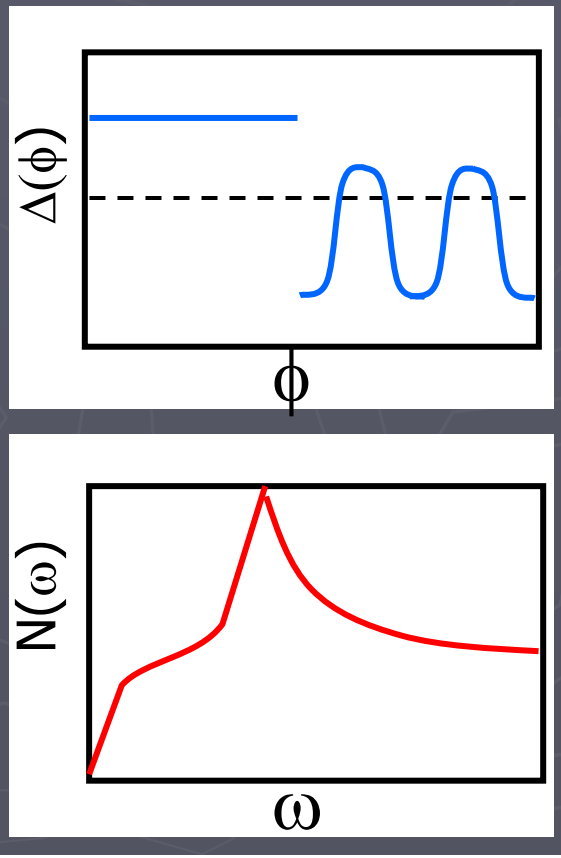
"sensitivity" to small changes in electronic structure, disorder

