Back to the Iron age – the physics of Fe-pnictides

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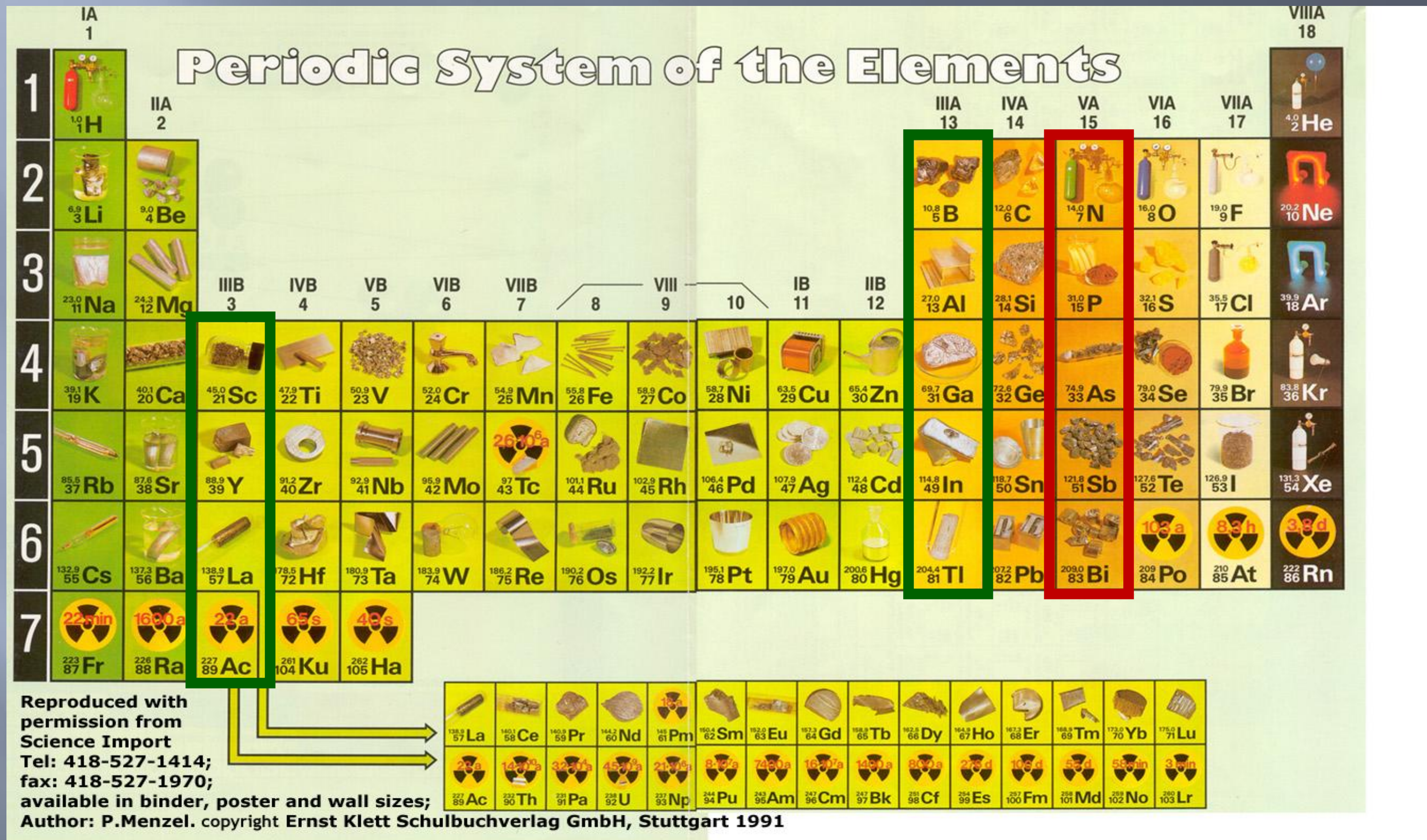
University of Wisconsin

KIAS, Dec. 16, 2009

Pnictides πνίγειν (Greek for chocking, suffocation):



Pnictides – elements from Group V of Periodic Table: nitrogen, phosphorus, arsenic, antimony and bismuth

III-V Semiconductors – formed by elements from Groups III and V:

Reviews:

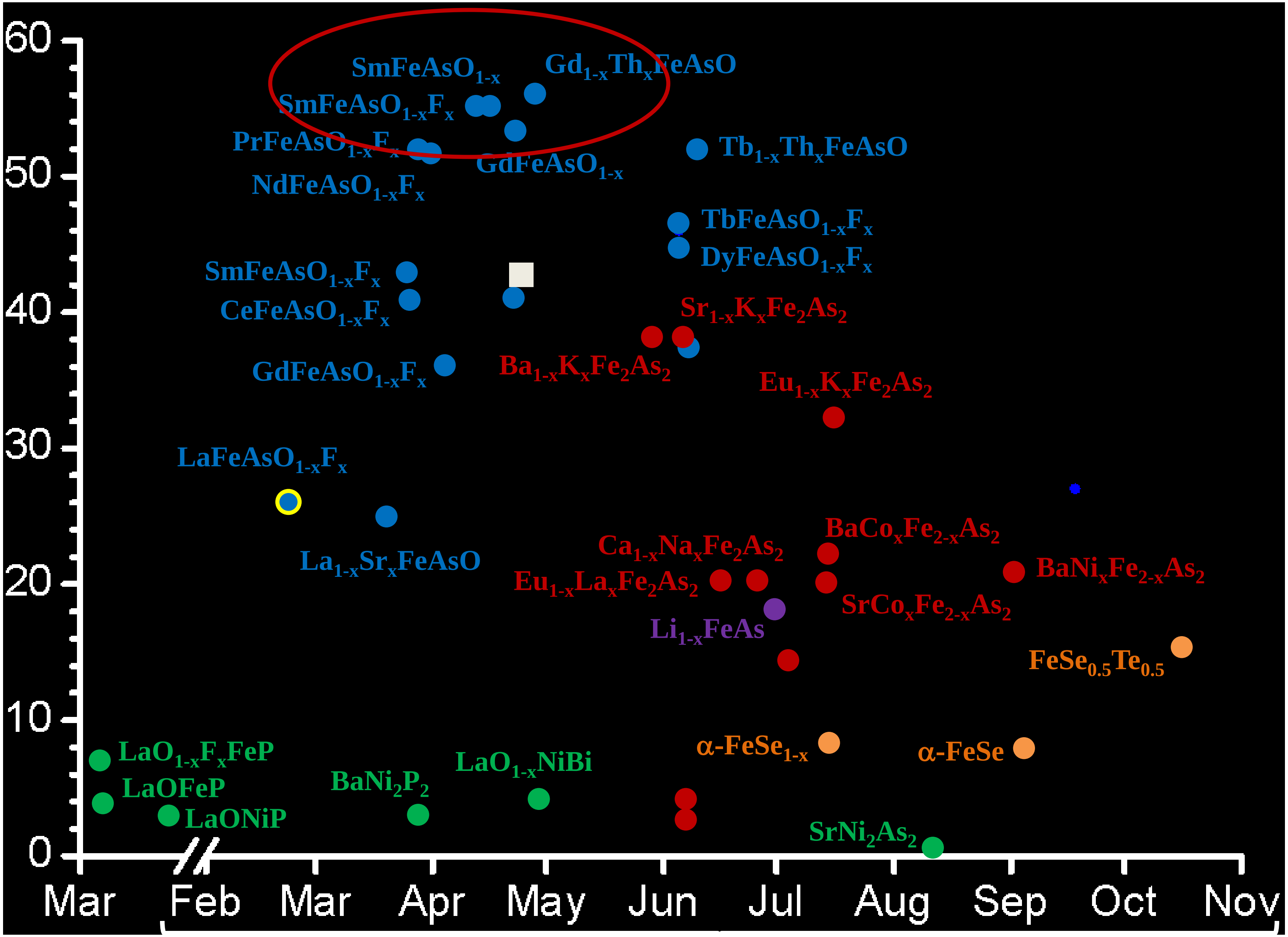
M.R. Norman, Physics **1**, 21 (2008); C. Xu and S. Sachdev, Nature Physics 4, 898 (2008); M.V. Sadovskii, Sov. Phys. Uspekhi.

I.I. Mazin and J. Schmalian, Physica C, 469, 614 (2009)

A.V. Chubukov, Physica C, **469**, 640 (2009).

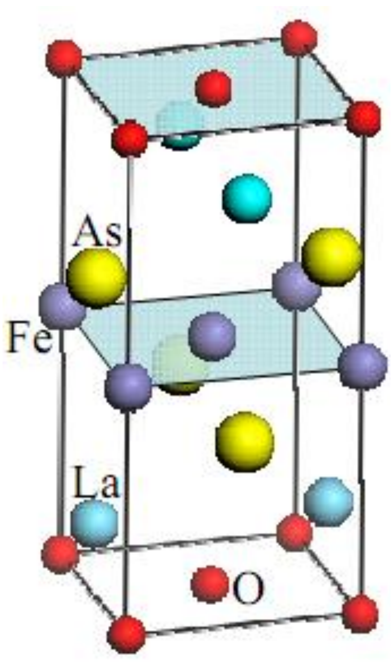
S. Graser, T. A. Maier, P.J. Hirschfeld and D.J. Scalapino, New J. Phys. **11**, 025016 (2009)

Fa Wang, Hui Zhai, Ying Ran, Ashvin Vishwanath, and Dung-Hai Lee, Phys. Rev. Lett. **102**, 047005 (2009).

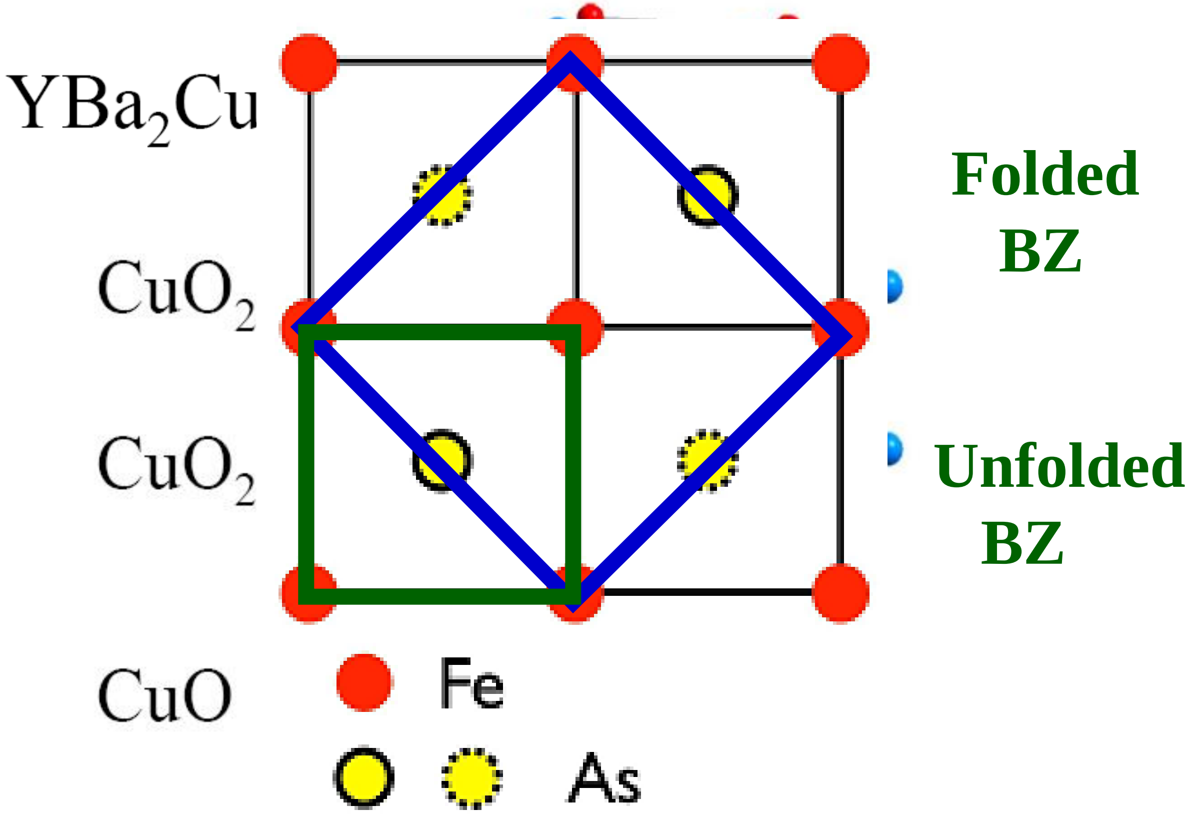


60
50
40
30
20
10
0
$SmFeAsO_{1-x}$
$Gd_{1-x}Th_xFeAsO$
$SmFeAsO_{1-x}F_x$
$PrFeAsO_{1-x}F_x$
$GdFeAsO_{1-x}$
$Tb_{1-x}Th_xFeAsO$
$NdFeAsO_{1-x}F_x$
$TbFeAsO_{1-x}F_x$
$DyFeAsO_{1-x}F_x$
$SmFeAsO_{1-x}F_x$
$CeFeAsO_{1-x}F_x$
$Sr_{1-x}K_xFe_2As_2$
$GdFeAsO_{1-x}F_x$
$Ba_{1-x}K_xFe_2As_2$
$Eu_{1-x}K_xFe_2As_2$
$LaFeAsO_{1-x}F_x$
$BaCo_xFe_{2-x}As_2$
$Ca_{1-x}Na_xFe_2As_2$
$La_{1-x}Sr_xFeAsO$
$Eu_{1-x}La_xFe_2As_2$
$BaNi_xFe_{2-x}As_2$
$SrCo_xFe_{2-x}As_2$
$Li_{1-x}FeAs$
$FeSe_{0.5}Te_{0.5}$
$LaO_{1-x}F_xFeP$
$LaO_{1-x}NiBi$
α-$FeSe_{1-x}$
α-FeSe
LaOFeP
$BaNi_2P_2$
LaONiP
$SrNi_2As_2$
Mar
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov

Crystal structure



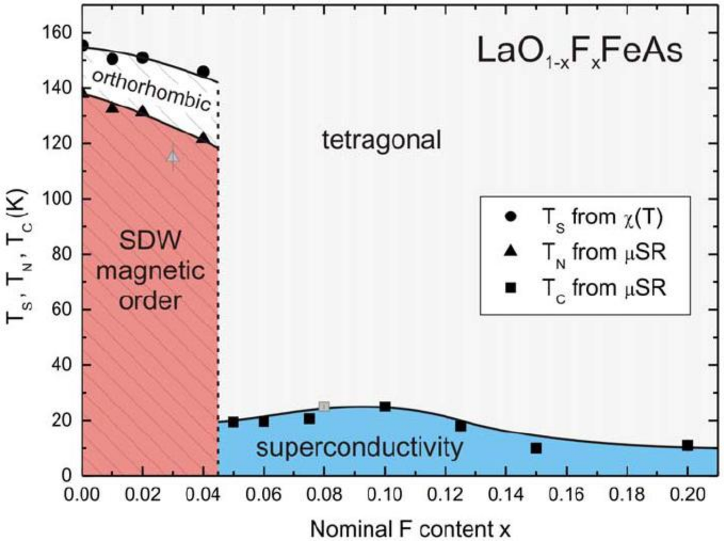
LaFeAsO



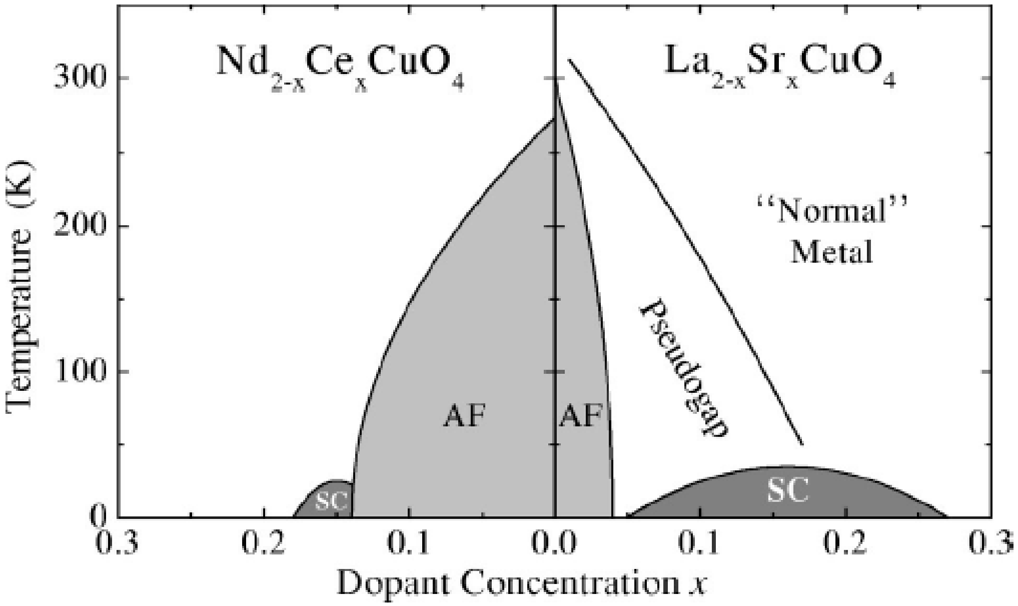
2D Fe-As layers with As above and below a square lattice formed by Fe

Are pnictides similar to cuprates?

