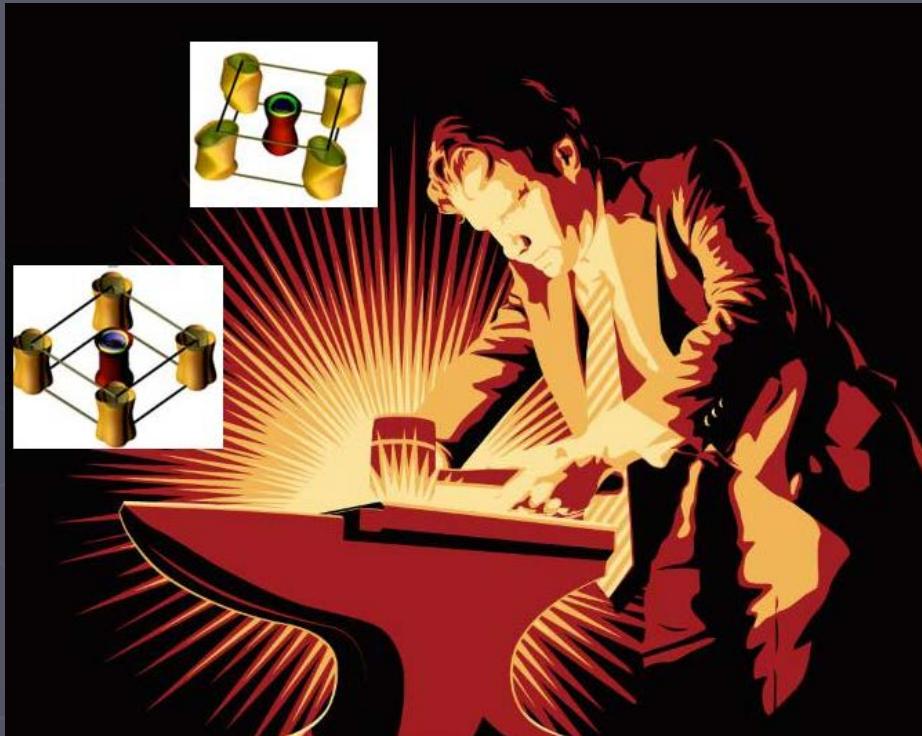


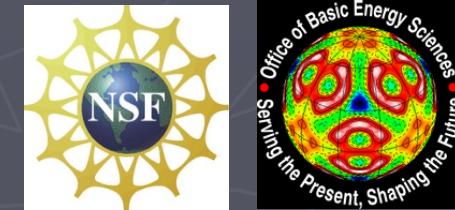
Forging an understanding of unconventional superconductivity: the iron age

P.J. Hirschfeld, U. Florida



PH, M.M. Korshunov & I.I. Mazin, Rep. Prog. Phys. 74, 124508 (2011)
PH, Comptes Rendus Physique 17, 197 (2016)

UAM November 2016



Collaborators

FeSC theory



from U. Florida Dept. of Physics:



Roser Valenti
(Frankfurt)



Brian Andersen
(Niels Bohr)



Vivek Mishra
(ORNL)



Maxim Korshunov
(Krasnoyarsk)



Lex Kemper
(NC State)



Hai-Ping
Cheng



Tom Berlijn
(ORNL)



Andreas Kreisel
(Leipzig)



Yan Wang
(U. Tenn.)



Saurabh Maiti



Andy
Linscheid



Peayush
Choubey



from rest of world:



Doug Scalapino
UCSB



Thomas Maier
ORNL



Andrey Chubukov
Igor Mazin, NRL
U. Minn.



Ilya Eremin,
Bochum

Experimentalists involved in recent work: [Sprau et al, arXiv:1611.02134](#)



Andrey
Kostin



Séamus
Davis



Anna E.
Böhmer



Valentin
Taufour



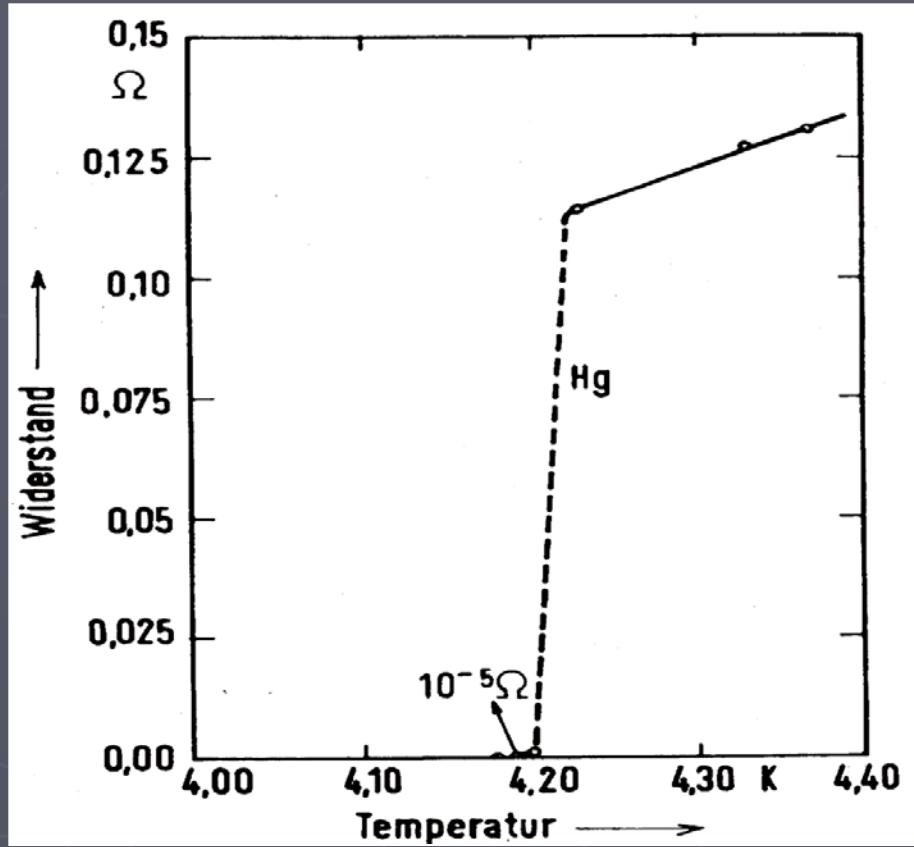
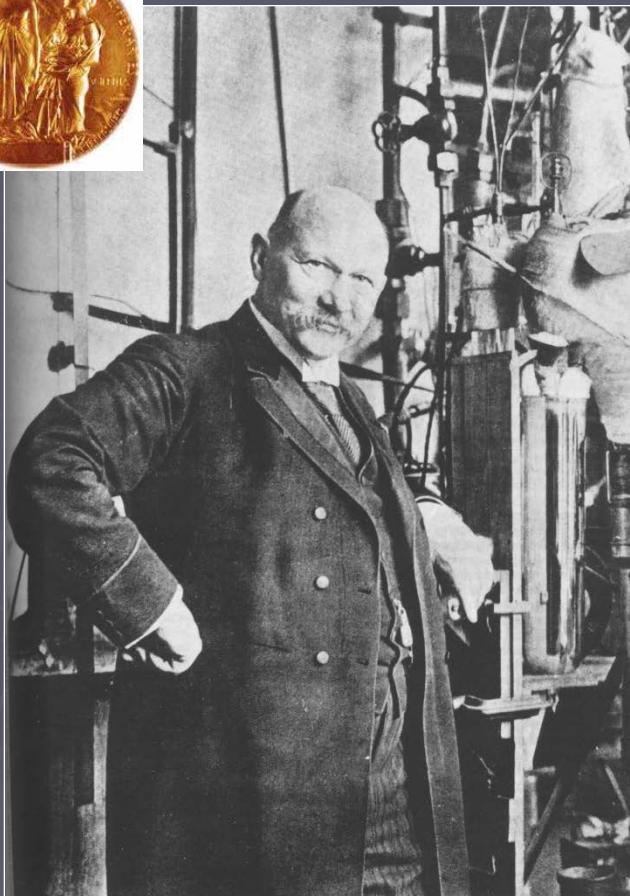
Paul C.
Canfield



Peter
Sprau

Cornell and Ames Labs, Iowa

Discovery of superconductivity



Heike Kammerling Onnes (1911)

Conventional superconductors

- During 46 years, from 1911 to 1957, superconductivity is recognized as one of the most important problems in theoretical physics
- Search for a theory of superconductivity: series of failures (see J. Schmalian in 50 Years of BCS)

Richard Feynman: “No one is brilliant enough to figure it out”



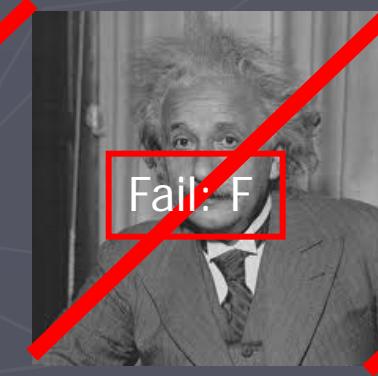
Bohr



Landau



Feynman



Einstein



Heisenberg

Conventional superconductors

- BCS theory (1957)

Quantum mechanical behavior at the macroscopic scale

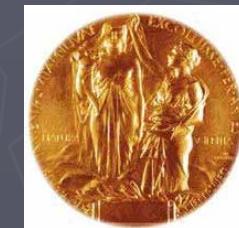
Leon Cooper



John Bardeen

Robert Schrieffer

Nobel prize : 1972



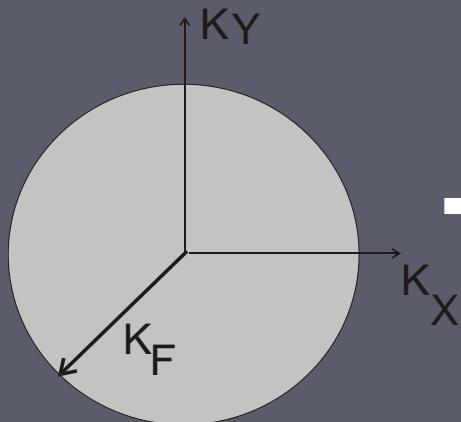
$$\text{Macro. Quantum State } \Psi_{BCS} = \prod_k \left(u_k + v_k c_{k\uparrow}^* c_{-k\downarrow}^* \right) |0\rangle$$

s-wave symmetry

$$\Delta \equiv V \langle c_{-k\downarrow} c_{k\uparrow} \rangle \sim \Delta_0 e^{i\phi}$$

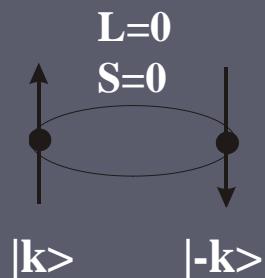
SC Ground State

Normal State (Metal)

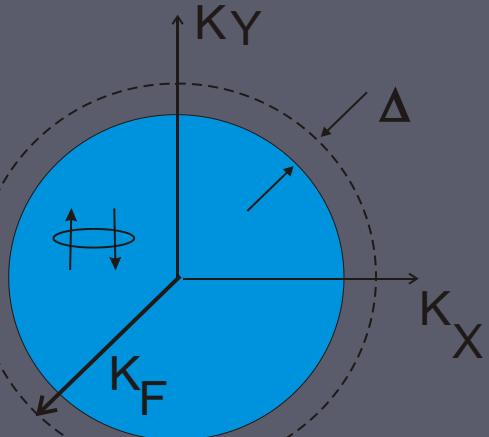


Degenerate ~free electron gas

Low Temp.
Cooper Pairing

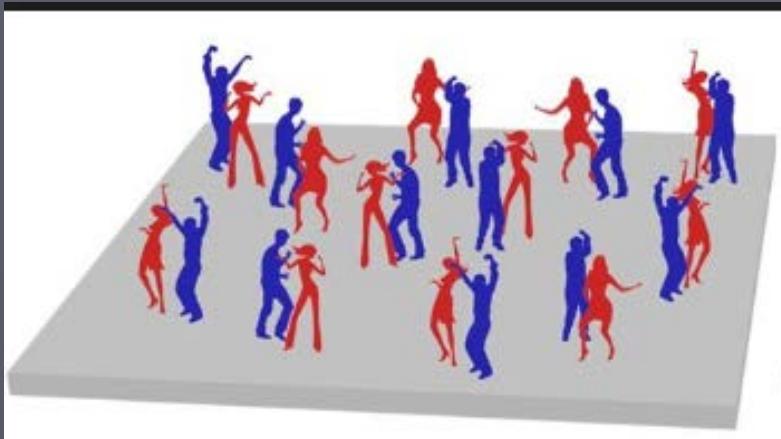


Superconducting
Ground State



~ Gas of Cooper Pairs

How can two electrons attract each other?

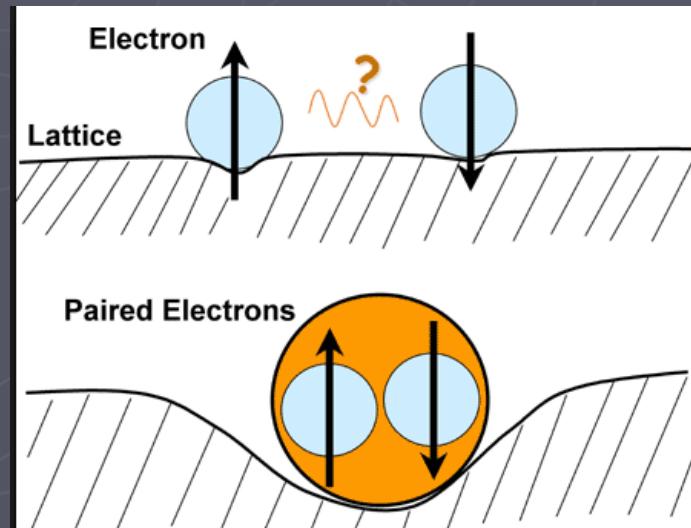


Dance analogy: coherent pairs

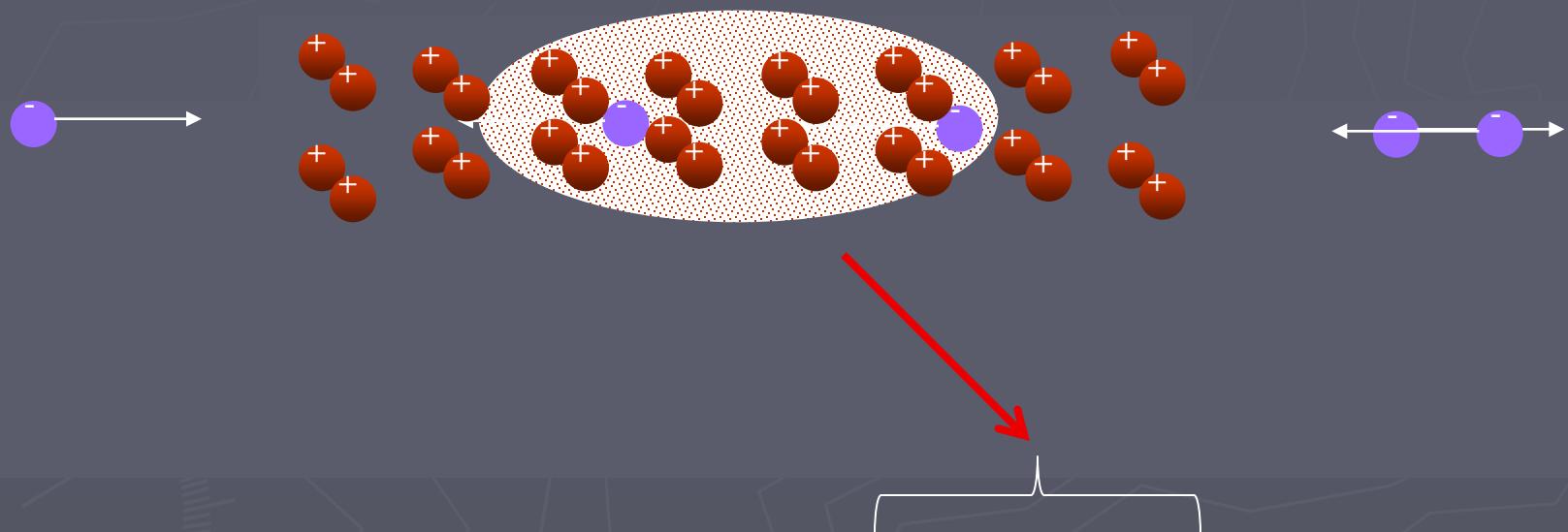


J. Robert Schrieffer:
"By dancing they lower their energy
or make themselves happier"

Another analogy:



How Cooper pairs form in conventional superconductors: the “glue”: electron-phonon interaction



Effective “residual”
e-e interaction
including Coulomb
 (“Jellium model”)

$$V(\mathbf{q}, \omega) = \frac{\mathbf{a} 4\pi e^2}{q^2 + k_s^2} + \frac{\mathbf{b} 4\pi e^2}{q^2 + k_s^2} \frac{\omega_q^2}{\omega^2 - \omega_q^2}$$

Screened Coulomb Electron-phonon attraction

For realistic system,
 $a \neq b$! Depends on details

Note: electrons avoid Coulomb repulsion in *time* (interaction is retarded)

Why do some elements superconduct, others not?

Periodic Table of Superconductivity

(dedicated to the memory of Bernd Matthias; compiled by James S. Schilling)

30 elements superconduct at ambient pressure, 23 more superconduct at high pressure.

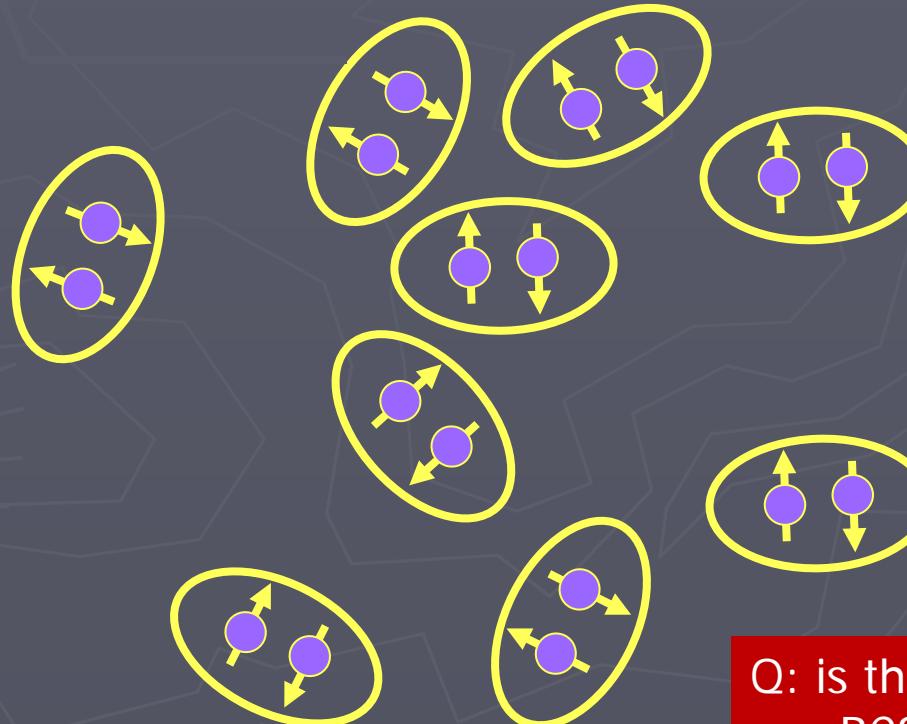
H	ambient pressure superconductor												high pressure superconductor												He	
Li 0.0004 14 30	Be 0.026 3.7 30												T _c (K) T _c ^{max} (K) P(GPa)												Ne	
Na	Mg													T _c ^{max} (K) P(GPa)												Ar
K	Ca 29 217	Sc 19.6 106	Ti 0.39 3.35 56.0	V 5.38 16.5 120	Cr	Mn	Fe 2.1 21	Co	Ni	Cu	Zn 0.875	Ga 1.091 7 1.4	Ge	As	Se	Br	Kr									
Rb	Sr 7 50	Y 19.5 115	Zr 0.546 11 30	Nb 9.50 9.9 10	Mo 0.92	Tc 7.77	Ru 0.51	Rh .00033	Pd	Ag	Cd 0.56	In 3.404	Sn 3.722 5.3 11.3	Sb	Te	I 1.2 25	Xe									
Cs	Ba 1.3 12	insert La-Lu 5 18	Hf 0.12 8.6 62	Ta 4.483 4.5 43	W 0.012	Re 1.4	Os 0.655	Ir 0.14	Pt	Au	Hg- α 4.153	Tl 2.39	Pb 7.193	Bi 8.5 9.1	Po	At	Rn									
Fr	Ra	insert Ac-Lr	Rf	Ha																						
			La-fcc 6.00 13 15	Ce 1.7 5	Pr	Nd	Pm	Sm	Eu 2.75 142	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu 12.4 174									
			Ac	Th 1.368	Pa 1.4	U 0.8(β) 2.4(α) 1.2	Np	Pu	Am 0.79 2.2 6	Cm	Bk	Cf	Es	Fm	Md	No	Lr									

a,b depend on details!

$$V(\mathbf{q}, \omega) = \frac{\textcolor{red}{a} 4\pi e^2}{q^2 + k_s^2} + \frac{\textcolor{blue}{b} 4\pi e^2}{q^2 + k_s^2} \frac{\omega_q^2}{\omega^2 - \omega_q^2}$$

Superconductivity: why is pairing good?