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

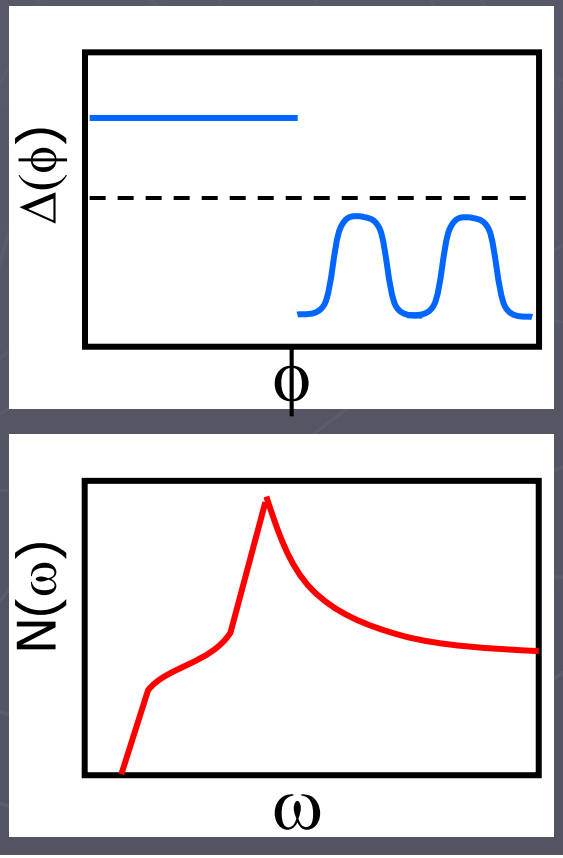
a) isotropic $s_{+/-}$



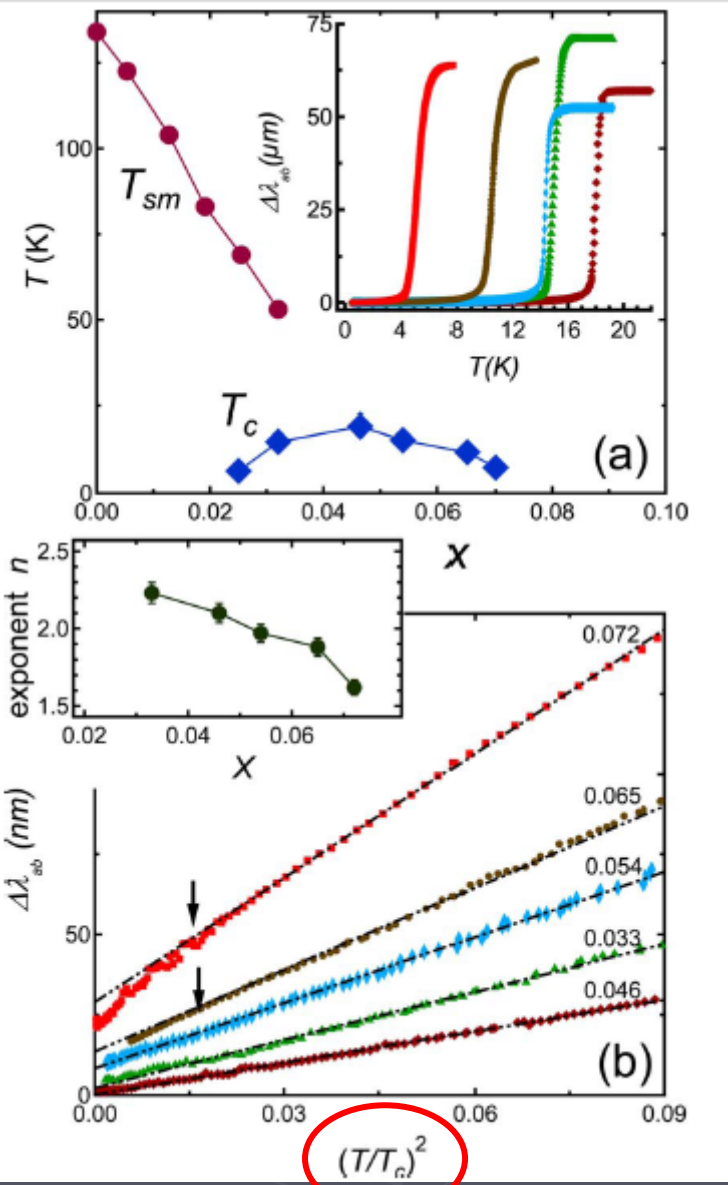
b) nodes



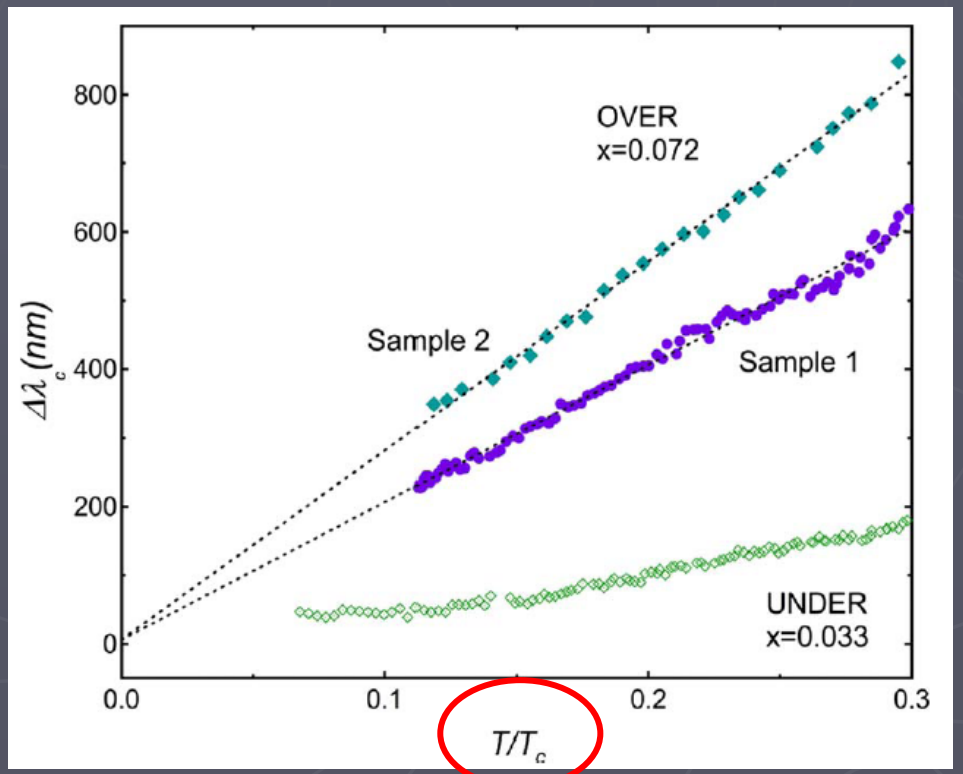
c) deep minima



3D superconductivity in 122 systems



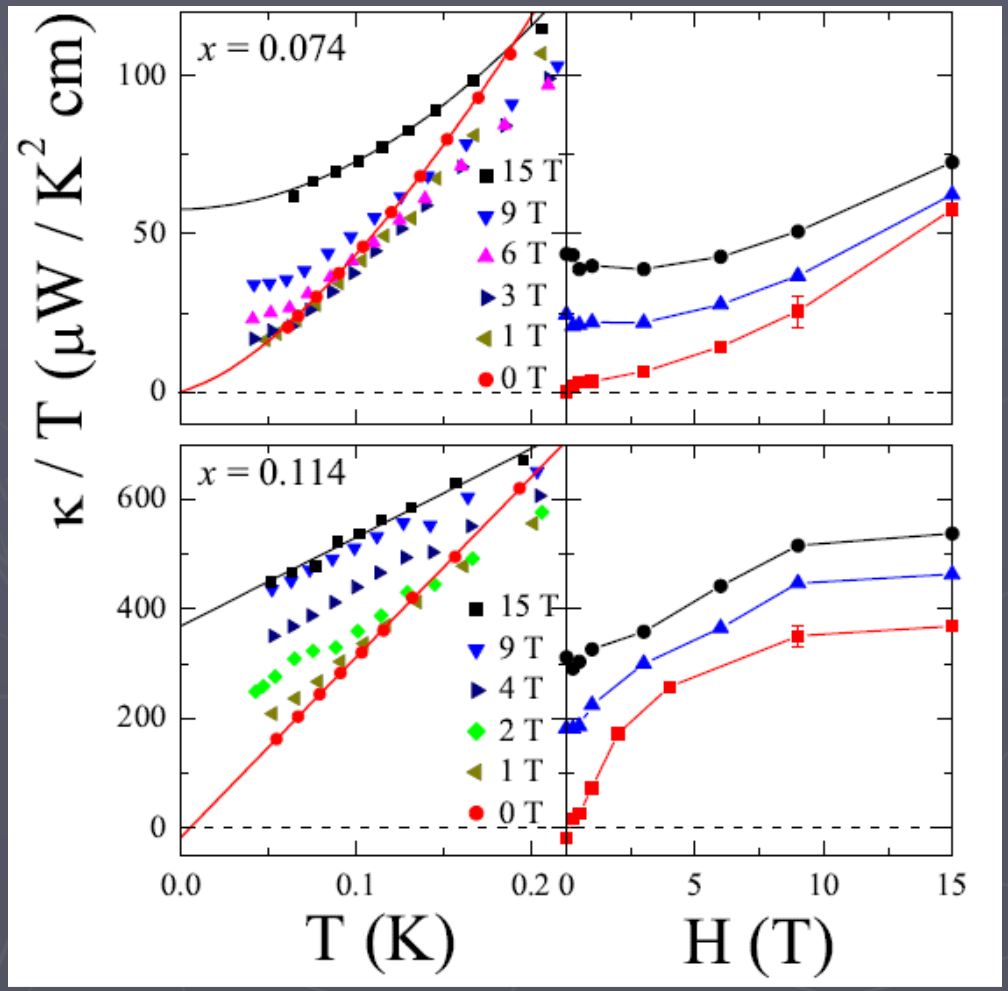
Martin et al 2010



ab- and c-axis responses have different T dependences!

3D superconductivity in 122 systems cont'd: recall: ab plane thermal conductivity

Co-doped Ba-122: Tanatar et al PRB 2009



Absent or tiny linear-T term corresponding to gap nodes!

Yet H-dependence is strong (Volovik effect?)