Pnictides



Cuprates



Parent compounds are antiferromagnets

Superconductivity emerges upon doping

TUG-OF-WAR

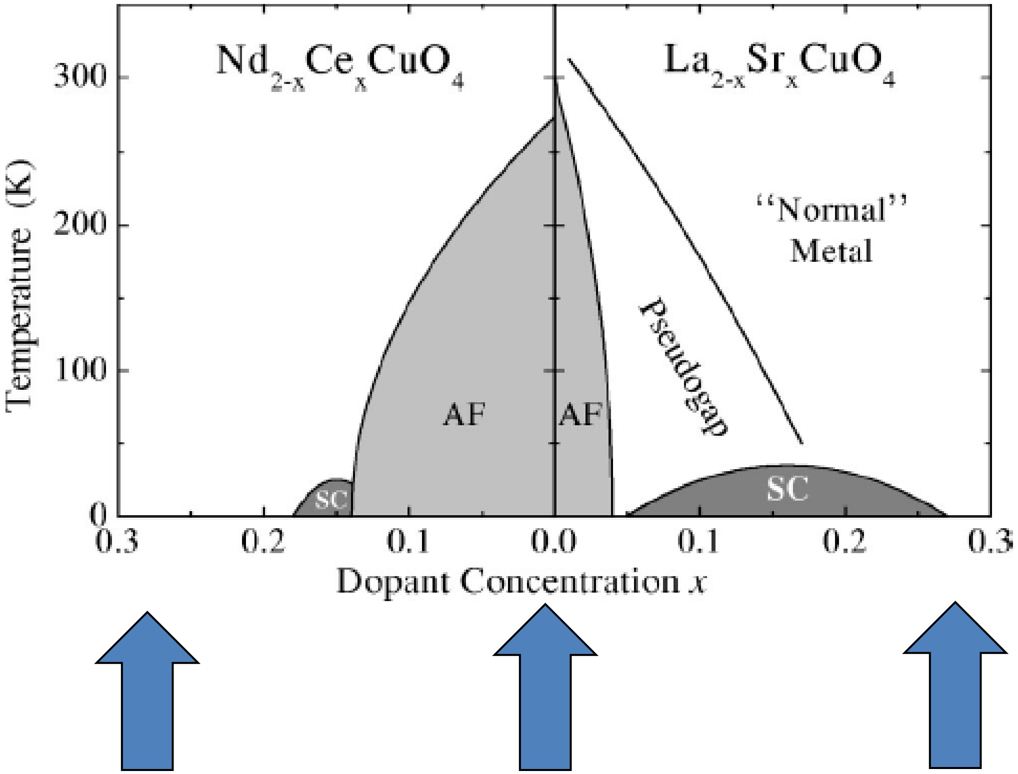
Similar

Abrahams, Bernevig, Haule, Kivelson, Kotliar, Phillips, Sachdev, Si, Sushkov, Xu ….

Different

Bang, Carbotte, Gorkov, Hirschfeld, D-H Lee, Mazin, Scalapino, Schmalian, Tesanovic, Vishwanath, ….

Cuprate high Tc superconductors

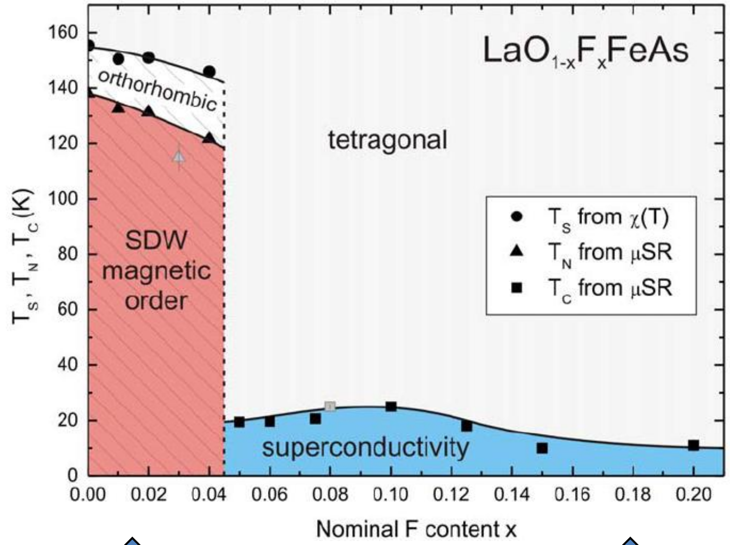


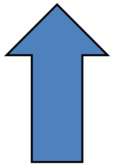
metal

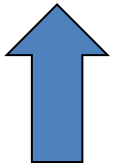
Mott insulator
Heisenberg
antiferromagnet

metal

Fe-Pnictides

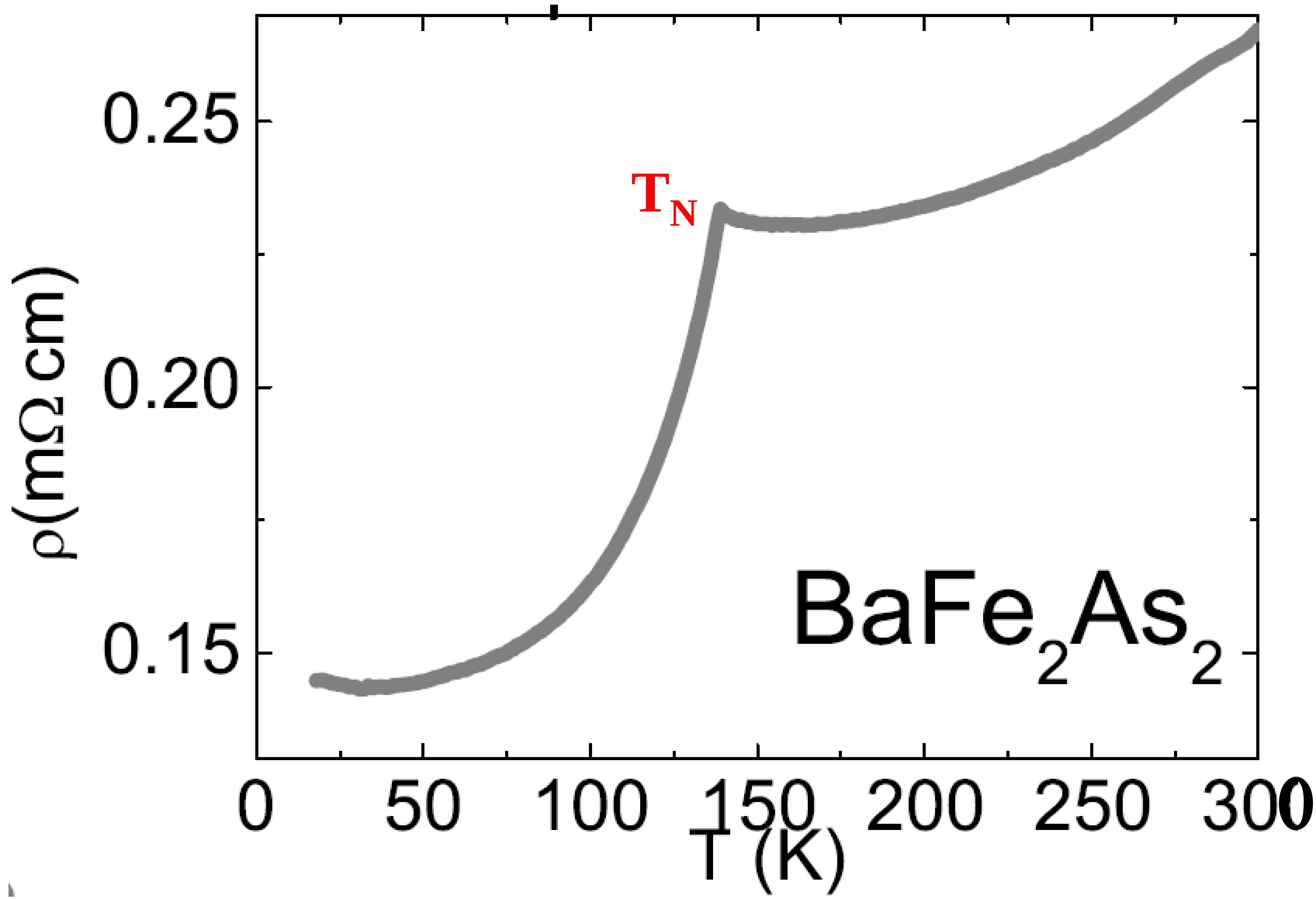






metal **metal**

I. Metallic behavior in the magnetic phase

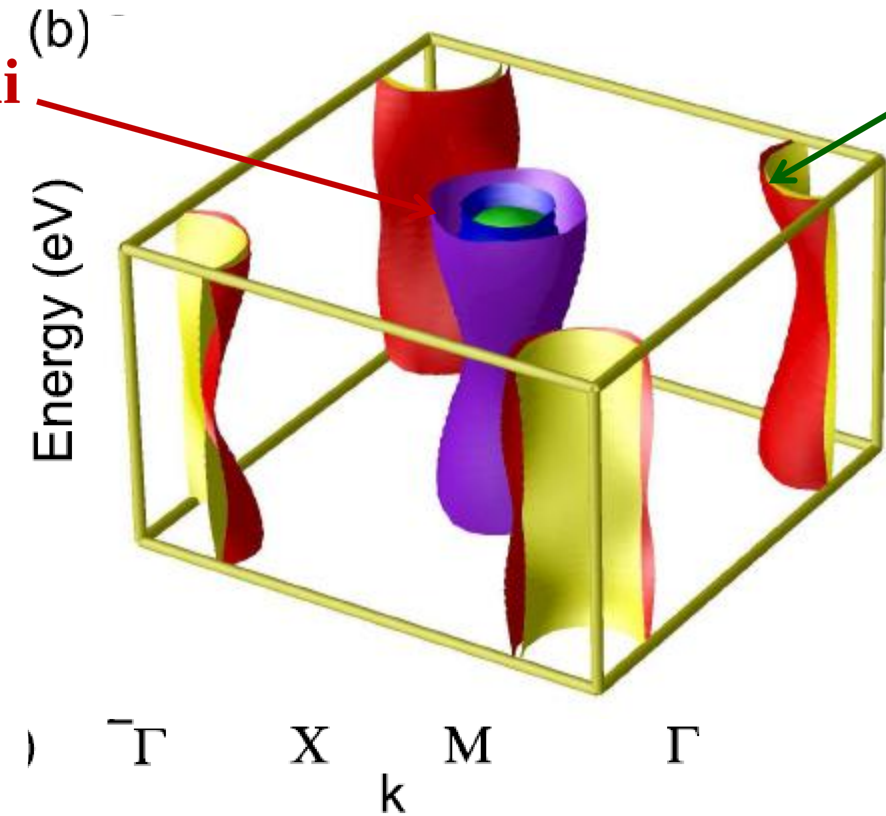


II. Band theory calculations agree with experiments

Lebegue, Mazin et al, Singh & Du, Cvetkovic & Tesanovic…

Hole Fermi surface

Electron Fermi surface



2 hole pockets around (0,0)

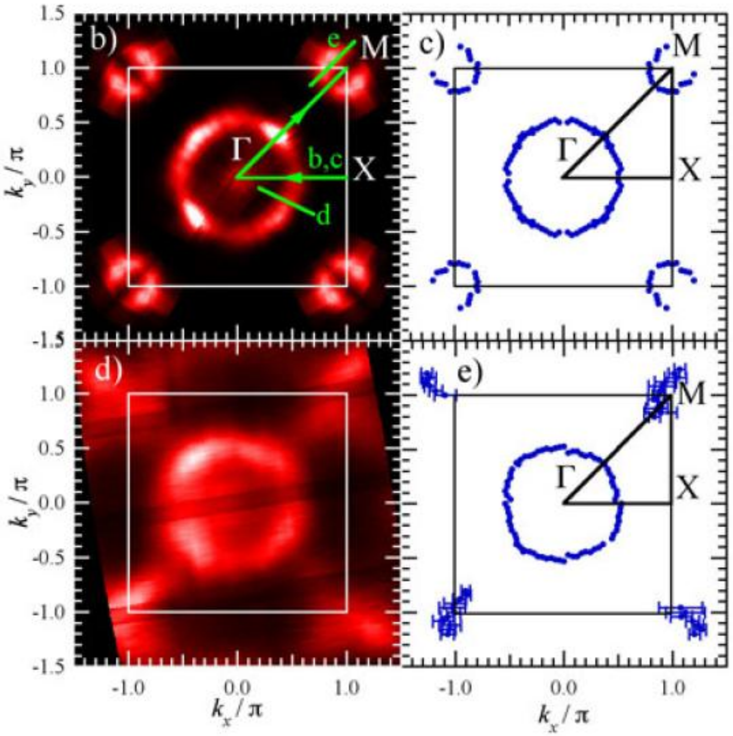
2 electron pockets around (π,π) (folded BZ), or $(0,\pi)$ and $(\pi,0)$ (unfolded BZ)

