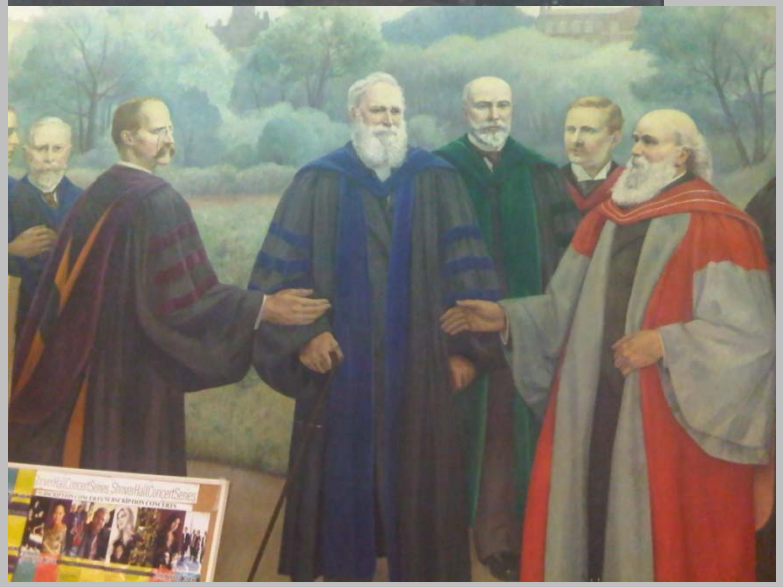


department of
PHYSICS

Colloquia & Seminars

home ›› this week in physics ›› Colloquia & Seminars

". . . To encourage the growth of any science, the best thing we can do is to meet together in its interest, to discuss its problems, to criticize each other's work and, best of all, to provide means by which the better portion of it may be made known to the world. . . ."

Henry A. Rowland, the first president of the American Physical Society

Henry A. Rowland Department of
Physics & Astronomy

Superconductivity at Dawn of the Iron Age

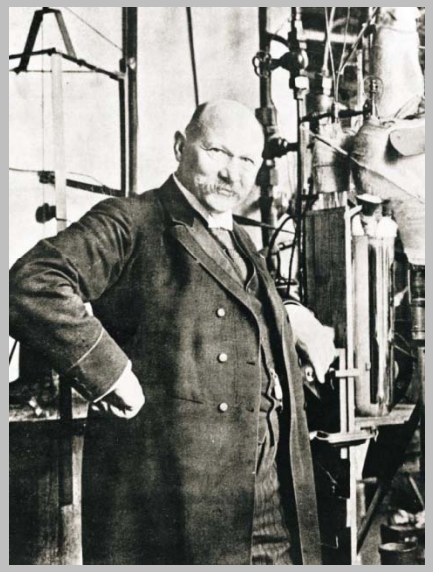
Zlatko Tesanovic, Johns Hopkins University
E-mail: zbt@pha.jhu.edu Web: http://www.pha.jhu.edu/~zbt

$ 100 question: What is the theory of iron-pnictides ?

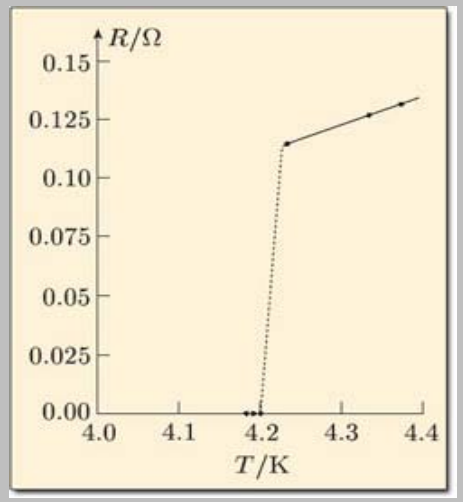
- LDA + RPA: Mazin, Kuroki et al, Scalapino et al, Schmalian et al, ...
- Weak coupling^{++}: Chubukov et al, DH Lee, Vishwanath et al, Cvetkovic et al, ...
- Mott limit: Si & Abrahams, Phillips et al, Sachdev et al, Kivelson et al, Zaanen & Sawatzky et al, Hu, Bernevig et al, Dagotto et al, ...
- Assorted insights: Haule & Kotliar, PA Lee & Wen, Raghu, SC Zhang, et al, Nagaosa & Ng, Gor'kov et al, Hirschfeld et al, FC Zhang & Rice, Castellani et al, ...

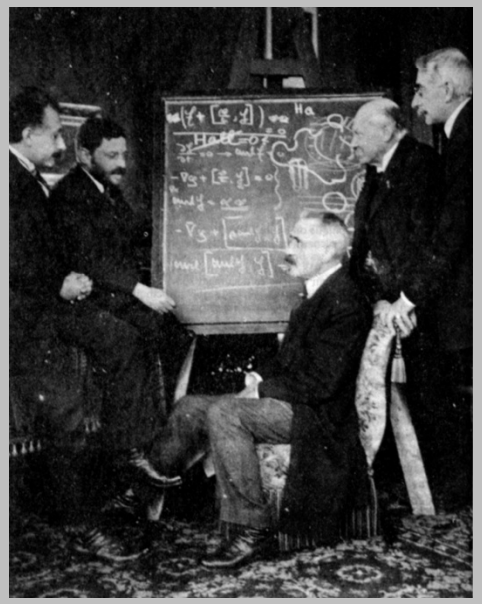
Summer Blockbuster of 2008

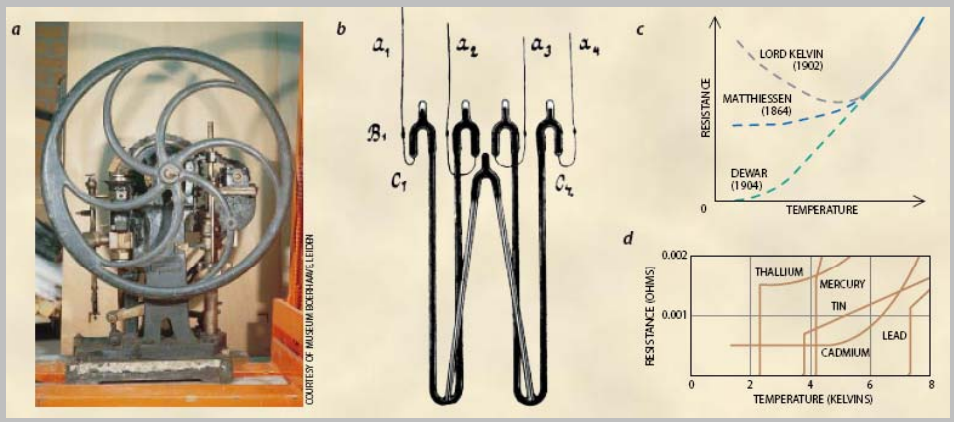
What is superconductivity ?



Heike Kamerlingh Onnes, Nov 1911

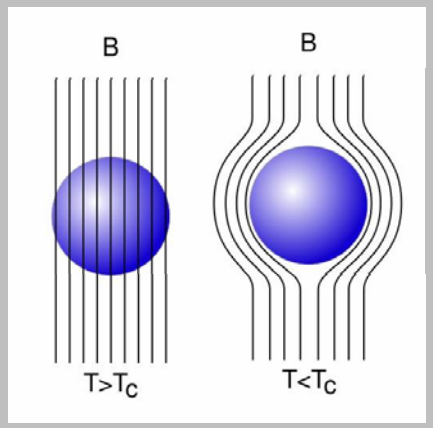






7. arXiv:physics/0510251 [ps, pdf, other]
Title: Theoretical remark on the superconductivity of metals
Authors: Albert Einstein
Comments: Translation of Albert Einstein's article "Theoretische Bemerkungen zur Supraleitung der Metalle", Gedenkboek aangeb. aan H. Kamerlingh Onnes, eaz. Leiden, E. IJdo, 1922 (page 435) Translated by Bjoern S. Schmekel with the courtesy of the Kamerlingh Onnes Laboratory, Leiden - Institute of Physics, Leiden University - A typo in the citation of the original article has been corrected
Subjects: History of Physics (physics.hist-ph); Superconductivity (cond-mat.supr-con)

What is superconductivity ?



Meissner-Ochsenfeld effect, 1933

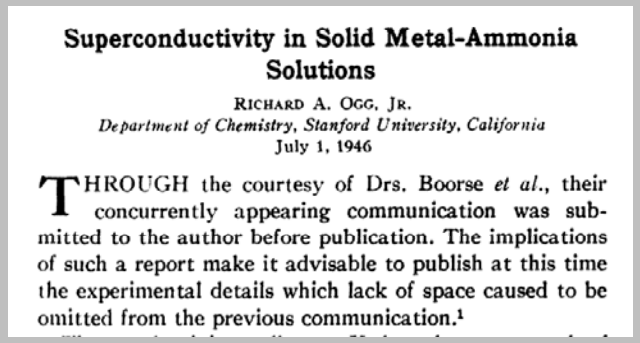
Superconductors are perfect diamagnets

$$\mathbf{j}_s = -\frac{n_s e_s^2}{mc}\mathbf{A}.$$

Heinz & Fritz London, 1935

Ginzburg-Landau theory, 1950-57

$$F = F_n + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m}\left|(-i\hbar\nabla - 2e\mathbf{A})\,\psi\right|^2 + \frac{|\mathbf{B}|^2}{2\mu_0}$$



Superconductivity in Solid Metal-Ammonia Solutions

RICHARD A. OGG, JR.
Department of Chemistry, Stanford University, California
July 1, 1946

THROUGH the courtesy of Drs. Boorse *et al.*, their concurrently appearing communication was submitted to the author before publication. The implications of such a report make it advisable to publish at this time the experimental details which lack of space caused to be omitted from the previous communication.[1]

GL theory explained much of superconducting phenomenology, including Meissner effect. GL leads Abrikosov to theory of type-II SC

Ogg pairs, 1945 were real-space "molecules" that underwent Bose-Einstein condensation

Bardeen-Cooper-Schrieffer (BCS) theory, 1957

$$|\phi_0\rangle = \prod_k \left(u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow}\right)|0\rangle$$

BCS introduce quantum mechanical wavefunction that captures the microscopic essence of superconductivity

What is superconductivity good for ?

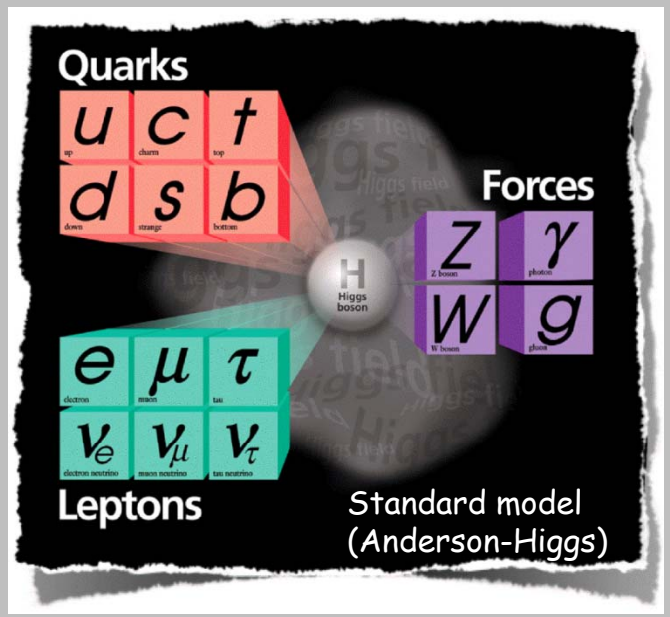
LHC magnets

Energy transmission & storage

Cell phone base stations

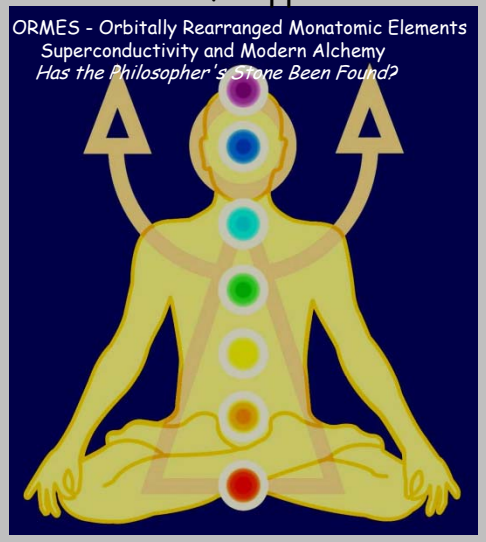
MRI medical imaging

Maglev trains



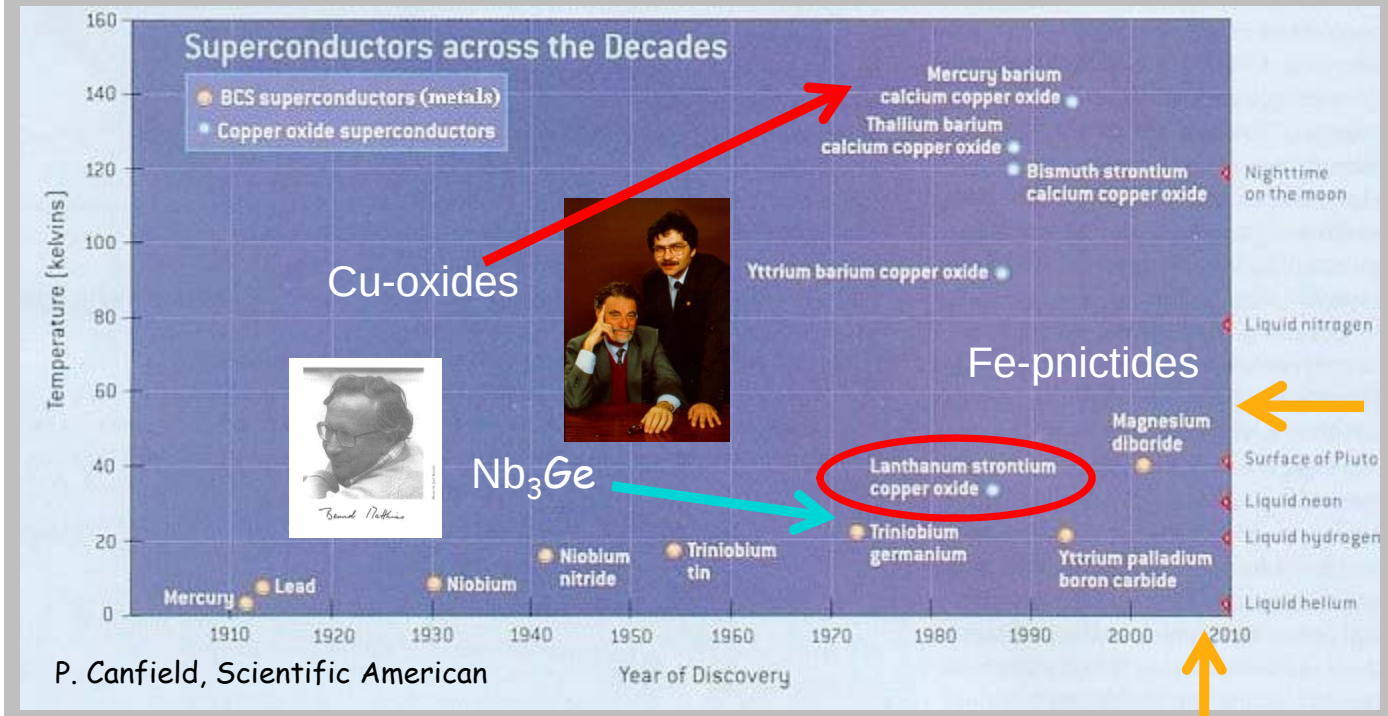
Standard model
(Anderson-Higgs)