Mishra et al 2009: deep gap minima on electron sheets

Mishra, Vorontsov, Vekhter and PH 2009: schematic

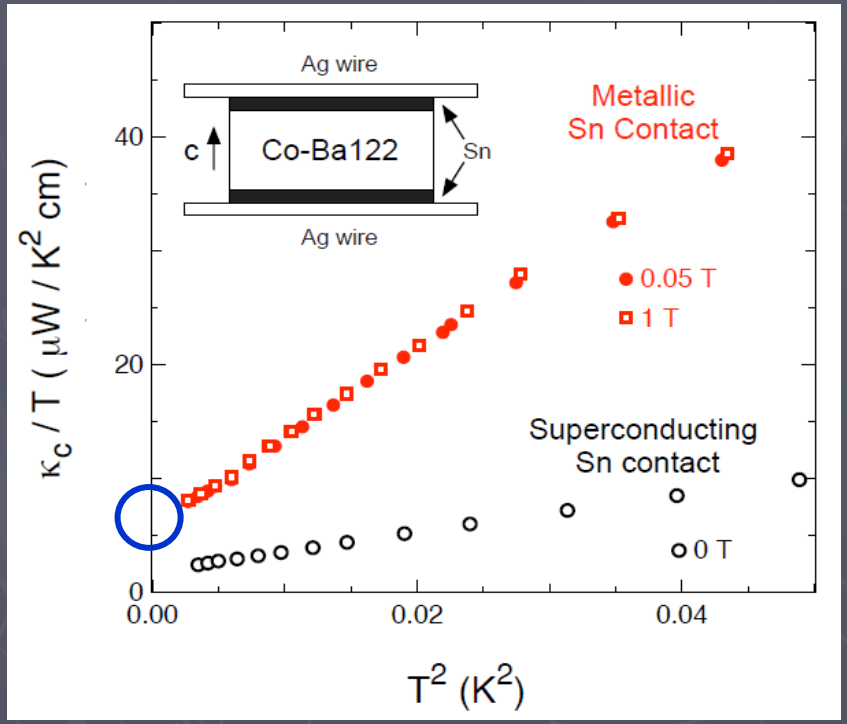
a) isotropic $s_{+/-}$

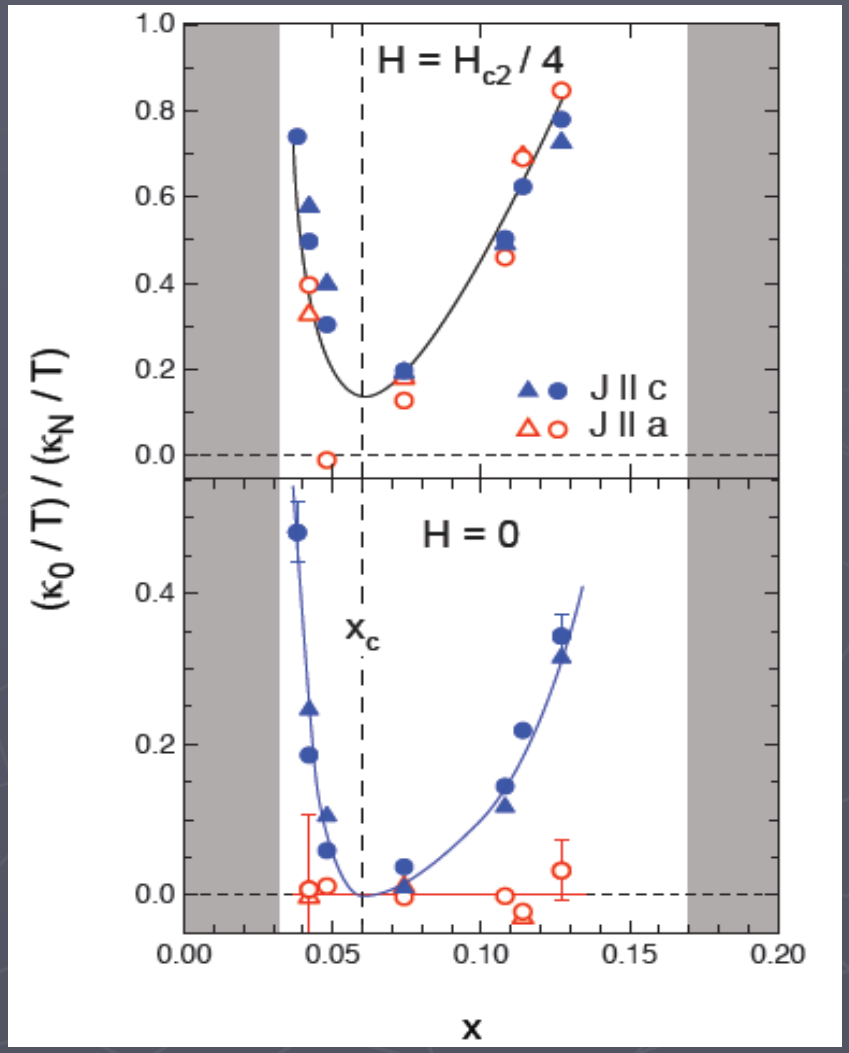
b) nodes

c) deep minima

c-axis transport: thermal conductivity

Reid et al 2010

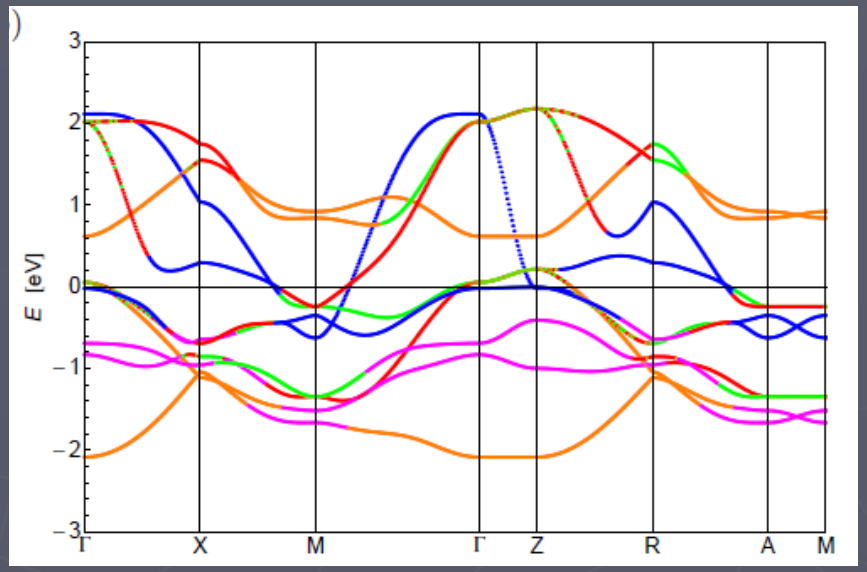




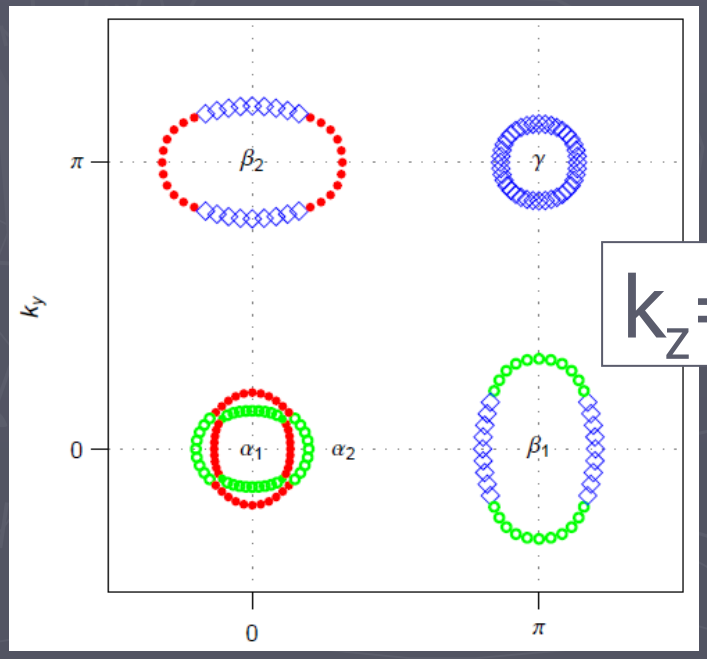
Their conclusion: deep gap minima on cylindridal sheet, nodes on corrugated sheet