ARPES

dHVa

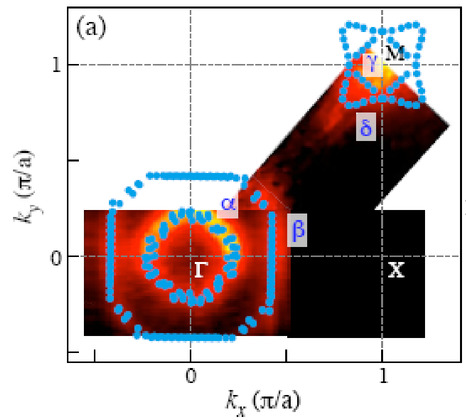
$NdFeAs(O_{1-x}F_x)$ (x=0.1)

A. Kaminski et al.

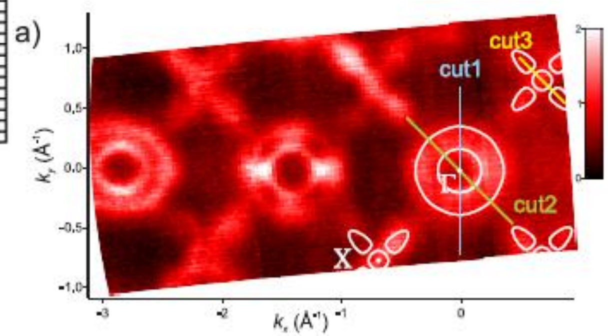


$Ba_{0.6}K_{0.4}Fe_2As_2$

H. Ding et al.

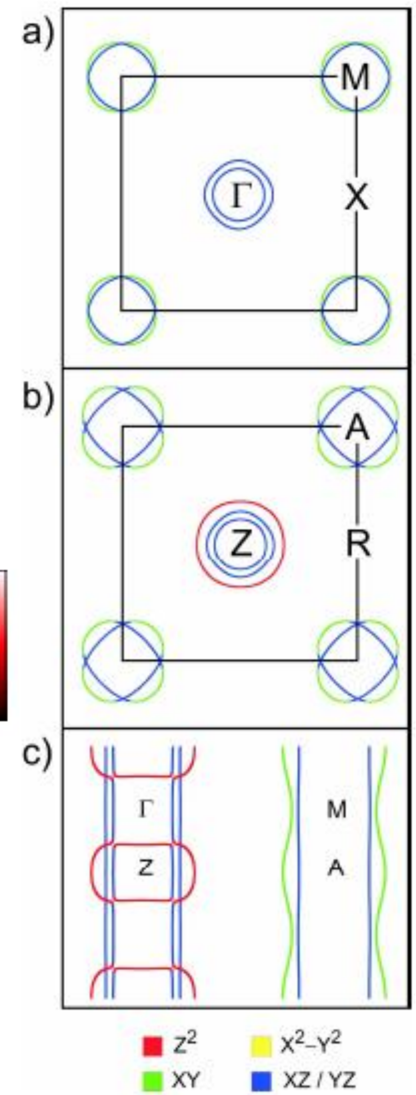


D. Evtushinsky et al



LaFeOP

A. Coldea et al,



Hole pockets near (0,0)

Electron pockets near (π,π)

A simple way to understand the difference between cuprates and pnictides

Tesanovic, Physics 2, 60 (2009)

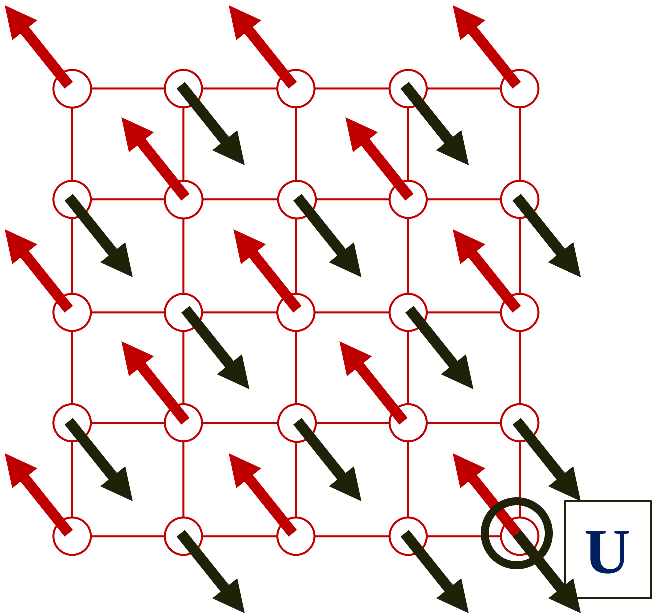
Fe : [Ar]3d^6 ~~4s^2~~, Cu : [Ar]3d^9 ~~4s^1~~

Fe^{2+}, Cu^{2+}

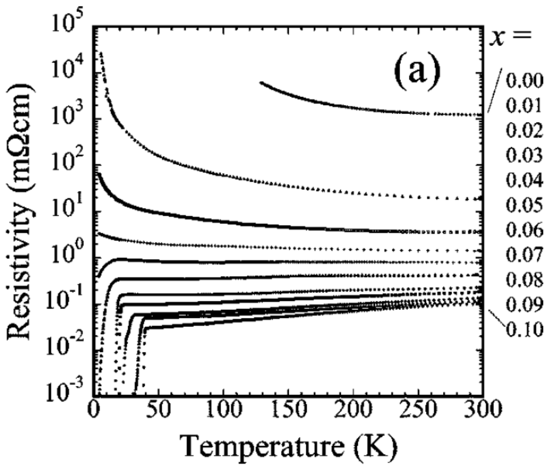
Cuprates: $Cu^{2+} \Rightarrow 3d^9$

one hole in a filled d-shell (1 "free" fermion per cite: half-filling)

In a half-filled band Coulomb repulsion $U n_{i\uparrow} n_{i\downarrow}$ $(U \gg t)$ keeps holes in place $\Rightarrow$ Mott insulator + Neel antiferomagnet !!



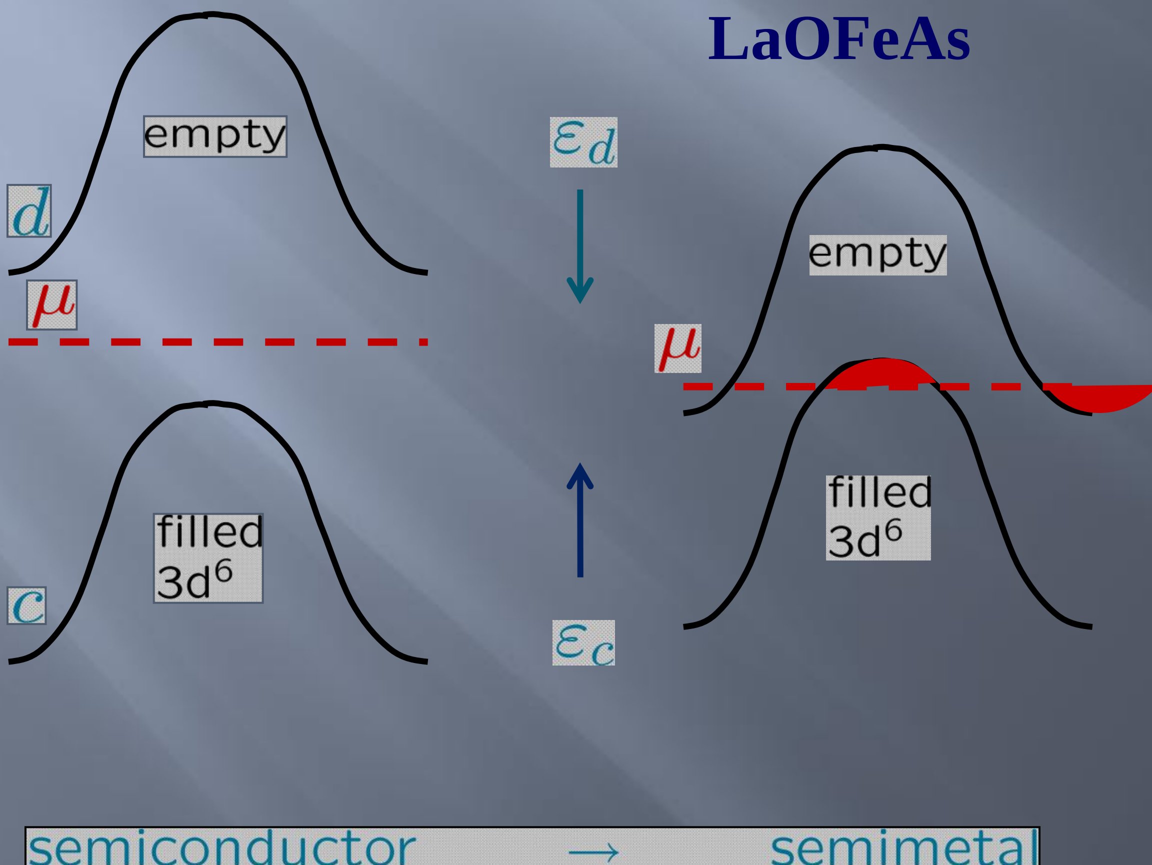
Only when doped with holes (or electrons) do cuprates turn into superconductors