Pursuit of happiness

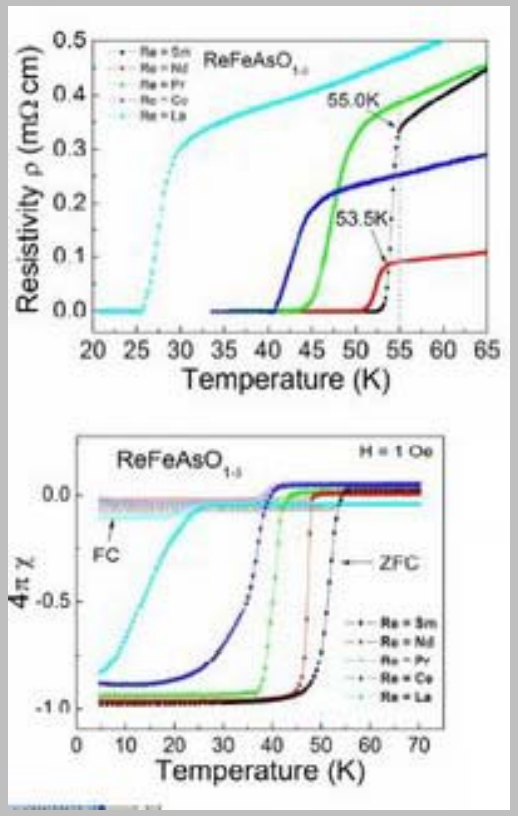


"Negative" gravity (Physics Fair)

Superconductors → Hg → Nb_3Ge → cuprates → pnictides



P. Canfield, Scientific American

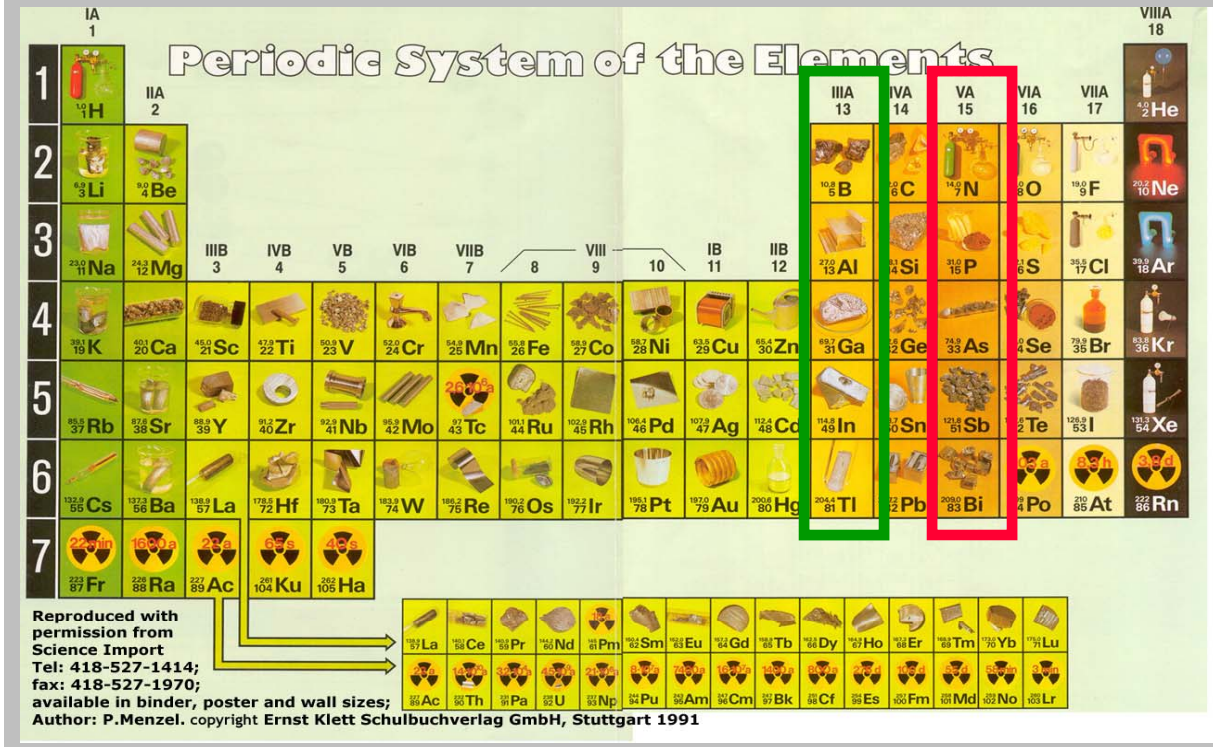


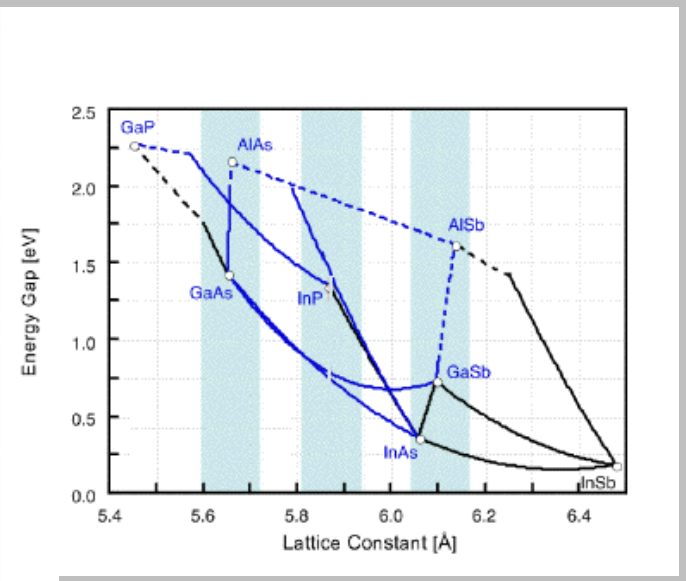
Spring 2008

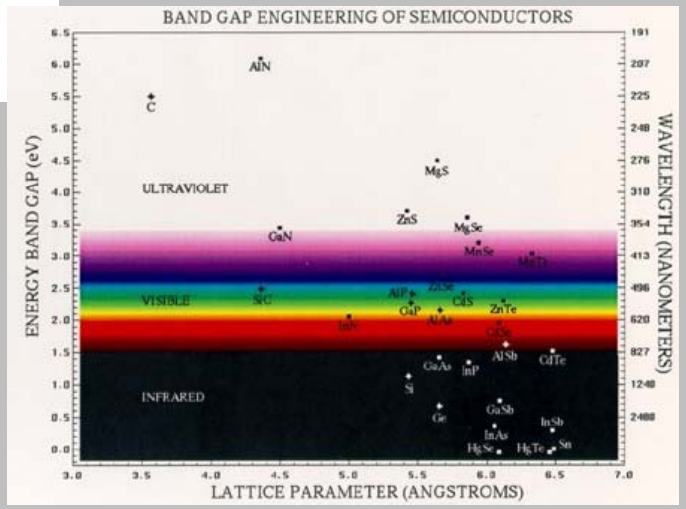
time

Greatest web-induced frenzy in history of condensed matter physics: 17 papers on arXiv in a single July '08 day. Comparable to the latest superstring "revolution" (Bagger-Lambert)

Pnictides πνίγειν (Greek for chocking, suffocation): Semiconductors → Semimetals → Superconductors







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: aluminium phosphide, aluminium arsenide, aluminium antimonide, gallium phosphide, gallium arsenide, gallium antimonide, indium phosphide, indium arsenide and indium antimonide plus numerous ternary and quaternary semiconductors.

Fe-pnictides: Semimetals → Superconductors

May 2006

J|A|C|S COMMUNICATIONS

Published on Web 07/15/2006

Iron-Based Layered Superconductor: LaOFeP

Yoichi Kamihara,† Hidenori Hiramatsu,† Masahiro Hirano,†,‡ Ryuto Kawamura,§ Hiroshi Yanagi,§ Toshio Kamiya,†,§ and Hideo Hosono*,†,‡

ERATO-SORST, JST, Frontier Collaborative Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan, Frontier Collaborative Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan, and Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-4, 4259 Nagatsuta, Yokohama 226-8503, Japan

Received May 15, 2006; E-mail: hosono@msl.titech.ac.jp

日経ナノビジネス R&Dから実用化へ NIKKEI NANO BUSINESS

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ナノテクノロジーの専門情報

日経ナノビジネスについて

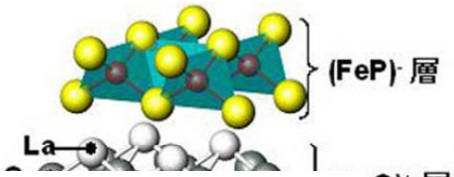
JSTと東工大、新しい酸化物超電導体LaOFePを発見

2006-07-18 (黒川 卓)

印刷用ページ

科学技術振興機構(JST)は東京工業大学と協同で、層状構造の新しい酸化物超電導体を発見した。酸化物超電導体としては遷移金属の銅(Cu)を含む物質がよく知られ、すでに産業界で実用化が始まっている。今回発見されたのは、Cuの代わりに遷移金属の鉄(Fe)を含む酸化超電導体。超電導転移する温度(Tc)は4Kと今のところ低いが、今後、構成元素の種類と組成比を変えることによってTcをさらに高められる可能性がある。

今回発見された超電導体の化学組成はLaOFeP(ランタン・鉄・リン酸化物)。JSTが進める「透明酸化物のナノ構造を活用した機能開拓と応用展開」プロジェクトで発見された。結晶構造は、LnOMPh(Ln=希土類元素、O=酸素、M=遷移金属、Ph=15族のP・As・Sbなど)で表記される物質群に属している。同プロジェクトの細野秀雄研究総括(東工大教授)らは、$(FeP)^-$層と$(LaO)^+$層が交互に積層したこの物質(Fig1)の超電導は$(FeP)^-$層が担っており、キャリアはFe^{2+}イオンの3d電子だと推定している。



Superconductivity at 43 K in Samarium-arsenide Oxides

$SmFeAsO_{1-x}F_x$

X. H. Chen* and T. Wu, G. Wu, R. H. Liu, H. Chen and D. F. Fang

Hefei National Laboratory for Physical Science at Microscale and Department of Physics,

University of Science and Technology of China,

Hefei, Anhui 230026,

People's Republic of China

arXiv:0803.3603v1 [cond-mat.supr-con] 25 Mar 2008

(Dated: March 25, 2008)

nature International weekly journal of science

go Advanced search

Letter

Nature 453, 761-762 (5 June 2008) | d

Superconductivity at

X. H. Chen[1 (#a1)], T. Wu[1 (#a1)]

1. Hefei National Laboratory for Phys

Correspondence to: X. H. Chen[1 (#a1)]

Since the discovery of hig
been devoted to exploring
from Bardeen–Cooper–Sc
copper oxide supercondu
(ref. 2 (/nature/journal/v453
La–Nd, Sm and Gd) are n
$LaO_{1-x}F_xFeAs$ (ref. 3 (/nat
superconductivity in the r
measurements reveal a tr
high-temperature superc

nature International weekly journal of science

Letter

Nature 459, 64-67 (7 May 2009) | doi:10.1038/nature07981; Received 4 November 2008; Accepted 13 March 2009

A large iron isotope effect in $SmFeAsO_{1-x}F_x$ and $Ba_{1-x}K_xFe_2As_2$

R. H. Liu[1], T. Wu[1], G. Wu[1], H. Chen[1], X. F. Wang[1], Y. L. Xie[1], J. J. Ying[1], Y. J. Yan[1], Q. J. Li[1], B. C. Shi[1], W. S. Chu[2,3], Z. Y. Wu[2,3] & X. H. Chen[1]

1. Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, China
2. Beijing Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China
3. National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei 230026, China

of science

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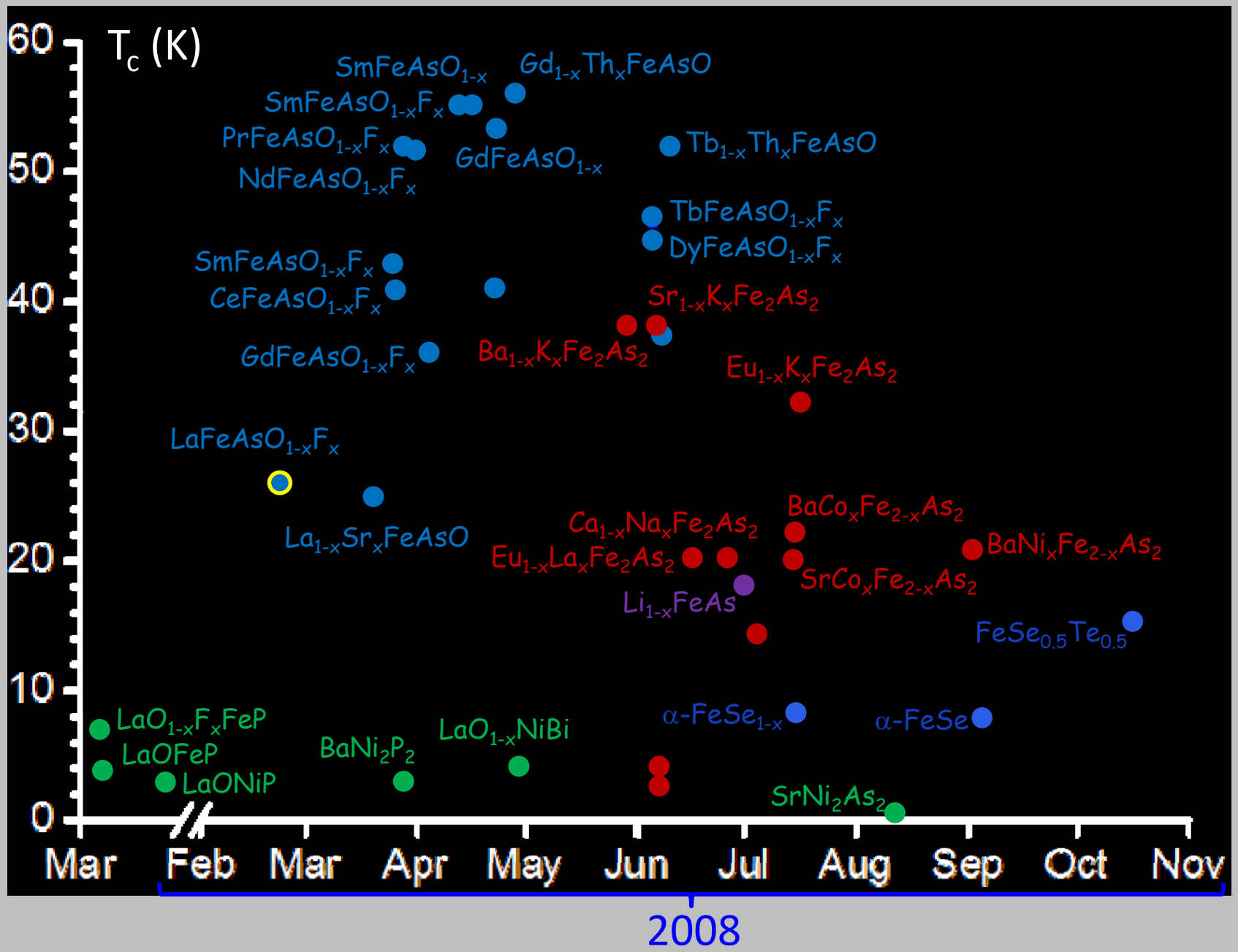
Accepted 5 May 2008; Published online 4 June 2008