Naive answer: once we have an attraction, we get pairs.
Pairs of fermions are *bosons*, so they can Bose condense
 \Rightarrow pair *superfluid*



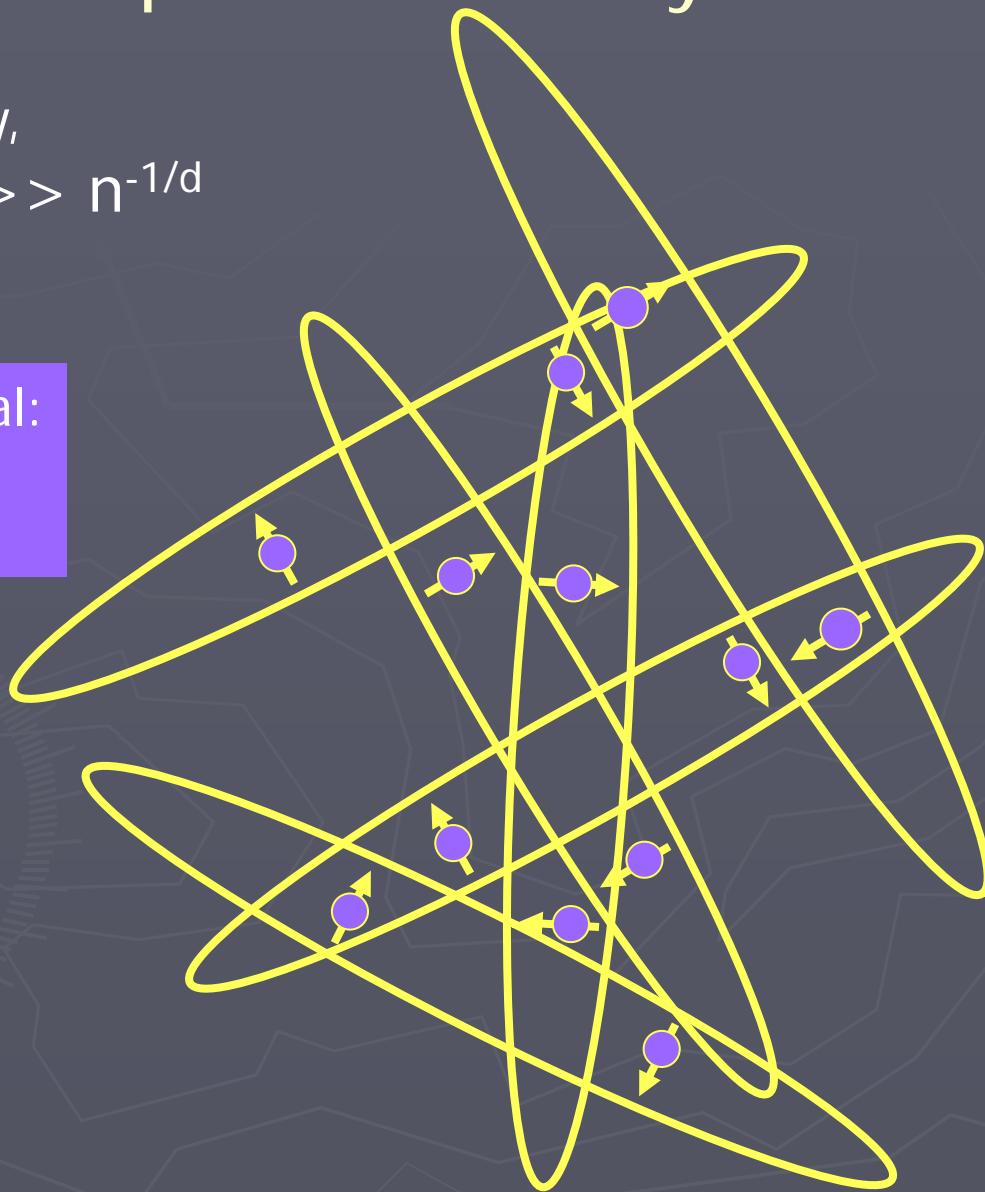
Q: is this the right picture of a
BCS superconductor?
A: No!

Superconductivity: Ground state

In reality,

$$\xi = v_F / \Delta \gg n^{-1/d}$$

Simple metal:
 $\xi \sim 10^3 \text{ Å}$
 $n^{-1/d} \sim 1 \text{ Å}$



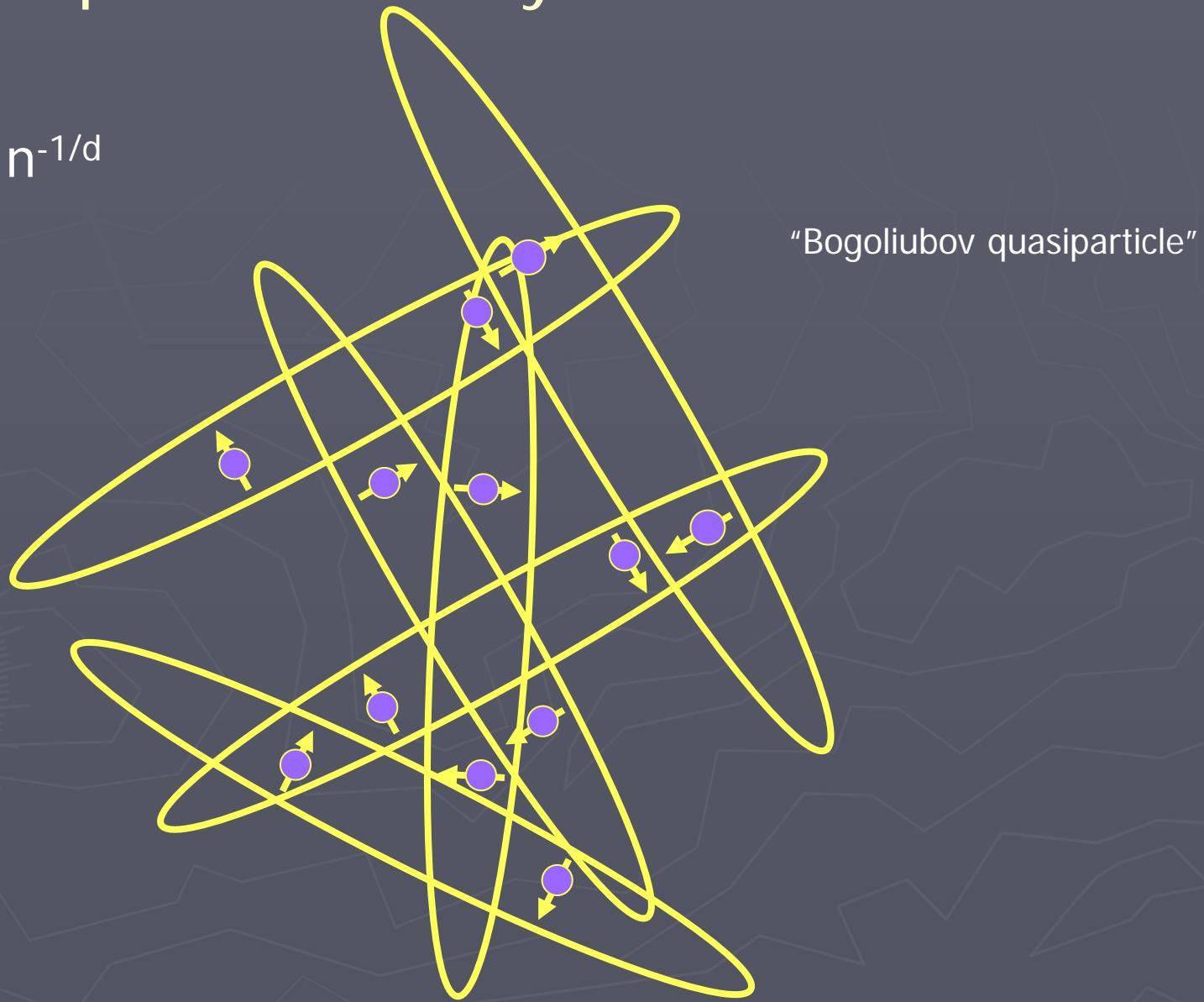
Remember that all pairs
are phase coherent!



St. Matthew's Passion
Oxford, UK

Superconductivity: Excited states

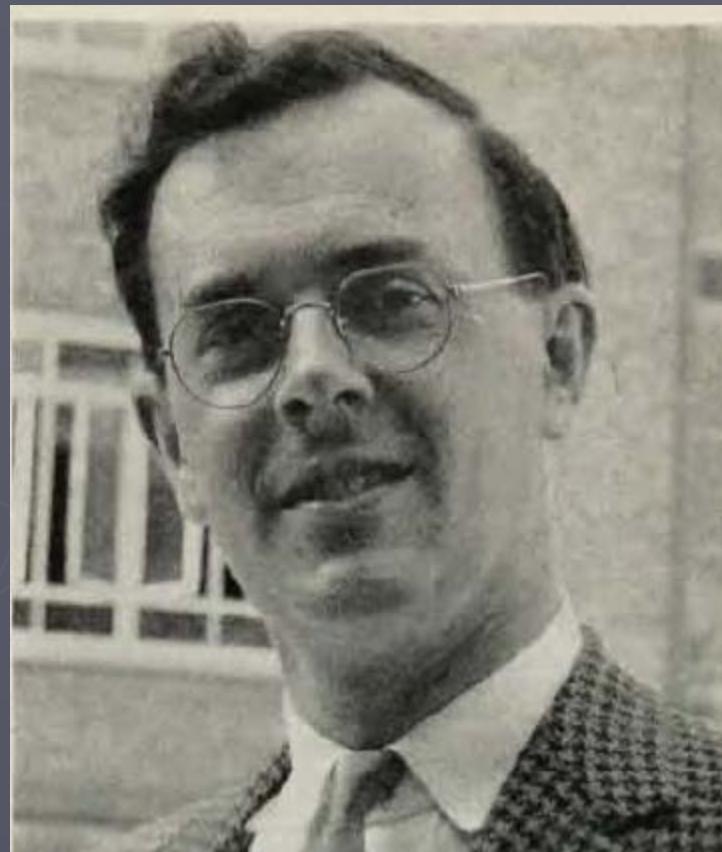
$$\xi = v_F / \Delta >> n^{-1/d}$$



Is that all there is? Brian Pippard and "The Cat and the Cream" speech IBM 1961



Is that all there is? Brian Pippard and "The Cat and the Cream" speech IBM 1961



"I think I might remark that in low-temperature physics the disappearance of liquid helium, superconductivity, and magneto-resistance from the list of major unsolved problems has left this branch of research looking pretty sick from the point of view of any young innocent who thinks he's going to break new ground."

High temperature superconductivity

Possible High T_c Superconductivity in the Ba – La – Cu – O System

J.G. Bednorz and K.A. Müller

IBM Zürich Research Laboratory, Rüschlikon, Switzerland

Received April 17, 1986

Z. Physik, June 1986



Alex Müller and Georg Bednorz

High temperature superconductivity

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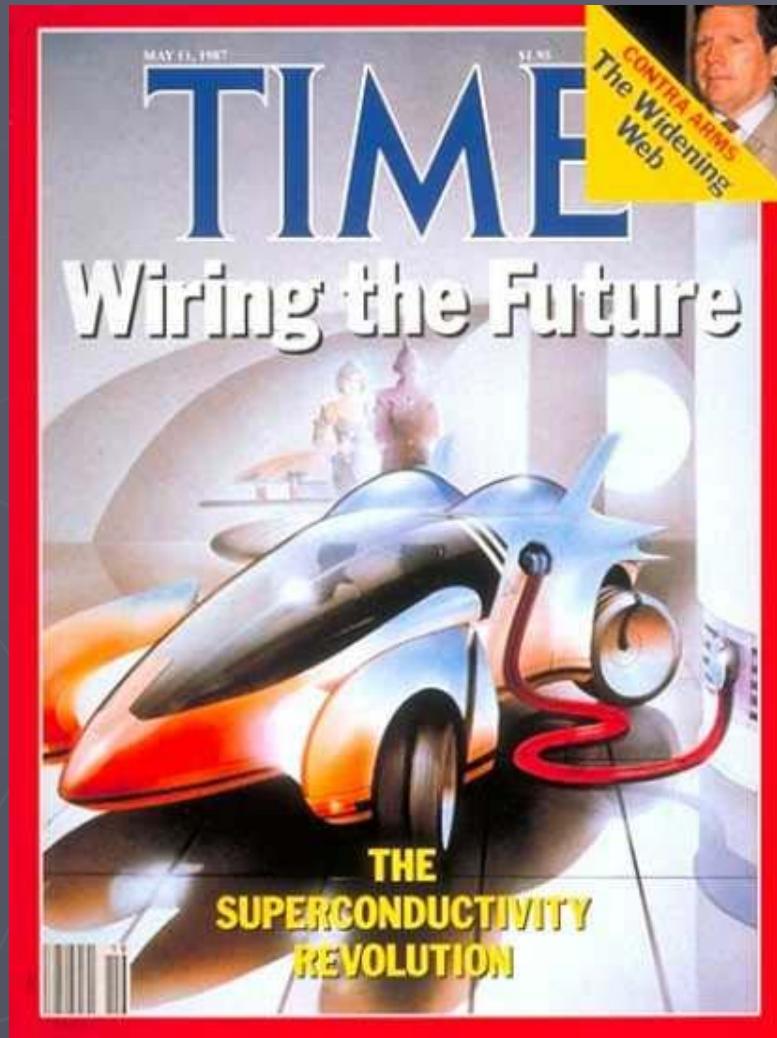
- Grüneisen parameter coupling in heavy fermion systems 169-174
DOI 10.1007/BF01303699
Authors M. Yoshizawa, B. Lüthi and K. D. Schotte
Text PDF (494 kb)
- Anomalous temperature dependence of the magnetic field penetration depth in superconducting UBe₁₃ 175-188
DOI 10.1007/BF01303700
Authors F. Gross, B. S. Chandrasekhar, D. Einzel, K. Andres, P. J. Hirschfeld, H. R. Ott, J. Beuers, Z. Fisk and J. L. Smith
Text PDF (1,206 kb)
- Possible high T_c superconductivity in the Ba–La–Cu–O system 189-193
DOI 10.1007/BF01303701
Authors J. G. Bednorz and K. A. Müller
Text PDF (396 kb)



20 Articles

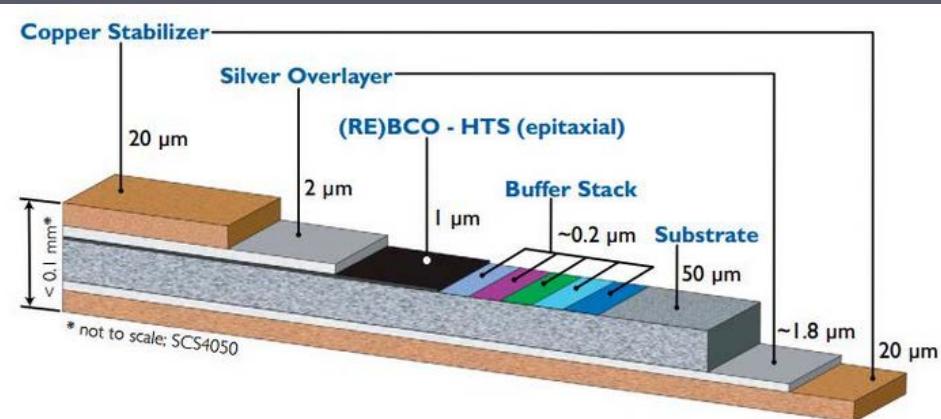
First | 1-10 | 11-20 | Next

Great expectations 1987

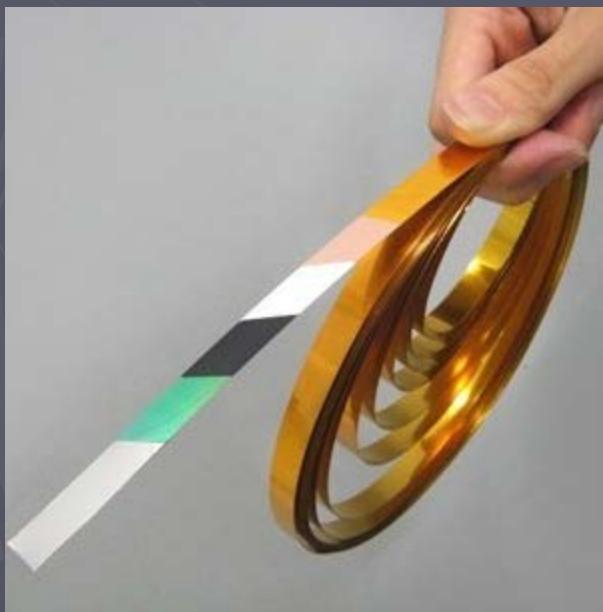


Applications 2016

Wires



transmission lines

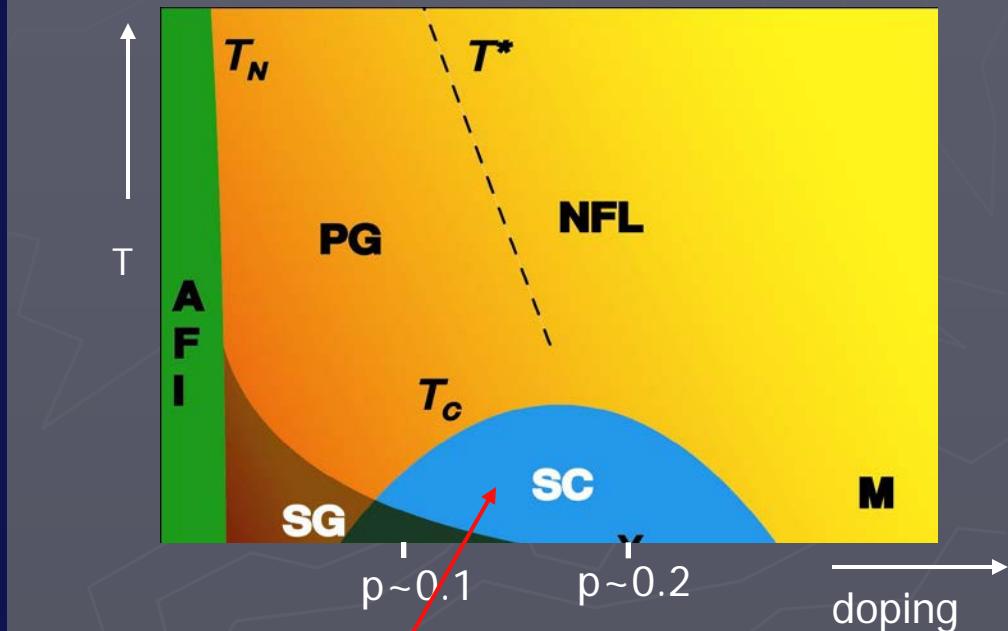
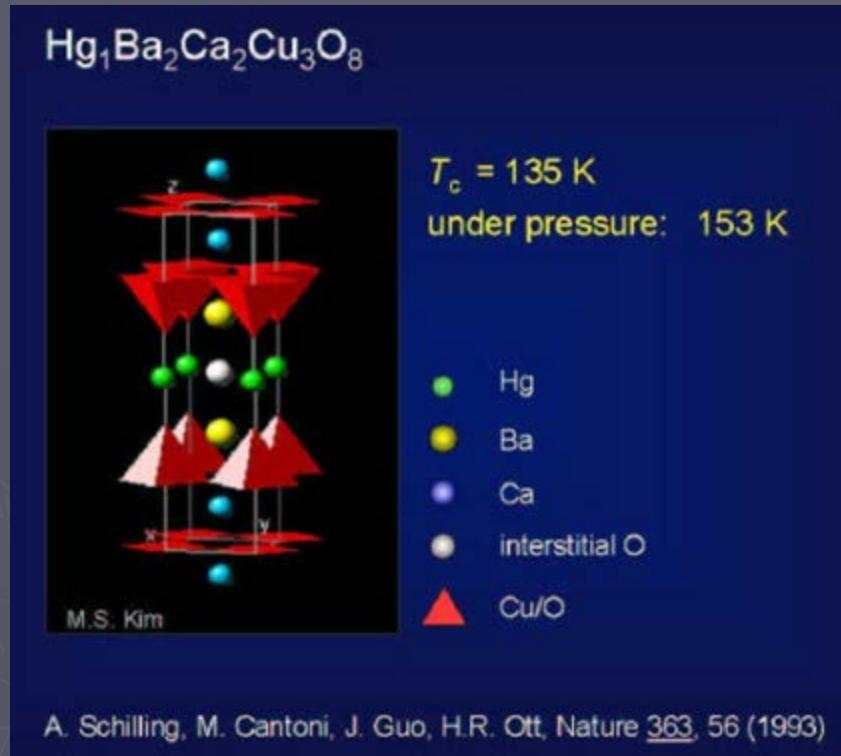


to make



large magnets – maglev technology...