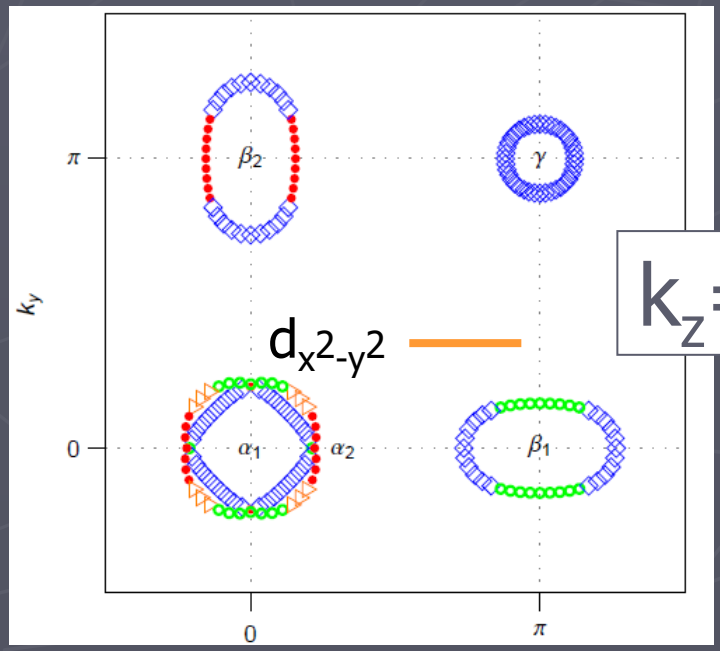
Effects of 3D: Ba-122 band structure

Graser et al PRB 2010
effective tight-binding
band structure for Ba-122



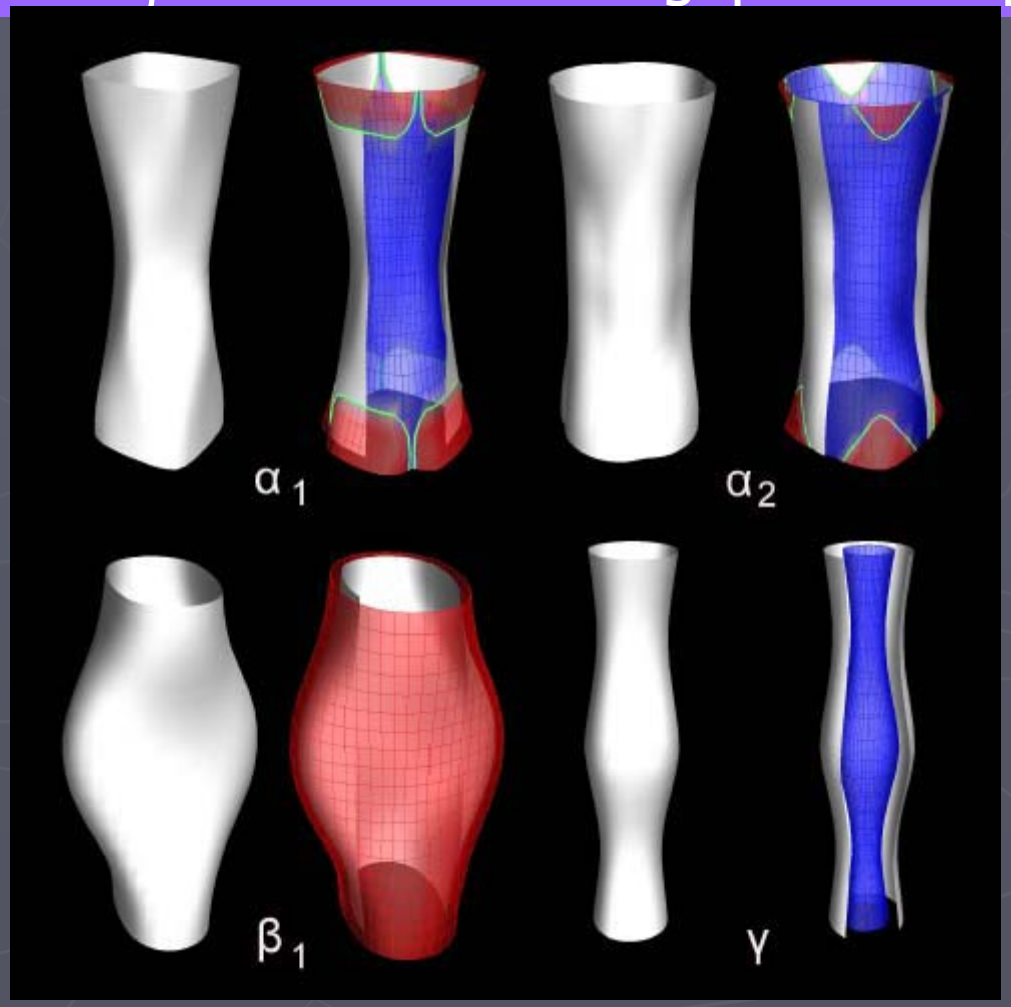
d_{xz} d_{yz} d_{xy}





Effects of 3D: Ba-122 order parameter

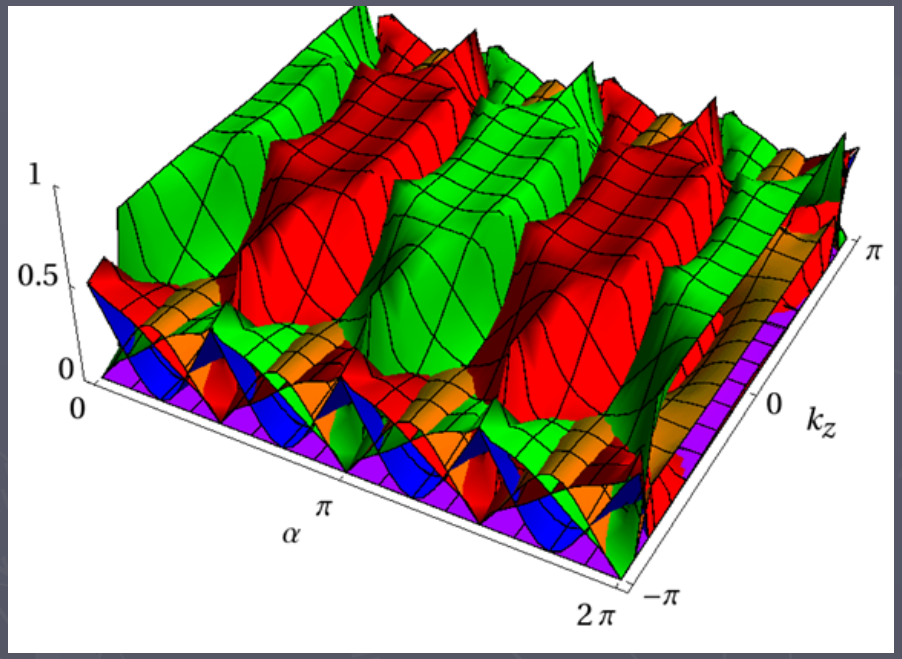
New possibility: nodes can appear on α sheets near *top* of BZ!
(while β sheets have full gap but deep minima)



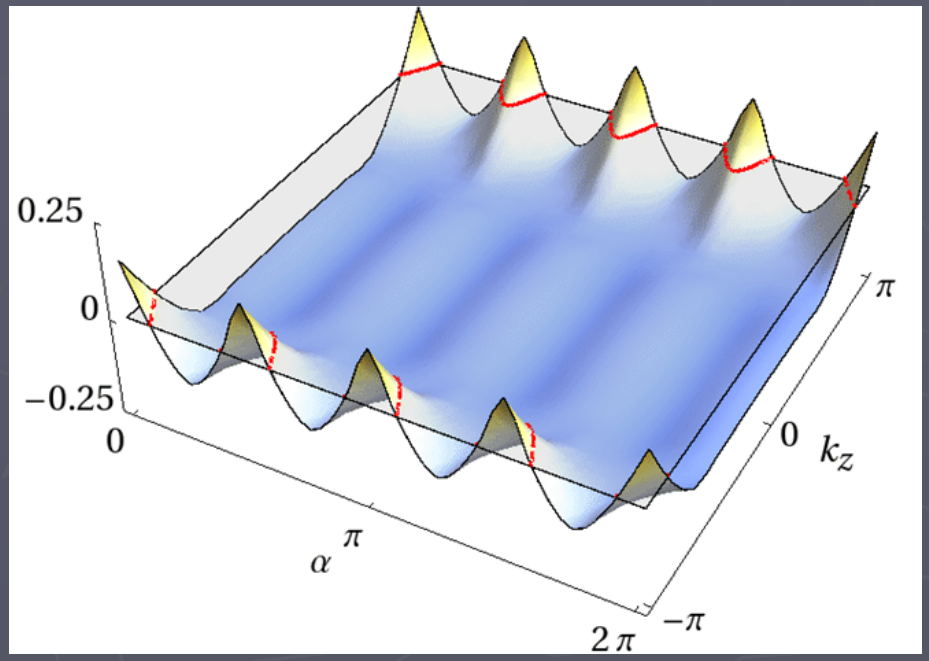
Implications for ab/c-axis pen. depth measurements (Martin et al 2009) and for ARPES

Why are nodes near $k_z=\pi$?

α_2 sheet



Orbital content



Order parameter

Theory of thermal conductivity in multiband systems Mishra et al 2009

$$\frac{\kappa_\alpha}{T} = n\frac{k_B^2 m}{16\pi\hbar d}\sum_i \int_0^\infty \frac{d\omega}{T}\,\frac{\omega^2}{T^2}\,\mathrm{sech}^2\left(\frac{\omega}{2T}\right) \times \left\langle (\mathbf{v}_{Fi}\cdot\hat{\alpha})^2 \frac{1}{Re\sqrt{\tilde{\Delta}_i^2-\tilde{\omega}_i^2}}\left[1+\frac{|\tilde{\omega}_i|^2-|\tilde{\Delta}_i|^2}{|\tilde{\omega}_i^2-\tilde{\Delta}_i^2|}\right]\right\rangle_{k_z,\phi}$$

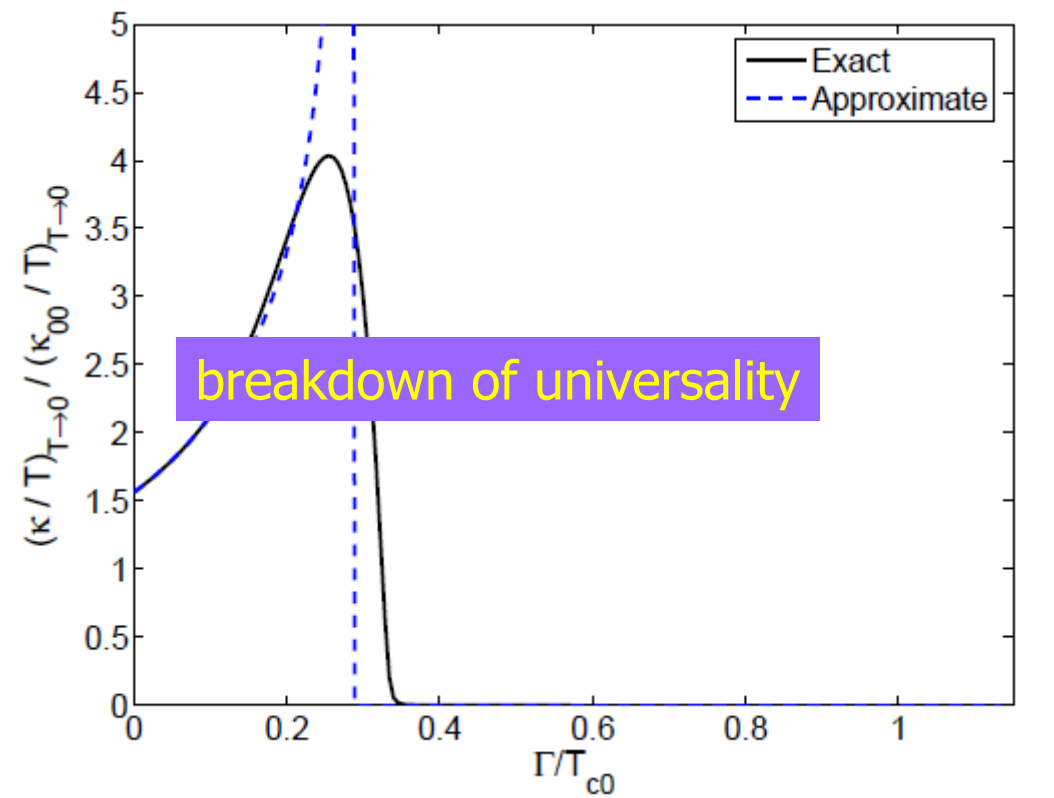
Both ω and Δ are renormalized by disorder