;Fo.15

& C. L. Chien[1 (#a1)]

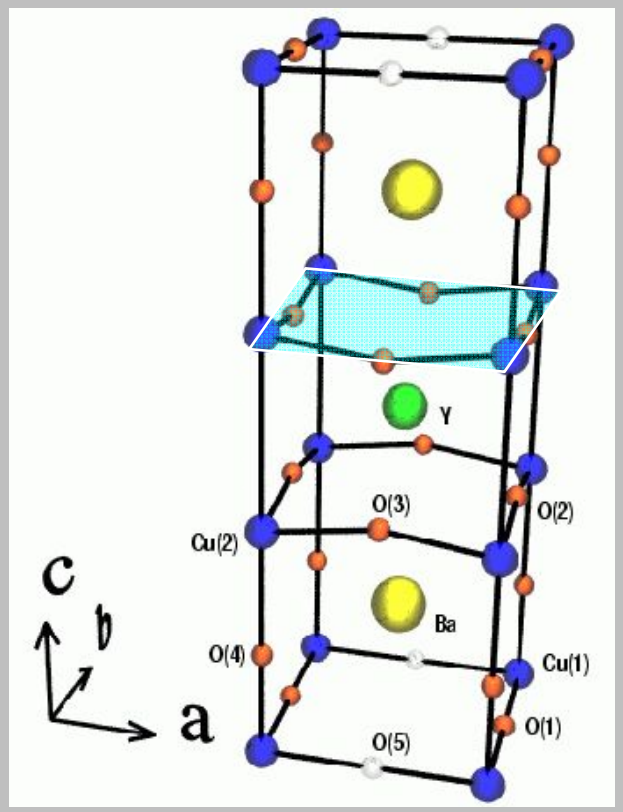
1218, USA

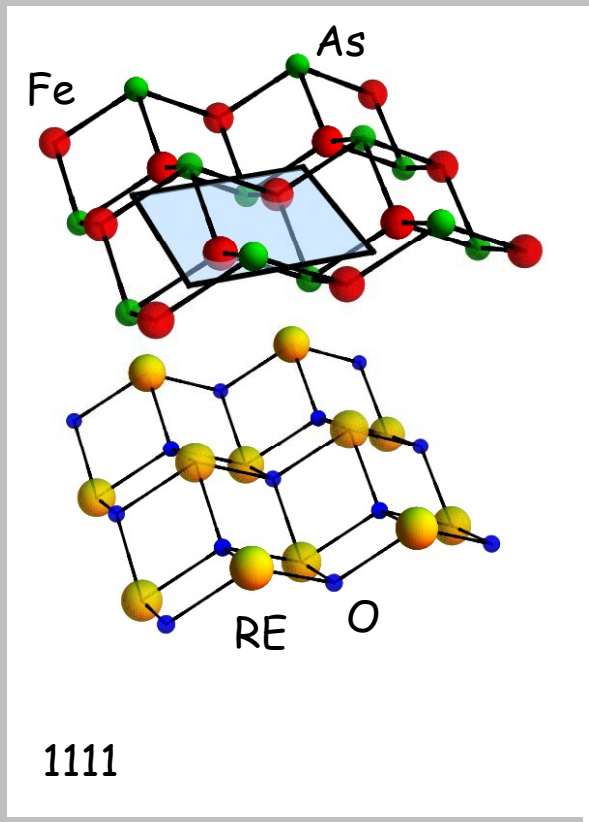
2. Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

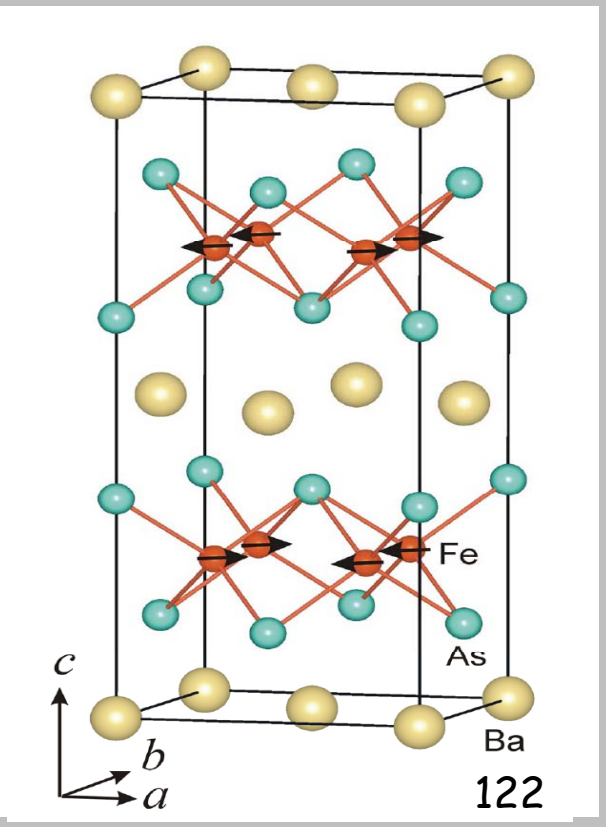


courtesy of J. Hoffman

Cu-oxides versus Fe-pnictides







Both have d-electrons in key role (Cu vs Fe)

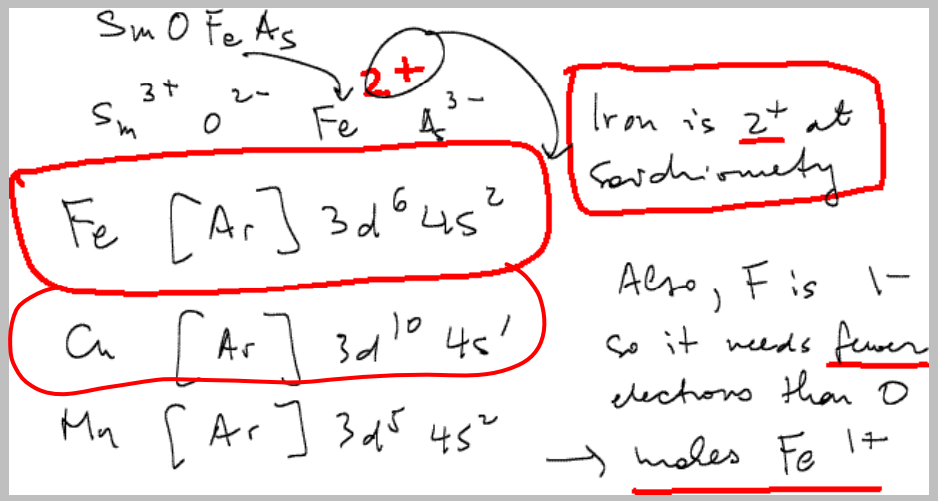
Both are layered (CuO_2 vs FeAs)

Both have AF and SC in close proximity

However, there are also many differences! This may add up to new and interesting physics

Key Difference: 9 versus 6 d-electrons

ZT, Physics **2**, 60 (2009)



$Fe^{2+} \longrightarrow 3d^6$

$Cu^{2+} \longrightarrow 3d^9$

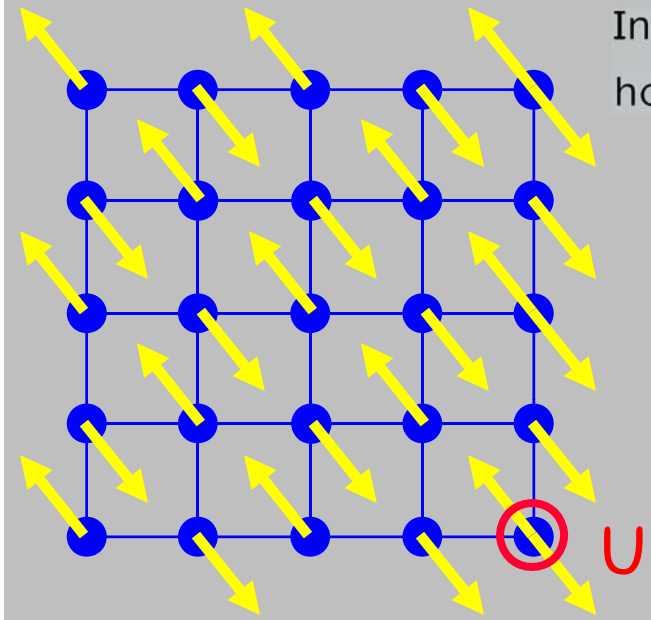
In CuO_2 a **single** hole in a filled 3d orbital shell

→ A suitable single band model might work

In FeAs large and **even** number of d-holes

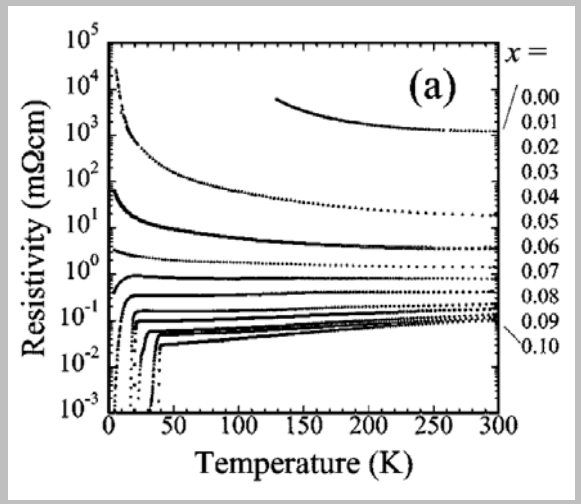
→ A multiband model is likely necessary

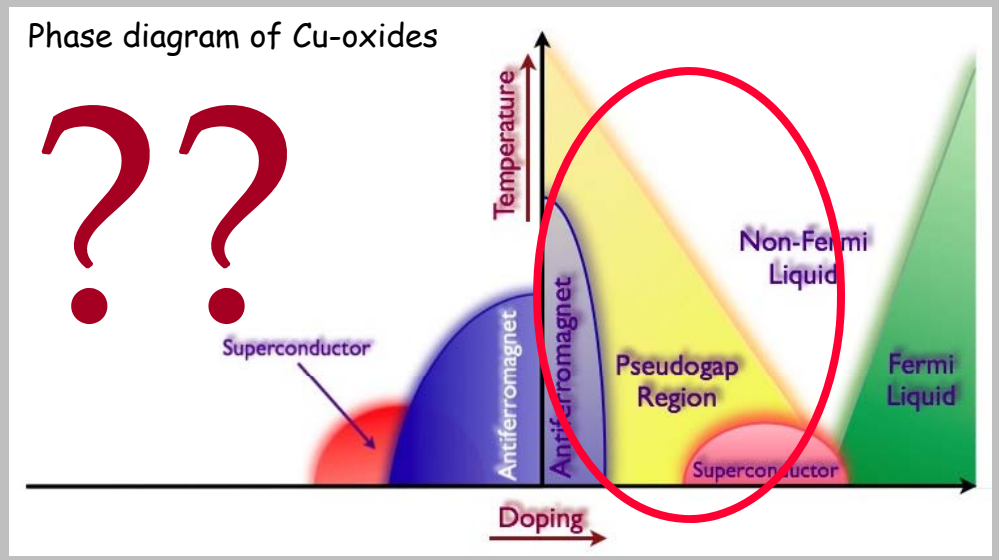
Cu-oxides: Mott Insulators → Superconductors



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

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

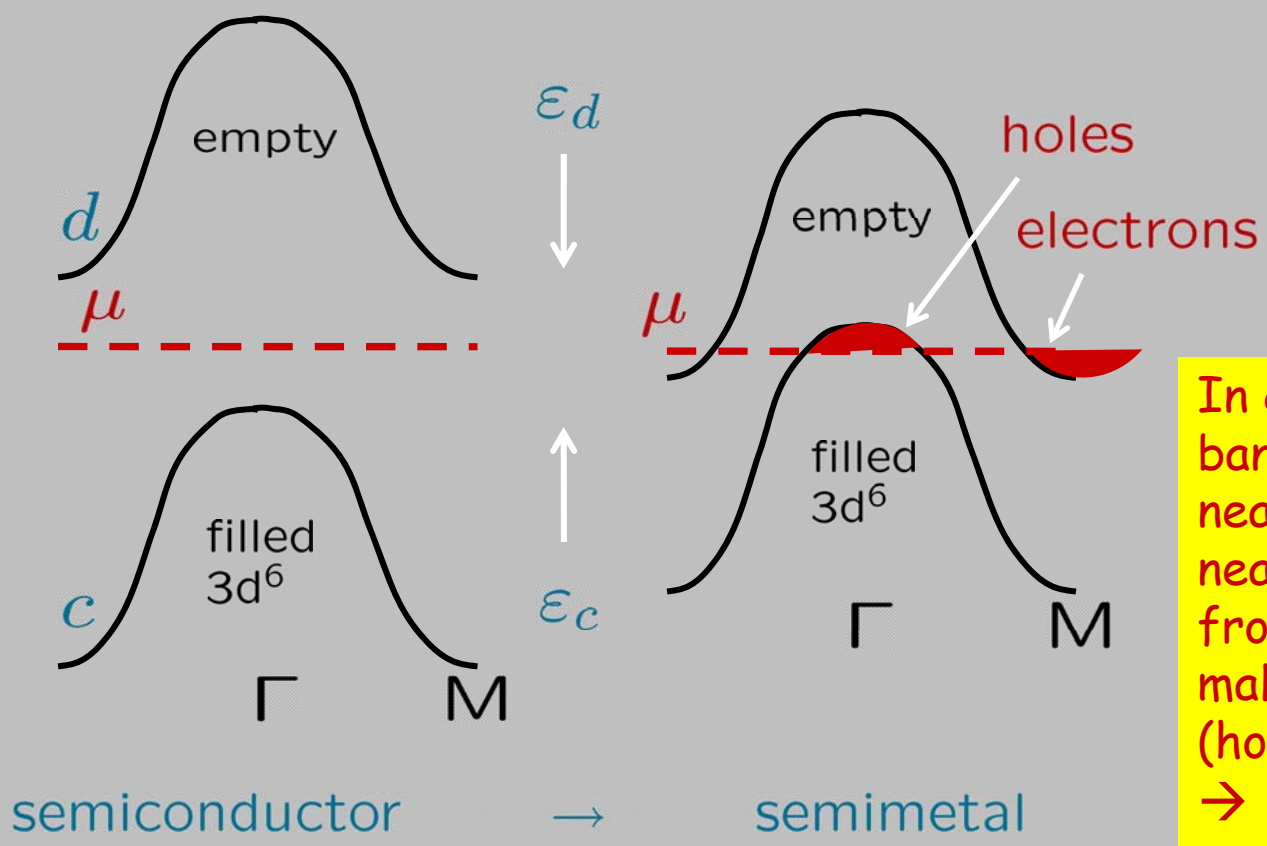




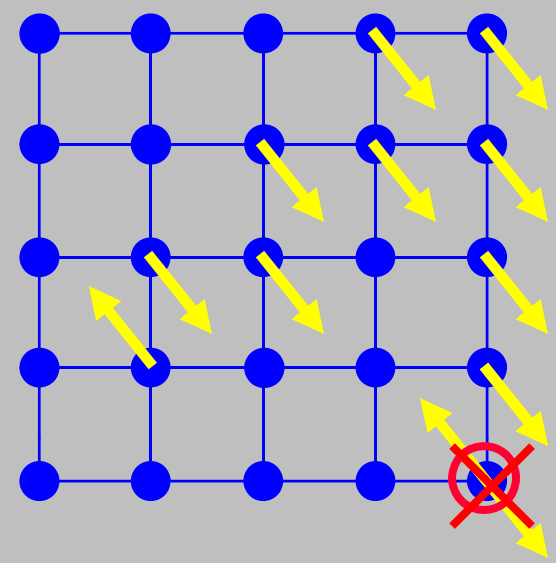
How Mott insulators turn into superconductors, particularly in the pseudogap region, remains one of great intellectual challenges of condensed matter physics