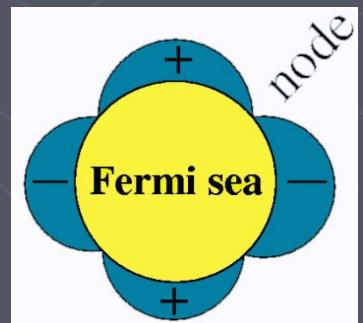
Cuprates: status report



T_c is too high for electron-phonon "glue" to work!
What holds pairs together?



$$\Delta_k = \frac{\Delta_0}{2} (\cos k_x - \cos k_y)$$

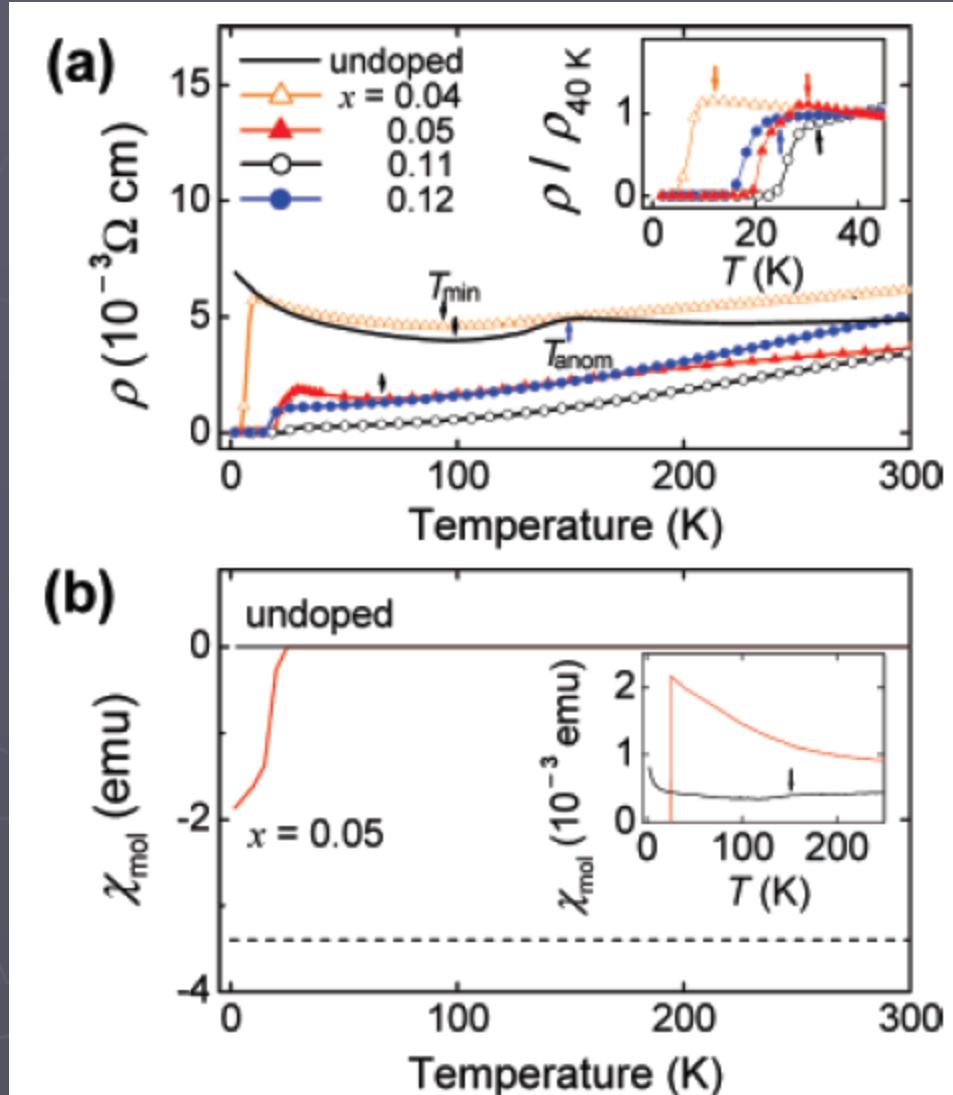
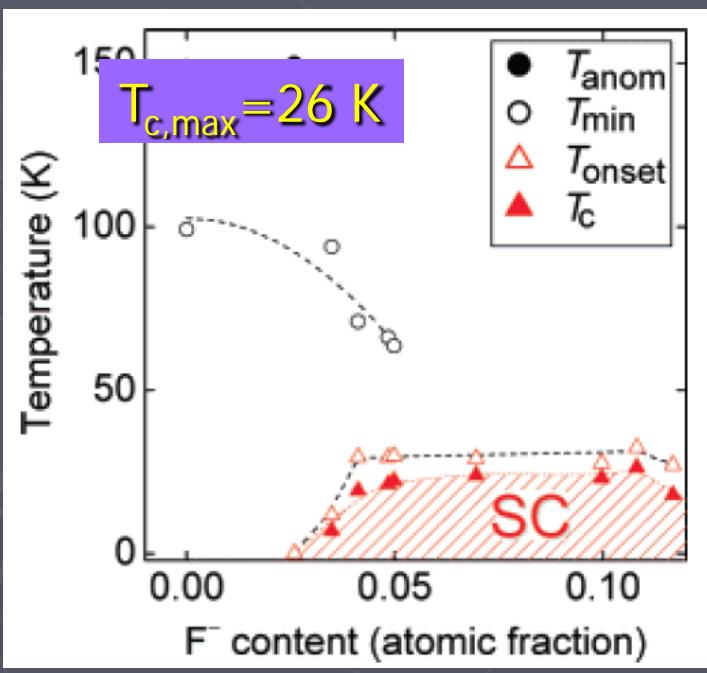


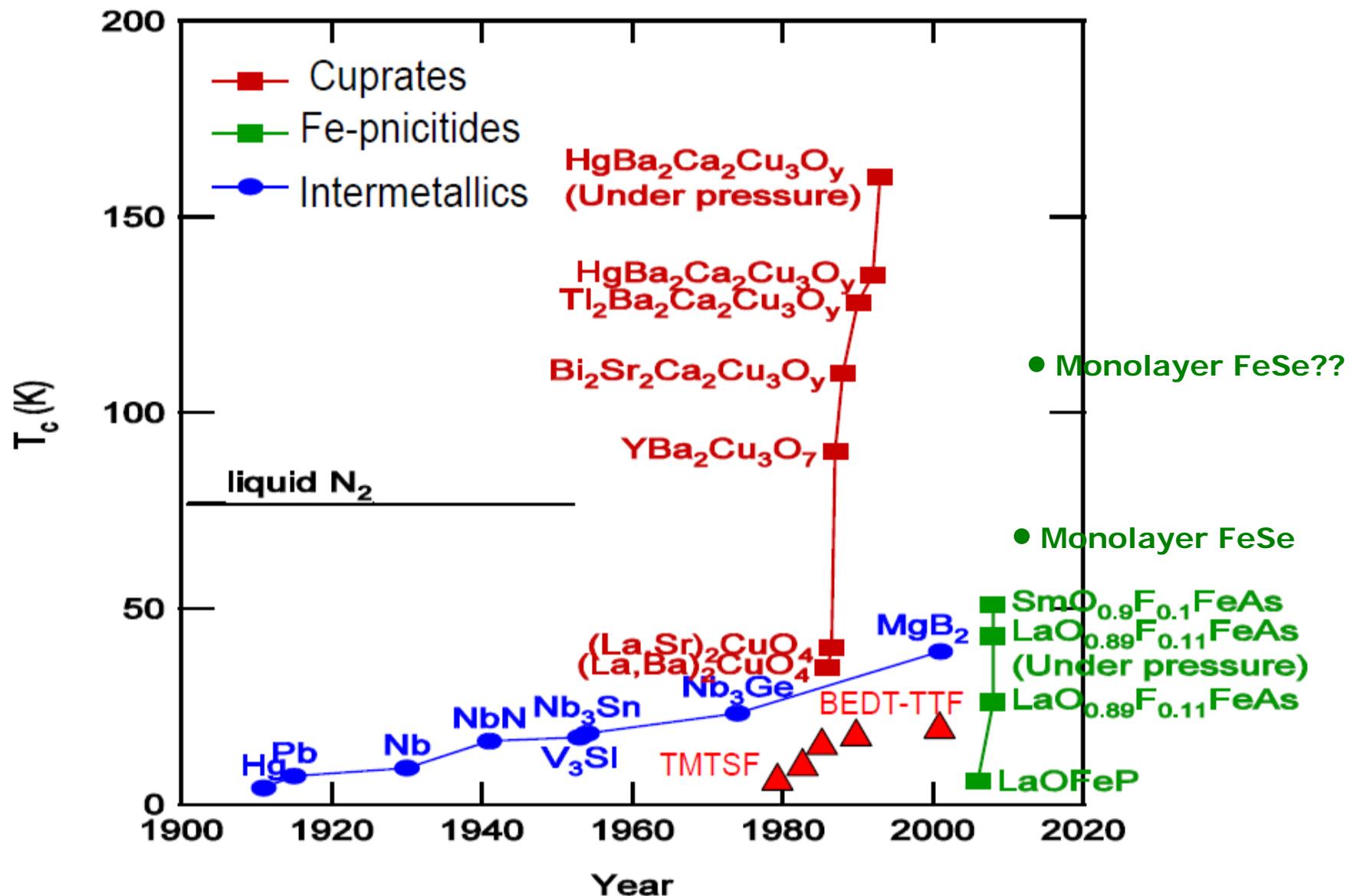
Discovery of $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$

Kamihara et al JACS 2008



H. Hosono

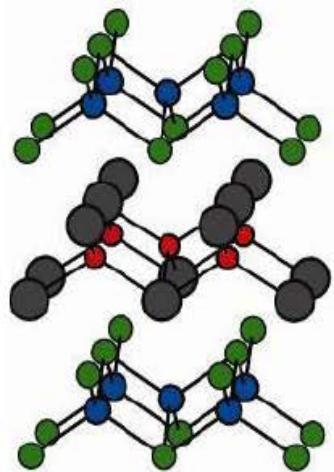




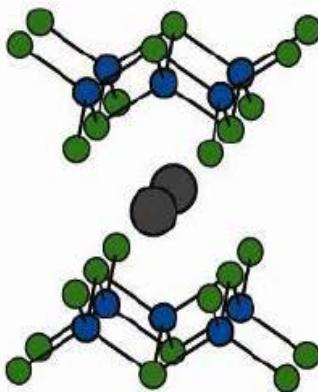
Iron-based superconductors

Recent reviews: Paglione & Greene Nat Phys 2010; Johnston Adv. Phys. 2010

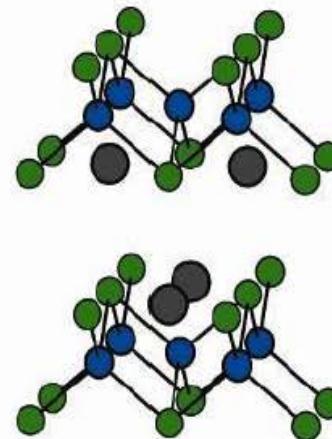
LaFeAsO



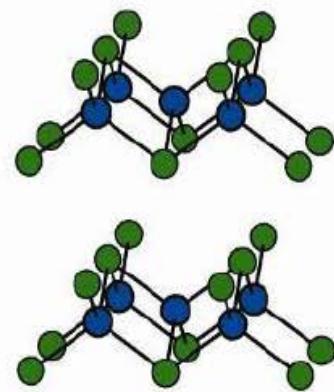
BaFe₂As₂



LiFeAs



FeSe



$T_c = 28K$
(55K for Sm)

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

$T_c = 38K$

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

$T_c = 18K$

Wang et al
Sol. St. Comm. 2008

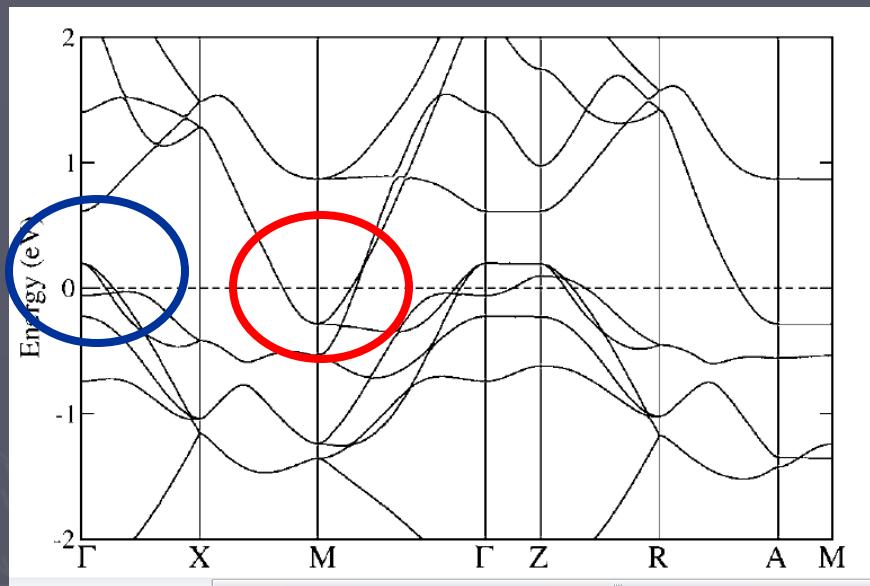
$T_c = 8K$

Hsu et al
PNAS 2008

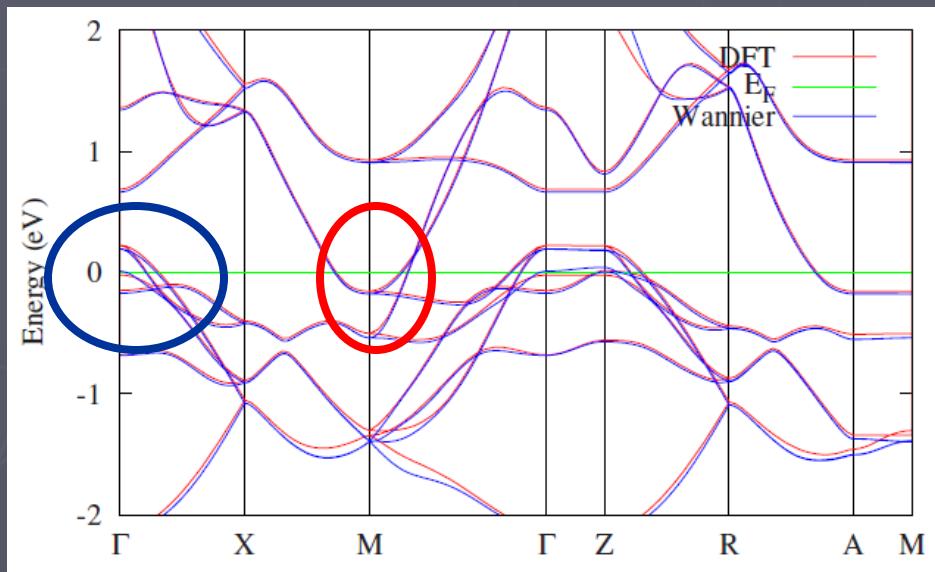
No arsenic ☺!

Electronic structure calculations

LaFePO Lebegue 2007 ($T_c=6\text{K}$)

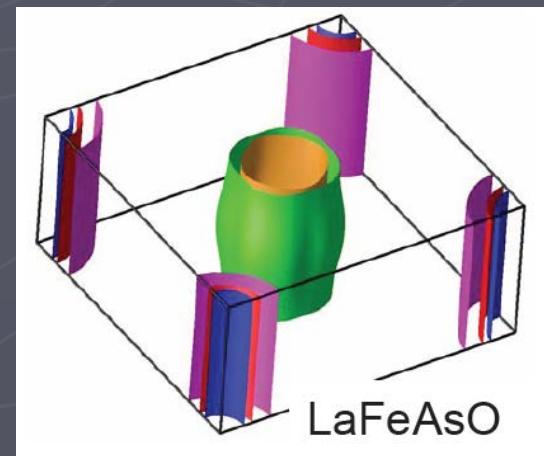


LaFAsO Cao et al 2008 ($T_c=26\text{K}$)



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

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

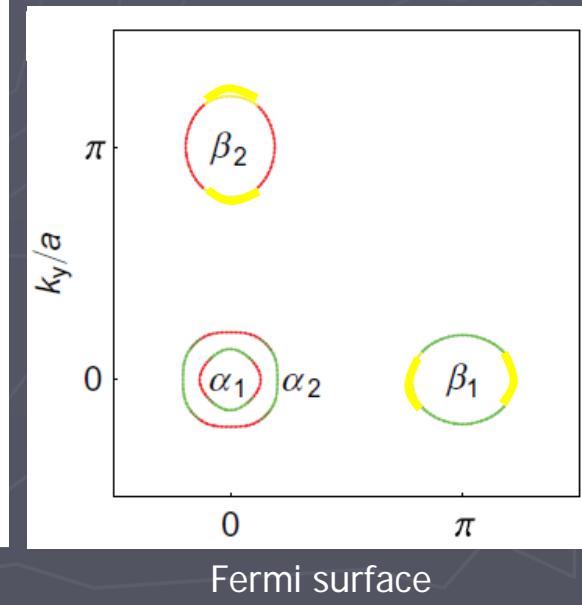
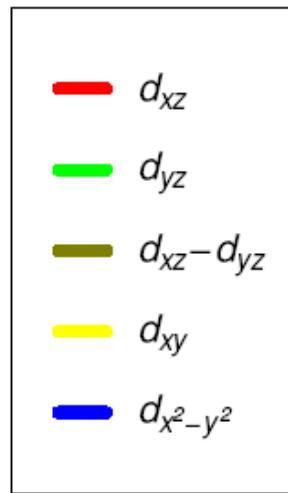
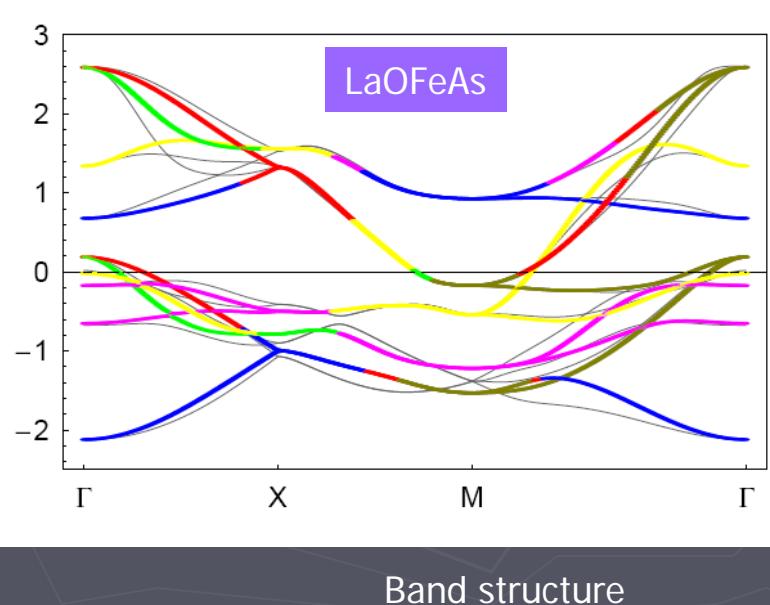
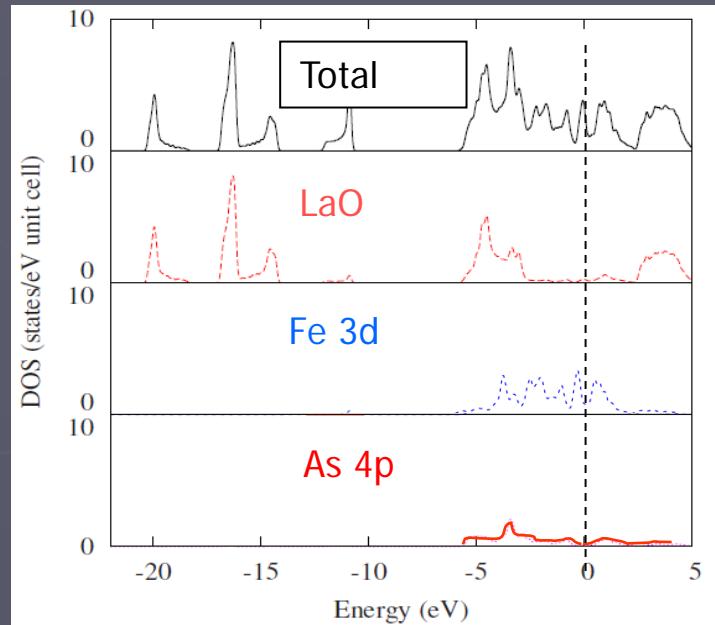