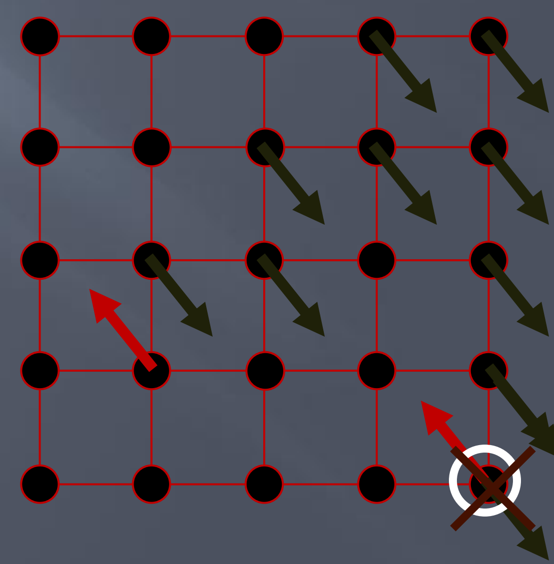


Pnictides: $Fe^{2+} \Rightarrow 3d^6$

4 holes per cite – multiband structure.
chemical potential lies in the gap

LaOFeAs

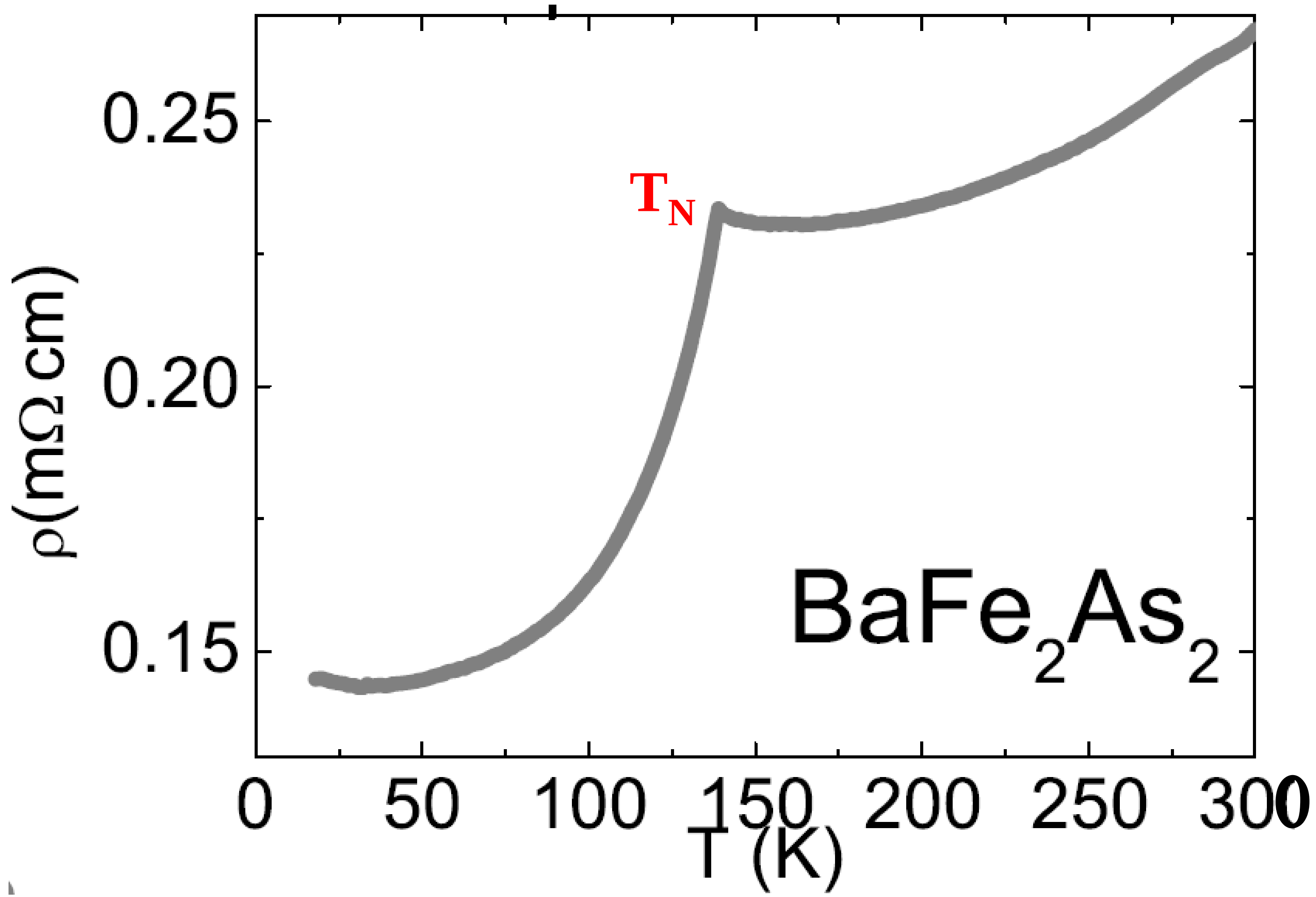




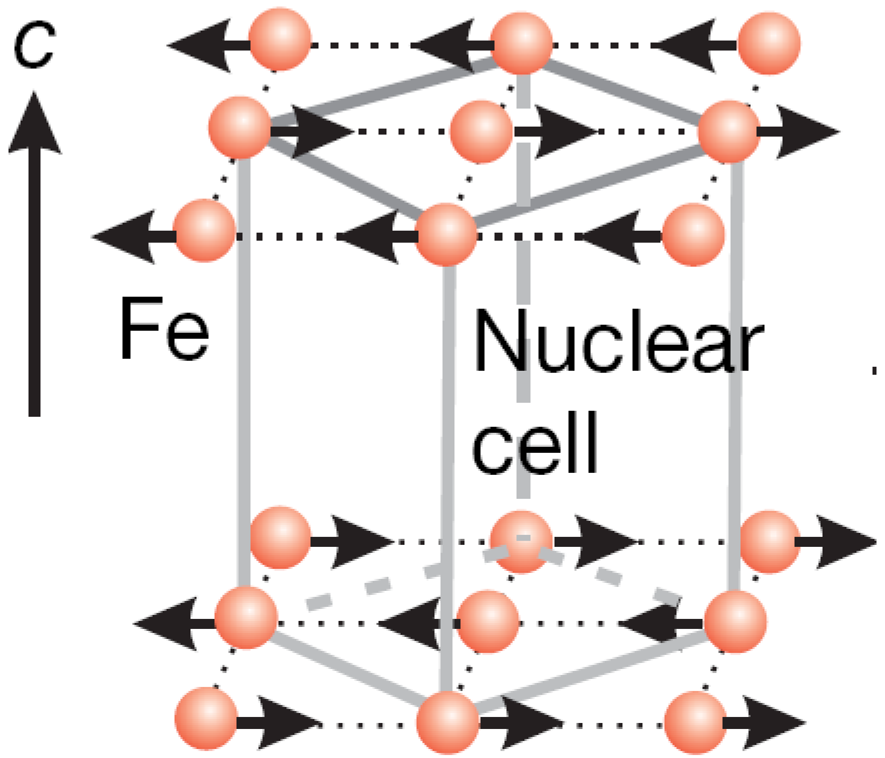
Itinerant approach

Magnetism

The system remains a metal the magnetic phase



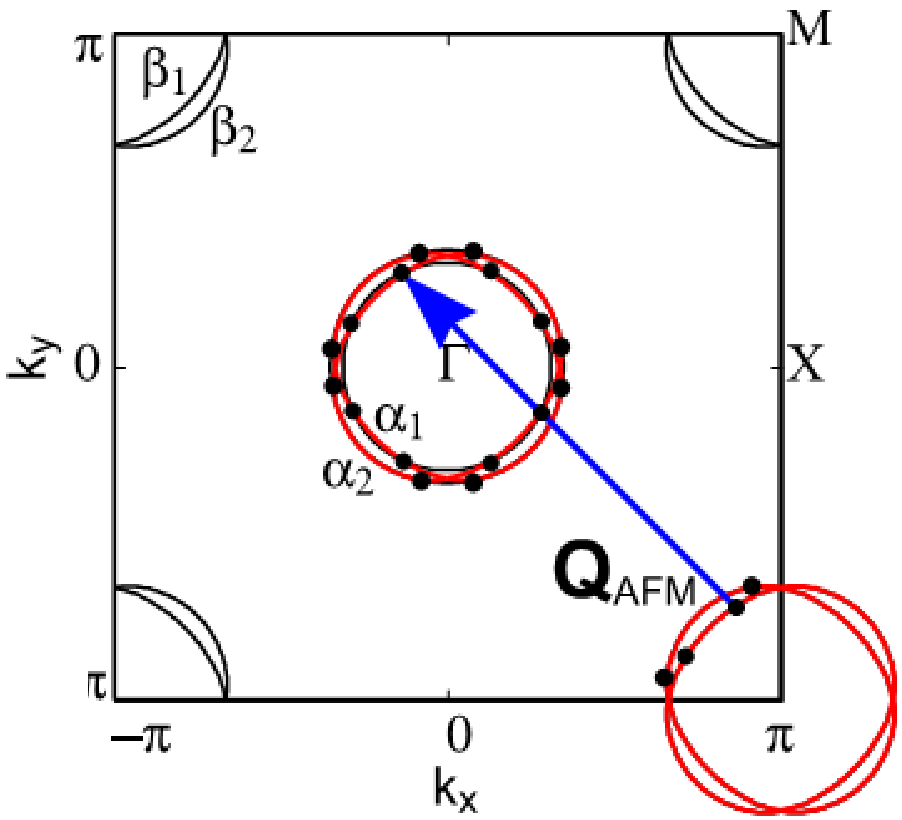
Magnetic order



(π,0) or (0,π) in the unfolded BZ

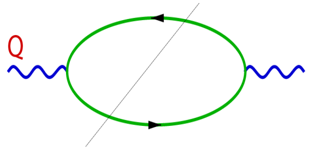
(π,π) in the folded BZ

Itinerant description: magnetism comes from nesting



Dong et al, Korshunov & Eremin,
Raghu et al., K. Kuroki et al, …

Nesting is a boost for an SDW antiferromagnetism

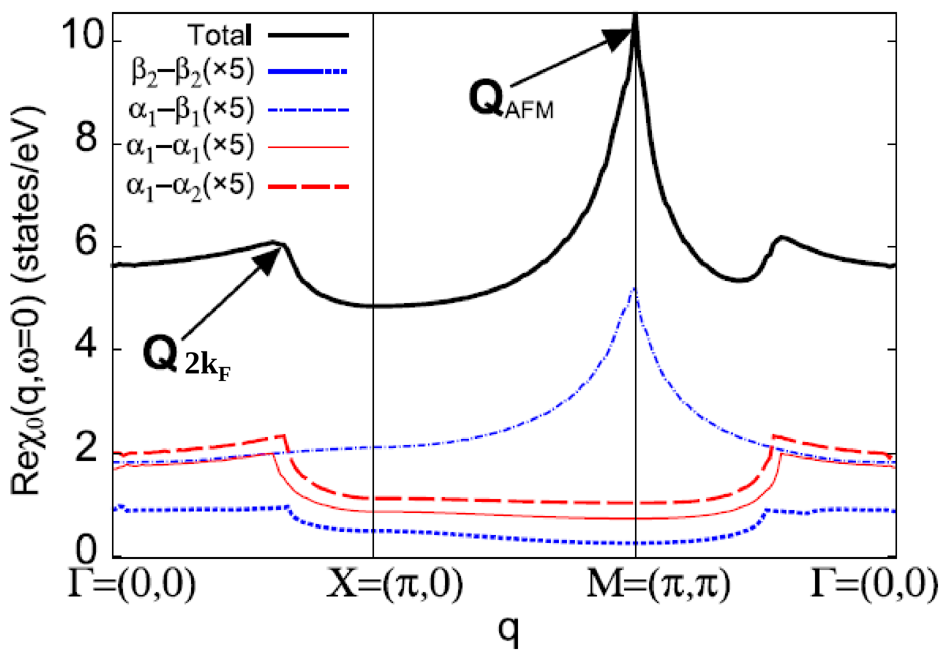
$\chi_0(Q) =$ 

$= \iint_T \frac{d\omega\, d\varepsilon_k}{\omega^2 + \varepsilon_k^2} = \log \frac{E_F}{T}$

(ellipticity of electron FSs is not an obstacle)

For a perfect nesting, AFM instability occurs already at small U

M. Rice (for Cr), V. Cvetkovic and Z.Tesanovic, ….

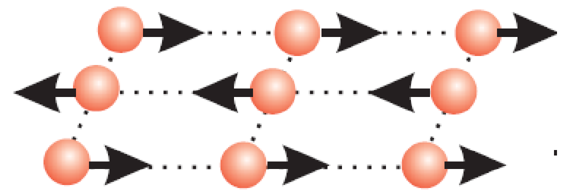


(π,π) in the folded BZ

Eremin & Korshunov

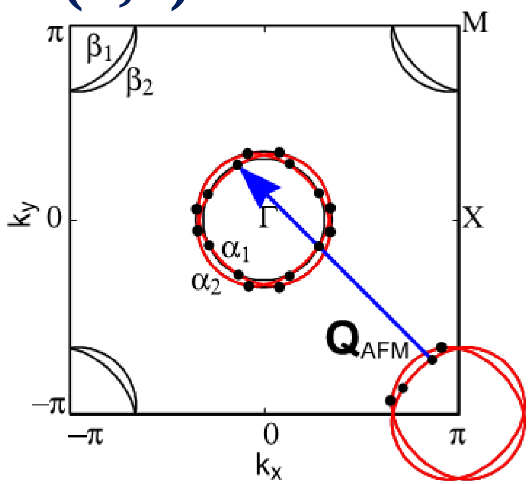
Questions

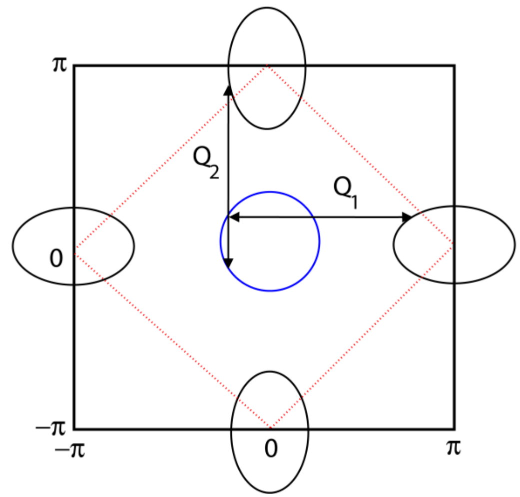
1. The actual order is



$(\pi,0)$

(π,π) folded BZ



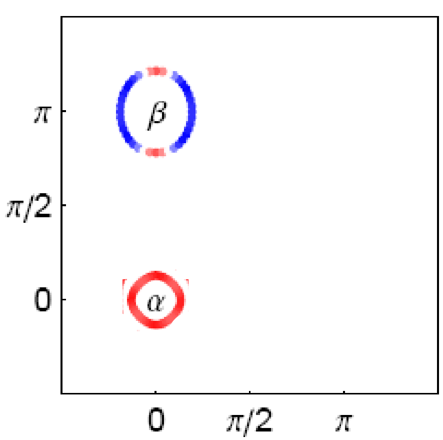


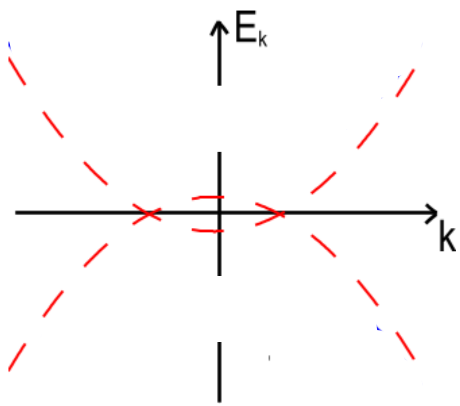
$$\mathbf{Q_1 = (\pi,0)}$$

$$\mathbf{Q_2 = (0,\pi)}$$

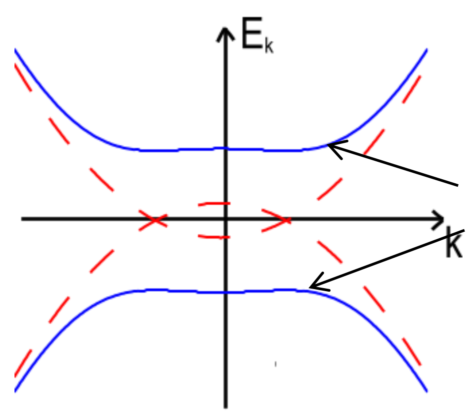
$$\vec{S} = \vec{S}_1\, e^{i\vec{Q}_1\vec{r}} + \vec{S}_2\, e^{i\vec{Q}_2\vec{r}}$$

2. Why the system remains a metal?





SDW

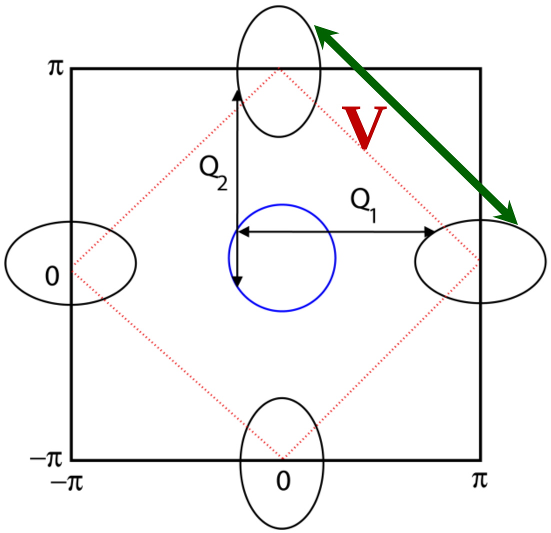


SDW gaps

1. Selection of a magnetic order

Introduction two SDW order parameters

$$\vec{W}_1 \text{ with } Q_1 = (0,\pi),$$
$$\vec{W}_2 \text{ with } Q_2 = (\pi,0)$$

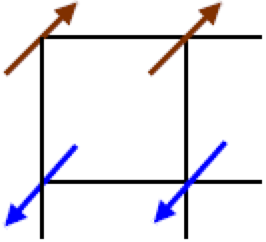


$$E_{gr} = F\left(\vec{W}_1^{\,2} + \vec{W}_2^{\,2}\right)$$

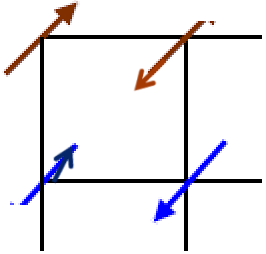
O(6) symmetry

$$E_{gr} = F\left(\vec{W}_1^{\,2} + \vec{W}_2^{\,2}\right) + a\,V\,(\vec{W}_1)^2\,(\vec{W}_2)^2, \quad a > 0$$