Fe-pnictides: Semimetals → Superconductors

$$\epsilon^c_{\vec{k}} = \varepsilon_c + t_c \cos(k_x a) + t_c \cos(k_y a)$$
$$\epsilon^d_{\vec{k}} = \varepsilon_d + t_d \cos(k_x a) + t_d \cos(k_y a)$$



$Fe^{2+} \longrightarrow 3d^6$

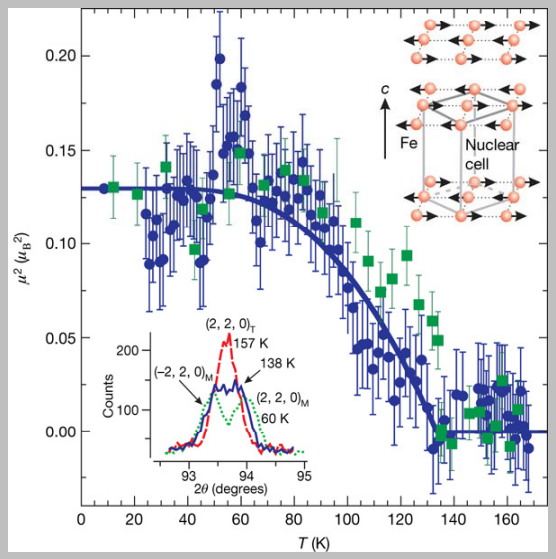


In contrast to CuO_2, all d-bands in FeAs are either nearly **empty** (electrons) or nearly **full** (holes) and far from being **half-filled.** This makes it easier for electrons (holes) to avoid each other.

→ **FeAs are less correlated than CuO_2 (correlations are still important !!)**

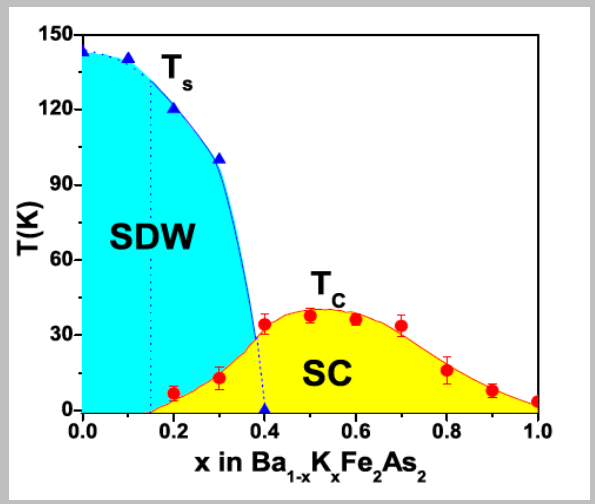
Phase diagram of Fe-pnictides

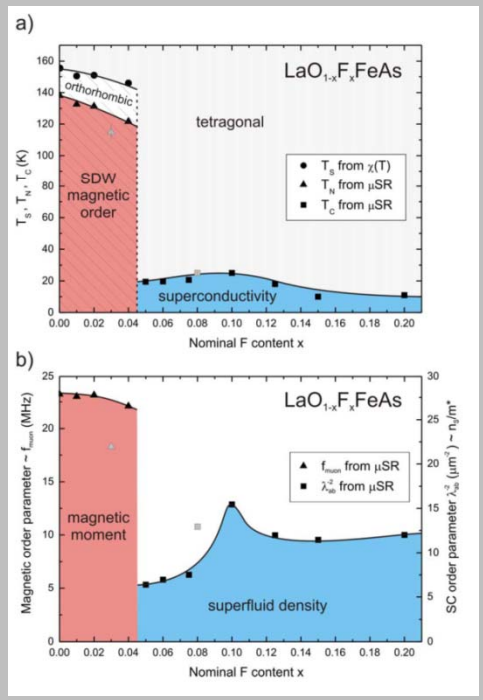
C. de la Cruz, *et al.*, Nature **453**, 899 (2008)



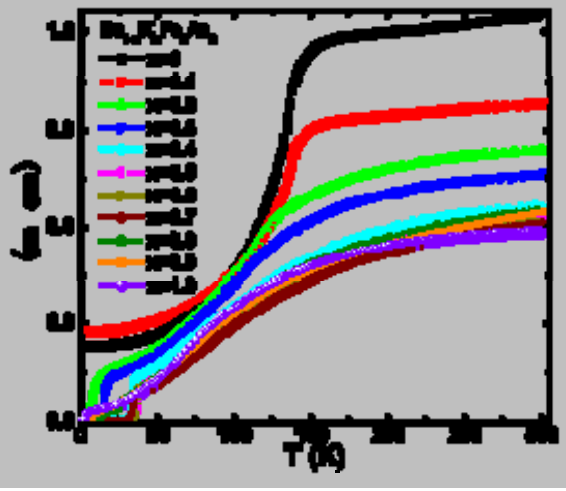
Like CuO_2, phase diagram of FeAs has SDW (AF) in proximity to the SC state.

H. Chen, *et al.*, arXiv/0807.3950



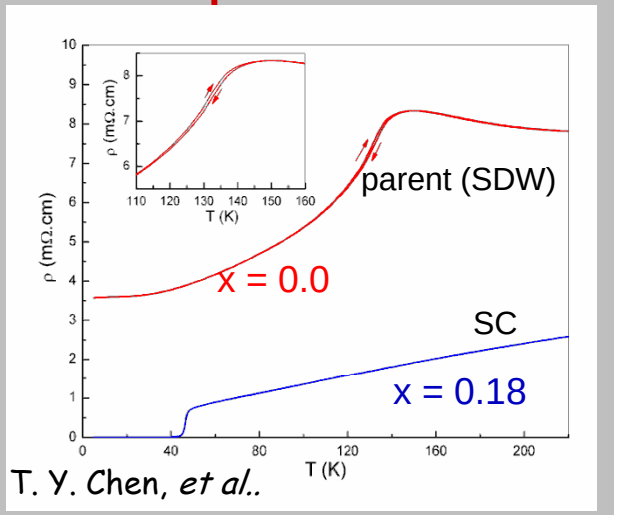


SC coexists with SDW (AF) in 122 compounds →



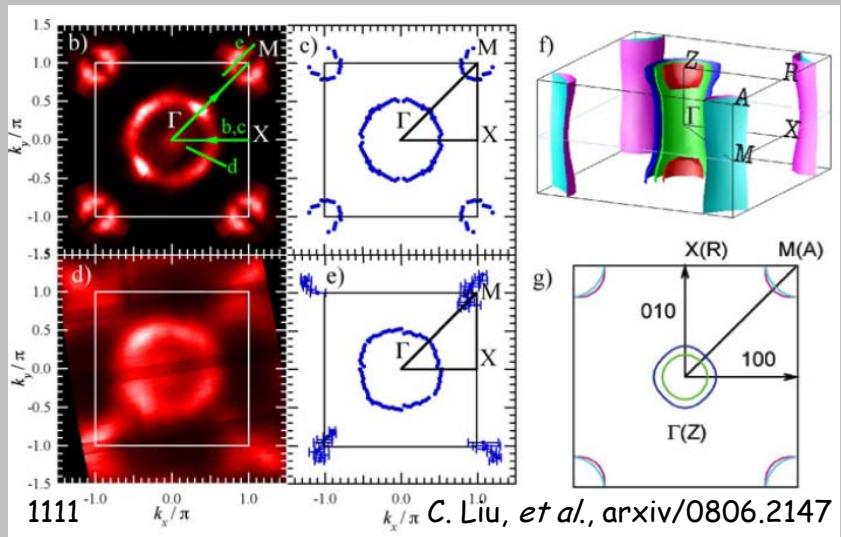
However, unlike CuO_2, all regions of FeAs phase diagram are (bad) metals !!

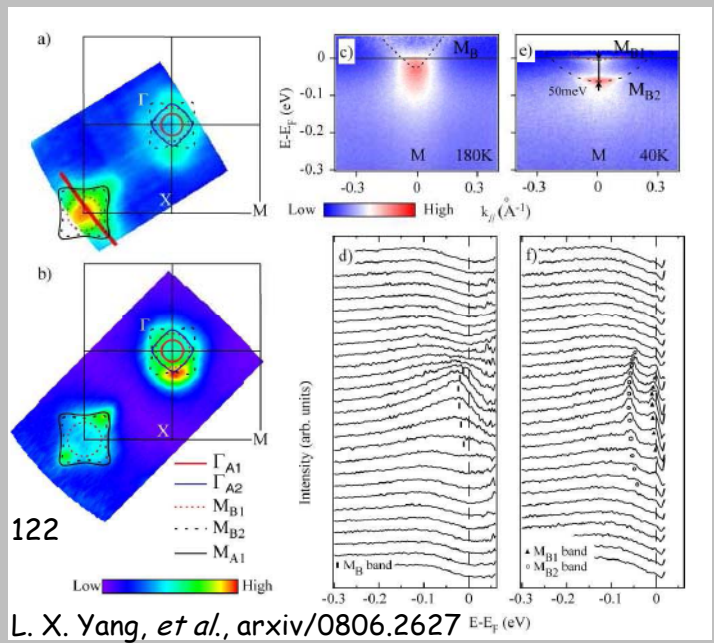
$SmFeAsO_{1-x}F_x$

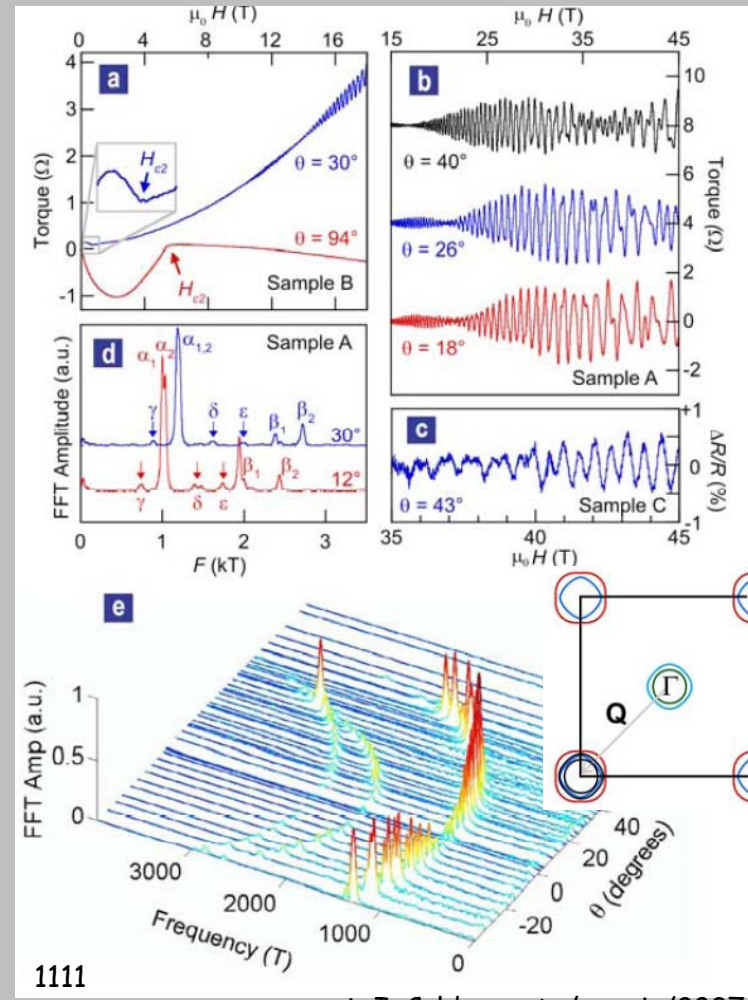


T. Y. Chen, *et al.*.

ARPES + dHvA



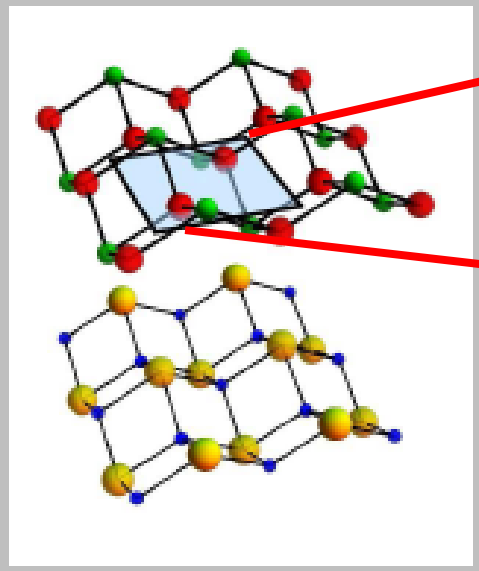


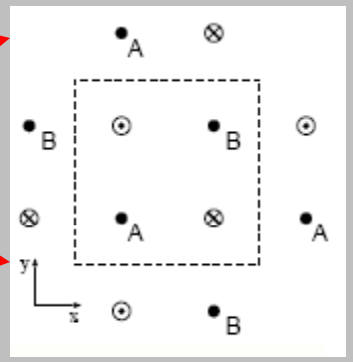


ARPES and dHvA see coherent (metallic) bands in rough agreement with LDA.