Multiorbital physics

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

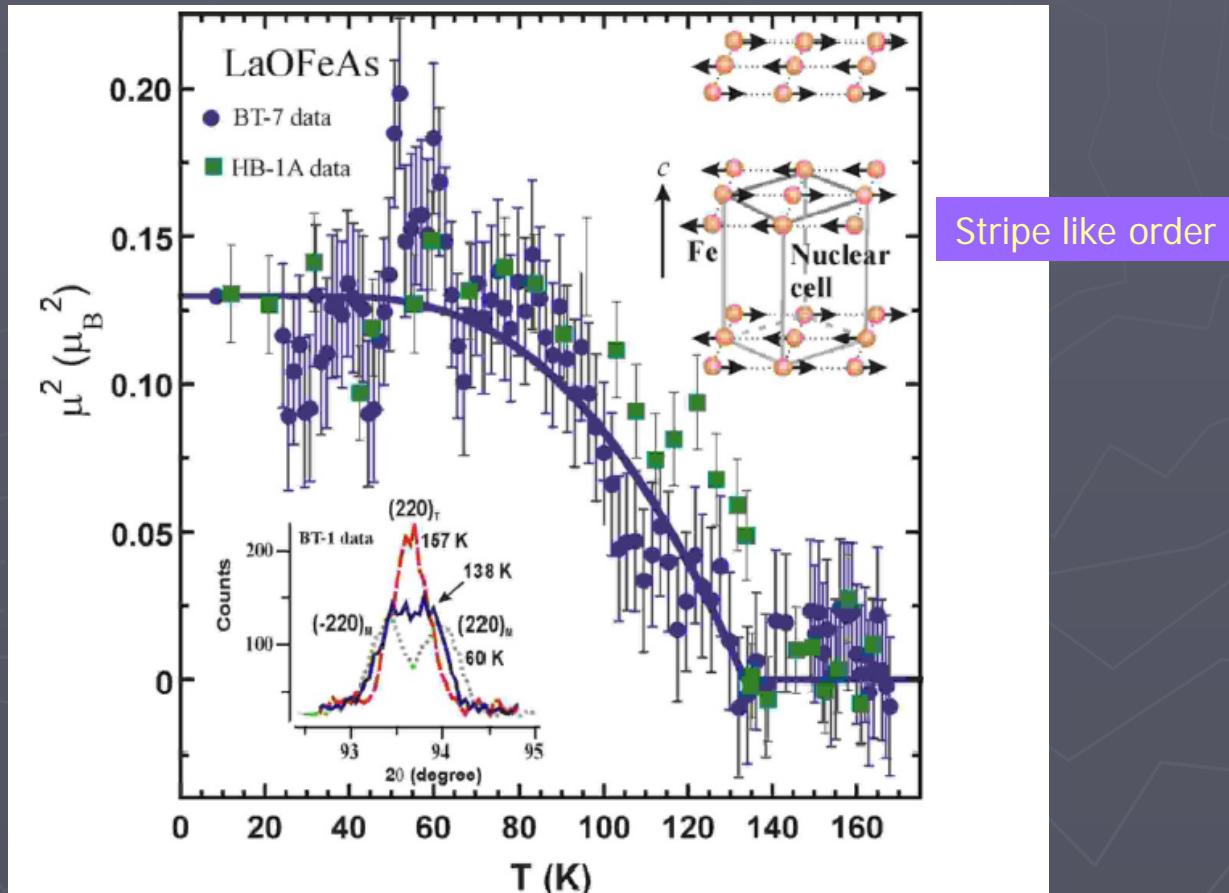
Complications: calculations will be harder

Novelty: surprising new aspects of multiorbital/multiband physics



Magnetic order in most (not all) parent compounds

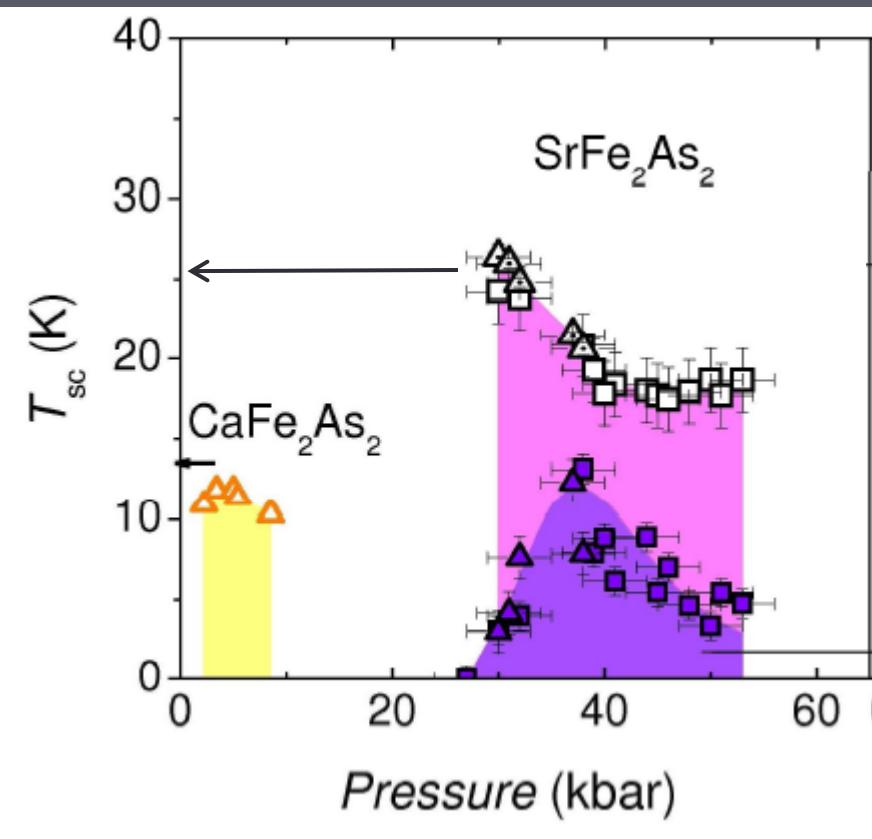
de la Cruz et al Nature 453, 899 (2008)



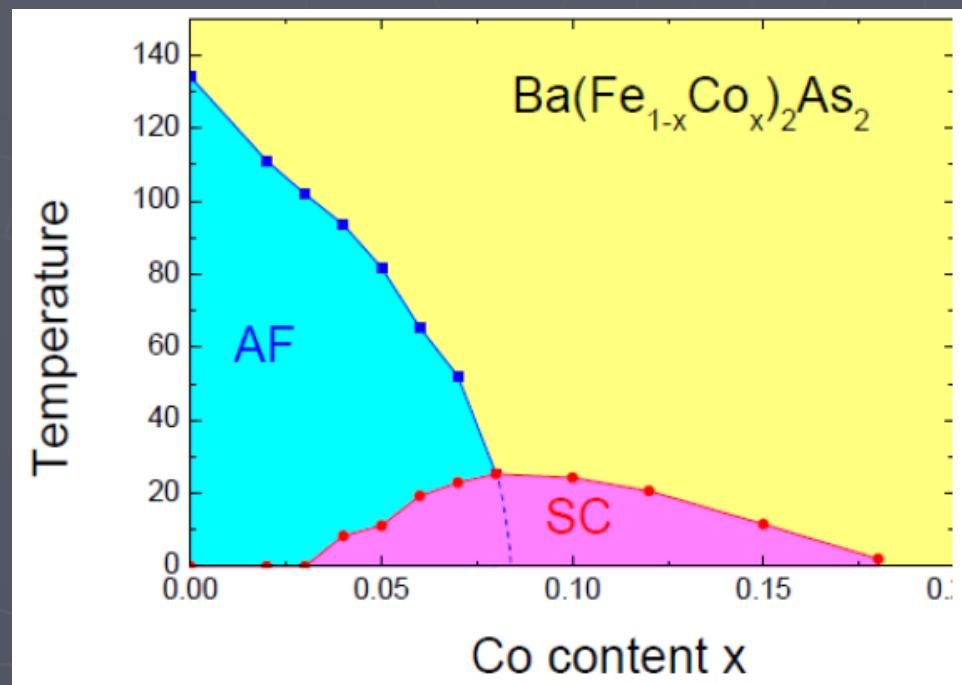
Review: E. Bascones, B. Valenzuela, M. J. Calderon, Comptes Rendus Physique (2016)

“Doping” the parent compound

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

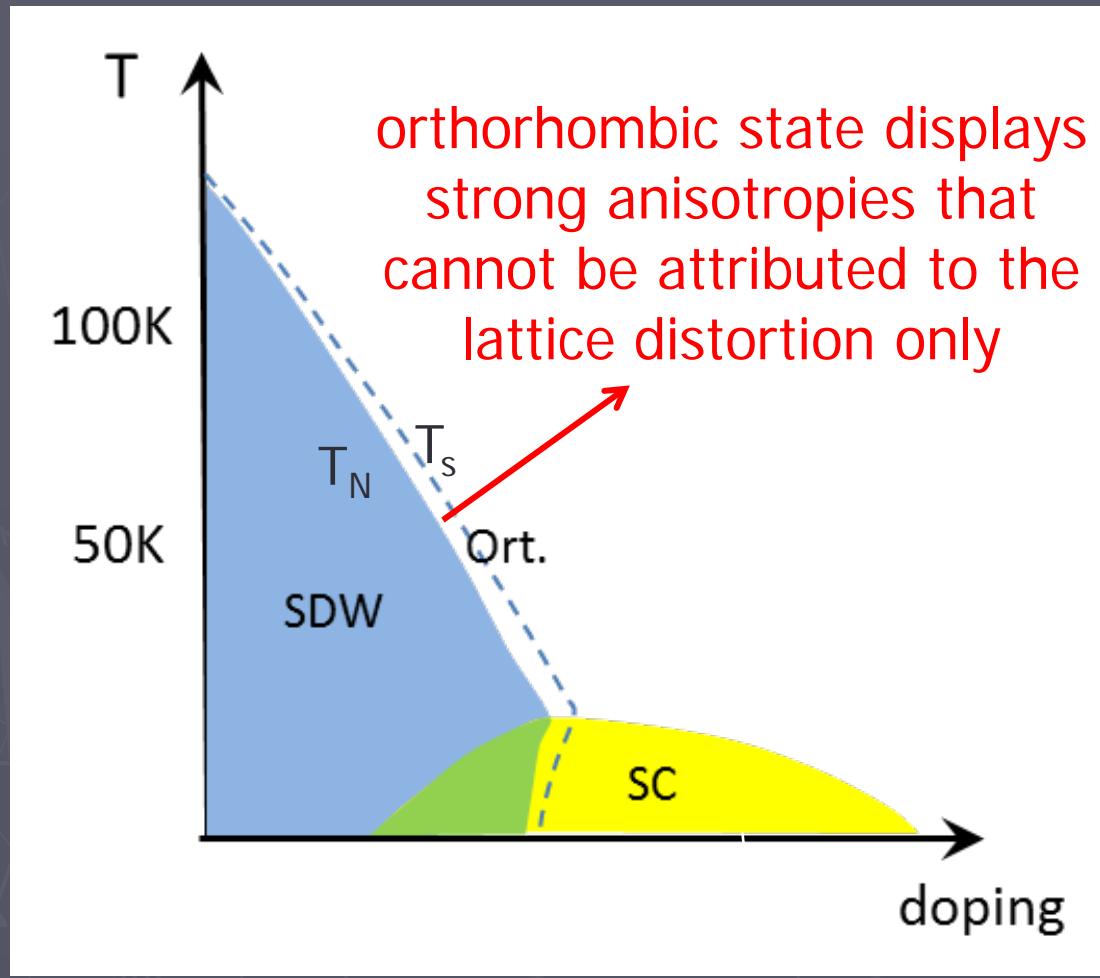


Alireza *et al.* (2008)

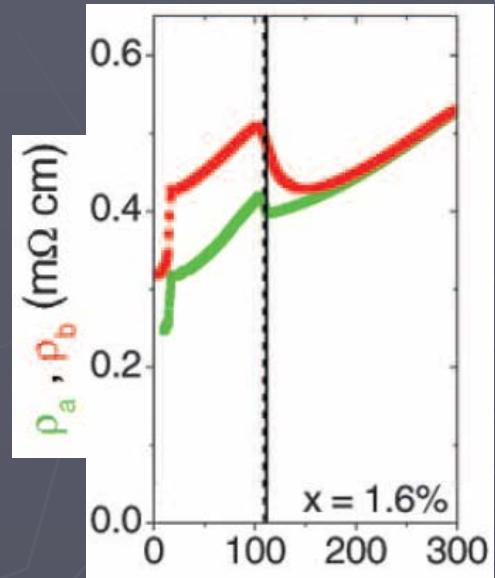


Fang *et al.* (2009)

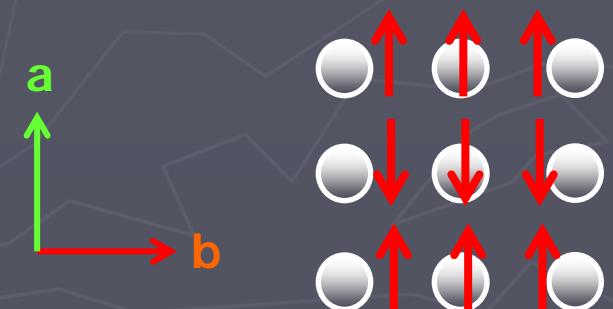
Nematic behavior



- resistivity

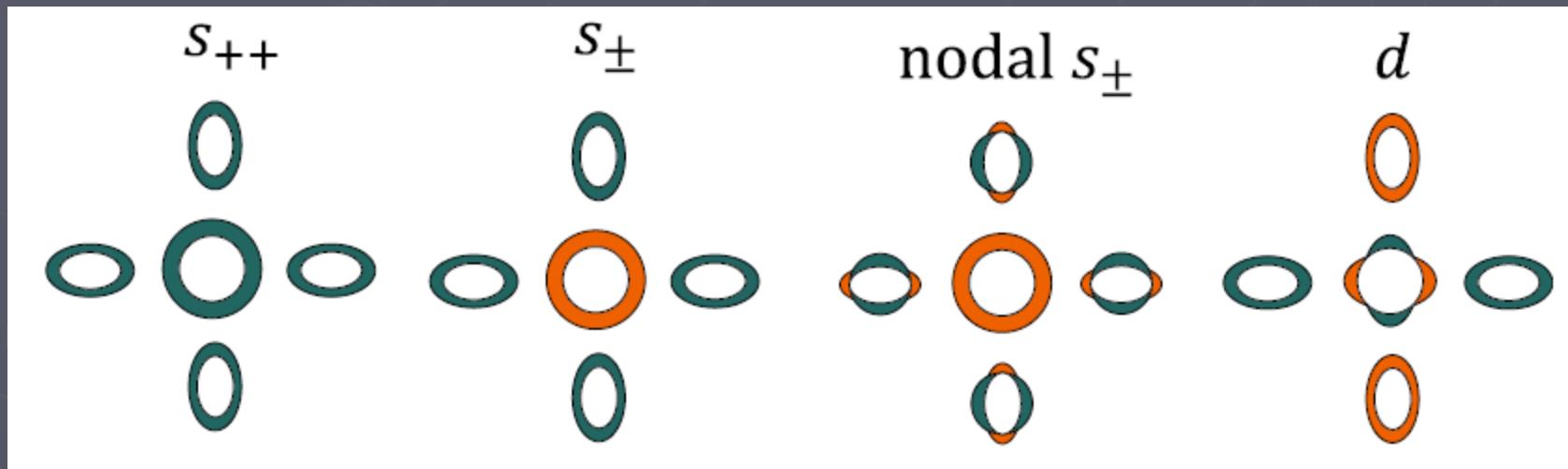


Chu et al, Science (2010)
Tanatar et al, PRB (2010)



SC gap symmetry and structure

$\Delta(\mathbf{k})$ = "energy gap" or "order parameter" or "pair wave function"

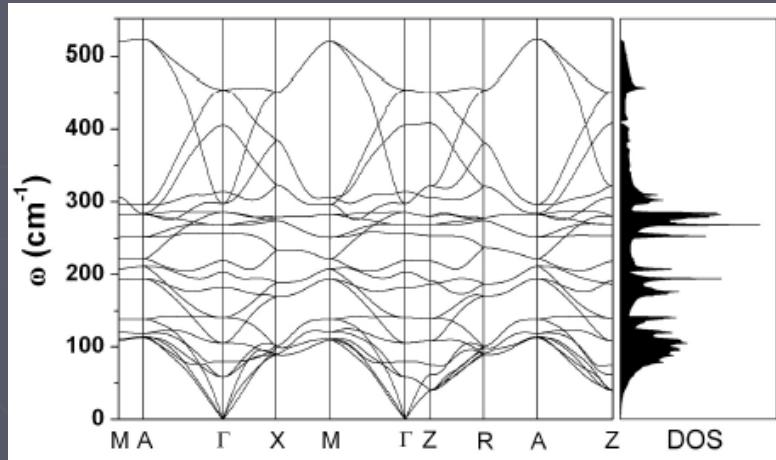


A_{1g}

B_{1g}

e-ph interaction is too weak

Phonon spectrum, density of states



Singh & Du PRL 2008

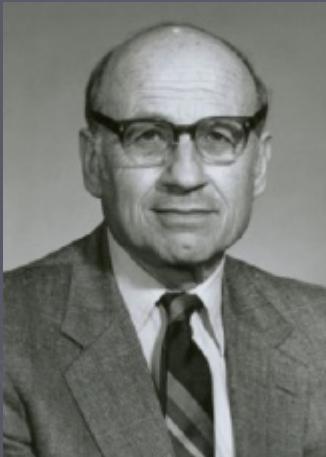
We have calculated *ab initio* the electron-phonon spectral function, $\alpha^2 F(\omega)$, and coupling, λ , for the stoichiometric compound [9]. Some moderate coupling exists, mostly to As modes, but the total λ appears to be ~ 0.2 , with $\omega_{log} \sim 250$ K, which can in no way explain $T_c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

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

superconductivity from e-e interactions

Pairing by exchange of spin, charge/orbital, nematic... fluctuations?