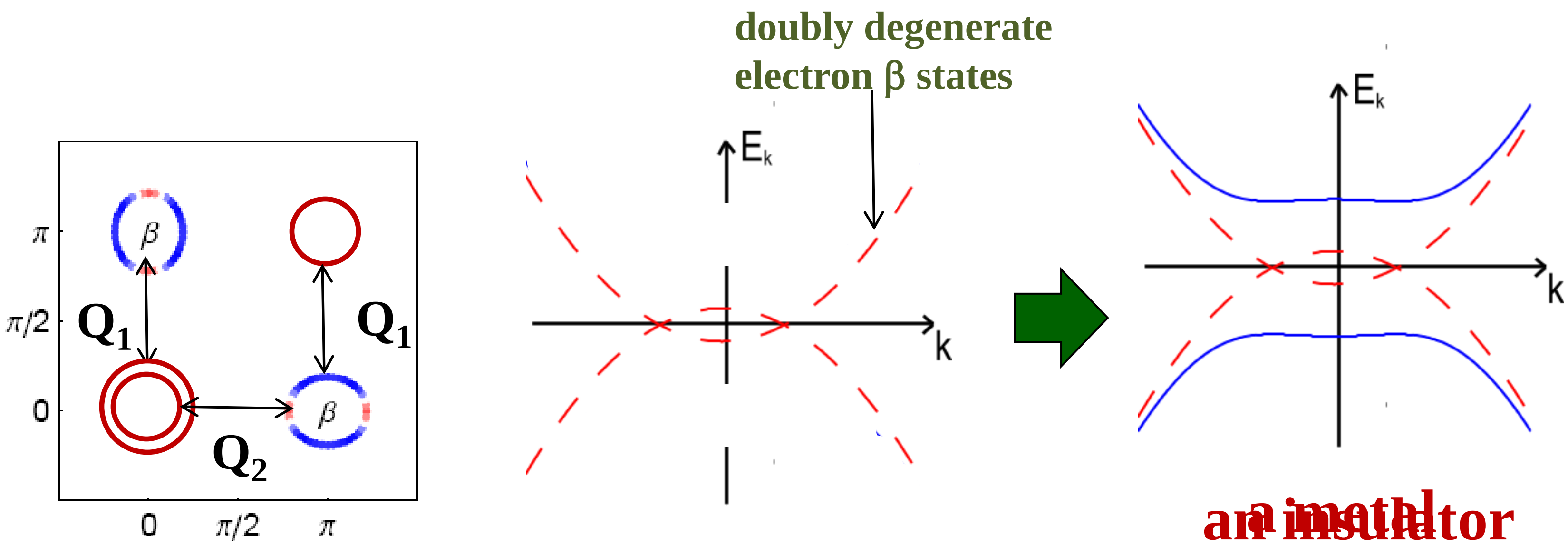
Either $W_1 = 0$, $(0,\pi)$ state



Or $W_2 = 0$, $(\pi,0)$ state



2. Metallicity

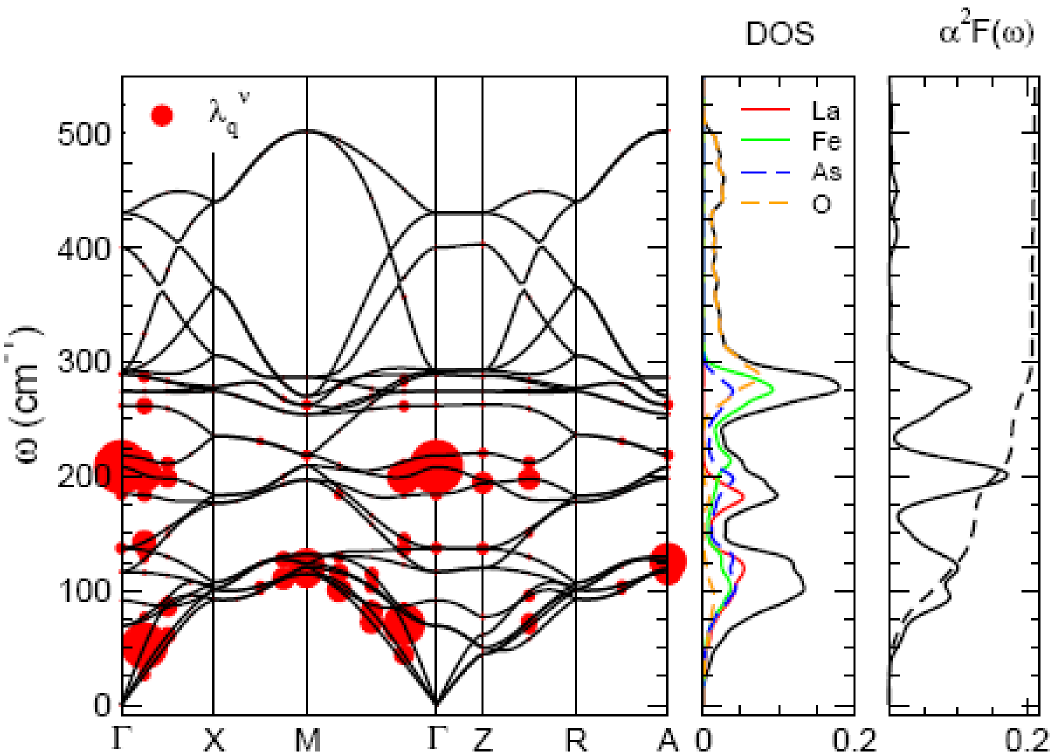


Angular dependence of the interaction also plays an essential role (nodes, even when SDW order affects all Fermi surfaces) **(Vishwanath et al, 2008)**

Itinerant approach

Superconductivity

Electron-phonon interaction is too weak



Boeri, Dolgov, & Golubov,
Singh & Du

$$\alpha^2F(\omega) = \frac{1}{N(0)} \sum_{nm\mathbf{k}} \delta(\varepsilon_{n\mathbf{k}})\delta(\varepsilon_{m\mathbf{k+q}}) \times$$
$$\times \sum_{\nu\mathbf{q}} |g_{\nu,n\mathbf{k},m(\mathbf{k+q})}|^2 \delta(\omega - \omega_{\nu\mathbf{q}});$$
$$\lambda(\omega) = 2\int_0^\omega d\Omega \alpha^2 F(\Omega)/\Omega$$

$$\lambda = 0.21$$

λ=0.44 for Al

Too small to account
for Tc =50K

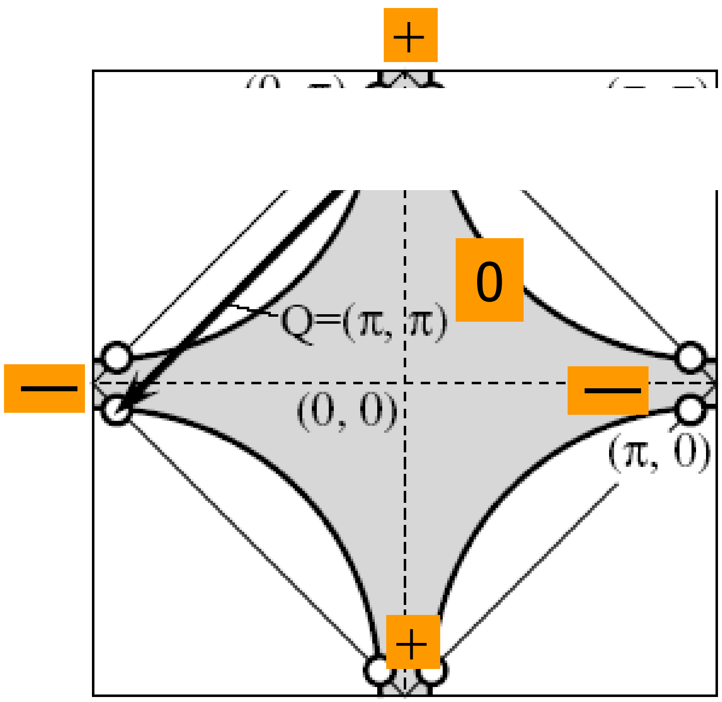
Pairing due to el-el interaction

How about using the "analogy" with overdoped cuprates and assume that the pairing is mediated by spin fluctuations

peaked at (π,π)

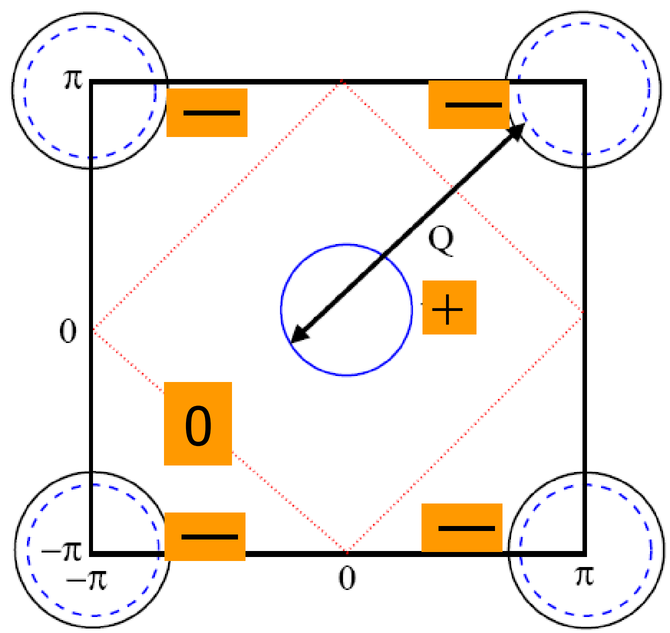
Mazin et al,
Kuroki et al....

Cuprates



$$\Delta(\theta) = \Delta_0 \, (\cos k_x - \cos k_y)$$

Pnictides



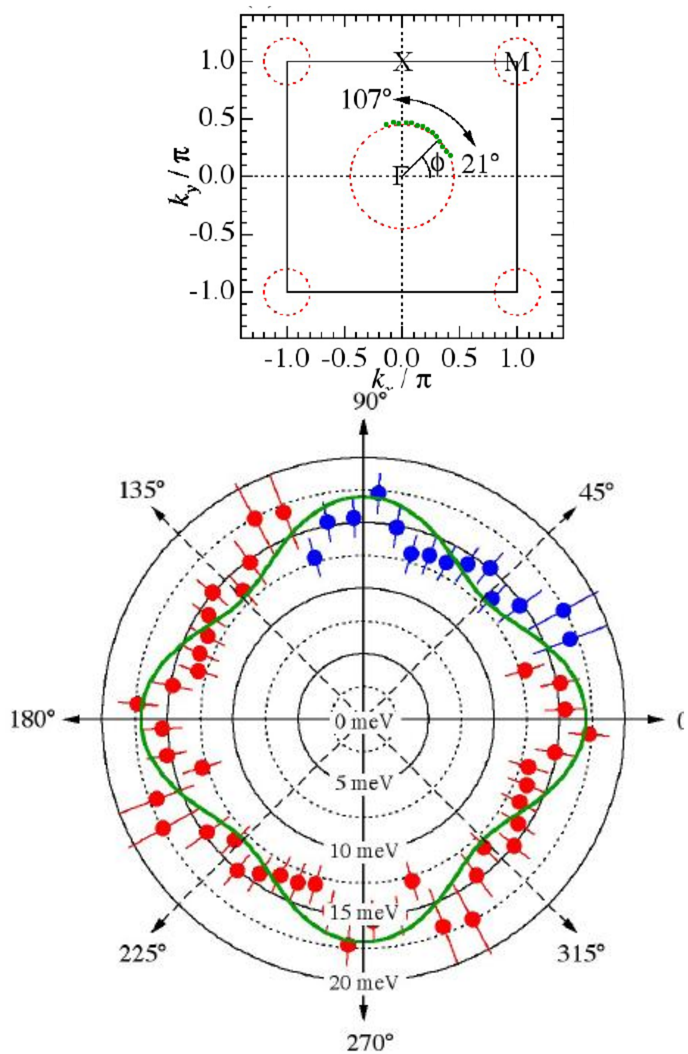
$$\Delta(\theta) = \Delta_0 \, (\cos k_x + \cos k_y)$$

sign-changing extended s-wave gap

Experiments

Some experiments are consistent with no-nodal s^{+-} gap

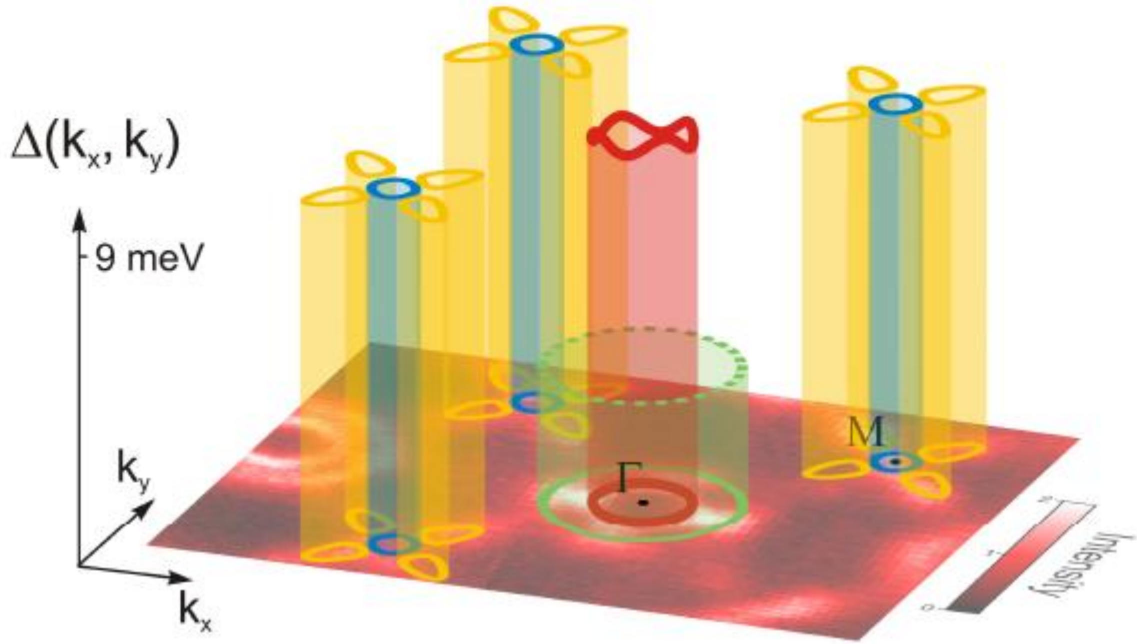
1. Photoemission in 1111 and 122 FeAs



$NdFeAsO_{1-x}F_x$

T. Kondo et al., arXiv:0807.0815

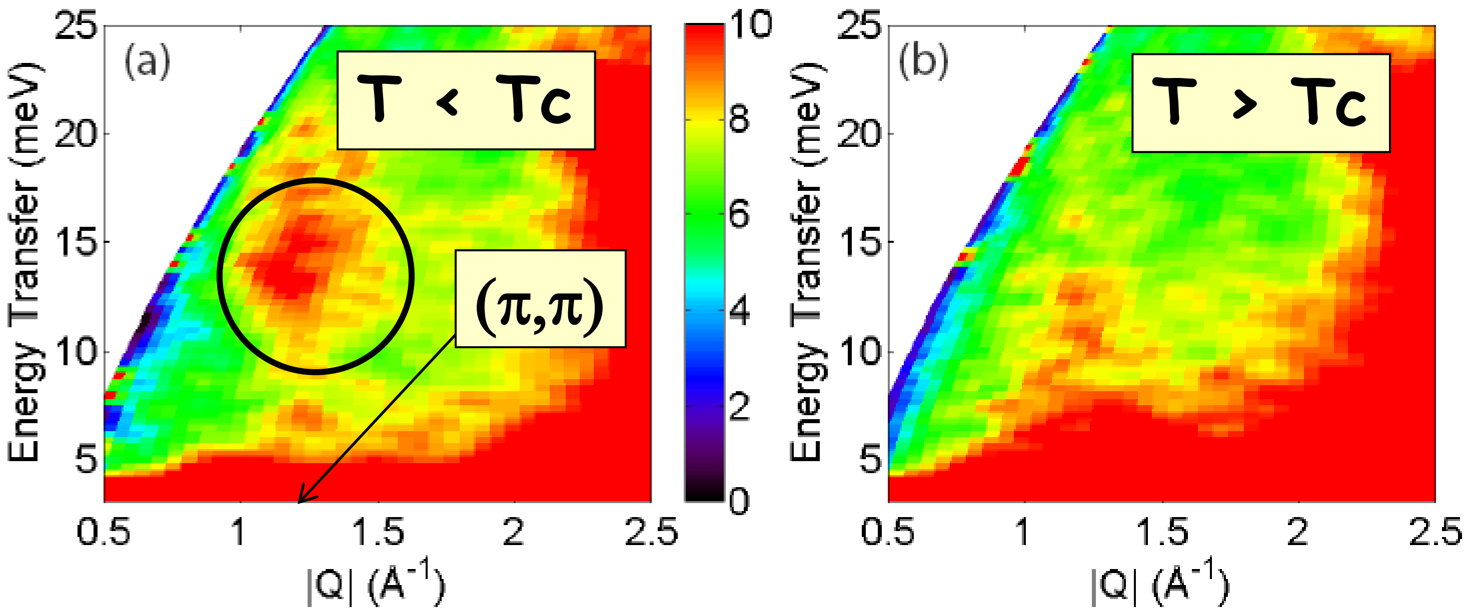
$Ba_{1-x}K_xFe_2As_2$



D. Evtushinsky et al

Almost angle-independent gap

2. Neutron scattering – resonance peak below 2D

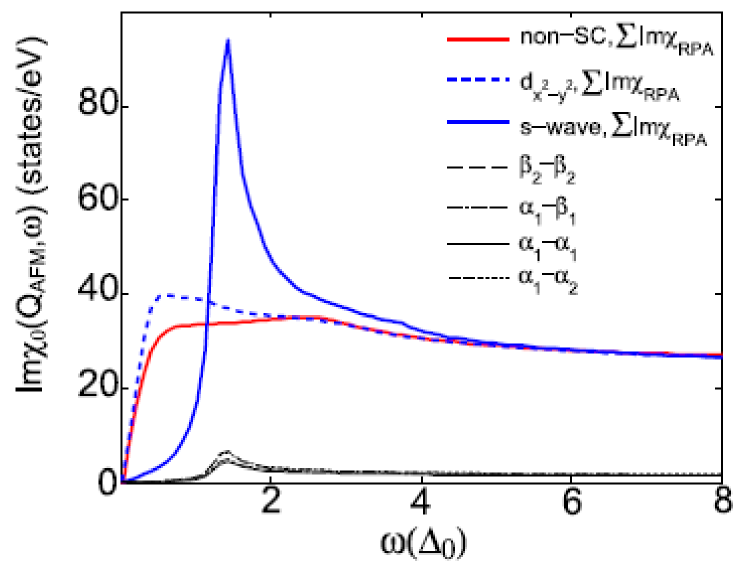


Christianson etal.