Minimal Model of FeAs Layers I

V. Cvetkovic and ZT, EPL **85**, 37002 (2009)



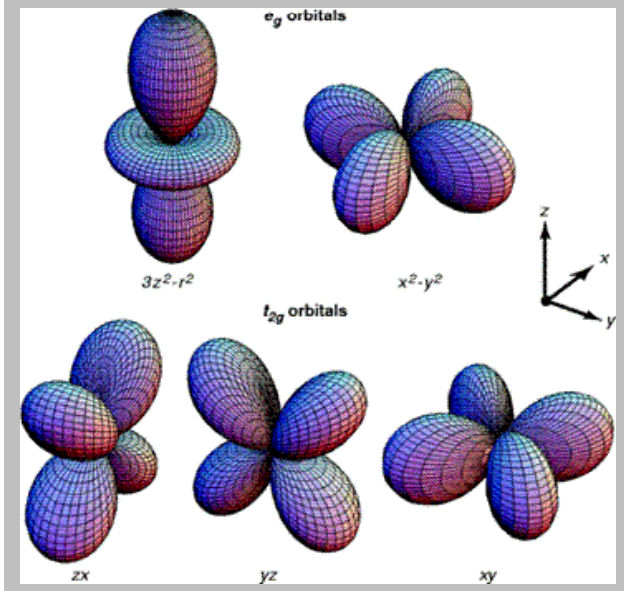


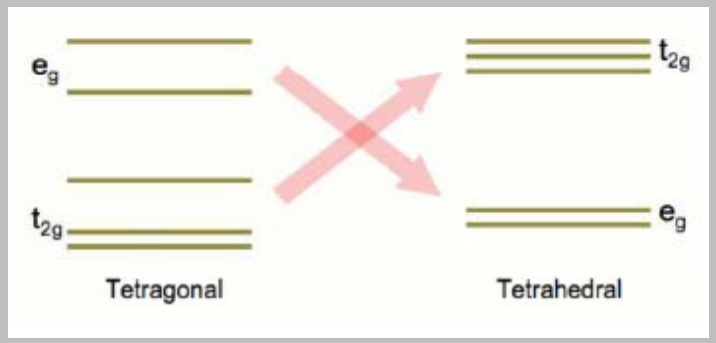
We consider effective 2D Fe model, with all 5 d-orbitals. As bands are below E_F but they contribute crucial terms to the "minimal" model

"Puckering" of FeAs planes is essential:

i) All d-orbitals are near E_F

ii) Large overlap with As p-orbitals below E_F
→ enhanced itinerancy of d electrons
defeats Hund's rule and large local moment



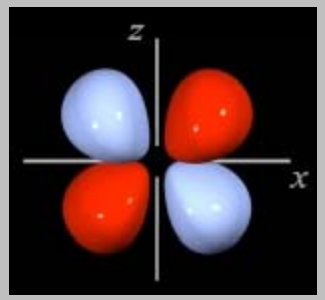


$(5+3)\times 2 = 16\ (\div 2)$ Wannier orbitals

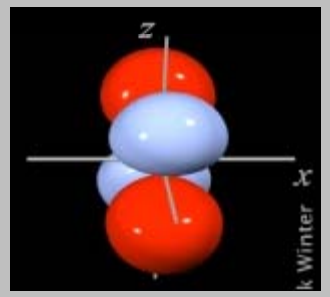
$\Rightarrow$ "minimal" model $\Rightarrow$

Minimal Model of FeAs Layers II

We consider an effective 2D model with 5 Fe + 3 As orbitals

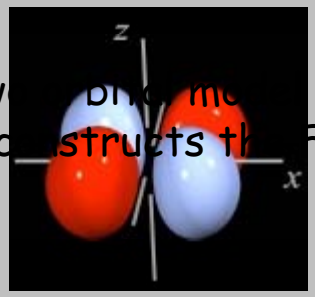


d_{xz}

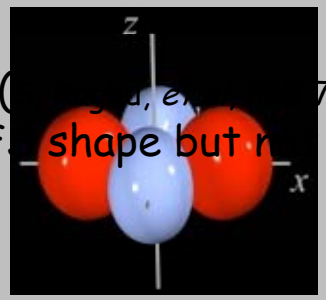


d_{yz}

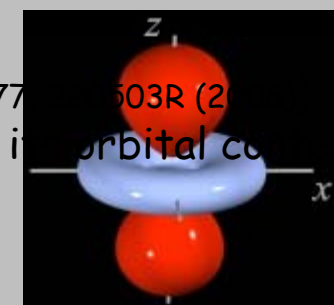
Tw[illegible] bri[illegible] mo[illegible] ([illegible] 77[illegible] 503R (2[illegible]
rec[illegible]structs th[illegible] F[illegible] shape but n[illegible] i[illegible] orbital co[illegible]nt



d_{xy}



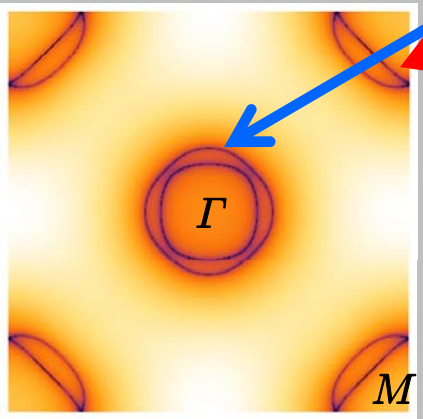
d_{xx-yy}



$d_{2zz-xx-yy}$

odd parity

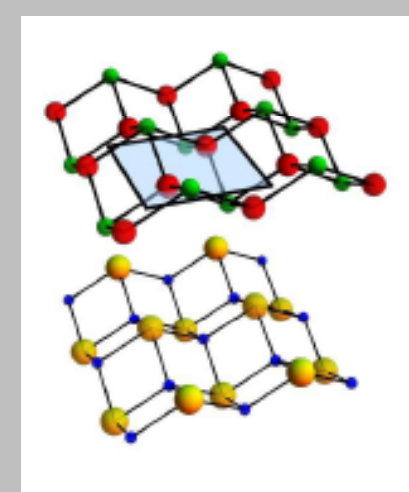
even parity



The importance of Fe 3d – As 4p hybridization:

Without pnictide atoms many hopping processes would vanish by symmetry.

These symmetries are violated by pnictide puckering.



Hund's Rule Defeated

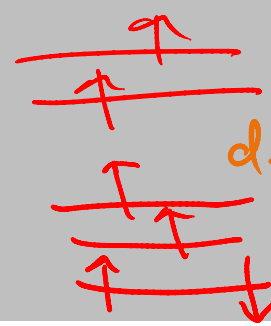
Hund's rule rules for Mn^{2+} :
all five d-electrons line up to minimize
Coulomb repulsion → S = 5/2

Y. Singh *et al.*, arXiv/0907.4094 (MnAs)

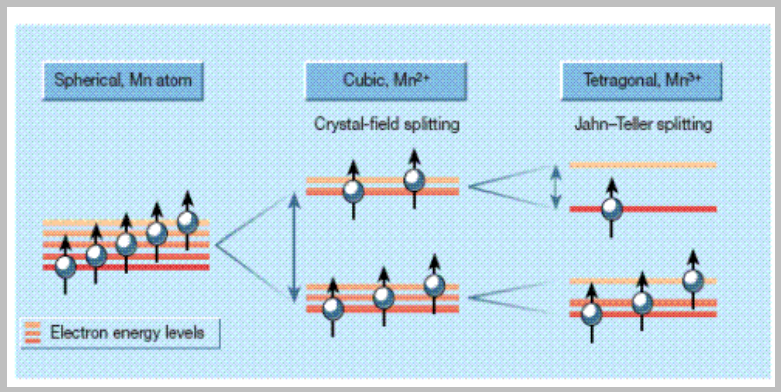
Fe^{2+}

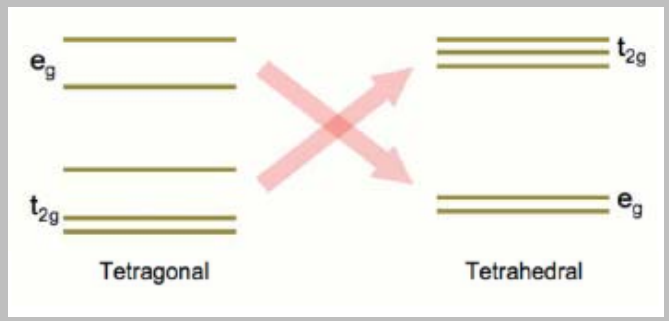
⇓

S = 2



6 d-electrons





SmOFeAs

Sm^{3+} O^{2-} Fe^{2+} As^{3-}

Iron is 2^+ at Sarchiometry

Fe [Ar] $3d^6 4s^2$

Cu [Ar] $3d^{10} 4s^1$

Mn [Ar] $3d^5 4s^2$

Also, F is 1− so it needs fewer electrons than O → makes Fe^{1+}

FeAs is away from Mott limit ($U < U_c$)

"Puckering" of FeAs planes is essential:

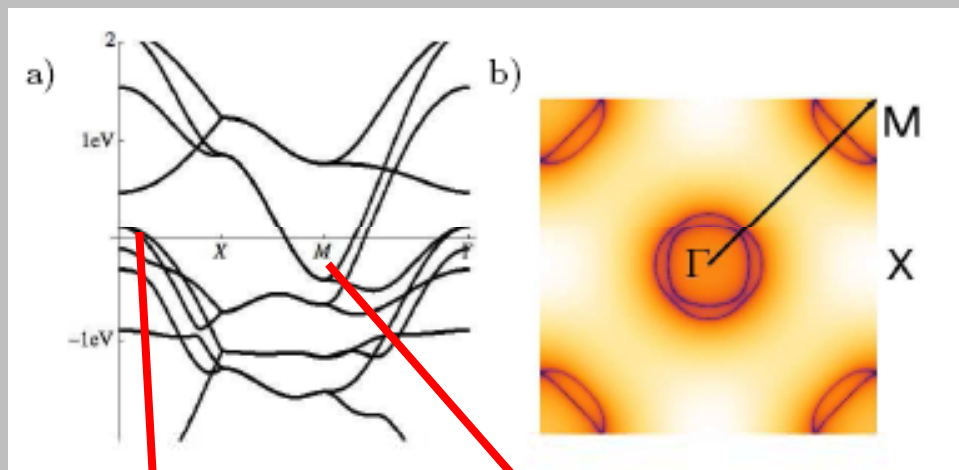
i) All d-orbitals are near E_F

ii) Large overlap with As p-orbitals below E_F → enhanced itinerancy of d electrons defeats Hund's rule and large local moment

Haule, Shim and Kotliar, PRL **100**, 226402 (2008)

Minimal Model of FeAs Layers III

V. Cvetkovic and ZT, EPL **85**, 37002 (2009); arXiv/0804.4678



hole FS
2 pockets (valleys)

electron FS
2 pockets (valleys)

Tight-binding model optimized for band structure + exps.
Only nearest neighbor Fe-As, Fe-Fe and As-As hoppings are used.

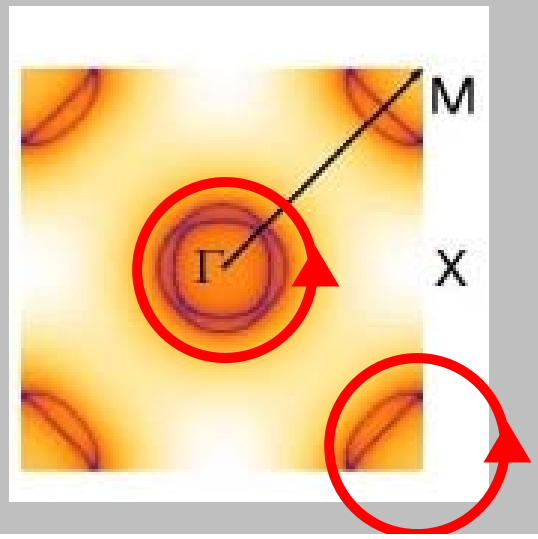
α	x^2-y^2	z^2	xy	xz
ϵ_α	-0.85	-1.4	-1.1	-1.15
$t^{Fe}_{\alpha,\alpha}$	-0.55	-0.5	-1.6	-0.55
$t_{\alpha,x/y}$	0.65	-1.4	1.5	3.2
$t_{\alpha,z}$	2.1	1.25		0.7

β	x	z
ϵ_β	-4.0	-4.0
$t^{As}_{\beta,\beta}$	-0.8	-0.45

$t^{Fe}_{z^2,xy} = 0.1$, $t^{Fe}_{xz,yz} = -0.75$, and $t^{As}_{x,y} = 0.8$.

Important: Near E_F e and h bands contain significant admixture of **all** five Wannier d-orbitals, d_{xz} and d_{yz} of **odd** parity (in FeAs plane) and the remaining three d-orbitals of **even** parity in FeAs plane →

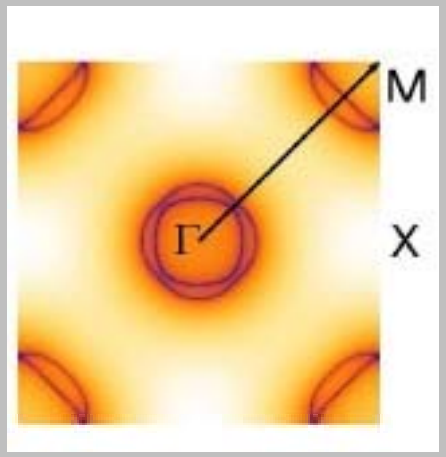
As one goes around the FS there is strong mixing of odd and even d-orbitals
⇒ no simple orbital "topology"



Nesting and Valley Density-Wave (VDW) in Fe-pnictides I

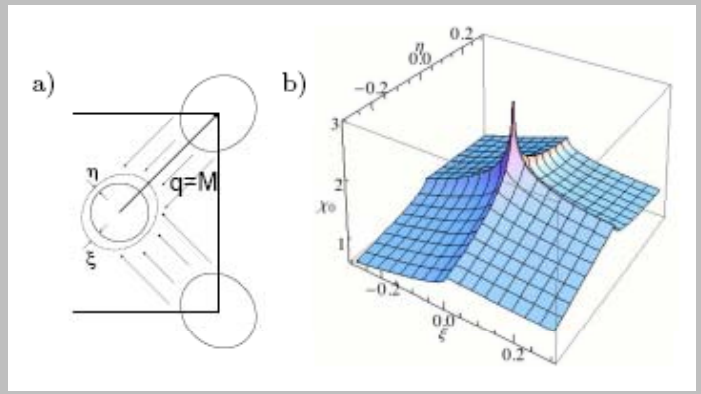
V. Cvetkovic and ZT, EPL **85**, 37002 (2009); arXiv/0804.4678