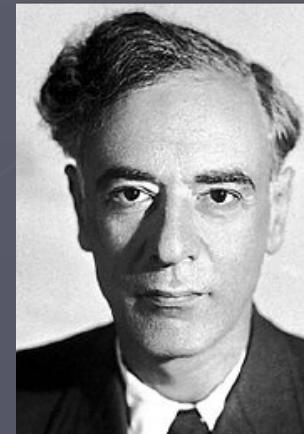
Prehistory: Kohn-Luttinger 1965



Walter Kohn



Quinn Luttinger



Also: Landau and Pitaevskii

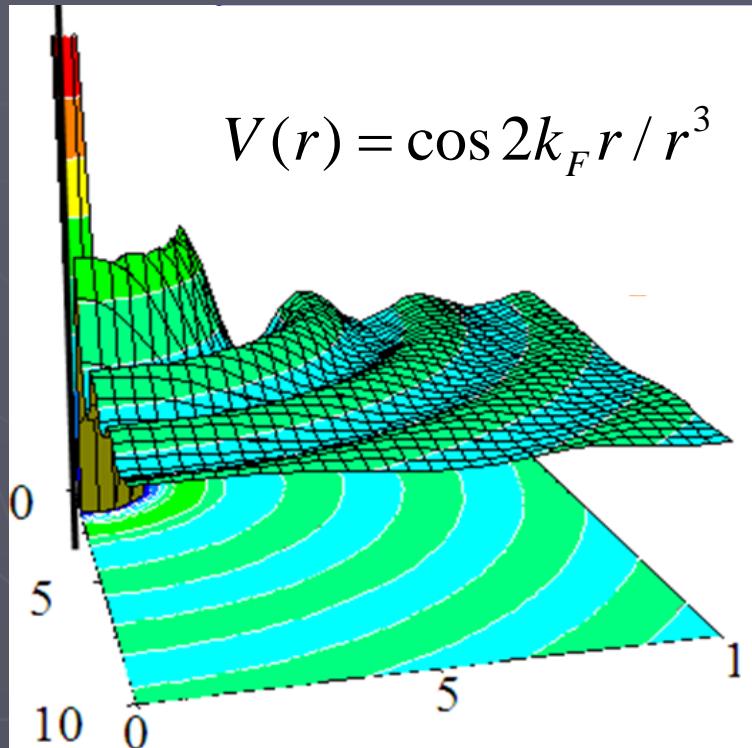


KL (1962): an electron gas with no phonons and only repulsive Coulomb interactions can be a superconductor!

A new paradigm: electrons avoid repulsive part of Coulomb interaction in space rather than time!

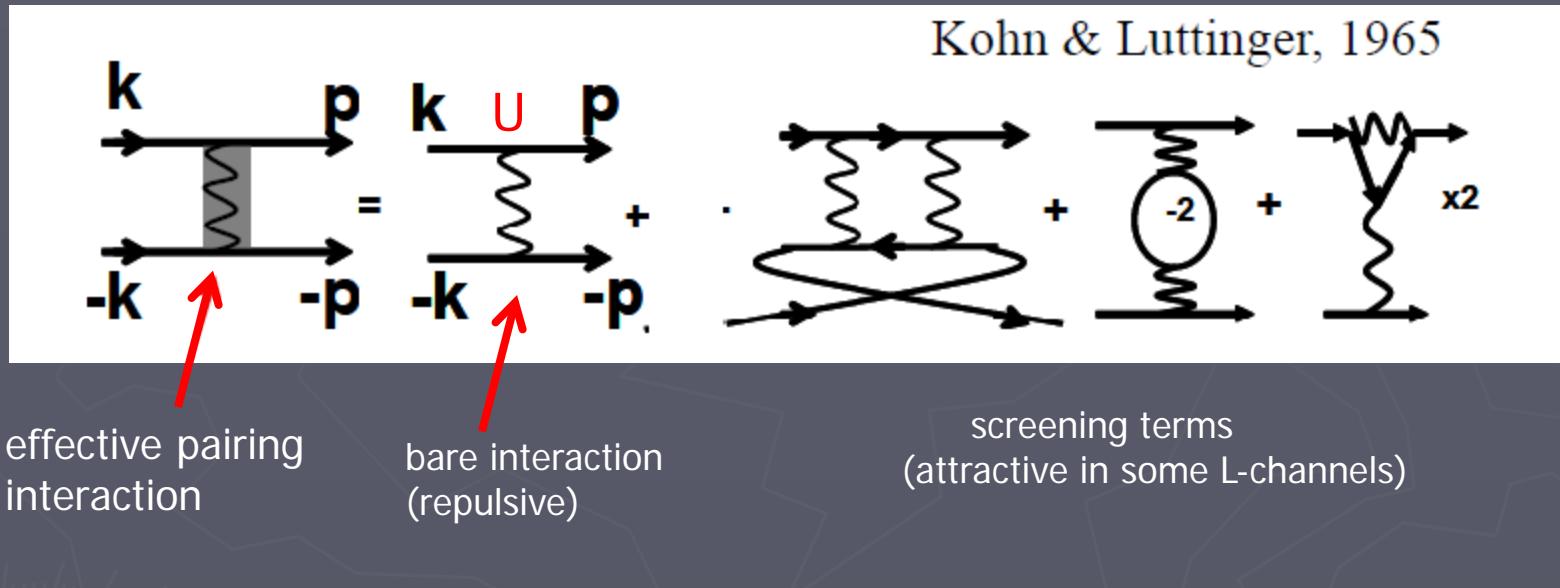
Prehistory: Kohn-Luttinger 1965

Friedel: screened Coulomb interaction



At finite distances, screened Coulomb interaction becomes attractive: finite-L pairing

Prehistory: Kohn-Luttinger 1965



Example: short range $U>0$ for rotationally invariant system ($\approx {}^3\text{He}$)

$$T_c \approx E_F \exp(-2.5L^4)$$

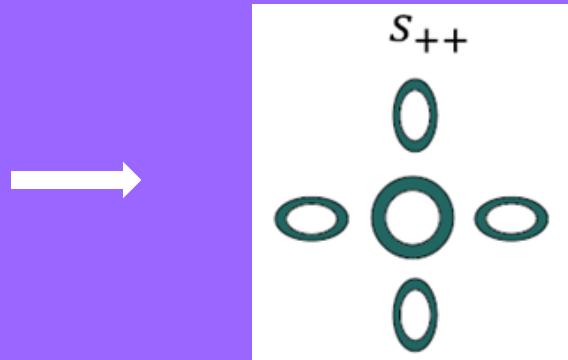
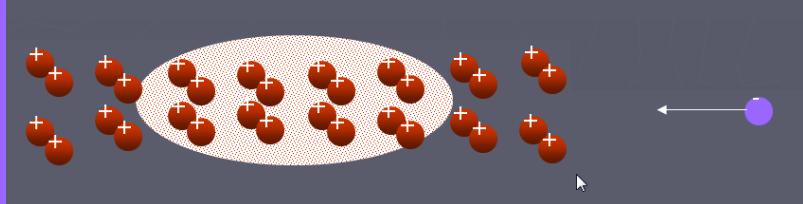
Best calculation in 1965: Brueckner Soda Anderson Morel PR 1960 :
predicted $L=2$ for ${}^3\text{He} \Rightarrow T_c \sim 10^{-17}\text{K}$

But had they taken $L=1$ they would have gotten $T_c \sim 1 \text{ mK!}$

2 paradigms for superconductivity

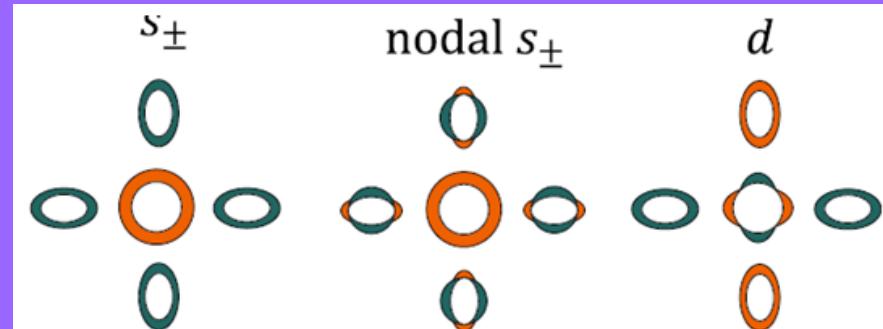
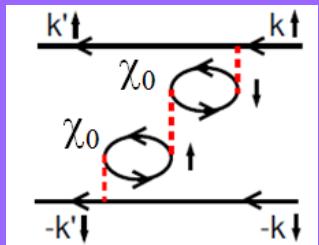
according to how pairs choose to avoid Coulomb interaction

"conventional" : isotropic s-wave pair wave fctn, interaction retarded in time



Overall effective interaction *attractive*

"unconventional": anisotropic or sign-changing pair wave fctn,



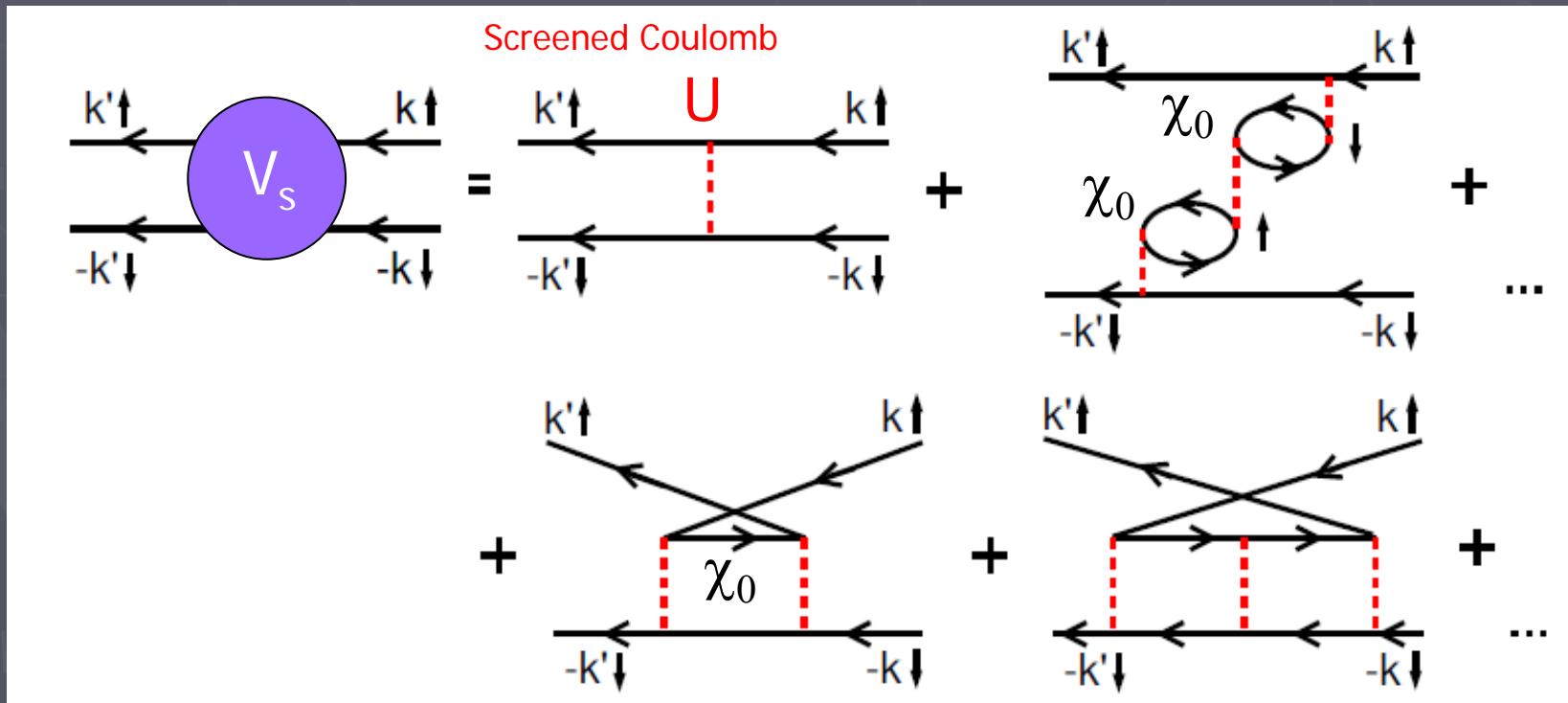
Overall effective interaction *repulsive*

Spin fluctuation theories of pairing

Effective singlet interaction from spin fluctuations (Berk-Schrieffer 1966)

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

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



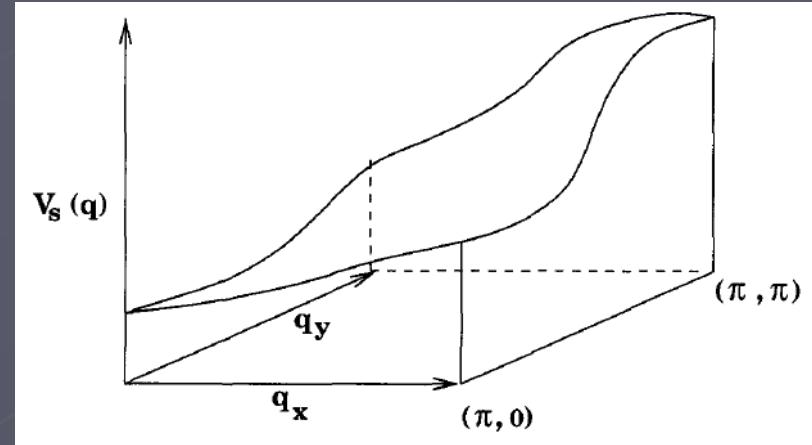
Spin fluctuation theories of pairing

Effective interaction from spin fluctuations (Berk-Schrieffer 1966)

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

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

paradigm: d -wave in cuprates from antiferromagnetic spin fluctuations



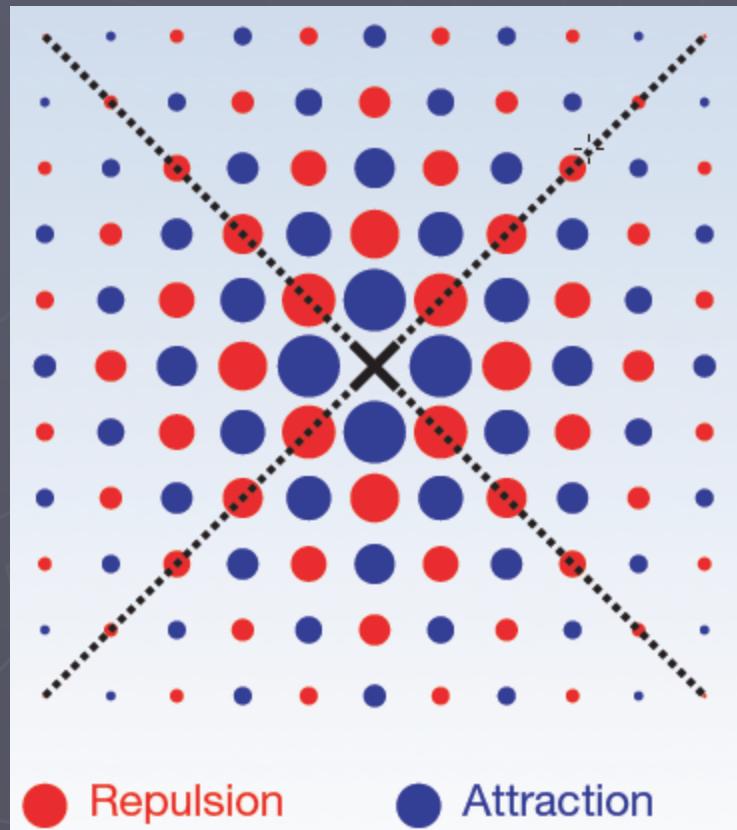
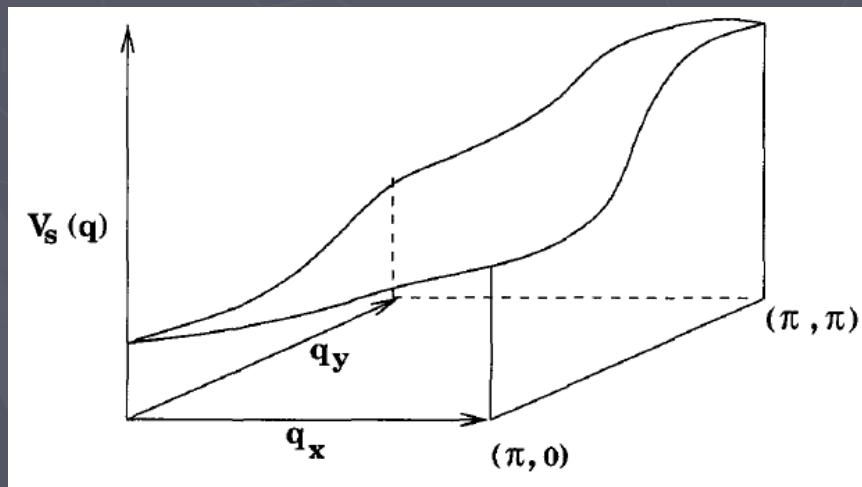
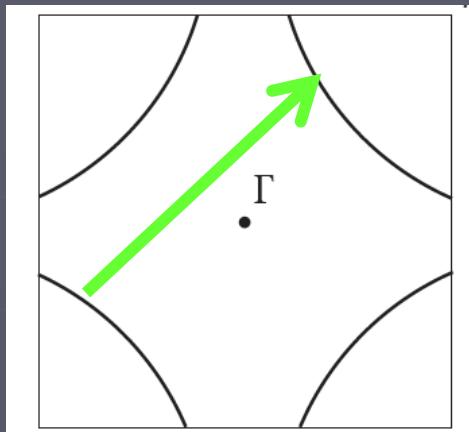
From DJ Scalapino, Phys Rep 1995

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

d -wave takes advantage of peak in spin susceptibility at $q=(\pi, \pi)!$

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

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

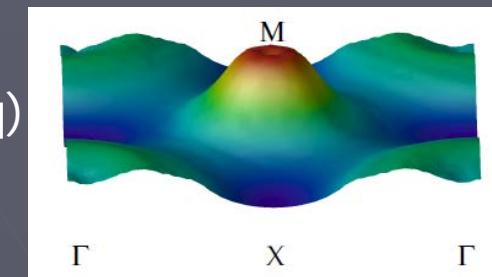
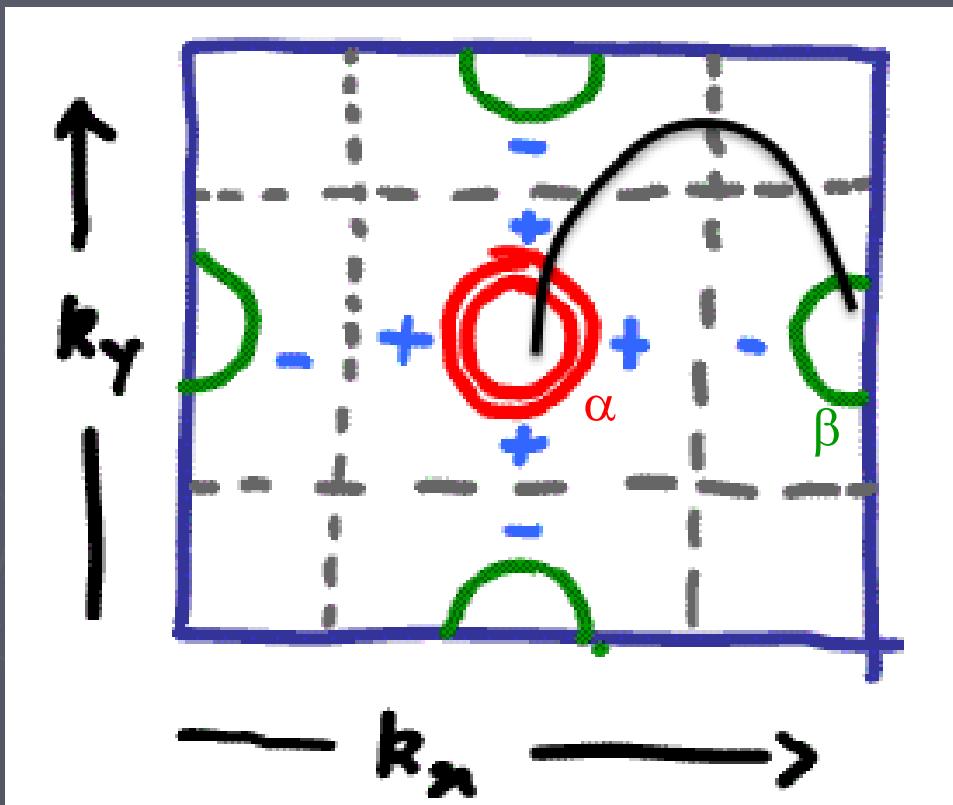


k -space:

$$V_s(k-k') \sim V_0 + V_2 \phi_d(k) \phi_d(k') + \dots$$

r -space

Similar argument from Mazin et al PRL 2008 for FeSC:
electron-hole pocket pair scattering dominates