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

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

Theory of thermal conductivity cont'd

intraband scattering



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

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

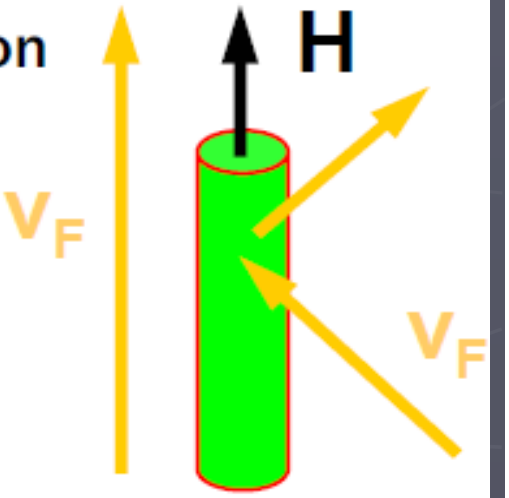
Field dependence of thermal conductivity: BPT method

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

Input: vortex lattice

- Brandt-Pesch-Tewordt approximation: $g \rightarrow$ 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

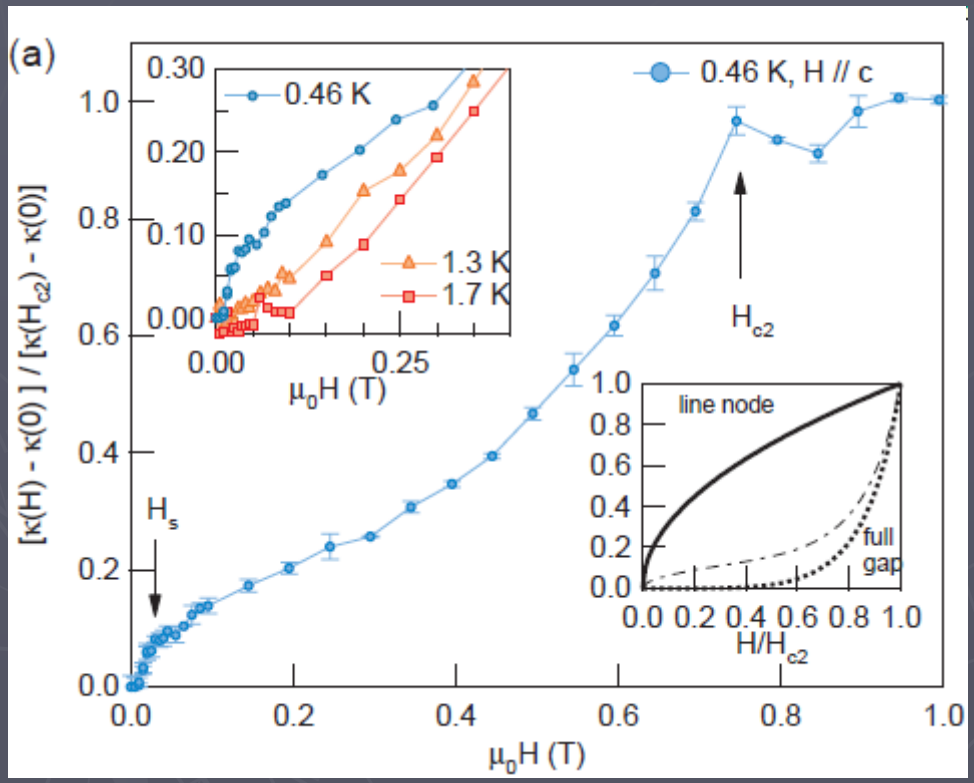
– DOS, specific heat, thermal conductivity

– angle-dependent scattering on the vortices

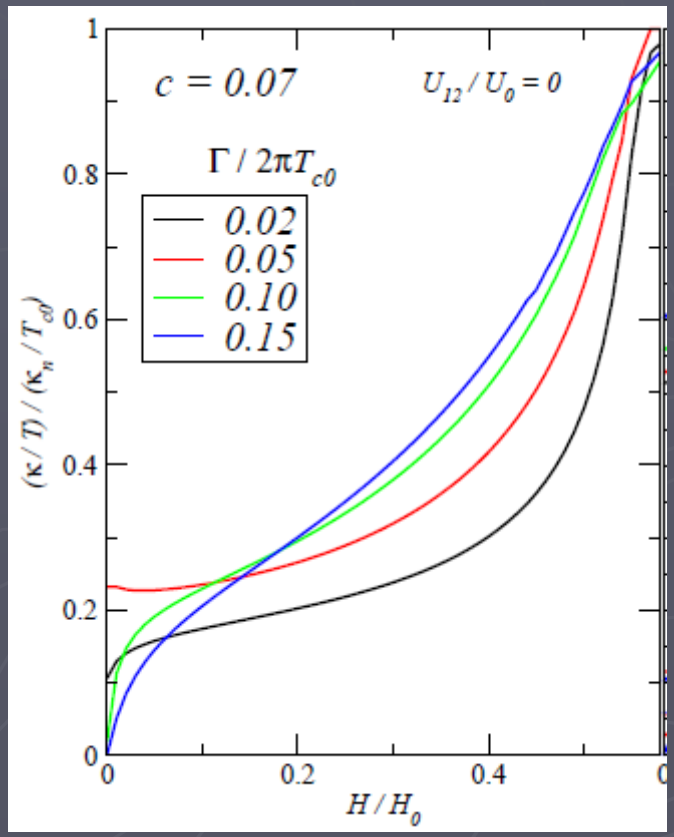
A. Houghton and I. Vekhter '98, H. Kusunose '04, A. Vorontsov and I.Vekhter, '06