V. Cvetkovic and ZT, PRB **80**, 024512 (2009); arXiv/0808.3742

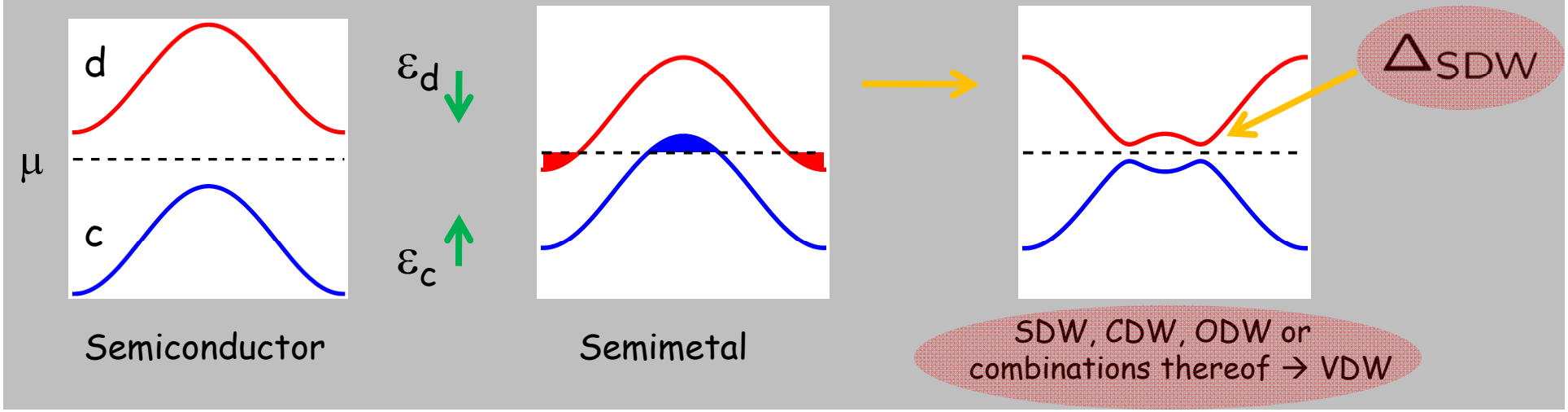


If hole (Γ) and electron bands (M) are identical
$\Rightarrow$ perfect nesting at $\mathbf{q} = \mathbf{M} = (\pi, \pi)$ $\Rightarrow$
strongly enhanced electron-hole excitations

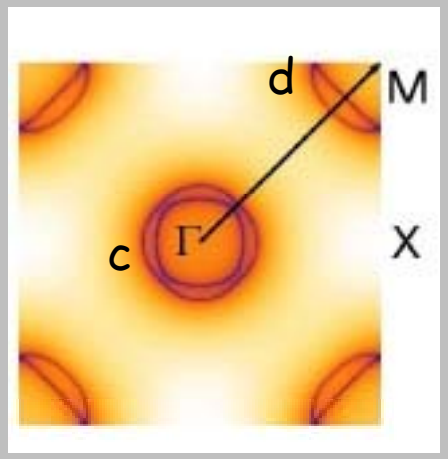
$$\chi_0'(\mathbf{q}, \omega = 0) = 2\frac{m_e}{2\pi} \log \frac{\Lambda}{|\mathbf{q} - \mathbf{M}|},$$

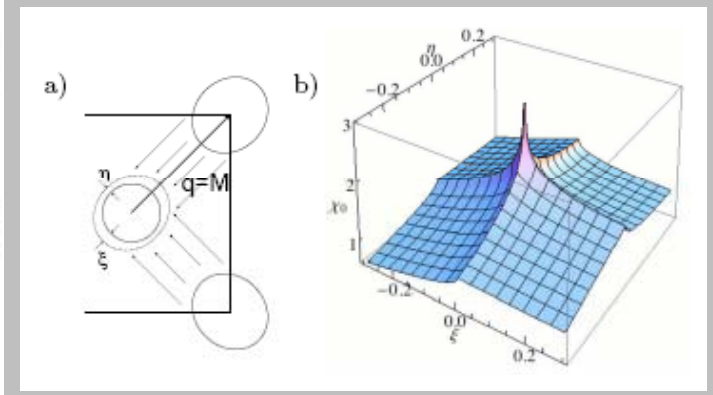


Turning on moderate interactions →
VDW = itinerant multiband CDW (structural), SDW (AF) and orbital orders at **q** = **M** = (π,π)



Nesting and Valley Density-Wave (VDW) in Fe-pnictides II



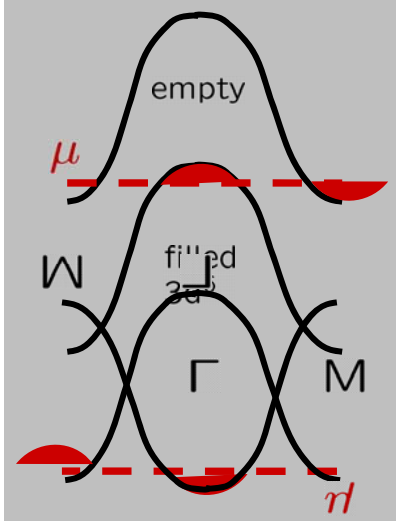


$$\chi_0'(\mathbf{q},\omega=0) = 2\frac{m_e}{2\pi}\log\frac{\Lambda}{|\mathbf{q}-\mathbf{M}|},$$

Consider the bare-bones model for interactions:

$$H = -\varepsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \varepsilon_{\mathbf{k}} d_{\mathbf{k}}^\dagger d_{\mathbf{k}} + U n_c^2 + U n_d^2 + W n_c n_d + (\cdots)$$

spinless fermions — Intraband — Interband



→ Particle-hole transformation

$$c \to h^\dagger \ , d \to e \ , n_c \to 1 - n_h \ , n_d \to n_e$$

$$H \to \varepsilon_{\mathbf{k}} h_{\mathbf{k}}^\dagger h_{\mathbf{k}} + \varepsilon_{\mathbf{k}} e_{\mathbf{k}}^\dagger e_{\mathbf{k}} - W n_h n_e + (\cdots)$$

Negative U Hubbard model: $(h, e) \leftrightarrow (f_\uparrow, f_\downarrow)$

Fictitious "Superconductor" → VDW in Fe-pnictides

$H \to \varepsilon_{\mathbf{k}} h^\dagger_{\mathbf{k}} h_{\mathbf{k}} + \varepsilon_{\mathbf{k}} e^\dagger_{\mathbf{k}} e_{\mathbf{k}} - W n_h n_e$

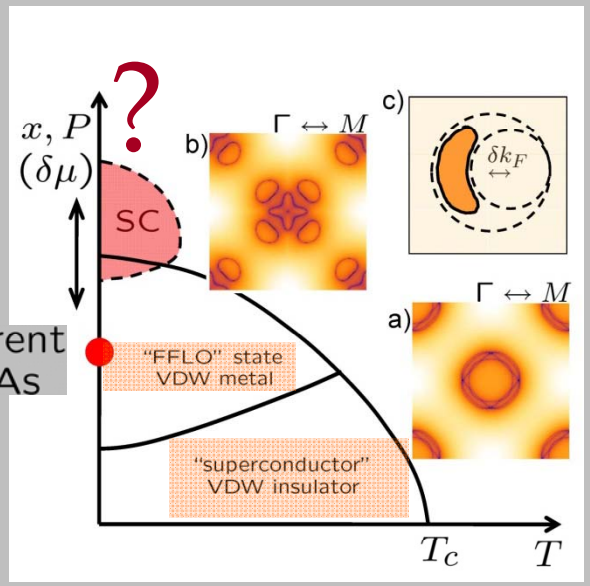
Negative U Hubbard model: $(h, e) \leftrightarrow (f_\uparrow, f_\downarrow)$

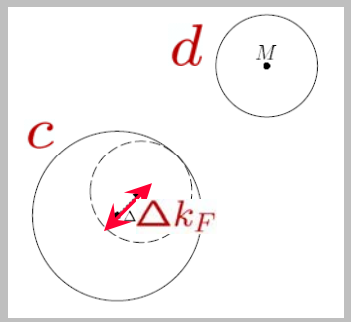
$\to \quad H = \sum_\sigma \varepsilon_{\mathbf{k}} f^\dagger_{\mathbf{k},\sigma} f_{\mathbf{k},\sigma} - W n_{f\uparrow} n_{f\downarrow}$

Ground state is a "superconductor":

$\langle f_\uparrow f_\downarrow \rangle \neq 0 \quad \Rightarrow \quad \langle c^\dagger d \rangle \neq 0$

$\Rightarrow$ insulating VDW (SDW/ODW/CDW)





Generically, the c and d bands are different:

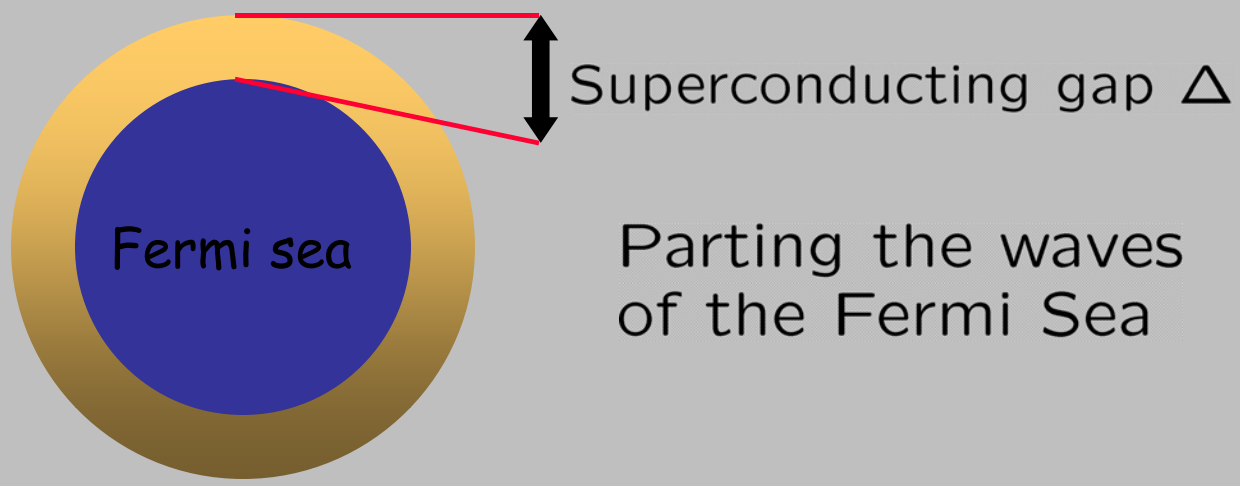
$k_{Fc} - k_{Fd} = \Delta k_F \neq 0 \quad \Rightarrow$ fictitious Zeeman magnetic field

$\Rightarrow$ "Fulde-Ferrell-Larkin-Ovchinikov", "breached pairing" states

$\Rightarrow$ metallic VDW (SDW/ODW/CDW)

What about real superconductivity ? (. . .)

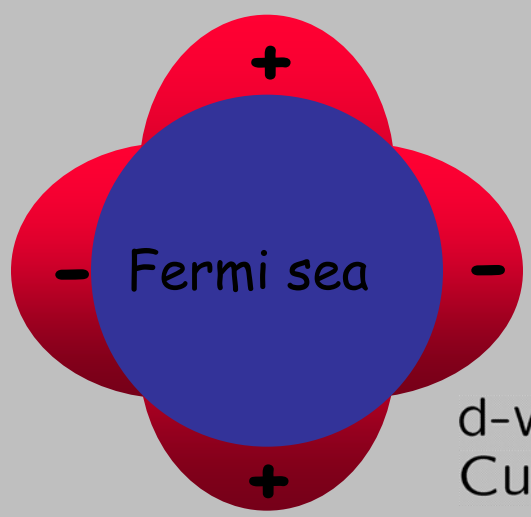
Pairing Gap Δ - Coastline of the Fermi Sea



Parting the waves
of the Fermi Sea

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

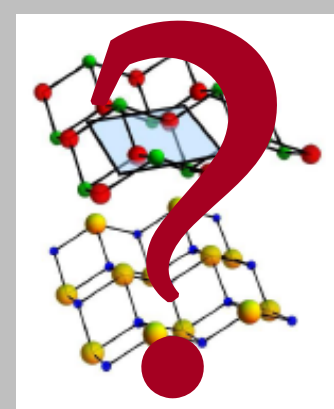
p-wave
Superfluid ^{3}He, SrRu (?)
$T_c \sim$ 1mK - 1K



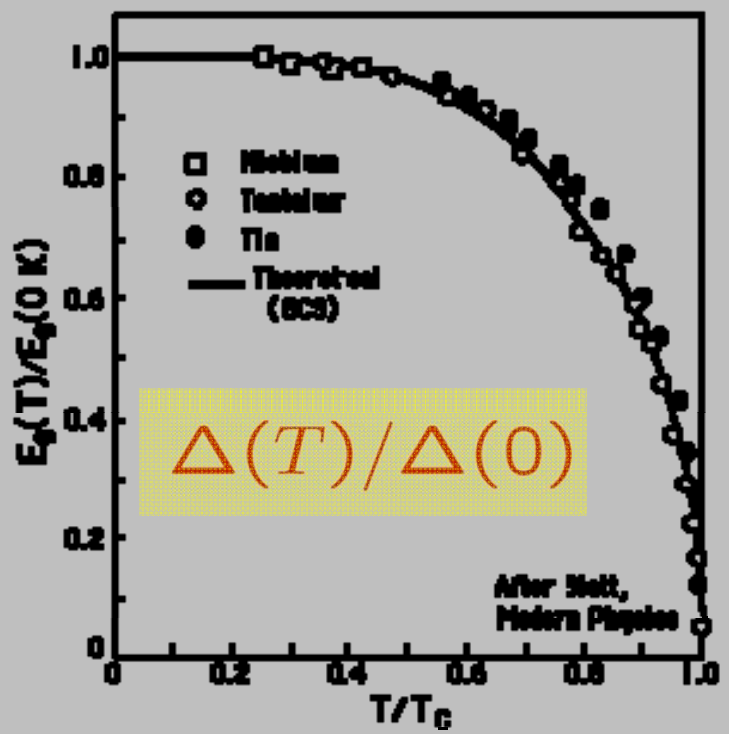
d-wave
Cuprate SC $T_c \sim 160$K

New REOFeAs SC
$T_c \sim 57$ K

$\Delta = ?$



What can Δ tell us about superconducting state ?

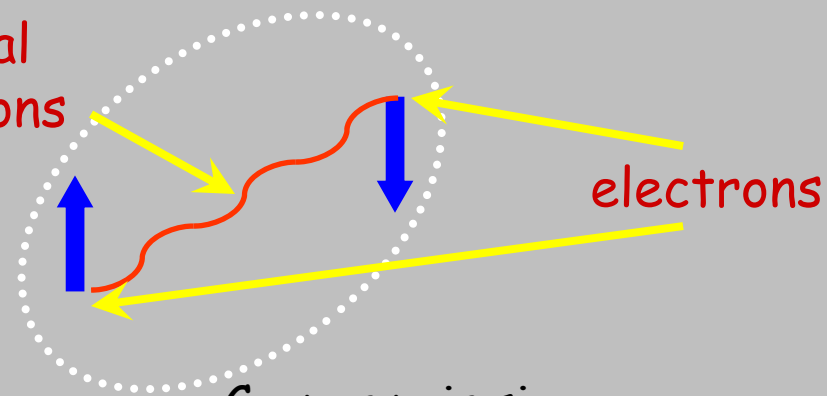


$$\Delta(T)/\Delta(0)$$

$$2\Delta(0)/k_B T_c = 3.53$$

Universal BCS behavior

In conventional superconductors Δ is uniform along Fermi sea (s-wave)
This reflects the pairing interaction being attractive !!
Its origin is electron-electron interaction mediated by phonons !!