$\chi(q)$

also:

Kuroki et al 2008

Seo et al. 2008

Chubukov et al 2008

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

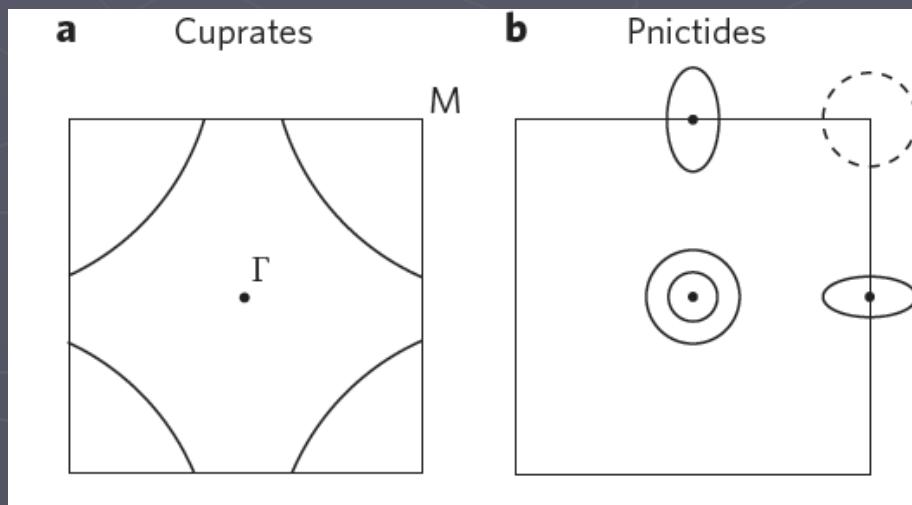
- nesting peaks interaction V_s at $\pi,0$ in 1-Fe zone.
- interaction is constant over sheet since they are small.
- therefore *isotropic* sign-changing $s_{+/-}$ state solves gap eqn

Comparing cuprates and FeSC

Table 1 | Properties of different classes of superconductor

Property	Conventional superconductors	Copper oxides	MgB ₂	Iron-based superconductors
T_c (maximum)	<30 K	134 K	39 K	56 K
Correlation effects	None (nearly-free electrons)	Strong local electronic interaction	None (nearly-free electrons)	Long-range (non-local) magnetic correlations
Relationship to magnetism	No magnetism	Parent compounds are magnetic insulators	No magnetism	Parent compounds are magnetic metals
Order parameter	One band, same-sign s wave	One band, sign-changing d wave	Two band, same-sign s wave	Two band, presumably sign-changing s wave
Pairing interaction	Electron-phonon	Probably magnetic (no consensus)	Electron-phonon	Presumably magnetic
Dimensionality	Three dimensional	Two dimensional	Three dimensional	Variable

I. Mazin, Nature 2010

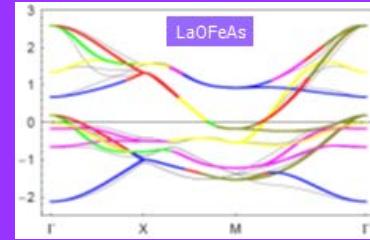


Different symmetry of superconducting order may be driven by *morphology of Fermi surface*
--- need not imply a different pairing mechanism

Spin fluctuation pairing theories in Fe-pnictides

$$H=H_0+H_{int}$$

H_0 =5-band tight-binding model

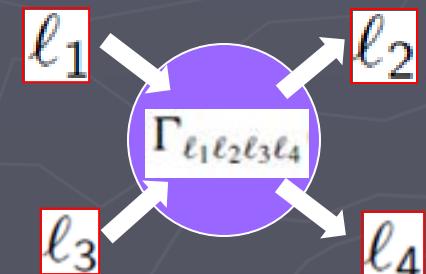


$$H = H_0 + \bar{U} \sum_{i,\ell} n_{i\ell\uparrow} n_{i\ell\downarrow} + \bar{U}' \sum_{i,\ell' < \ell} n_{i\ell} n_{i\ell'}$$

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

most general 2-body Hamiltonian
with **intrisite** interactions only!

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

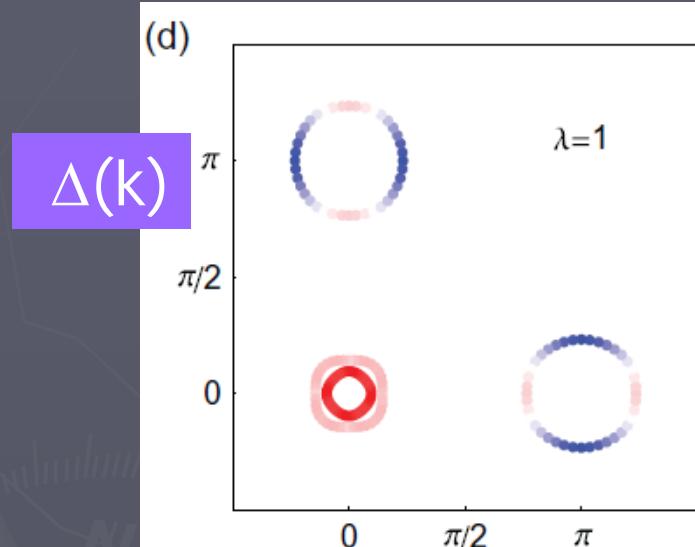


$$\Gamma_{\ell_1 \ell_2 \ell_3 \ell_4}(\mathbf{k}, \mathbf{k}', \omega) = \left[\frac{3}{2} \bar{U}^s \chi_1^{\text{RPA}}(\mathbf{k} - \mathbf{k}', \omega) \bar{U}^s + \frac{1}{2} \bar{U}^s - \frac{1}{2} \bar{U}^c \chi_0^{\text{RPA}}(\mathbf{k} - \mathbf{k}', \omega) \bar{U}^c + \frac{1}{2} \bar{U}^c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

Realistic theories: realistic gaps display strong anisotropy/ nodes

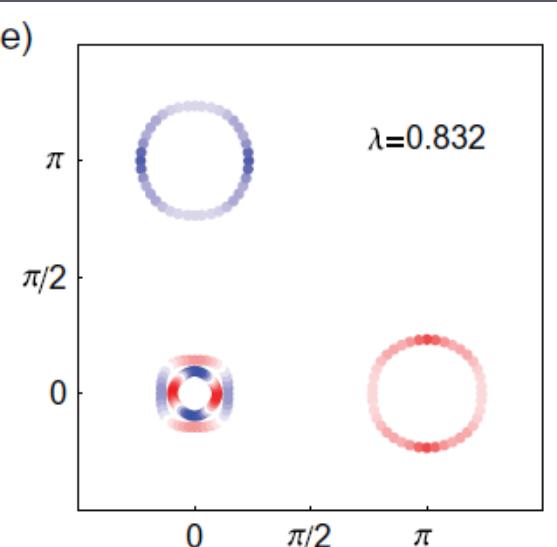
$$\Gamma_{\ell_1 \ell_2 \ell_3 \ell_4}(\mathbf{k}, \mathbf{k}', \omega) = \left[\frac{3}{2} \bar{U}^s \chi_1^{\text{RPA}}(\mathbf{k} - \mathbf{k}', \omega) \bar{U}^s + \frac{1}{2} \bar{U}^c \chi_0^{\text{RPA}}(\mathbf{k} - \mathbf{k}', \omega) \bar{U}^c + \frac{1}{2} \bar{U}^c \right]_{\ell_3 \ell_4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

"anisotropic extended-s"-wave



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

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



Graser, PJH et al 09, 10

similar:

Kuroki et al '08, '09
Ikeda et al '09, '10

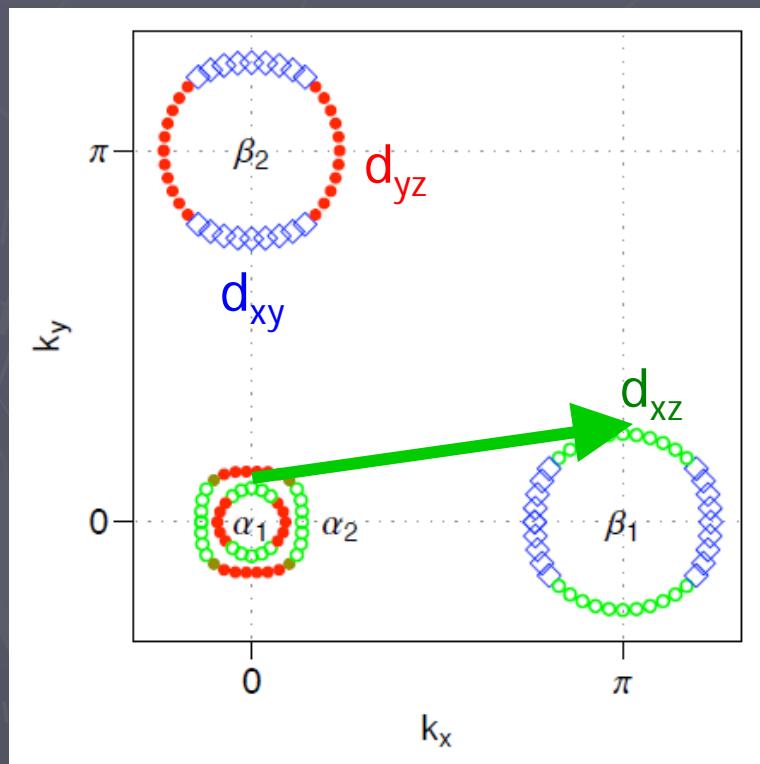
Two pairing channels nearly degenerate

- a) Can different FeAs materials have different symmetries?
- b) More likely: s-wave *symmetry*, differing gap *structures* for different materials

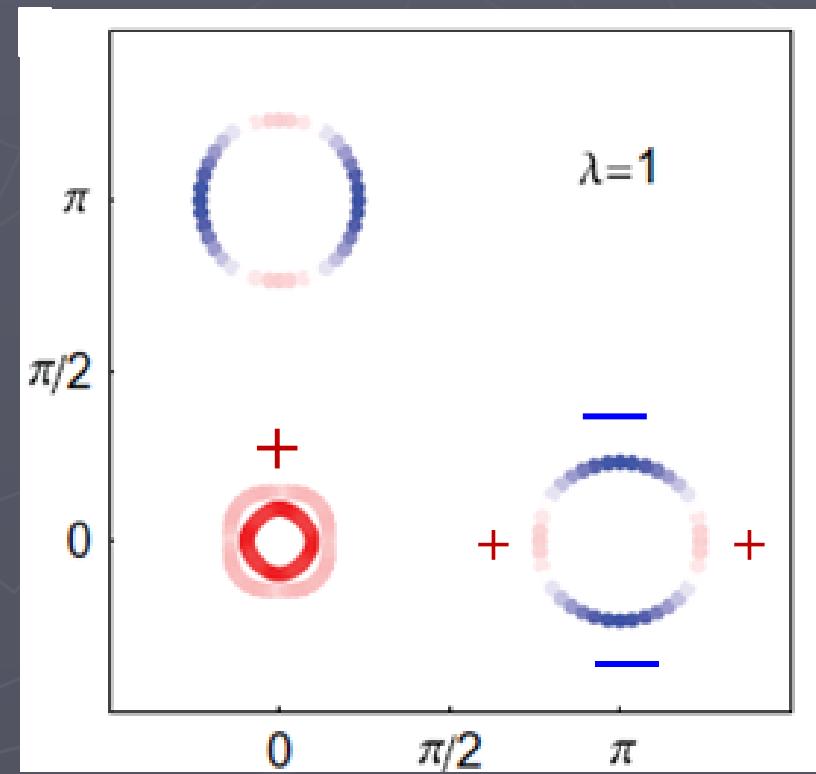
What is the origin of the gap anisotropy [Maier, PJH et al PRB 09]?

1. 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),
Zhang et al 2009 Thomale et al 2010, Kemper et al 2010



Fermi surface w/ orbital character



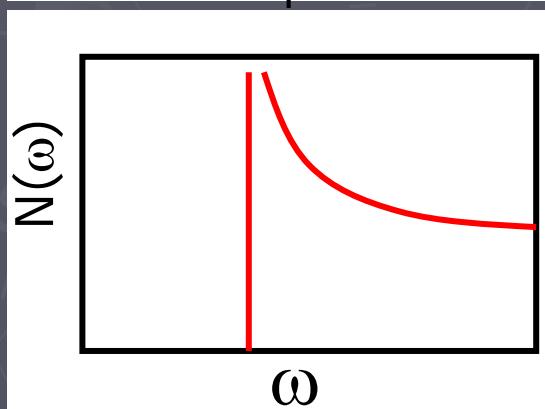
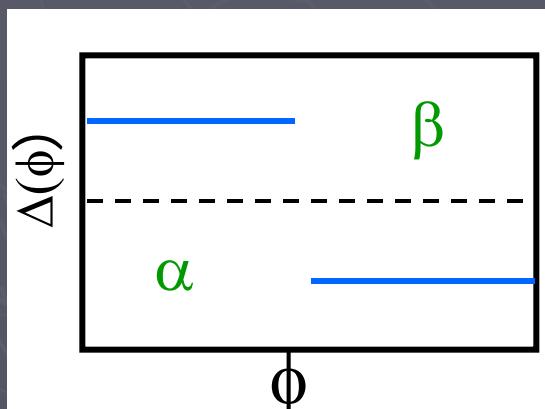
Gap

"sensitivity" to small changes in electronic structure

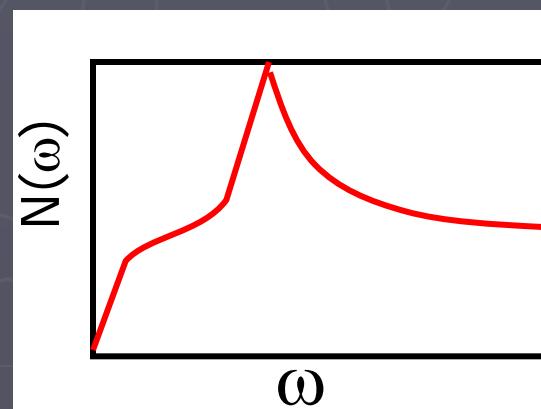
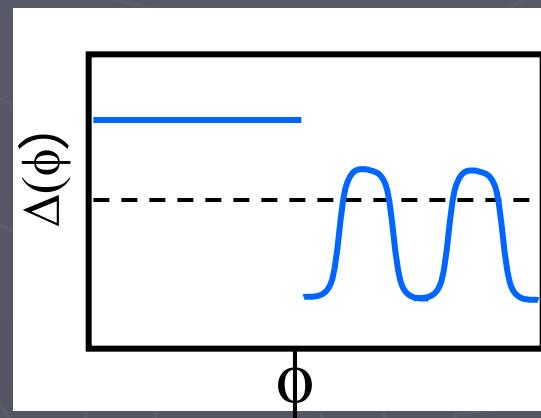
Kemper et al 2010

- a) changes to small Fermi pockets \Rightarrow big changes in gap
- b) any nodes are *accidental* rather than symmetry-enforced in ext.-s states

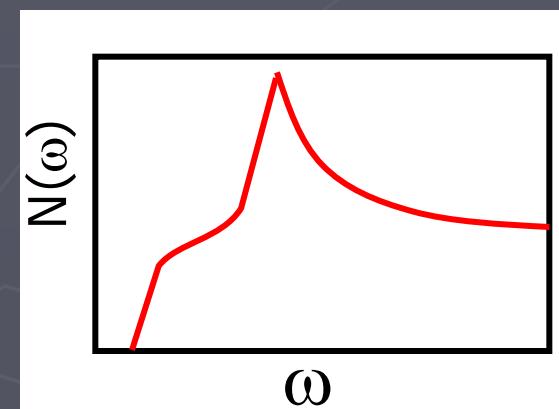
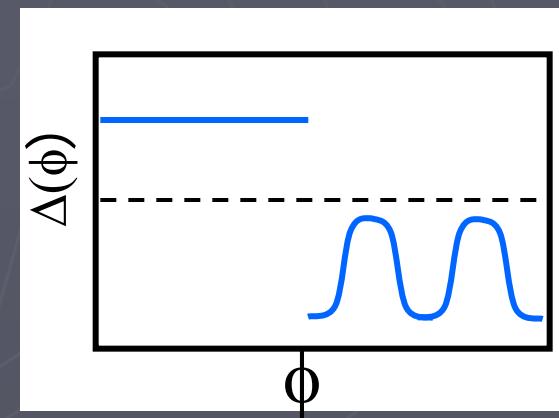
a) isotropic s_{+/−}