Field dependence of thermal conductivity: results

Expt: LaFePO Yamashita et al

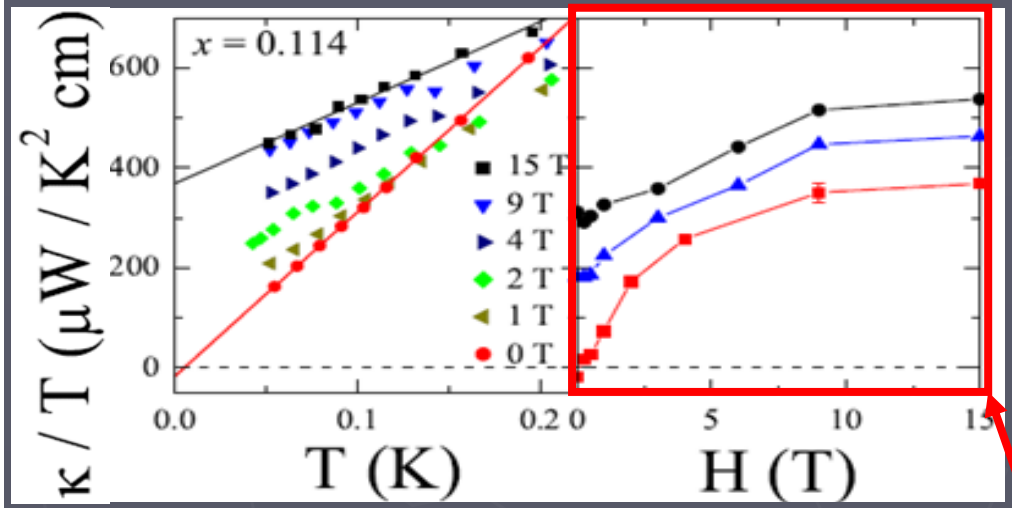


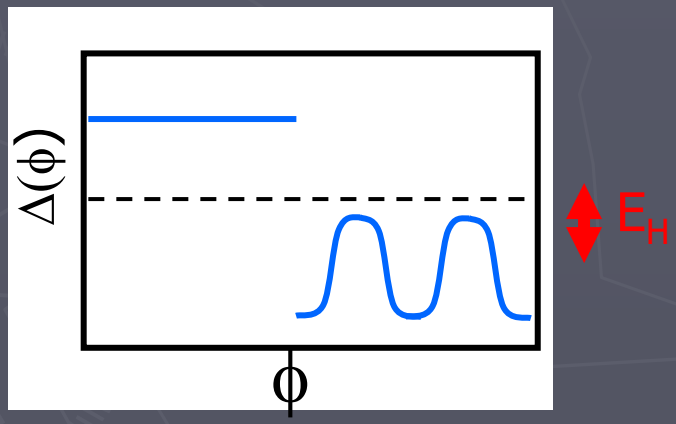
Theory: nodes, pure intraband scatt only



Field dependence of thermal conductivity: results cont'd

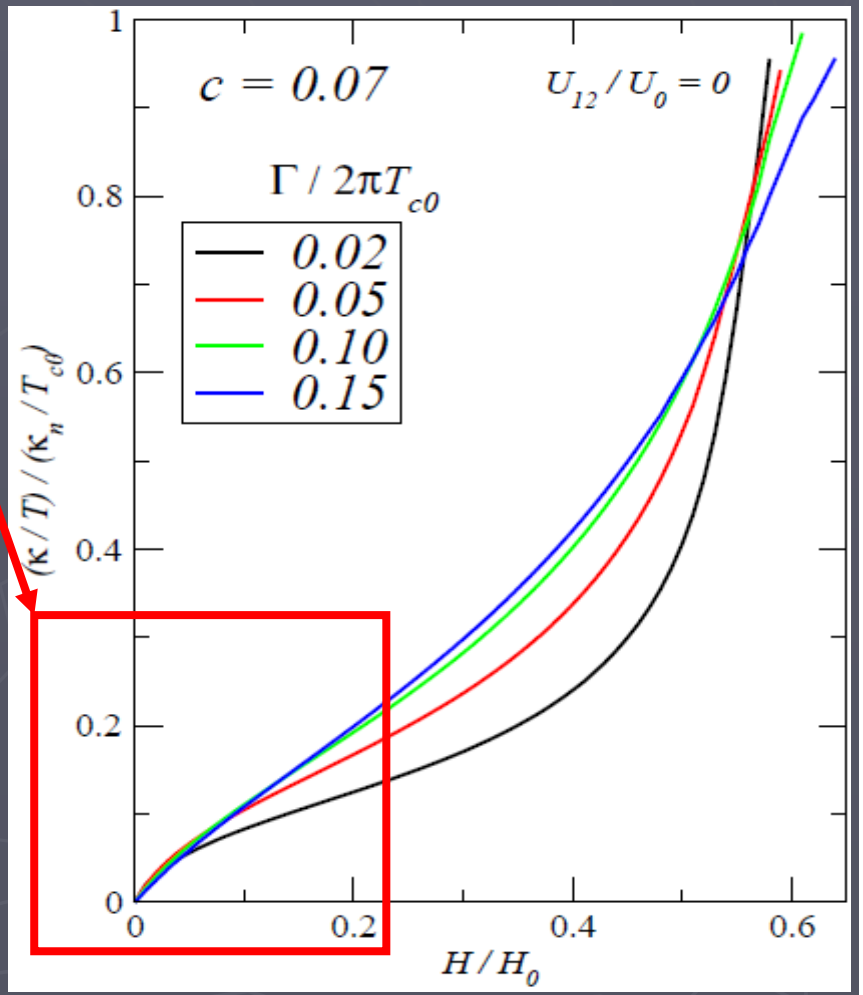
Expt: Co-doped Ba-122 Tanatar et al



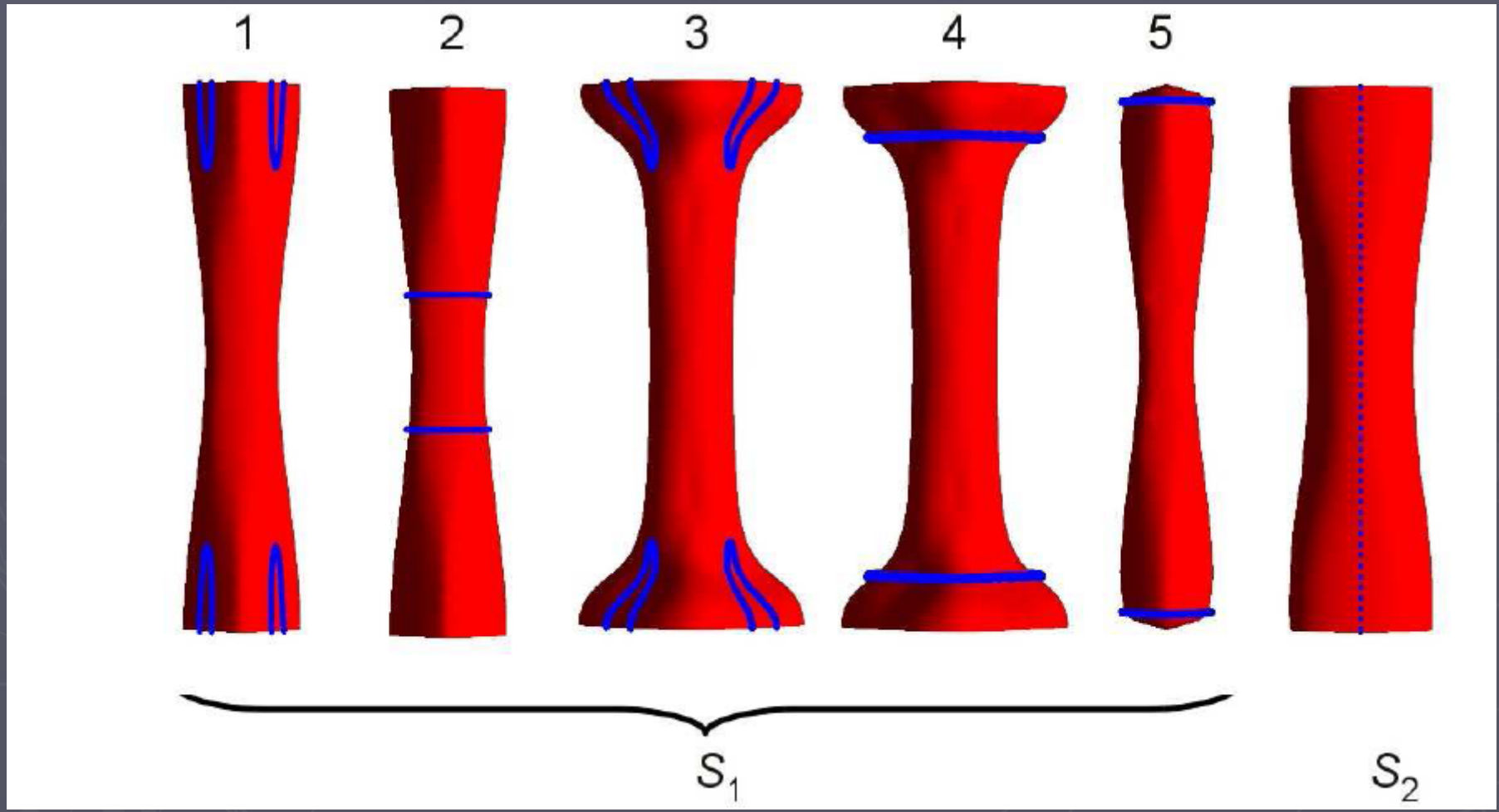


Field dependence with deep gap minima not qualitatively different from nodes!