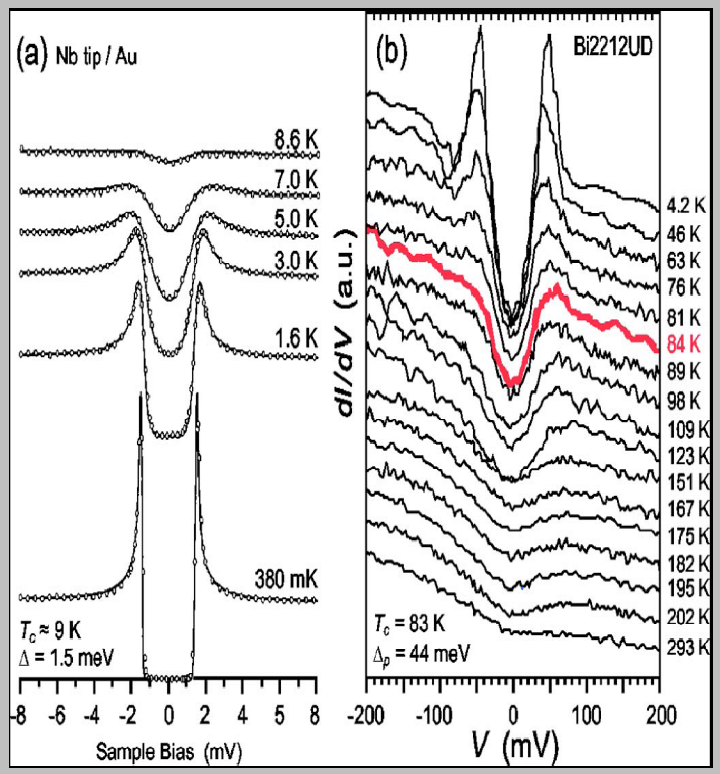


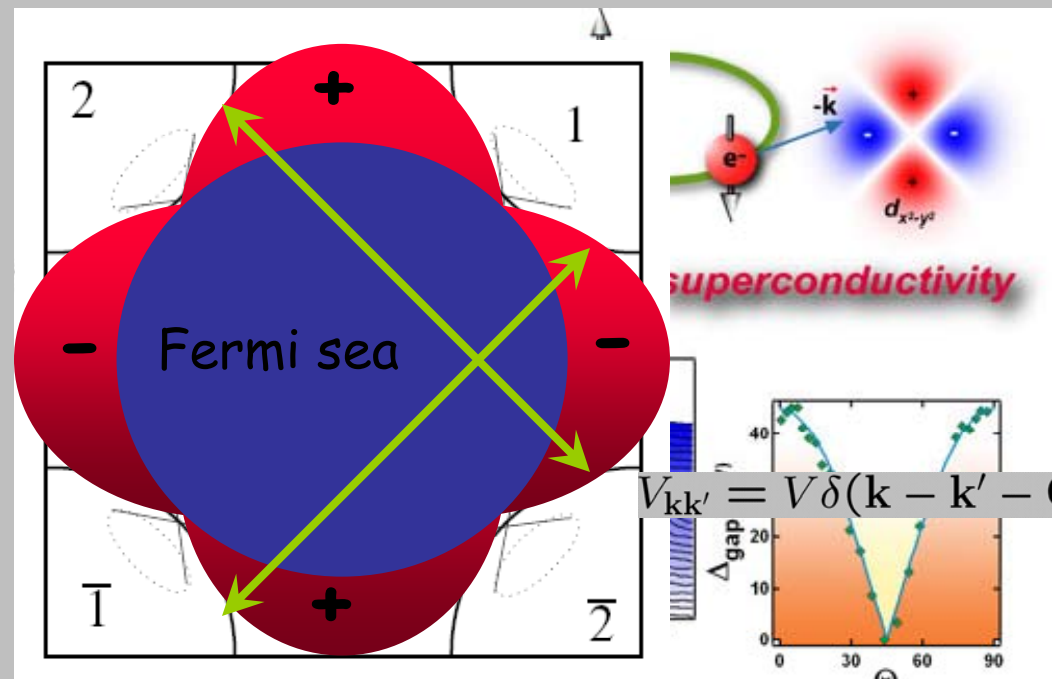
Cooper pair size
= coherence length ξ

Standard BCS theory works well in materials like Nb, Sn or Hg. In Pb and more complex systems (Nb_3Ge) one needs "strong coupling" theory ($2\Delta/T_c \sim 4$-6)

What can Δ tell us about superconducting state ?

In cuprate superconductors Δ has nodes and $d_{x^2-y^2}$ symmetry. This suggests the basic interaction is repulsive !! The same is true of other nodal SCs





$$V_{\mathbf{k}\mathbf{k}'} = V\delta(\mathbf{k} - \mathbf{k}' - \mathbf{Q})$$

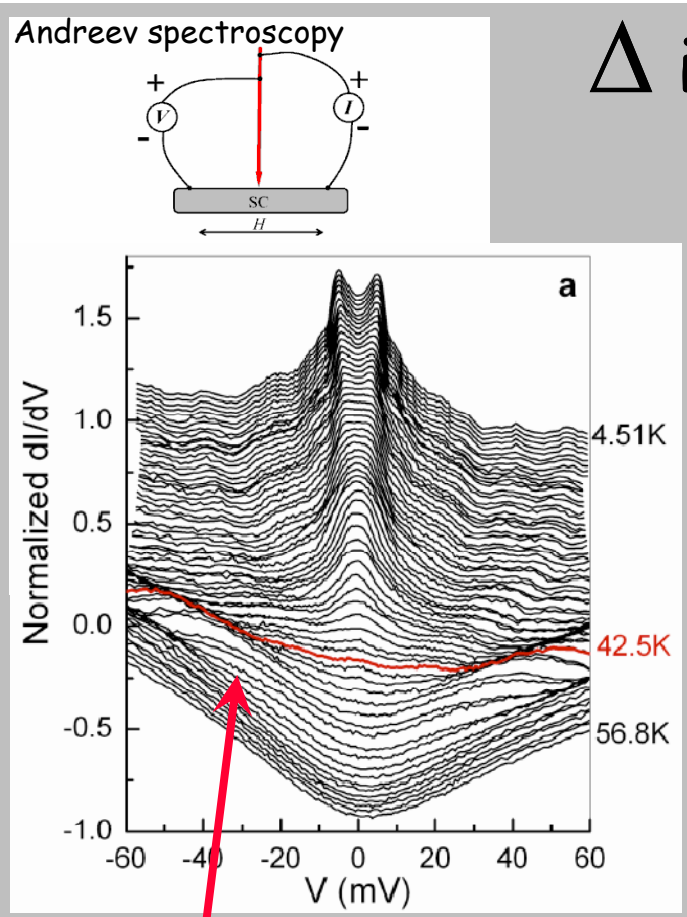
Gap equation $\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{\sqrt{\epsilon_{\mathbf{k}'}^2 + |\Delta_{\mathbf{k}'}|^2}}$

Furthermore, high temperature cuprate SCs exhibit a pseudogap behavior:
Δ remains finite even for $T > T_c$!
This reflects strong fluctuations !

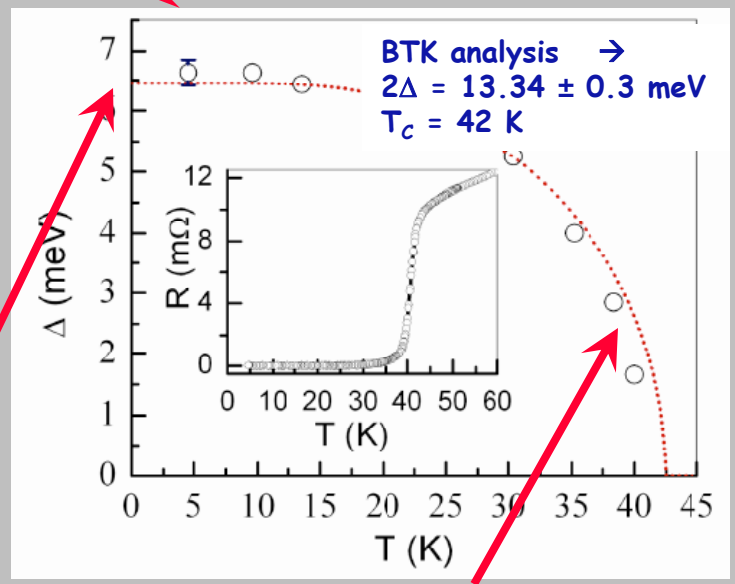
Results for FeAs mostly appear inconsistent with these features

Δ in FeAs superconductors I

T. Y. Chen *et al.*, Nature **453**, 1224 (2008)



$$\frac{2\Delta_{d(p)}(0)}{k_B T_c} = 4.28$$



No pseudogap !

Δ disappears at $T = T_c$

$2\Delta(0)/k_B T_c = 3.68 \sim 3.53$

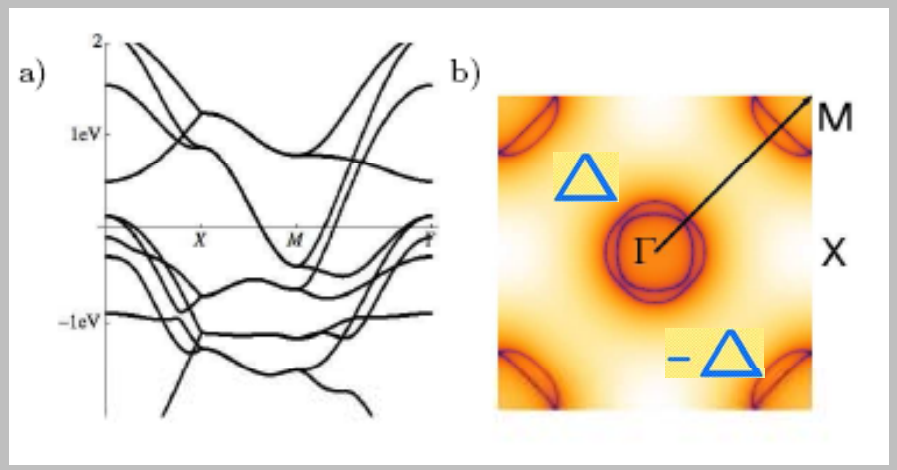
Nodeless isotropic gap !

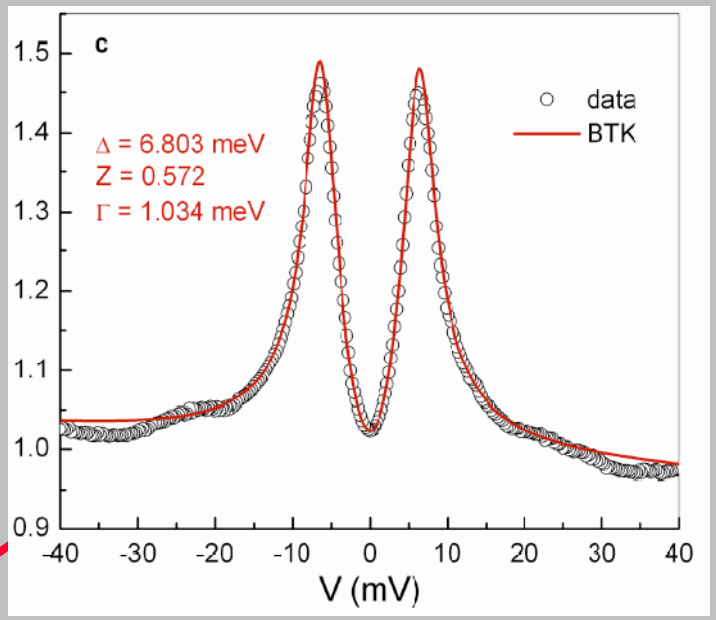
$\Delta(T)$ consistent with BCS theory (sign/phase variation still possible!)

Conclusions: Nodeless superconducting gap and no pseudogap behavior. Very different from high T_c cuprate superconductors !!

Δ in FeAs superconductors II

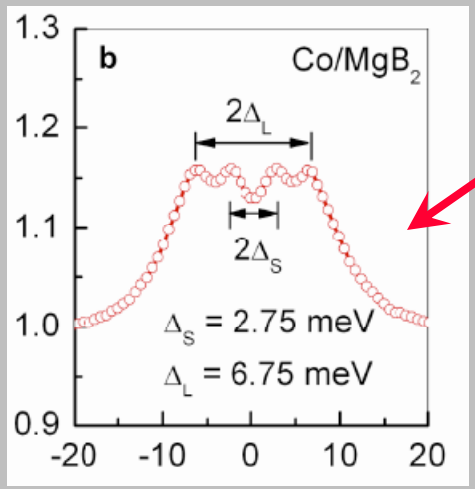
T. Y. Chen *et al.*, Nature **453**, 1224 (2008)





Fermi sea in FeAs materials is more like Land o'Lakes. It is multiply-connected.

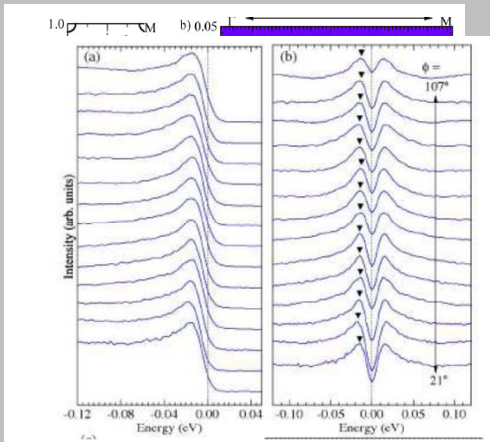
We see only a single isotropic gap
If different Fermi "lakes" had significantly different Δ we would see them

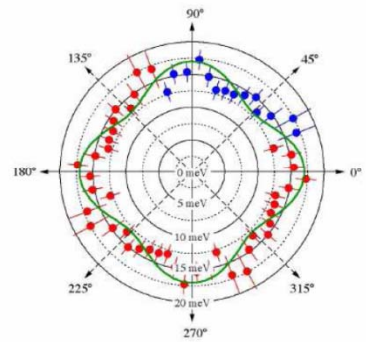


Only a "single" superconducting gap – sign/phase could be different for holes and electrons.

Conclusions: Conventional phonon-mechanism is unlikely but so is Mott limit-induced repulsion of the cuprate d-wave kind. We have something new !!

Emerging consensus (PCAR, ARPES, STM, μw, SQUID, …): nodeless "single" Δ in 1111, "two" Δ's in 122, nodes in lower T_c SC ??