b) nodes



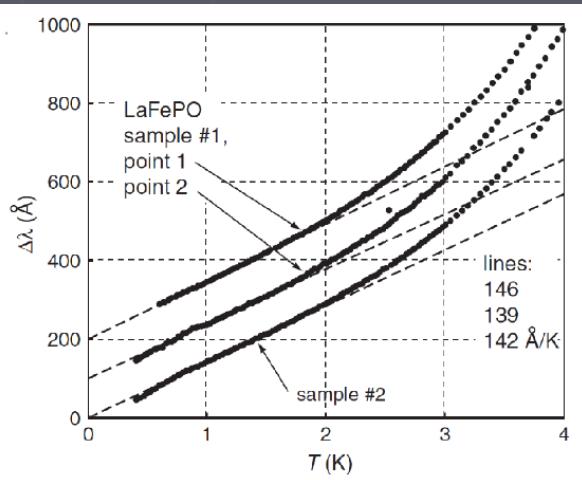
c) deep minima



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

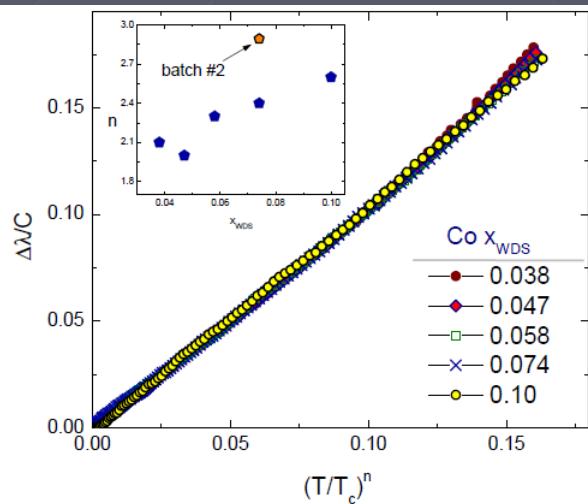
Hicks et al 2008

LaFePO $T_c=6\text{K}$



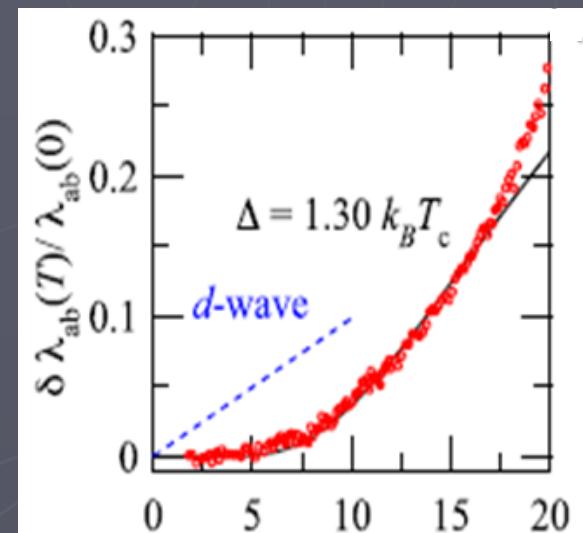
Prozorov, 2011

Co-doped Ba122 $T_c=25\text{K}$



Hashimoto et al 2009

K-doped Ba122 $T_c=40\text{K}$



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

dirty *nodal SC*
 clean *gapped SC*

$$N(\omega) \simeq N_0 + a\omega^2$$

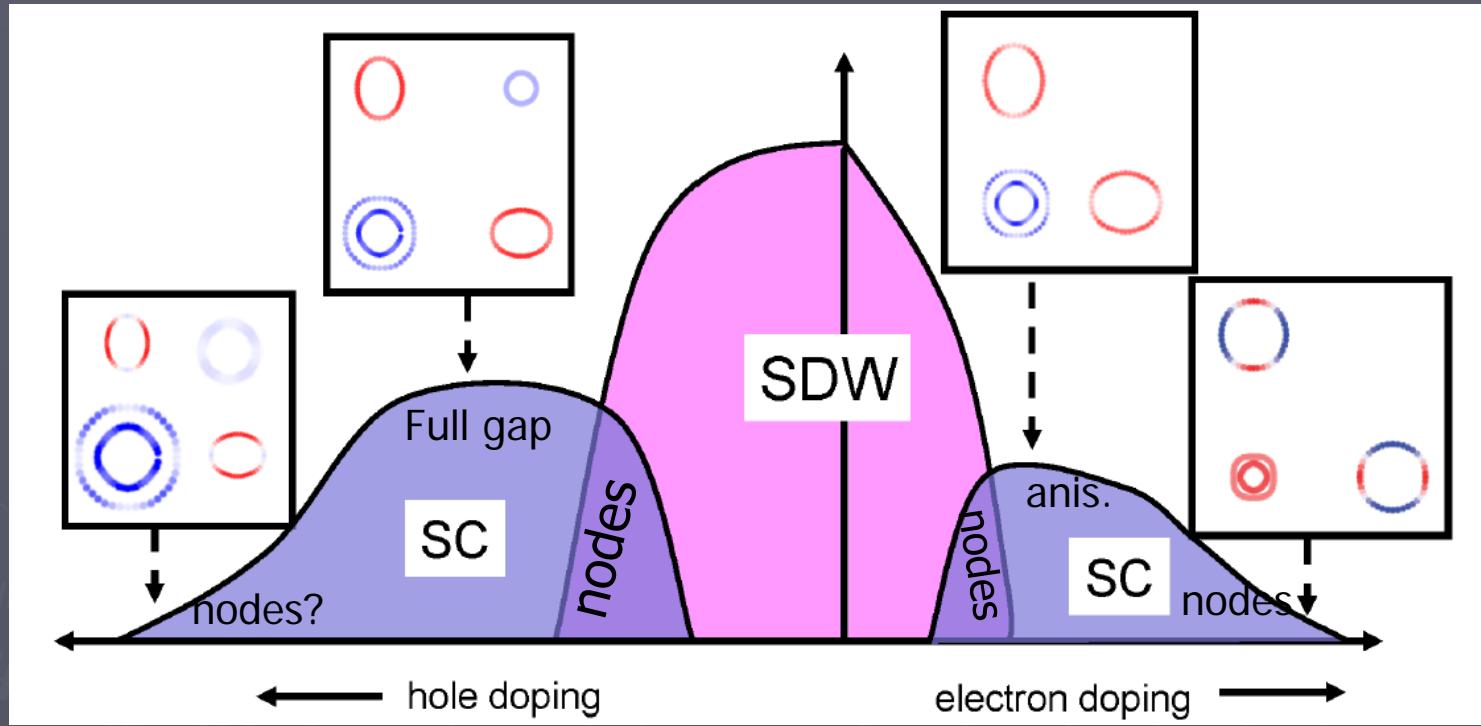
$$N(\omega) \simeq \omega$$

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

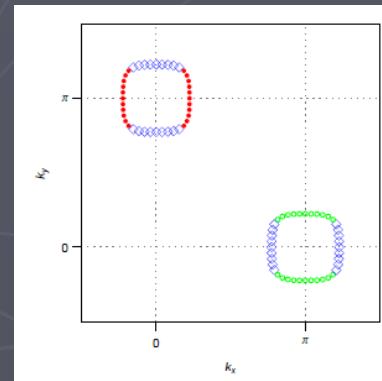
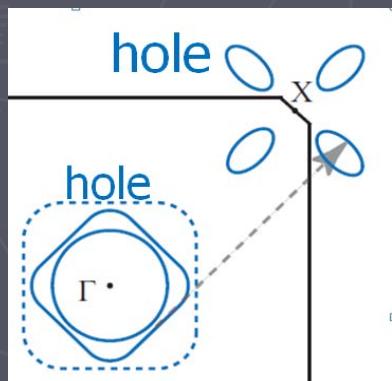
$$\text{so } \Delta\lambda \simeq e^{-\Delta/T}$$

Big picture: evolution of gap with doping

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

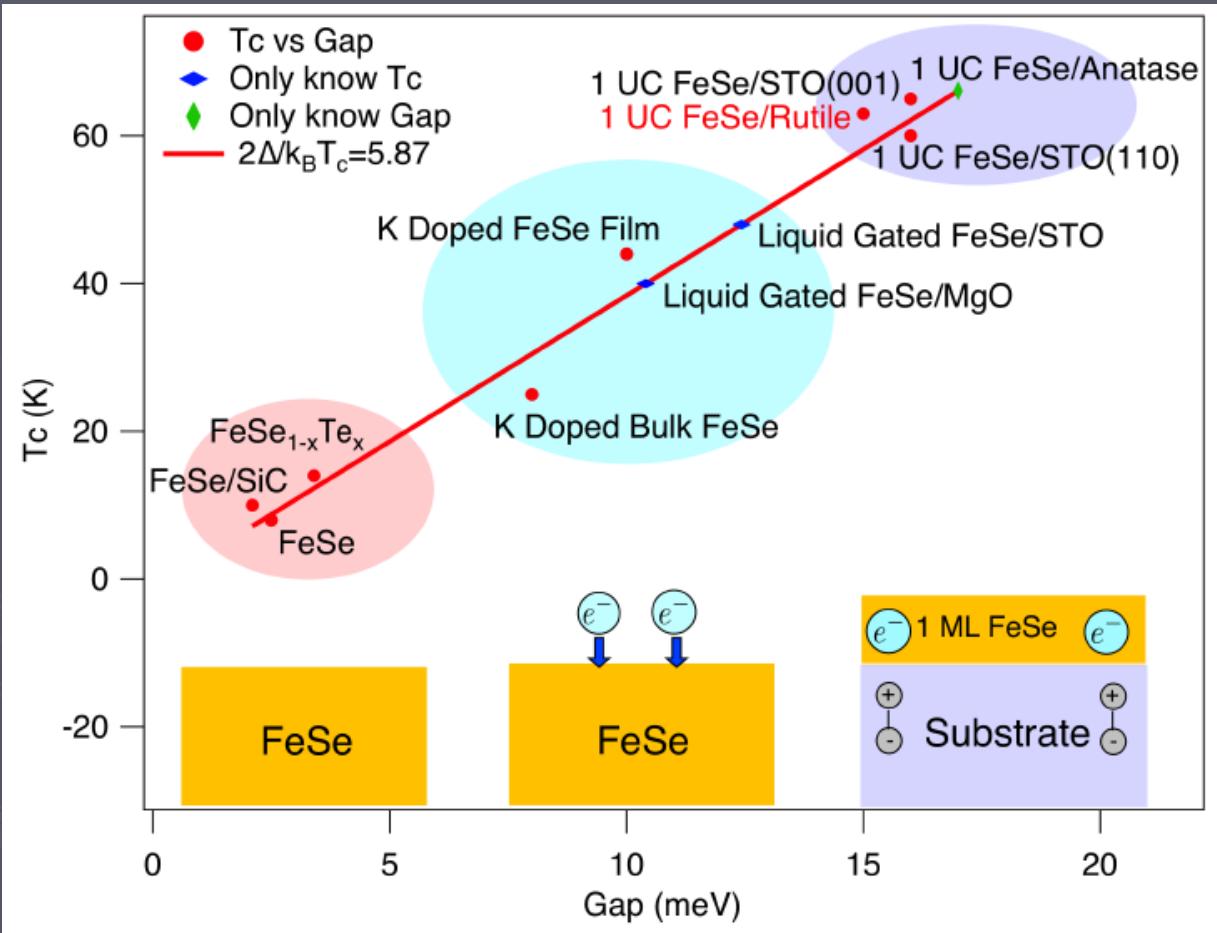


KFe_2As_2 :
No electron pockets: d-wave?
Thomale et al
S-wave:
Okazaki et al
(ARPES)



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

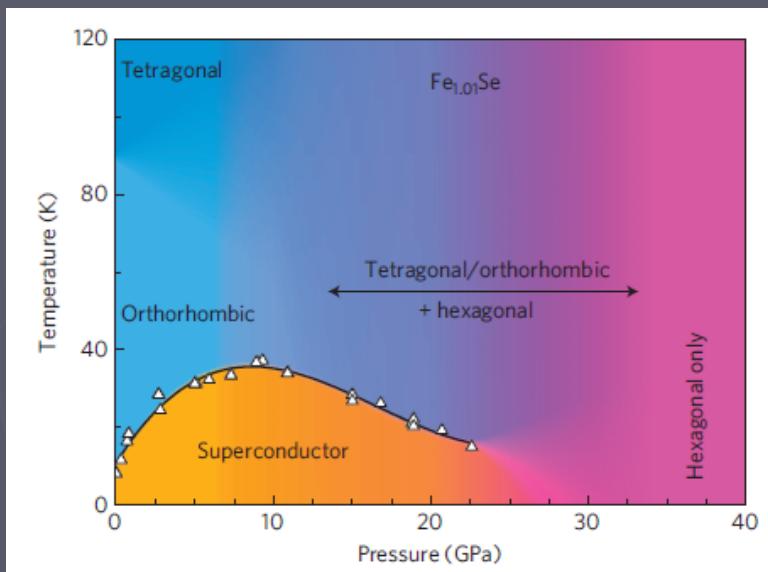
But: higher T_c from Fe chalcogenides



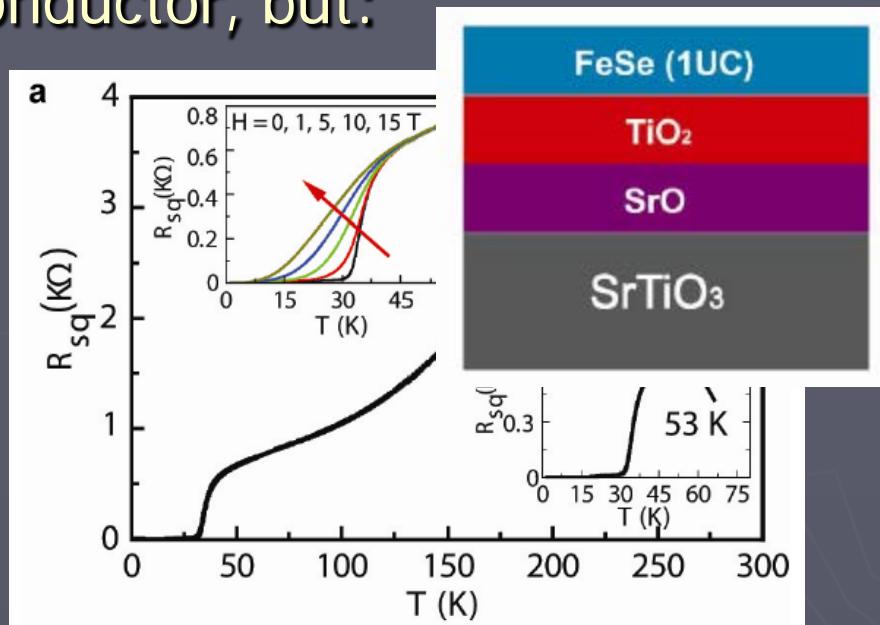
Rebec et al arXiv: 1606

see also PH, Comptes Rendus Physique 17, 197 (2016)
(Special focus issue on Fe-based superconductivity)

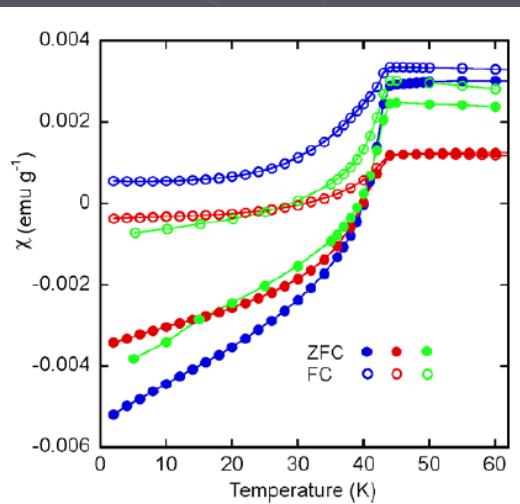
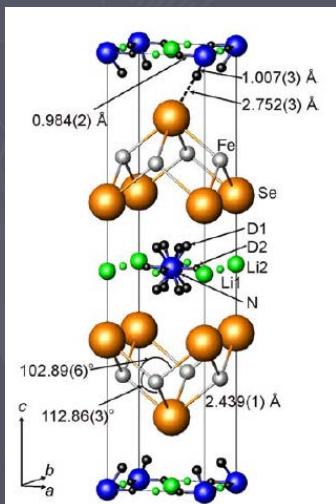
FeSe: nonmagnetic 8K superconductor, but:



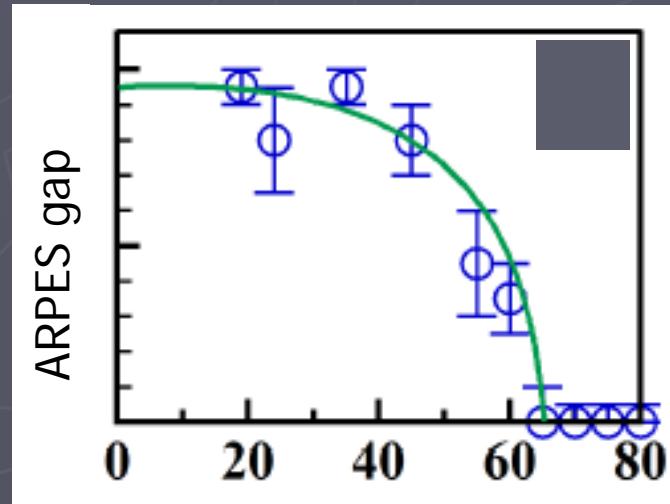
Medvedev et al 2010: $T_c \rightarrow 37\text{K}$ under pressure



Wang et al, Chin. Phys. Lett. 2012
1 layer $T_c \rightarrow 35\text{K}$ under tensile strain

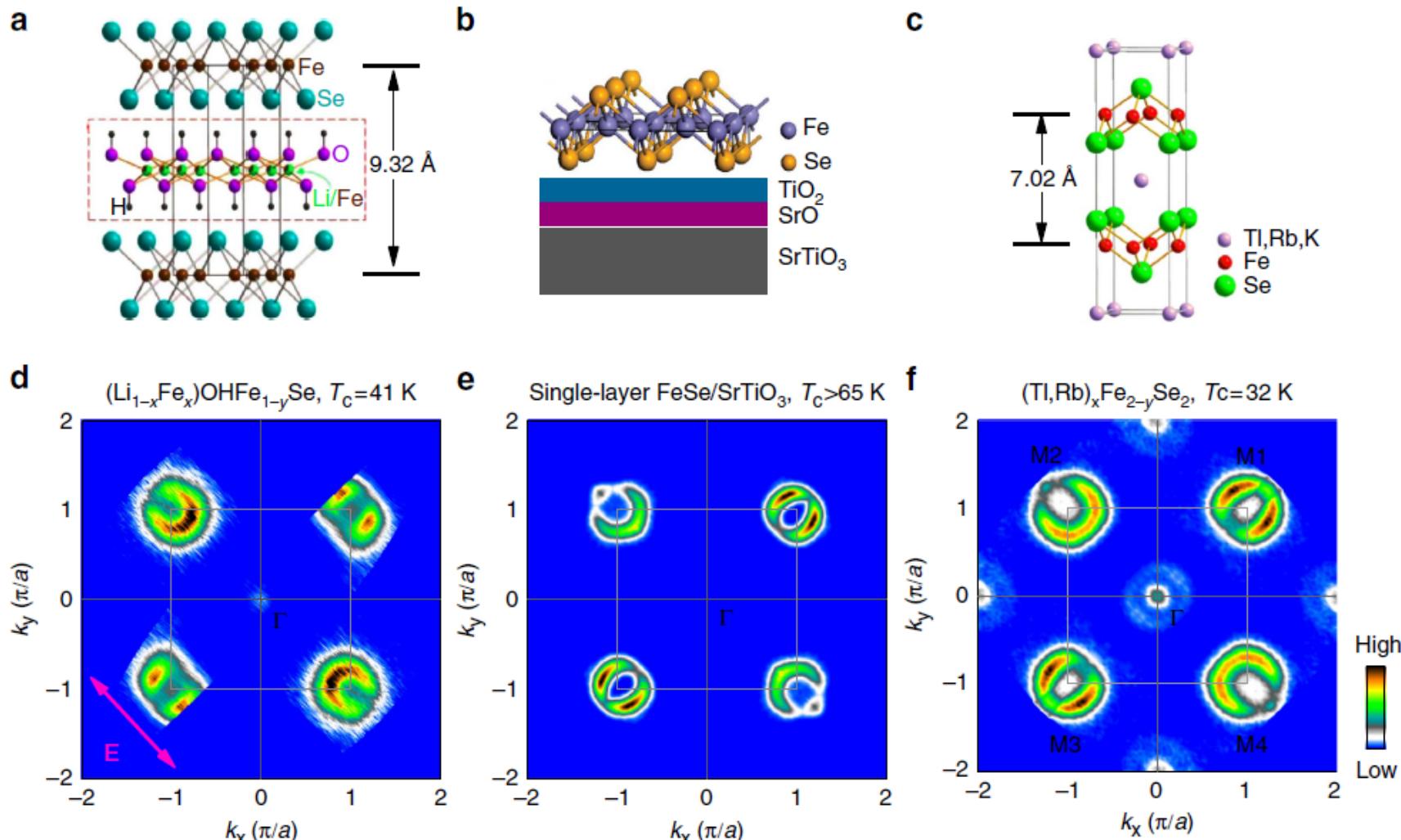


Burrard-Lucas et al 2012
 $T_c \rightarrow 43\text{K}$ molecular intercalation



S. He, Nat. Mat. 2013

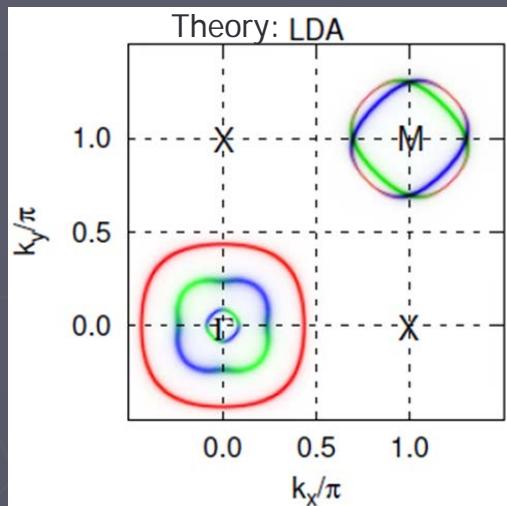
FeSC with electron pockets only goes against $s_{+/-}$ paradigm!