$Ba_{0.6}K_{0.4}Fe_2As_2$

$$\text{Theory : need } \Delta_{k+\pi} = -\Delta_k$$

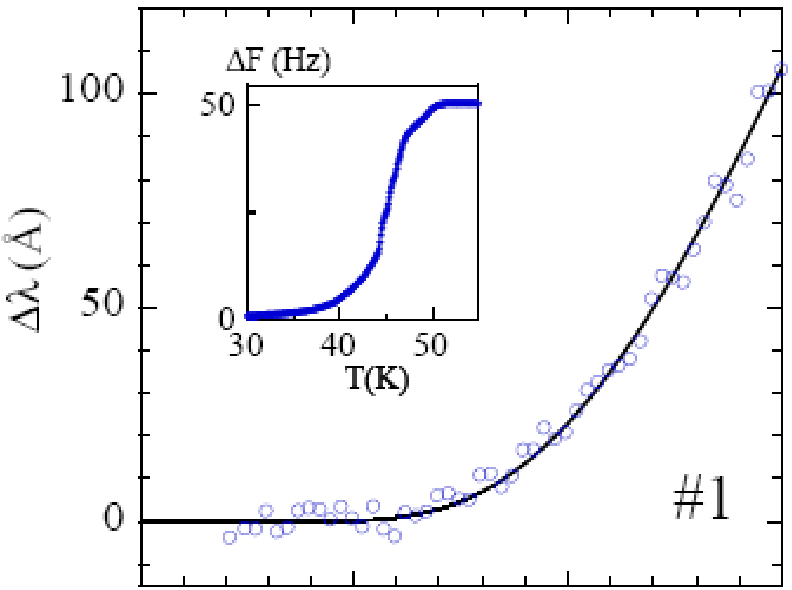
The “plus-minus” gap is the best candidate



Eremin & Korshunov
Scalapino & Maier

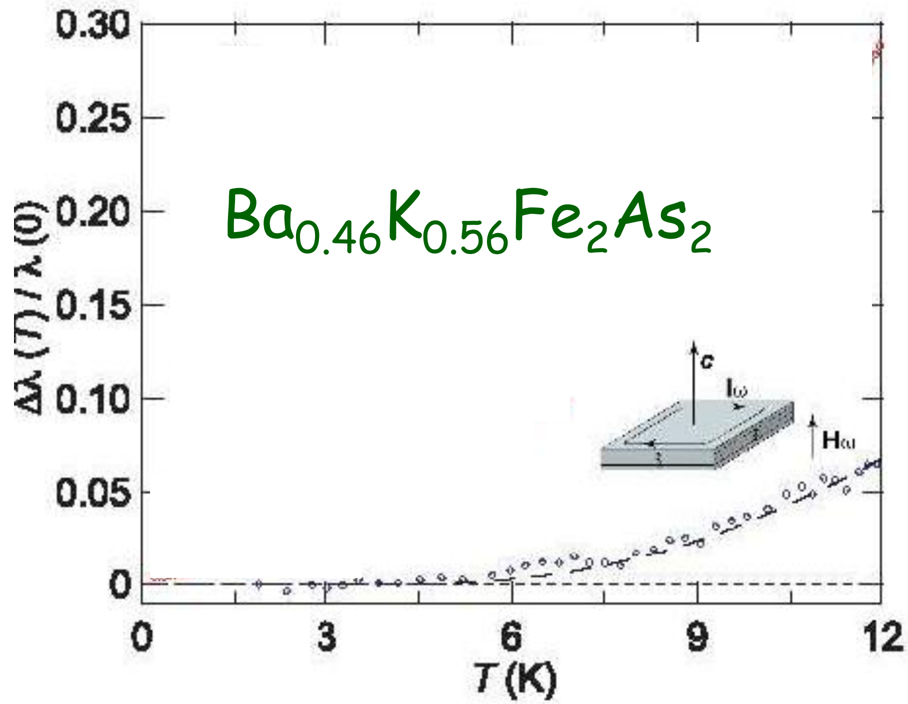
3. Penetration depth behavior in 1111 and 122 FeAs

SmOFeAs



Carrington et al

Ba1-xKxFe2As2



$Ba_{0.46}K_{0.56}Fe_2As_2$

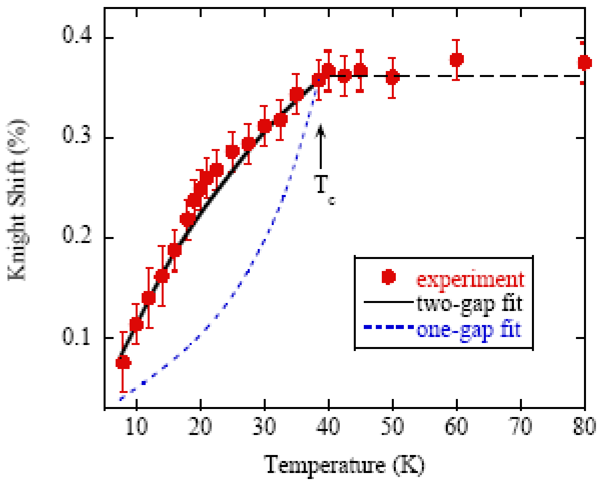
Y. Matsuda

"Exponential" behavior at low T
(or, at least, a very flat behavior)

Other experiments, howecver, indicate that the gap may have nodes

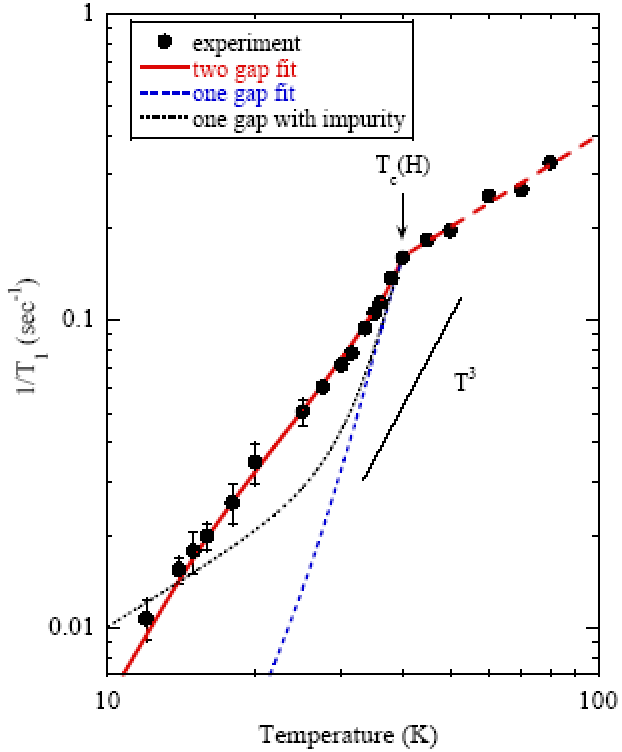
1. NMR and Knight shift in 1111 FeAs

Knight shift



Matano et al

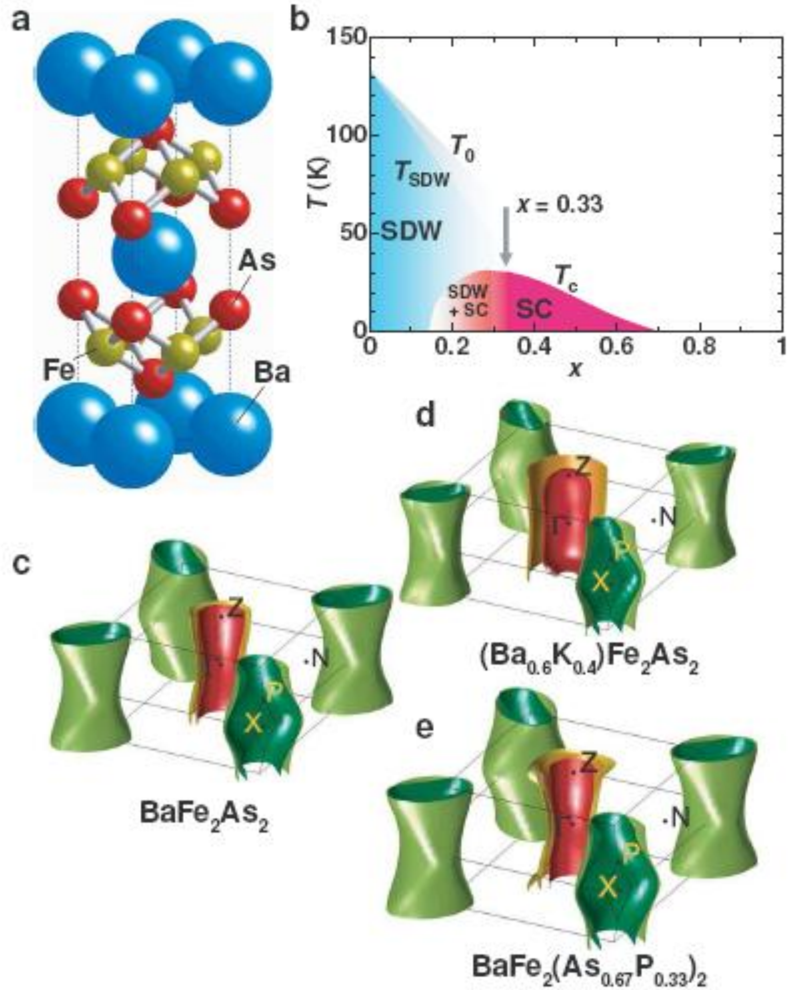
NMR relaxation rate

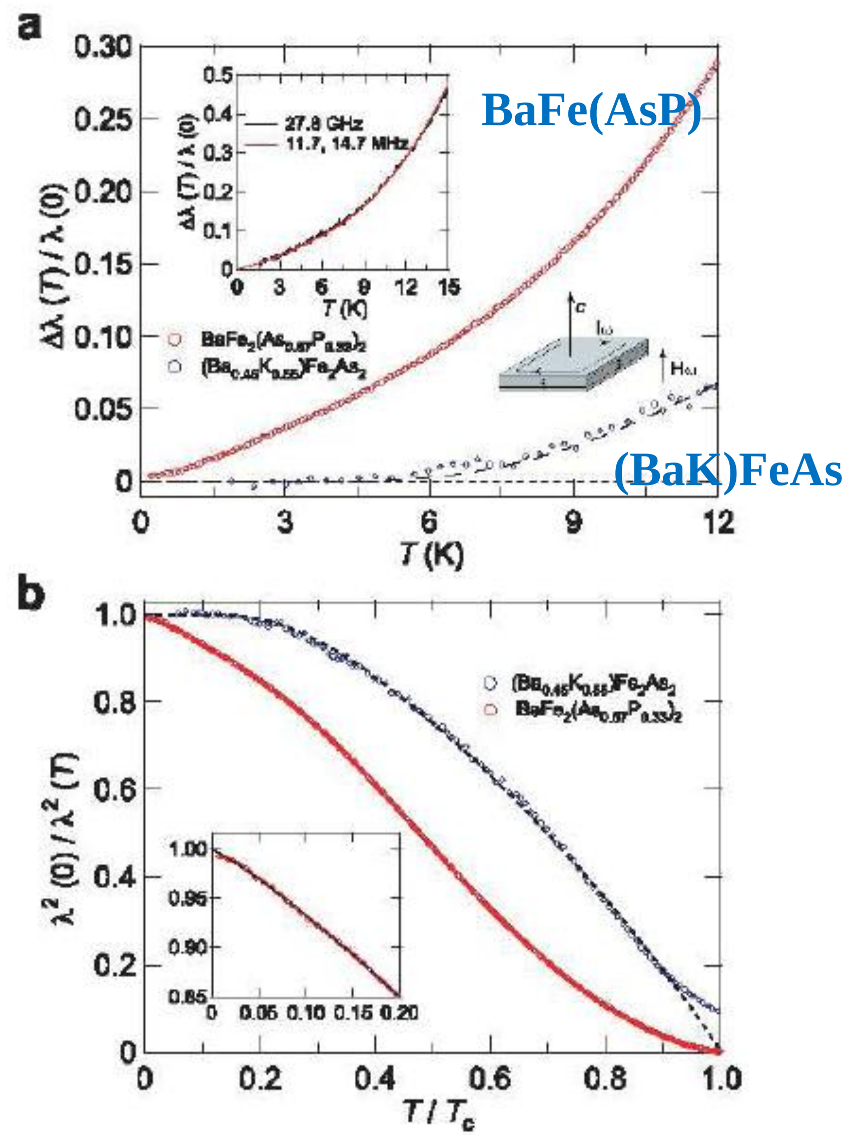


Non-exponential behavior!