Theory: deep gap minima



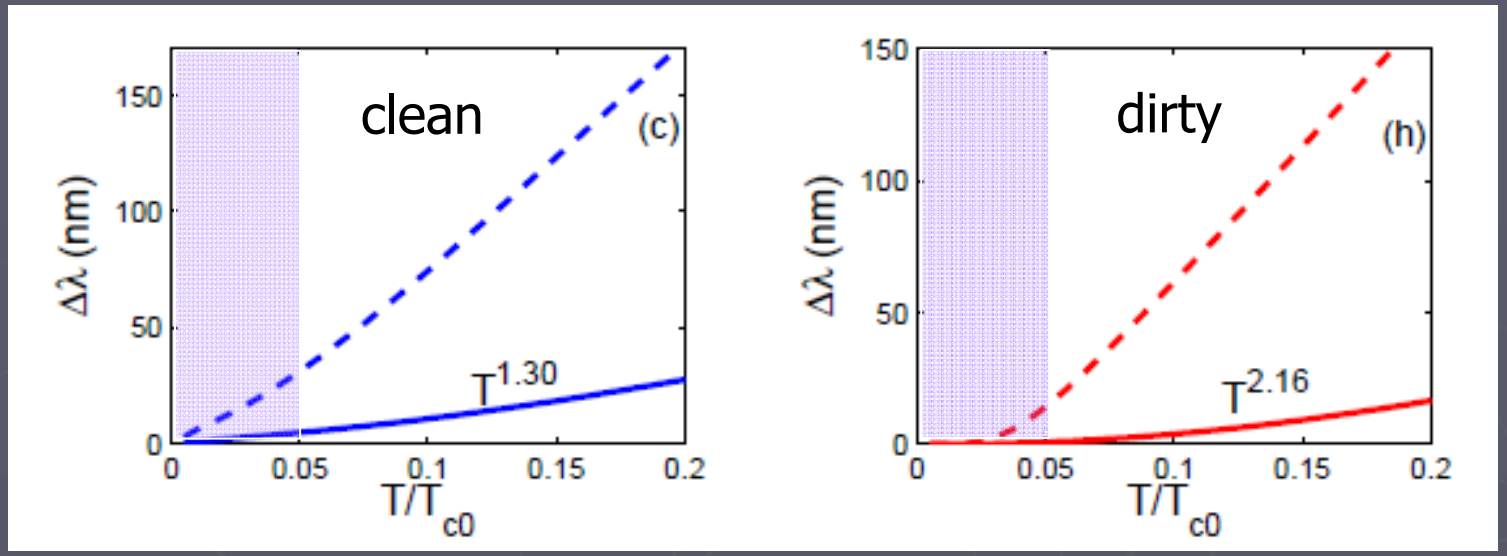
modelling c-axis transport

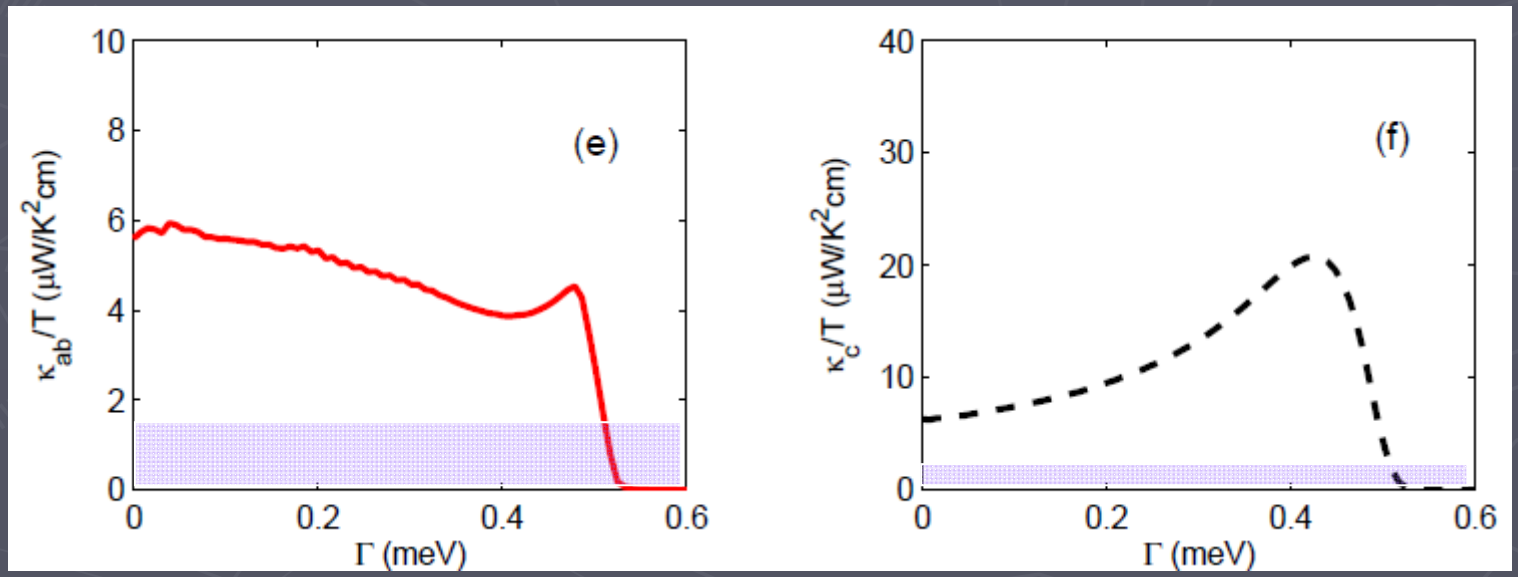


Some possibilites for hole sheet

Electron sheet

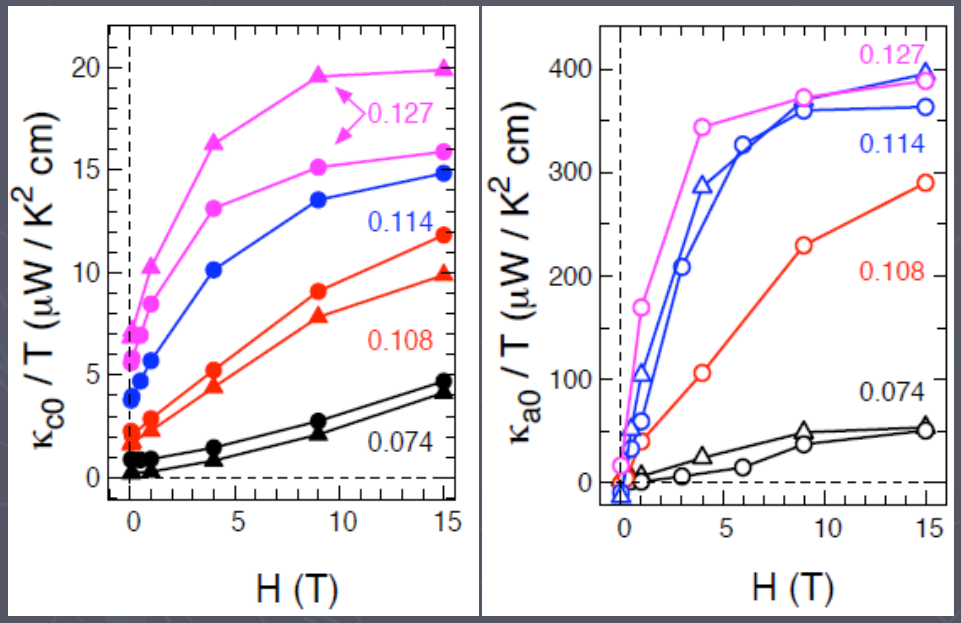
Modeling c-axis transport: results (e.g. case 3)