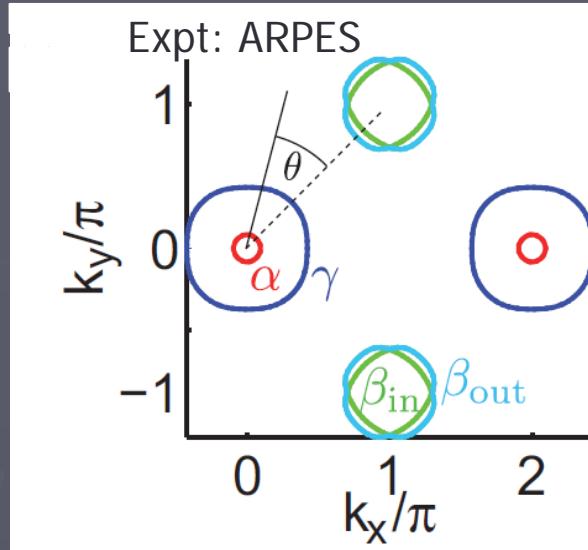
LiFeAs

$$k_z = \pi$$

Importance of correlations



Ferber et al PRB 2012



Wang et al 2013

Nearly compensated pockets *shrink* due to interband interactions



True to greater or lesser extent for all FeSC: Ortenzi et al PRL 2009

Quasiparticle renormalization factor: microscopic description of Landau theory

$$G(k, \omega) = [\omega - \epsilon_{k0} - \Sigma(k, \omega)]^{-1}$$

$$\epsilon_{k0} + \Sigma(k, \omega) = (k - k_F) \left[\frac{k_F}{m} + \frac{\partial \Sigma(k_F, 0)}{\partial k} \right] + \omega \frac{\partial \Sigma(k_F, 0)}{\partial \omega} + \dots$$

$$\begin{aligned}\epsilon_k &= (k - k_F)/m^* \\ m^{*-1} &= [m^{-1} + k_F^{-1} \partial \Sigma(k_F, 0)/\partial k] Z\end{aligned}$$

$$Z^{-1} = 1 - \partial \Sigma(k_F, 0)/\partial \omega$$

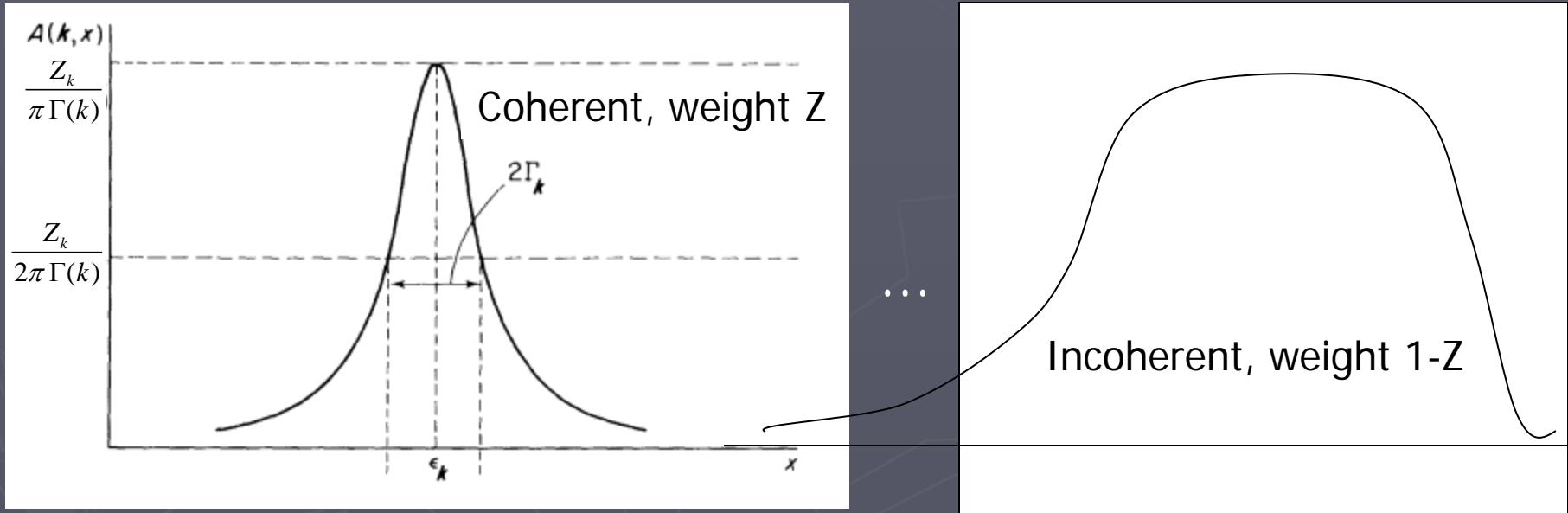
$$G(k, \omega) = Z (\omega - \epsilon_k)^{-1} + G'(k, \omega)$$

coherent quasiparticle

incoherent excitations

Quasiparticle renormalization factor: Landau theory

Z=quasiparticle residue



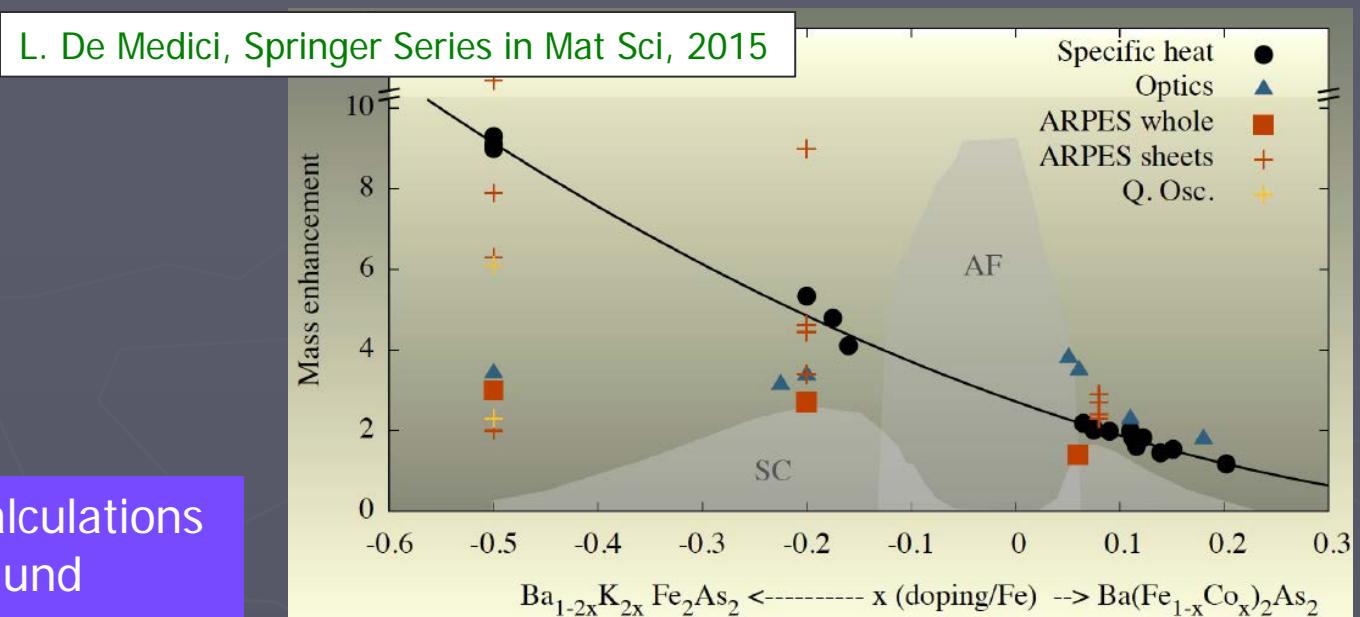
Orbital selective correlations: tendency for certain orbitals (d_{xy} !) to be more strongly renormalized than others

$\pi^{-1} \operatorname{Im}$

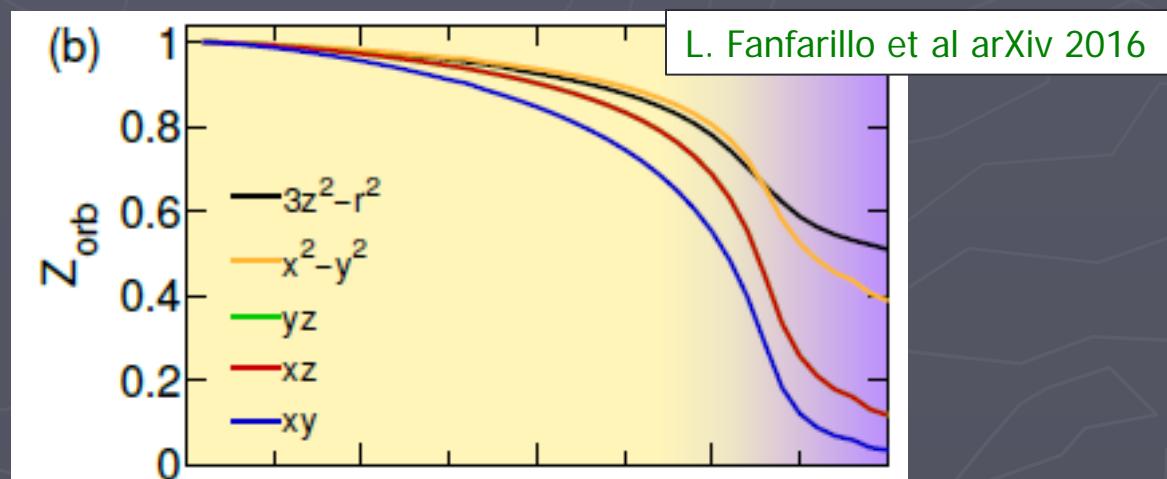
$$G(k, \omega) = Z (\omega - \epsilon_k)^{-1} + G'(k, \omega)$$

Orbitally selective correlations:

LDA+DMFT: Z.P. Yin et al, Nat. Mat. (2011)



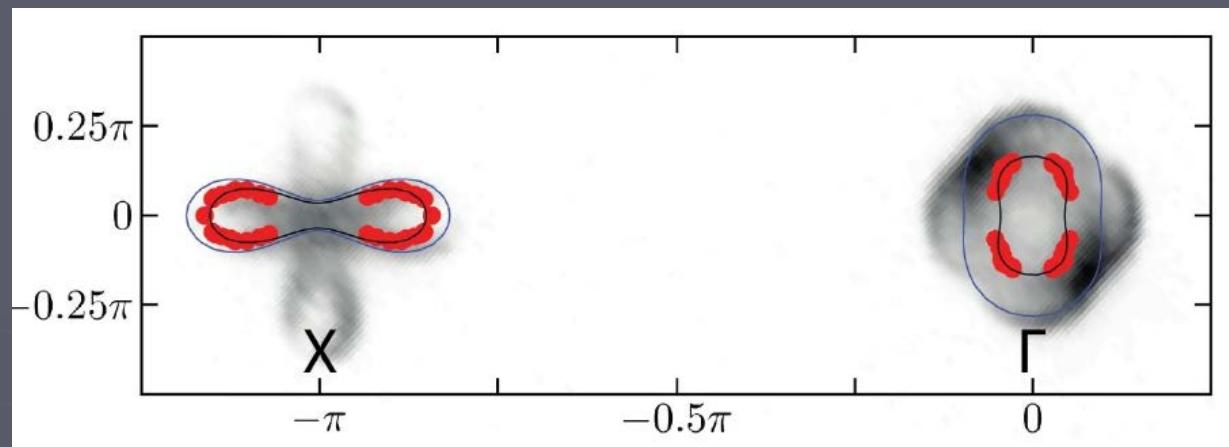
"slave spin" calculations
for Hubbard-Hund
Hamiltonian



What are the implications for pairing ???

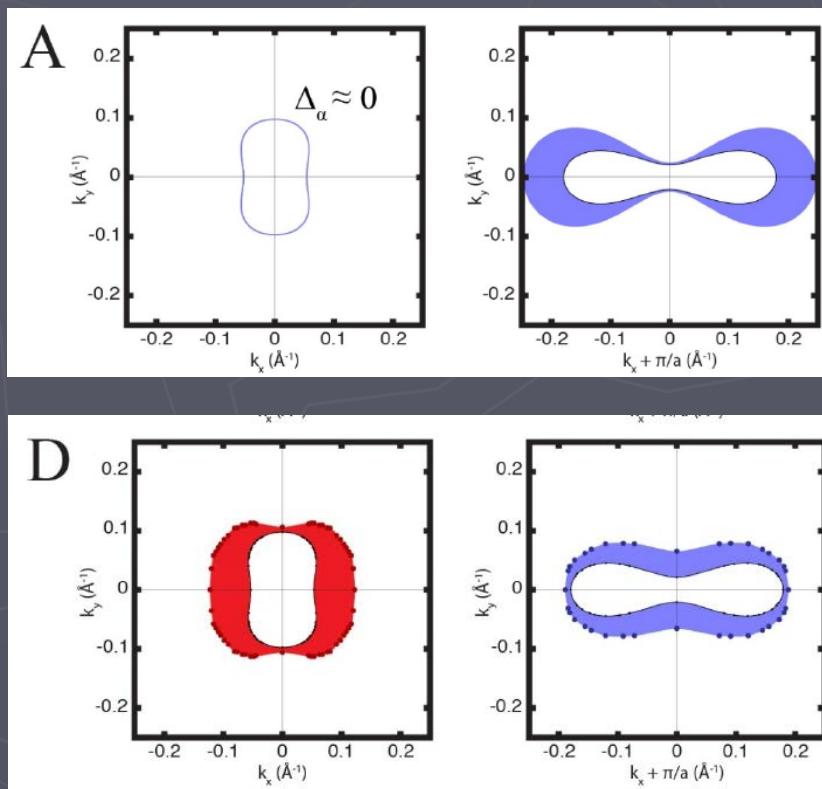
FeSe: 1st (QPI) gap measurements *disagree* with standard spin fluctuation pairing theory

Fit to ARPES Fermi surface also reproduces QPI Fermi surface



theory

However spin fluctuation theory gap is quite different from measurement



expt.

Sprau et al. arXiv 2016

Renormalize Green's function with qp weights

Sprau et al. arXiv 2016

$$G_{ab}(\mathbf{k}, \omega) = Z_{ab} G_{ab}^0(\mathbf{k}, \omega)$$

$$c_a \rightarrow \sqrt{Z_a} c_a$$

\Rightarrow

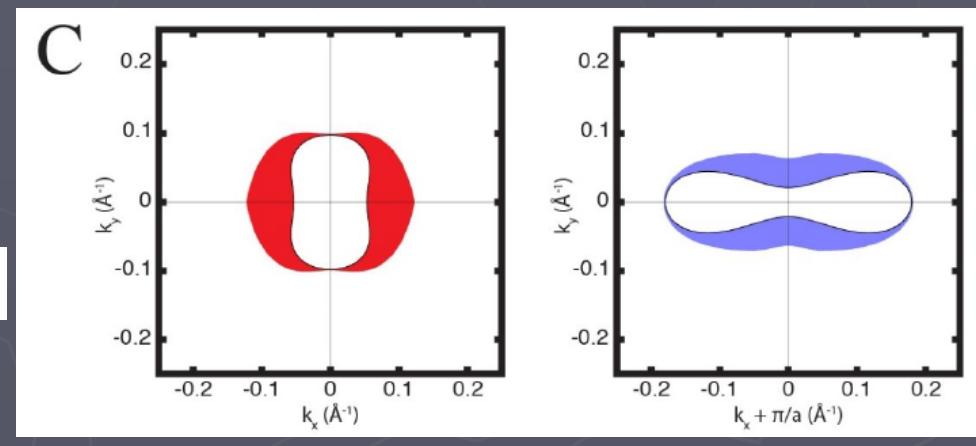
$$Z_{ab} = \sqrt{Z_a} \sqrt{Z_b}$$

Z-factors

theory

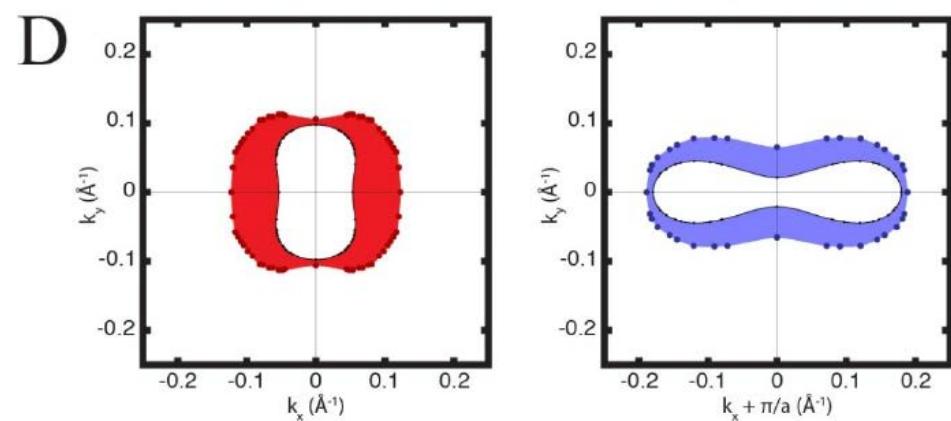
$$d_{xy}, d_{x^2-y^2}, d_{xz}, d_{yz}, d_{3z^2-r^2}$$

0:2715; 0:9717; 0:4048; 0:9236; 0:5916



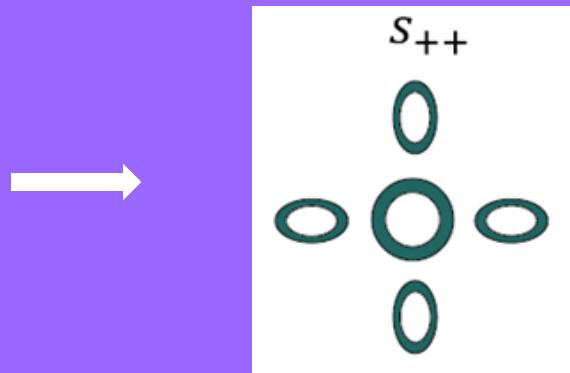
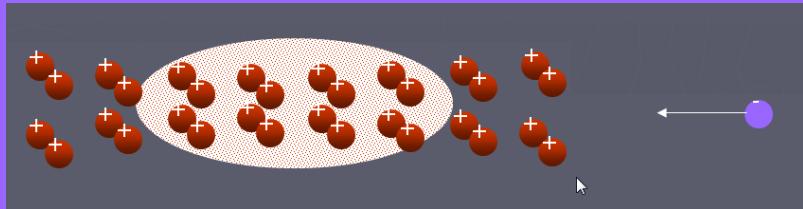
expt.

Also works well with LiFeAs,
monolayer FeSe
Kreisel et al arXiv: 2016



Conclusions I: 2 paradigms for superconductivity

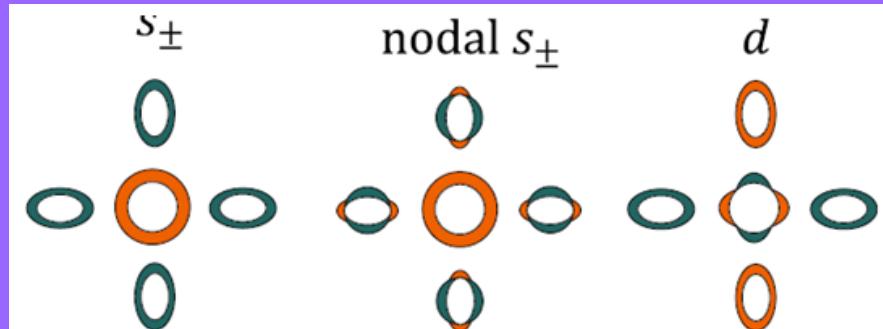
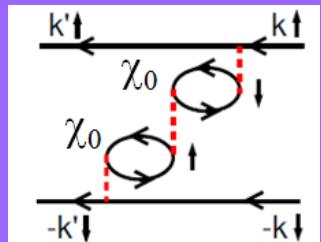
"conventional" : isotropic s-wave pair wave fctn, interaction retarded in time



Overall effective interaction *attractive*

Elements, A15s, MgB₂, borocarbides, A-doped C₆₀,

"unconventional": anisotropic or sign-changing pair wave fctn,



Overall effective interaction *repulsive*

Cuprates, Fe-based, heavy fermions, organics,

Conclusions II/questions

- Symmetry of SC order in systems with repulsive interactions often dictated by morphology of Fermi surface. FeSC appear to be A_{1g} ("s-wave"), probably with overall sign change-- nodes in some systems, not in others. What are the consequences of residual electronic correlations?
- Are there several families of SC linked by common pairing mechanism—"common thread"?
- Higher T_c ? Materials-specific calculations needed.
- Recent news: superconductivity at 200K in H_3S under pressure ([Drozdov, Nature 2015](#)). No limit on e-ph T_c , superconductivity reinvents itself again!
(see Cappelluti talk this afternoon)