2. The behavior of $BaFe_2(As_{1-x}P_x)_2$, Tc =30K

Y. Matsuda et al



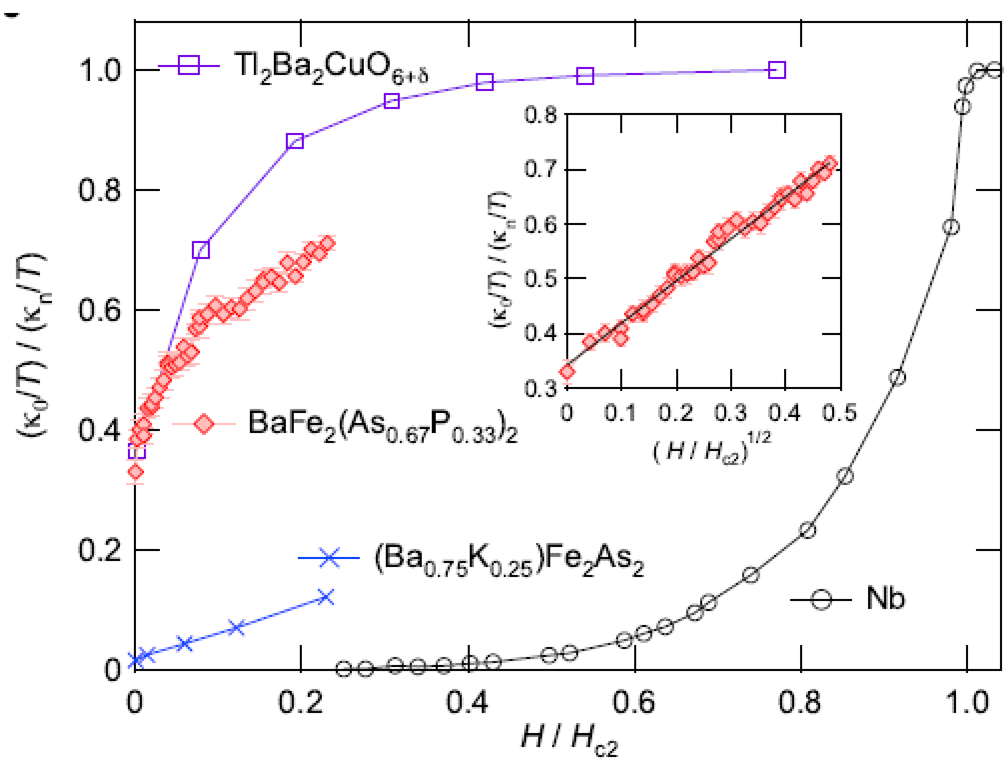


Nodes in $BaFe_2(As_{1-x}P_x)_2$,

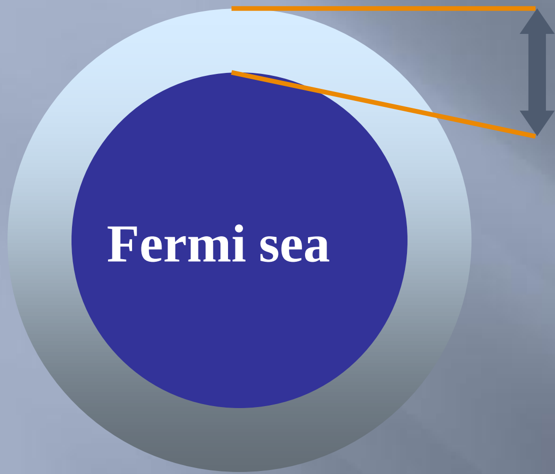
2. The behavior of $BaFe_2(As_{1-x}P_x)_2$, Tc =30K

Y. Matsuda et al

Thermal conductivity



Do nodes in the gap imply non-s-wave?

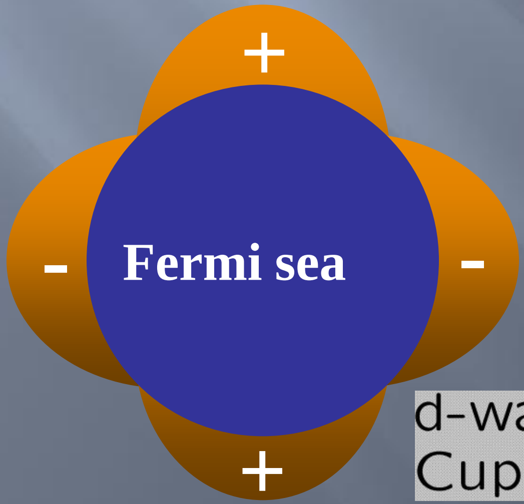


Superconducting gap Δ

One Fermi surface (open or close)

s-wave (isotropic)
Conventional SC (Nb, Pb, Al, $\cdots$)
$T_c < 25$K

p-wave
Superfluid ^{3}He, SrRu (?)
$T_c \sim$ 1mK - 1K



may have nodes

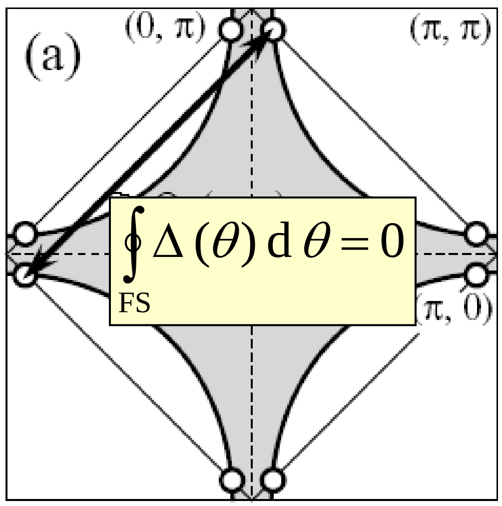
no nodes

d-wave
Cuprate SC $T_c \sim$ 160K

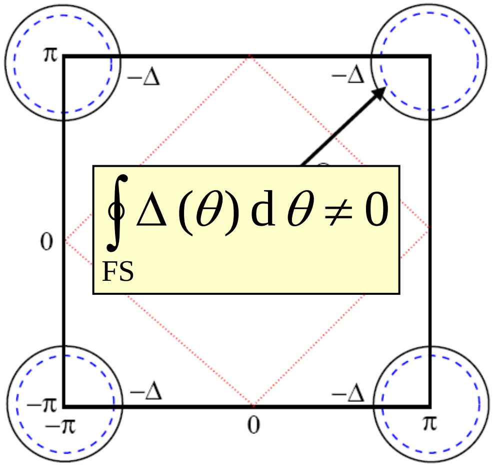
Back to simple reasoning

There is a problem: how to get rid of an intra-band Hubbard repulsion ?

Cuprates

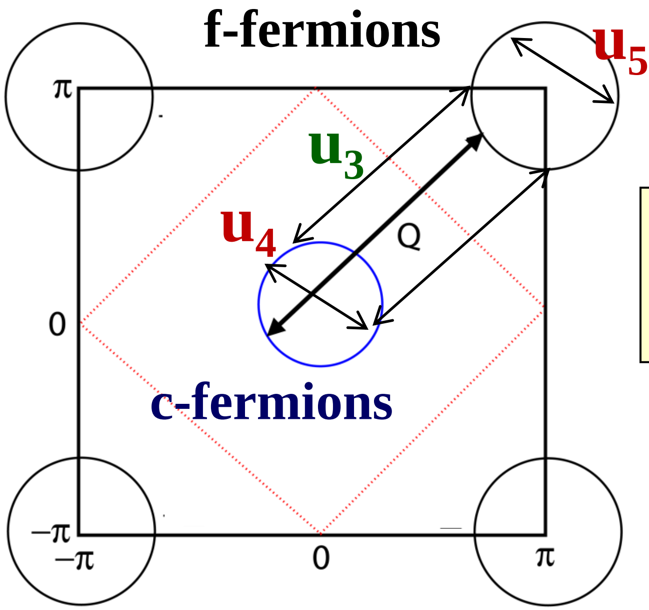


Pnictides



Hubbard repulsion cancels out, only d-wave, (π,π) interaction matters

Intra-band repulsion does not cancel and has to be overtaken by a (π,π) interaction



Theory

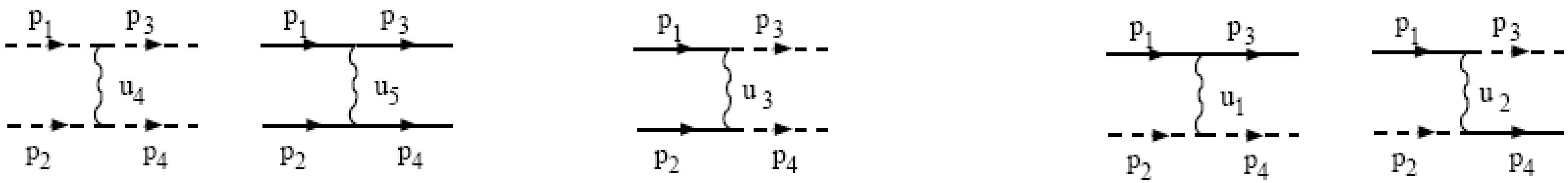
The two-band nested Fermi liquid with intra-band and inter-band interactions

$$\epsilon_p^c = E_F - \frac{p^2}{2m}, \quad \epsilon_{p+Q}^f = \frac{(p+Q)^2}{2m} - E_F$$

$$H = U_1^{(0)} \sum c^\dagger_{\mathbf{p}_3\sigma} f^\dagger_{\mathbf{p}_4\sigma'} f_{\mathbf{p}_2\sigma'} c_{\mathbf{p}_1\sigma} + U_2^{(0)} \sum f^\dagger_{\mathbf{p}_3\sigma} c^\dagger_{\mathbf{p}_4\sigma'} f_{\mathbf{p}_2\sigma'} c_{\mathbf{p}_1\sigma}$$

$$+ \frac{U_3^{(0)}}{2} \sum \left[f^\dagger_{\mathbf{p}_3\sigma} f^\dagger_{\mathbf{p}_4\sigma'} c_{\mathbf{p}_2\sigma'} c_{\mathbf{p}_1\sigma} + h.c \right] + \frac{U_4^{(0)}}{2} \sum f^\dagger_{\mathbf{p}_3\sigma} f^\dagger_{\mathbf{p}_4\sigma'} f_{\mathbf{p}_2\sigma'} f_{\mathbf{p}_1\sigma} + \frac{U_5^{(0)}}{2} \sum c^\dagger_{\mathbf{p}_3\sigma} c^\dagger_{\mathbf{p}_4\sigma'} c_{\mathbf{p}_2\sigma'} c_{\mathbf{p}_1\sigma}$$

$u_i^{(0)} = U_i^{(0)} N_0 \qquad N_0 = m/(2\pi)$ **= density of states in 2D**



Intra-band repulsion
$u_4 = u_5$

Pair hopping
(π,π) interaction

Inter-band forward
and “back-scattering”

Let's see how pair hoping and intra-band repulsion compete

1. Spin density wave

$$\chi^{SDW} = \frac{(\chi^{SDW})_0}{1-(\Gamma^{SDW})_0\,\Pi_{sdw}}$$

$$\Pi_{sdw} \propto \log\frac{E_F}{T}$$

nesting

$$\Gamma_0^{SDW} = u_3 + u_1 > 0,$$

The system surely favors an SDW instability

2. S+ superconductivity

$$\chi_{s+}^{SC} = \frac{(\chi_{s+}^{SC})_0}{1-(\Gamma_{s+}^{SC})_0\,\Pi_{sc}}$$

$$\Pi_{sc} \propto \log\frac{E_F}{T}$$

$$(\Gamma_{s+}^{SC})_0 = u_3 - u_4,$$

If intra-band repulsion (u_4) is stronger than the pair hopping (u_3), the pairing interaction is repulsive

Orbital model -> band model: $u_4 > u_3$

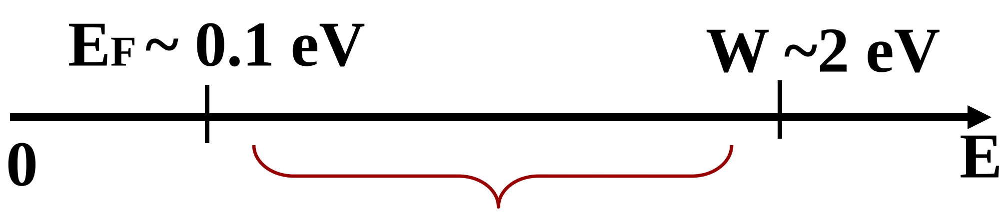
SDW magnetism, but no superconductivity (repulsion wins!)

Explore nesting AND the smallness of the pockets

Chubukov et al, Wang et al, Honerkamp et al, Tesanovic et al

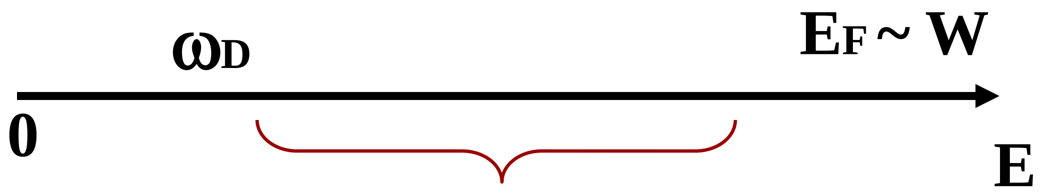
The terms in the Hamiltonian are bare interactions, at energies comparable to a fermionic bandwidth

We, however, need interactions at energies smaller than the Fermi energy [we have log E_F/T]



Couplings flow due to renormalizations by particle-particle and particle-hole bubbles

We know this story for conventional (phonon) superconductors



Coulomb repulsion is renormalized down by the renormalization in the particle-particle channel (McMillan-Tolmachev renormalization)

If only Cooper channel is involved, this cannot change a repulsion into an attraction

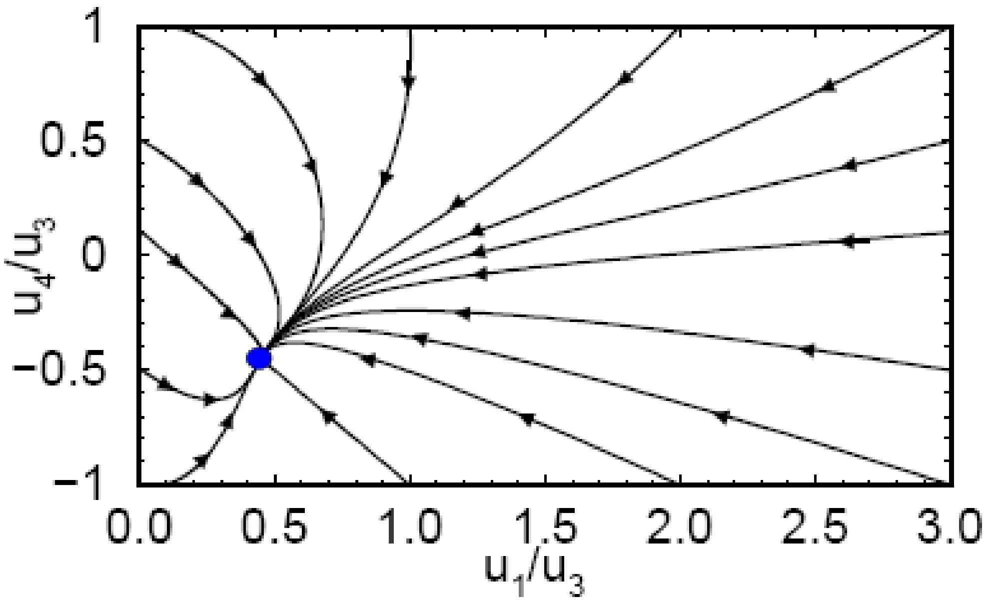
$$u_4 - u_3 = \frac{(u_4 - u_3)_0}{1 + (u_4 - u_3)_0 \log W/E}$$

In our case, there are renormalizations in both particle-particle AND particle hole channel. This implies that we need to construct parquet RG to analyze the system flow between W and E_F

(H. Shultz, Dzyaloshinskii & Yakovenko)

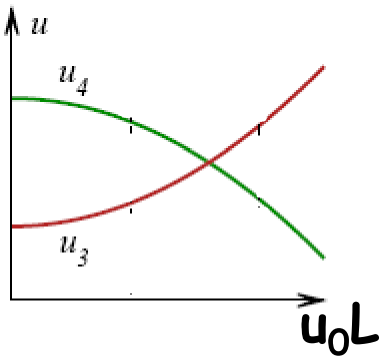
One-loop parquet RG

$$\dot{u}_1 = u_1^2 + u_3^2$$
$$\dot{u}_2 = 2u_2(u_1 - u_2)$$
$$\dot{u}_3 = 2u_3(2u_1 - u_2 - u_4)$$
$$\dot{u}_4 = -u_3^2 - u_4^2$$