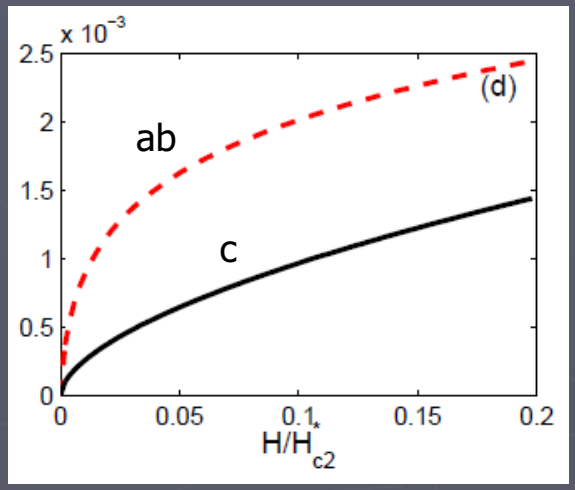




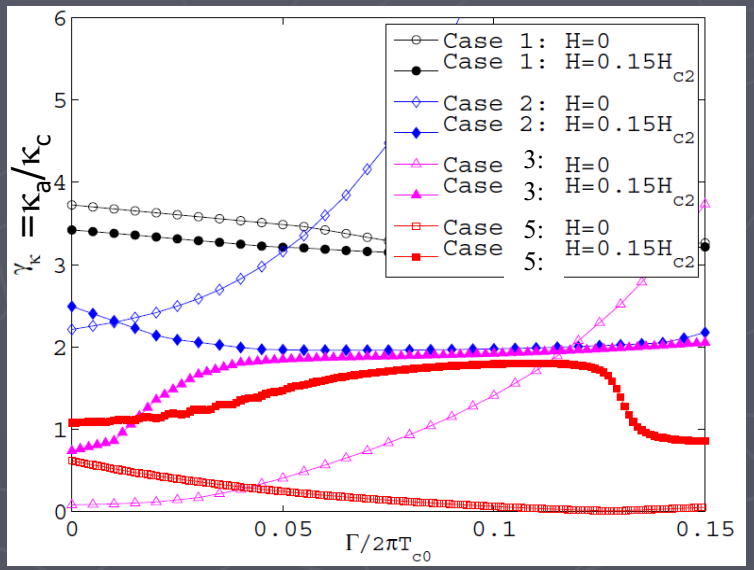
Field dependence

Reid et al 2010



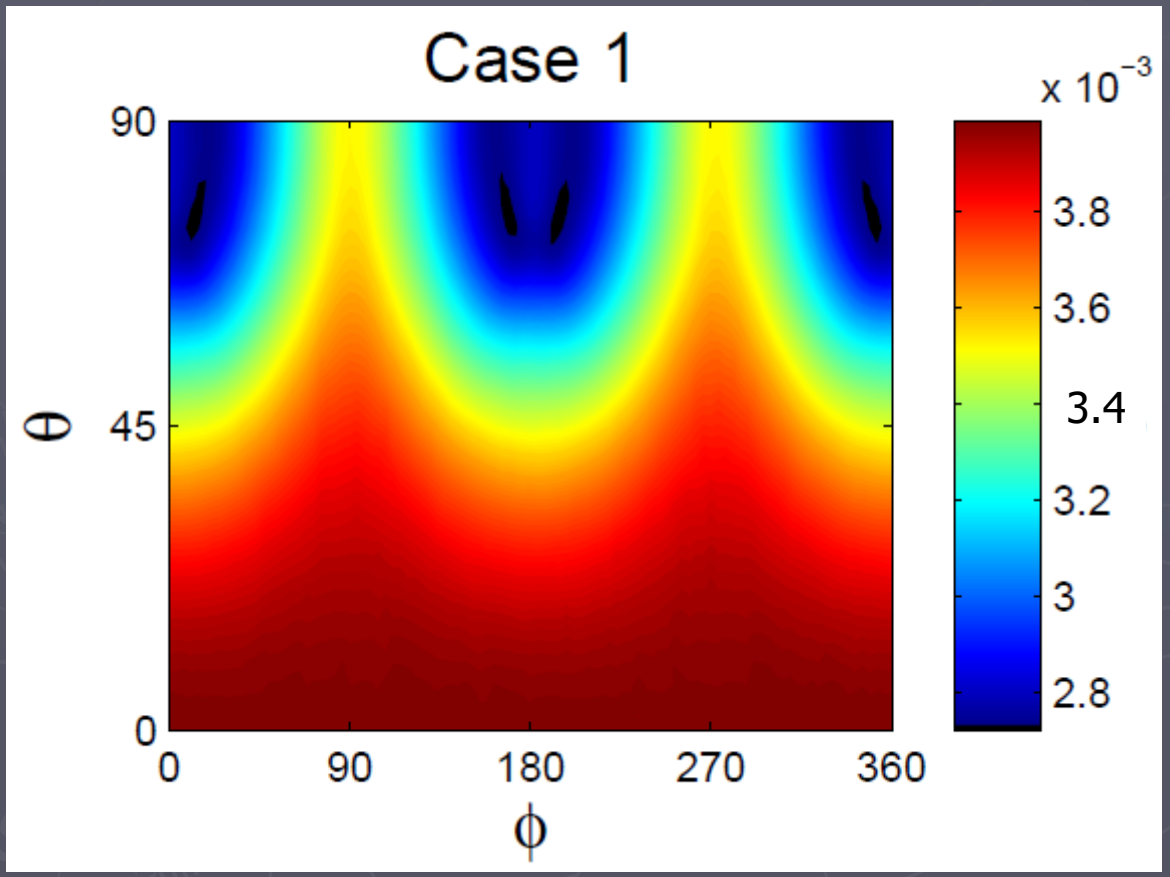


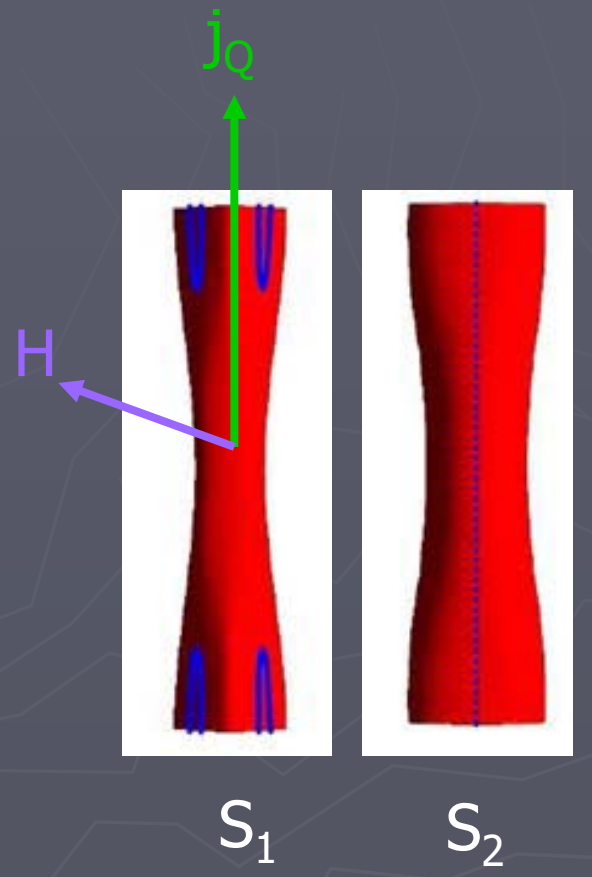
Case 3



Larger field dependence in ab plane due to long gap minima on electron sheets!

Proposal: 3D field oscillation expt:





Conclusions

- Order parameter form controversial, experiments disagree. Symmetry A_{1g} ("s-wave"), probably with overall sign change-- nodes in some systems, not in others
- Spin fluctuation calculations predict reasonable T_c, find dominant anisotropic $s_{+/-}$.
- anisotropic $s_{+/-}$ nodal structures show strong sensitivity to small changes in electronic structure (crystal structure, surfaces, strain, defects)
- 122 experiments appear to require 3D Fermi surface, nodes along c-axis---promising for applications
- Challenge: use such theories to predict *systematics* of T_c within family