The fixed point: the pair hopping term u_3 is the largest

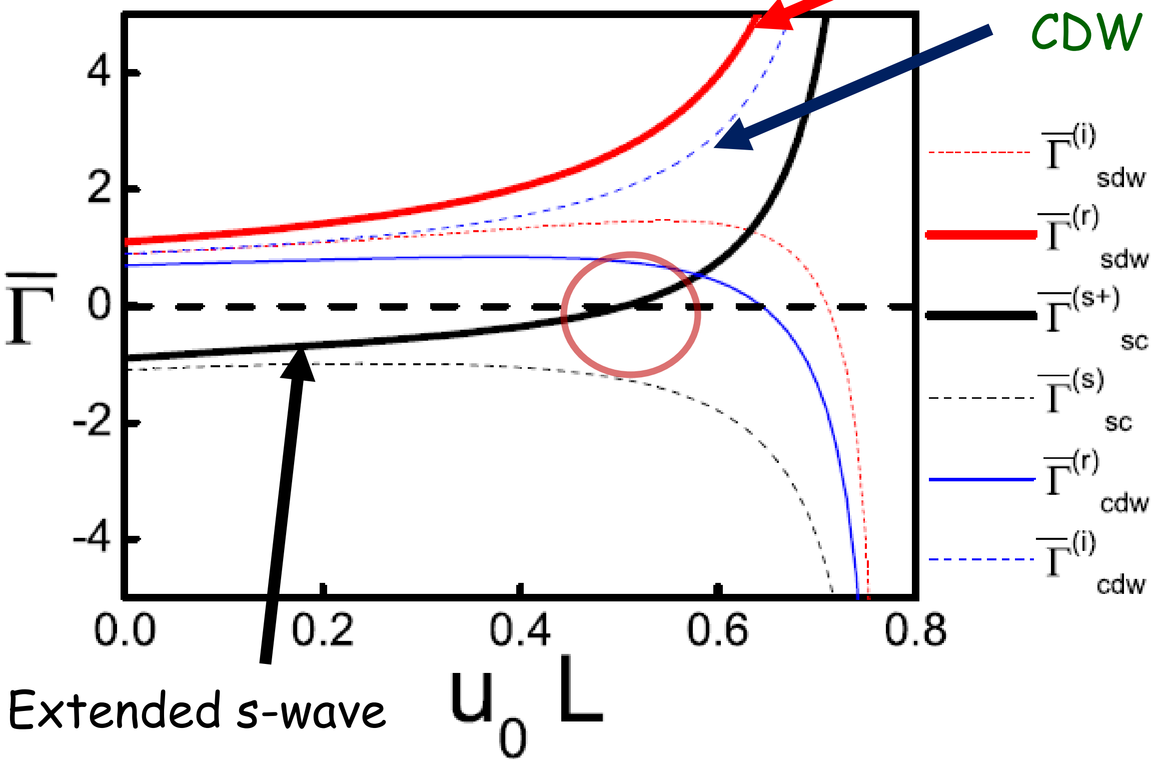
$$u_1 = -u_4 = -u_5 = \frac{|u_3|}{\sqrt{5}}, \quad u_2 \propto |u_3|^{1/3}$$



One-loop RG Flow

SDW with real order parameter

CDW with imaginary order parameter

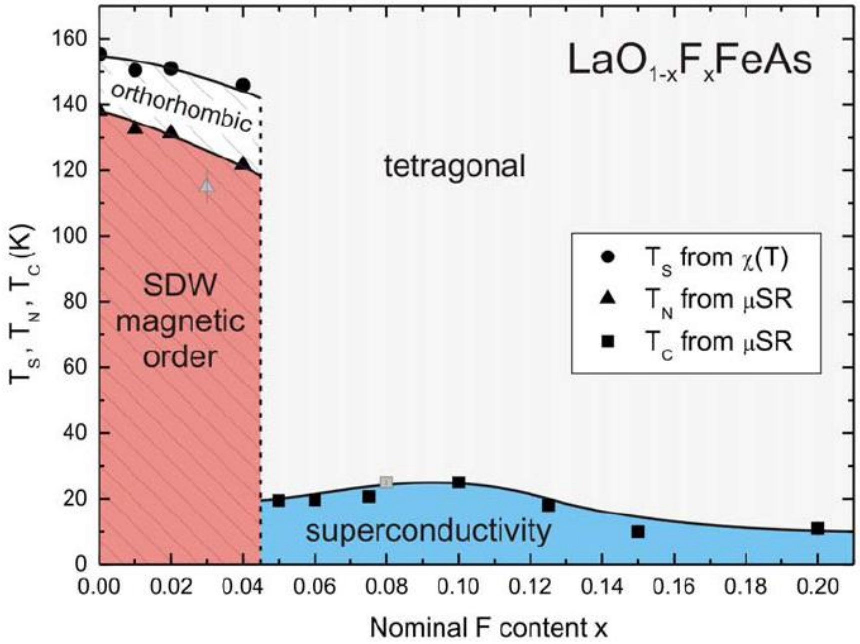


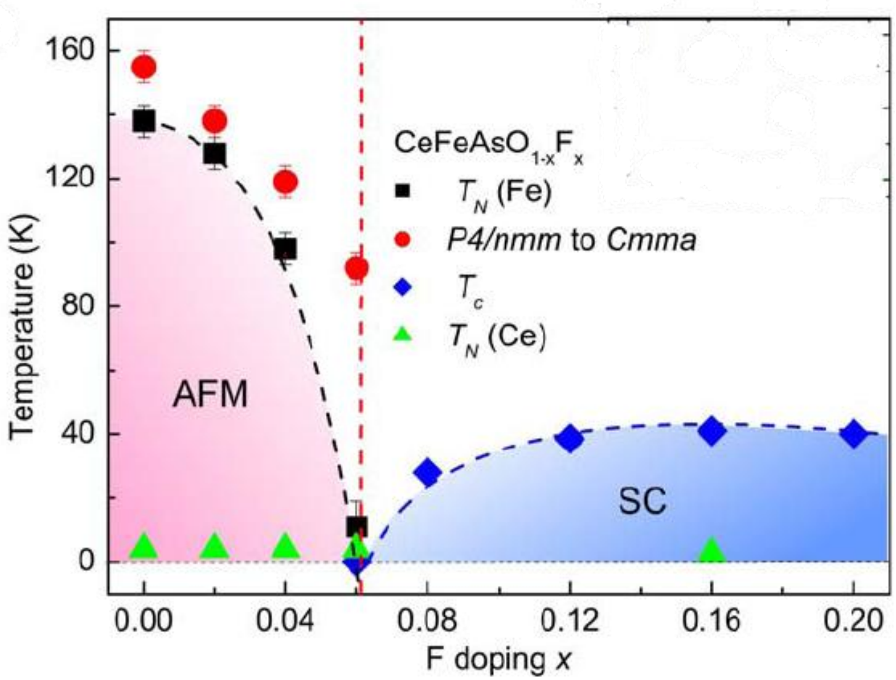
O(6) symmetry at the fixed point trajectory

Podolsky, Kee & Kim

In the process of RG flow, the interaction in the extended s-wave channel becomes attractive

Numerical RG : F. Wang, H. Zhai, Y. Ran, A. Vishwanath, and D.- H. Lee
C. Platt, C. Honerkamp, and W. Hanke





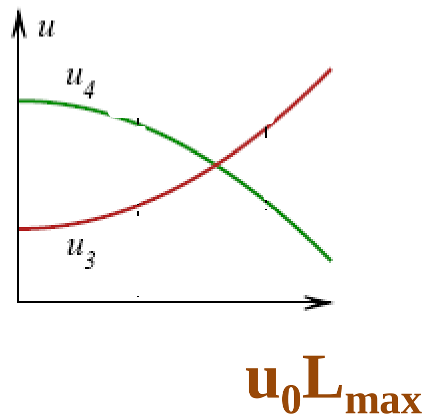
Perfect nesting –
SDW wins

Non-perfect nesting –SDW vertex remains the strongest, but the SDW instability is cut, and a node-less s+ SC wins

However,

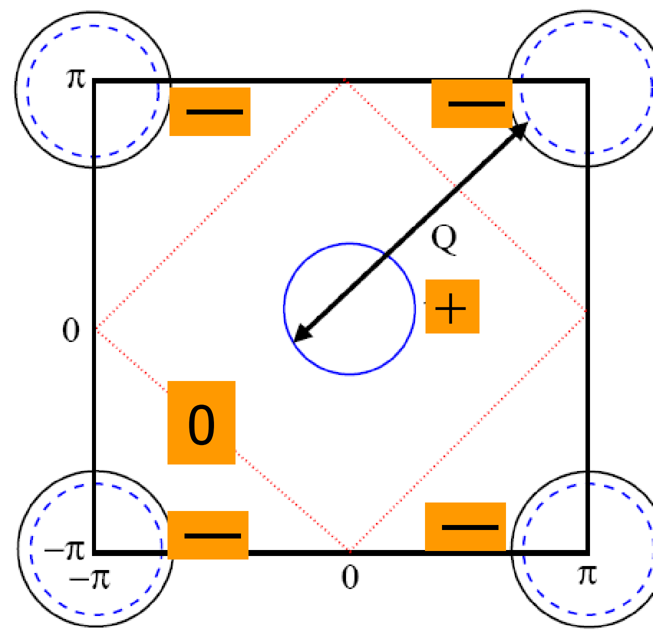
Parquet RG stops at $E \sim E_F$

$u_0 L_{max} = u_0 \log W/E_F$



A sign-changing, nodeless s+ gap does not emerge

No s+ pairing?



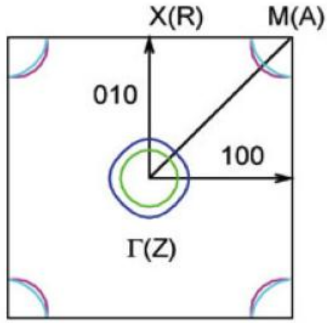
$$\Delta(\theta) = \Delta_0 (\cos k_x + \cos k_y)$$

Let's include momentum-dependent part of the pair hopping

The idea: if the gap averages to zero along either hole or electron FSs, or both, the effect of intra-pocket repulsion will be eliminated , at least partly

$$u_3(q-q')c^\dagger_q c^\dagger_{-q} f_{q'} f_{-q'}$$

$$u_3(p) = u_3 + 2\tilde{u}_3 \cos\frac{p_x}{2}\cos\frac{p_y}{2} + \tilde{\tilde{u}}_3(\cos p_x + \cos p_y) + \ldots$$



The expansion in the size of a Femi pocket

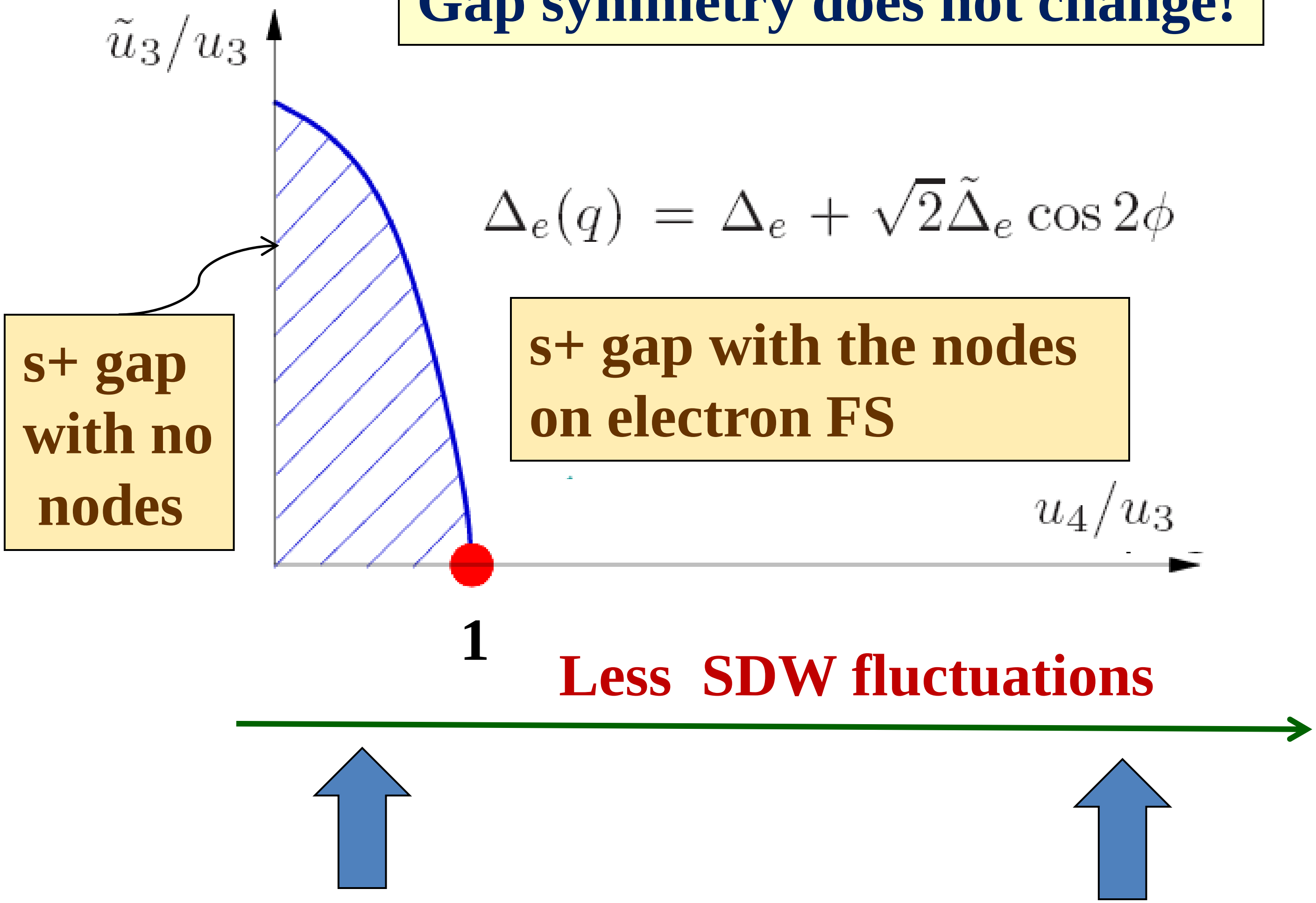
$$\Delta(q) = \Delta_0(\cos q_x + \cos q_y) + \Delta_1 \cos\frac{q_x}{2}\cos\frac{q_y}{2} + \Delta_2(\cos q_x - \cos q_y) + \ldots$$

a plus-minus gap

an s-wave gap with nodes on electron FSs

a d-wave gap with nodes on all FSs

Gap symmetry does not change!



Underdoped 1111, 122 FeAs

LaFeOP, $BaFe_2(As_{1-x}P_x)_2$
Overdoped 1111, 122 FeAs

Conclusions:

Fe-pnictides are itinerant systems,
no evidence for Mott physics

Magnetism is of SDW type, the system remains a metal

Superconductivity is the result of the interplay between intra-pocket repulsion and the pair hopping.

If the tendency towards SDW is strong, pair hopping increases in the RG flow, and the system develops an s^{+-} gap without nodes, once SDW order is eliminated by doping.

If the tendency towards SDW is weaker, intra-pocket repulsion remains the strongest. The system still becomes an s^{+-} supercnductor, but the gap has nodes along the two electron Fermi surfaces.

THANK YOU