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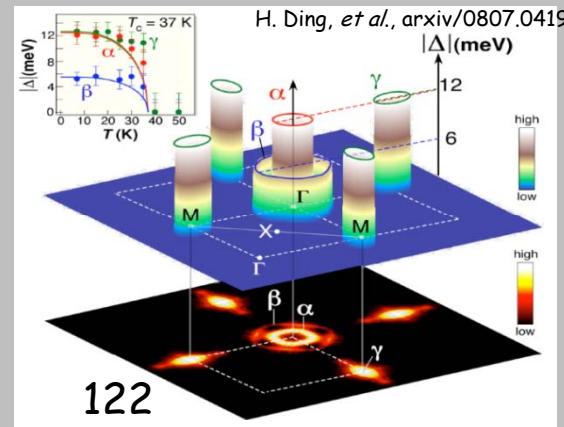
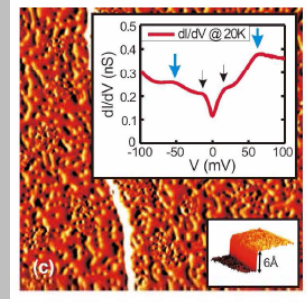
H. Ding, *et al.*, arxiv/0807.0419



NMR sees nodal behavior ($\sim T^2$) in 1111

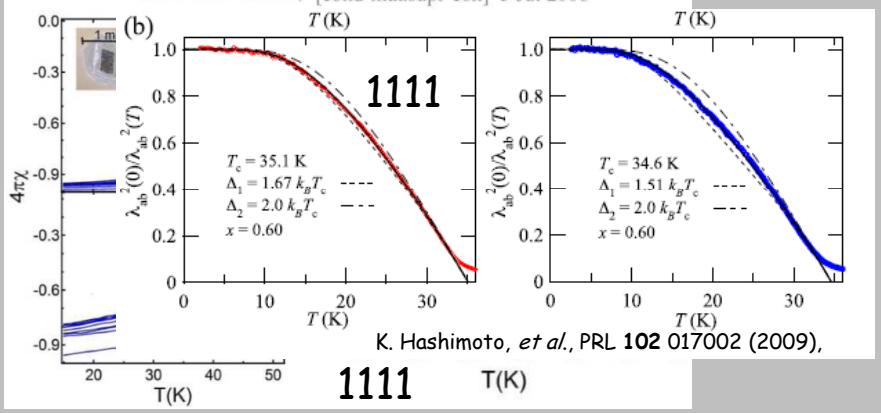


arXiv:0807.0815v1 [cond-mat.supr-con] 6 Jul 2008

Takeshi Kondo,[1] A. F. Santander-Syro,[2,3] O. Copie,[4] Chang Liu,[1] M. E. Tillman,[1] E. D. Mun,[1] J. Schmalian,[1] S. L. Bud'ko,[1] M. A. Tanatar,[1] P. C. Canfield,[1] and A. Kaminski[1]

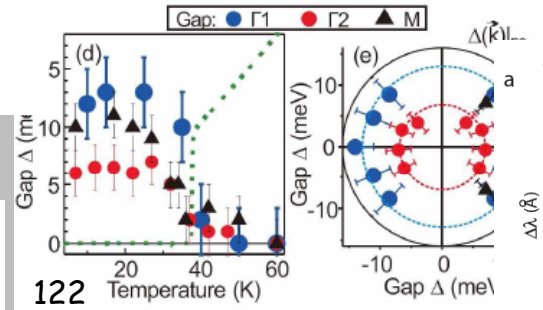
C. Martin, R. T. Gordon, M. A. Tanatar, M. D. Vannette, M. E. Tillman, E. D. Mun, P. C. Canfield, V. G. Kogan, G. D. Samolyuk, J. Schmalian, and R. Prozorov*

arXiv:0807.0876v1 [cond-mat.supr-con] 5 Jul 2008

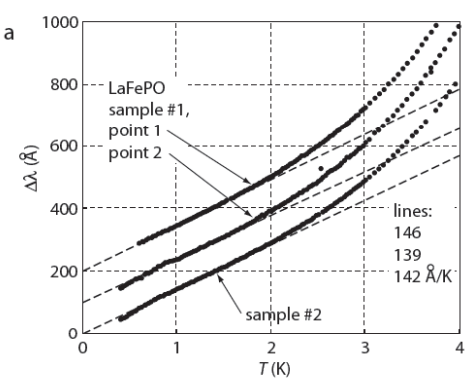


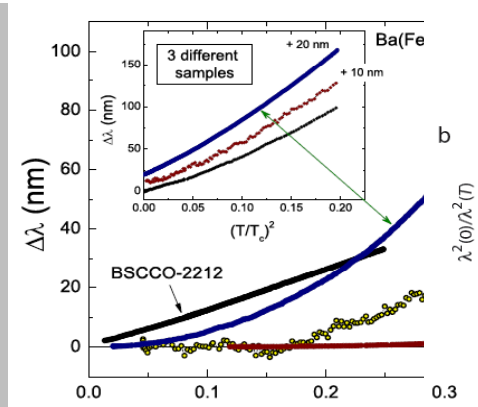
K. Hashimoto, *et al.*, PRL **102** 017002 (2009),

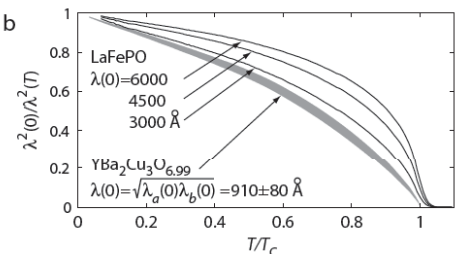
1111 T(K)



L. Wray, *et al.*, PRB **78** 184508 (2008),







C. Hicks, *et al.*, arxiv/0903.5260

R. T. Gordon *et al.*, arxiv/0810.2295

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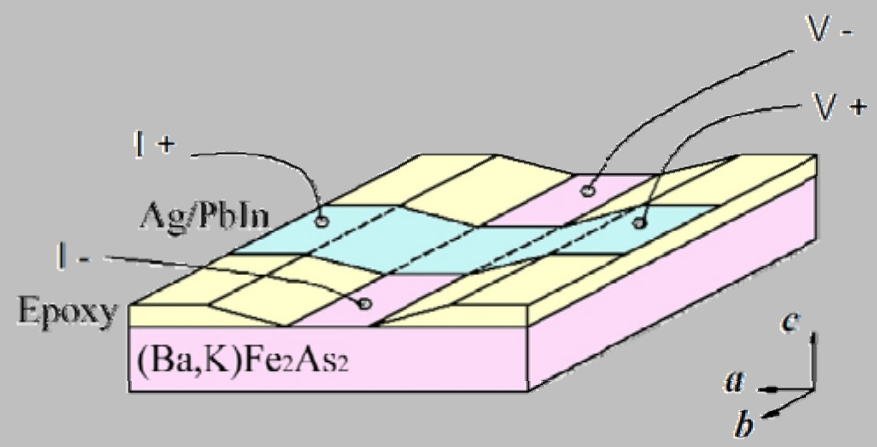
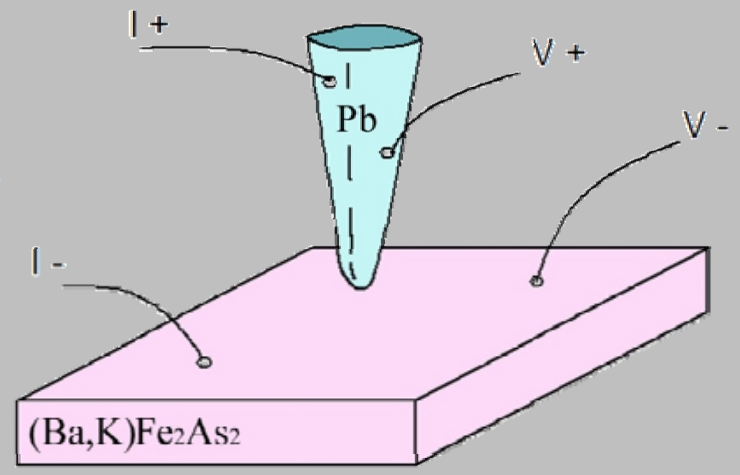
Multiband superconductivity in Fe-pnictides !?

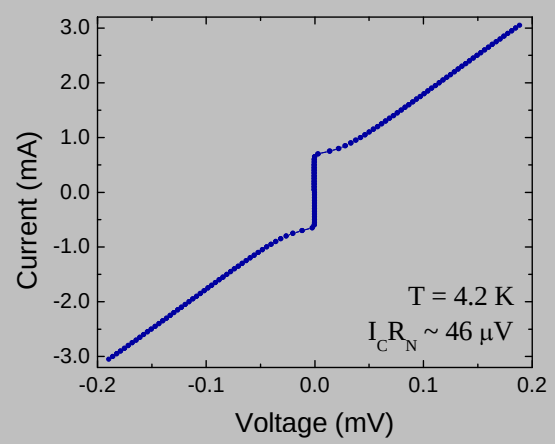
Josephson Effect Between FeAs and Pb

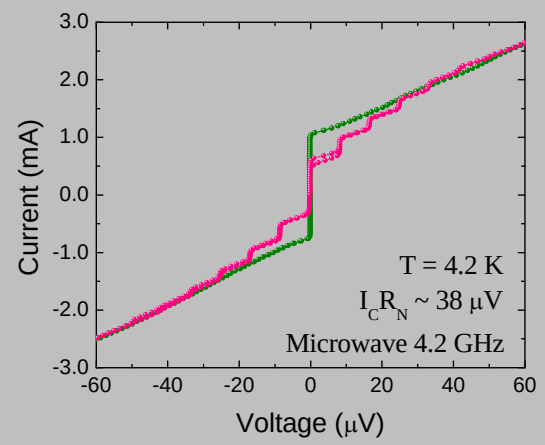
X. Zhang *et al.*, PRL **102**, 147002 (2009)





Point Contact Junction





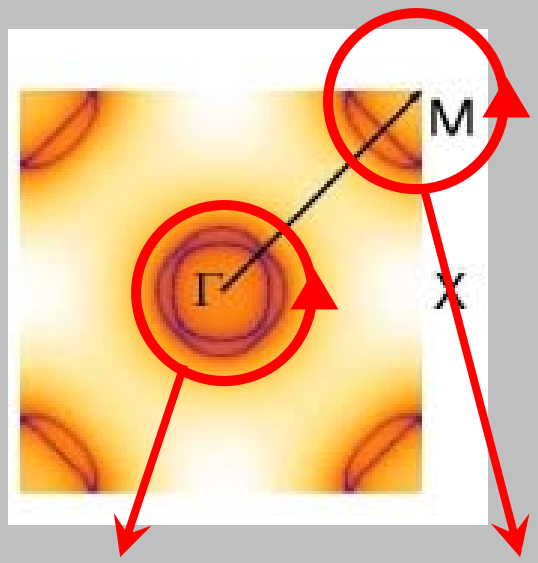
- I-V characteristics are resistively like a shunted junction
- Shapiro steps were observed under microwave irradiation

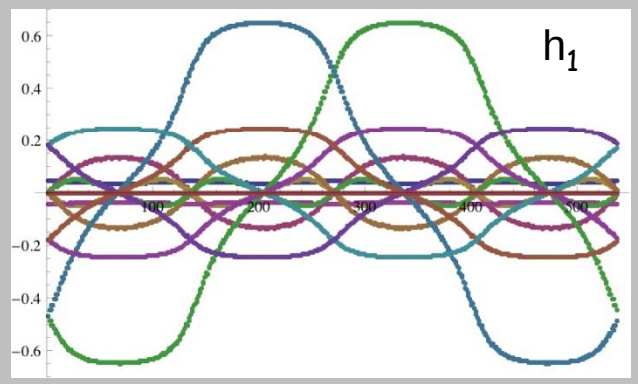
Strong indication of s-wave like SC state

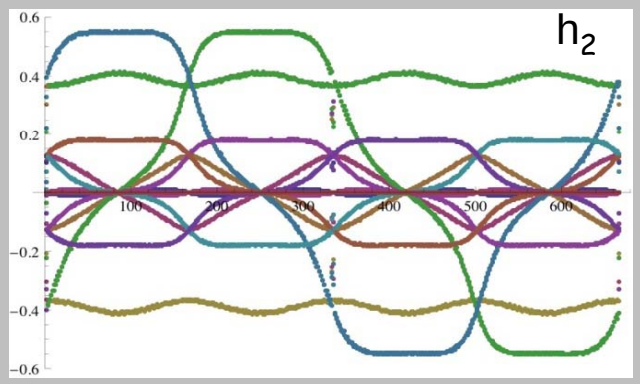
NAM center for nanophysics and advanced materials

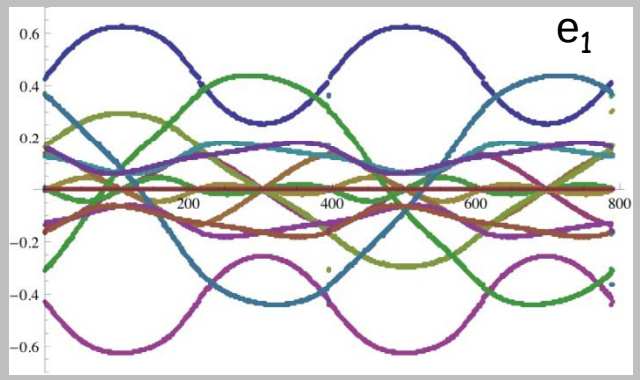
courtesy of R. Greene

Minimal Model of FeAs Layers IV









hole FS
2 pockets (valleys)

electron FS
2 pockets (valleys)

As one goes around the FS there is
strong mixing of odd and even d-orbitals
$\Rightarrow$ rich orbital content

FeAs are different from CuO_2

Charge carriers are more itinerant and less localized on atomic sites. Multiband description is necessary, unlike an effective single band model of cuprates

Interactions in FeAs I

High multiband itinerancy implies significant metallic screening

Yang *et al*, PRB **80**, 014508 (2009):
U_d not larger than $\sim$ 2 eV, $J_{\text{Hund}} \sim 0.8$ eV
from X-ray absorption
$\Rightarrow$ moderate correlations $U_d \sim t$, $J_{\text{Hund}} < U_d$

Consider $\frac{1}{2}\int d^2r d^2r' V(\mathbf{r},\mathbf{r}') n(\mathbf{r}) n(\mathbf{r}')$, where $V(\mathbf{r},\mathbf{r}')$ is the screened Coulomb repulsion $\Leftrightarrow$ Hubbard-like Hamiltonian with U_d and J_{Hund} reflecting atomic limit Coulomb correlations

$$H_{\text{FeAs}} = -\sum_{ij,\alpha\beta} t_{ij}^{\alpha\beta} c_{i\alpha}^\dagger c_{j\beta} + \sum_{i,\alpha} \epsilon_i^\alpha c_{i\alpha}^\dagger c_{i\alpha} + \frac{1}{2} U_d \sum_i n_{di}^2 - J_{\text{Hund}} \sum_i \mathbf{S}_{di}^2 + (\cdots)$$

Sawatzky *et al* discuss various interorbital interactions $(\cdots)$

Effective interaction at the Fermi surface:

$$\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \Gamma_{\alpha,\beta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q}) f_{\mathbf{k}+\mathbf{q},\alpha}^\dagger f_{\mathbf{k}'-\mathbf{q},\beta}^\dagger f_{\mathbf{k}',\delta} f_{\mathbf{k},\gamma}$$

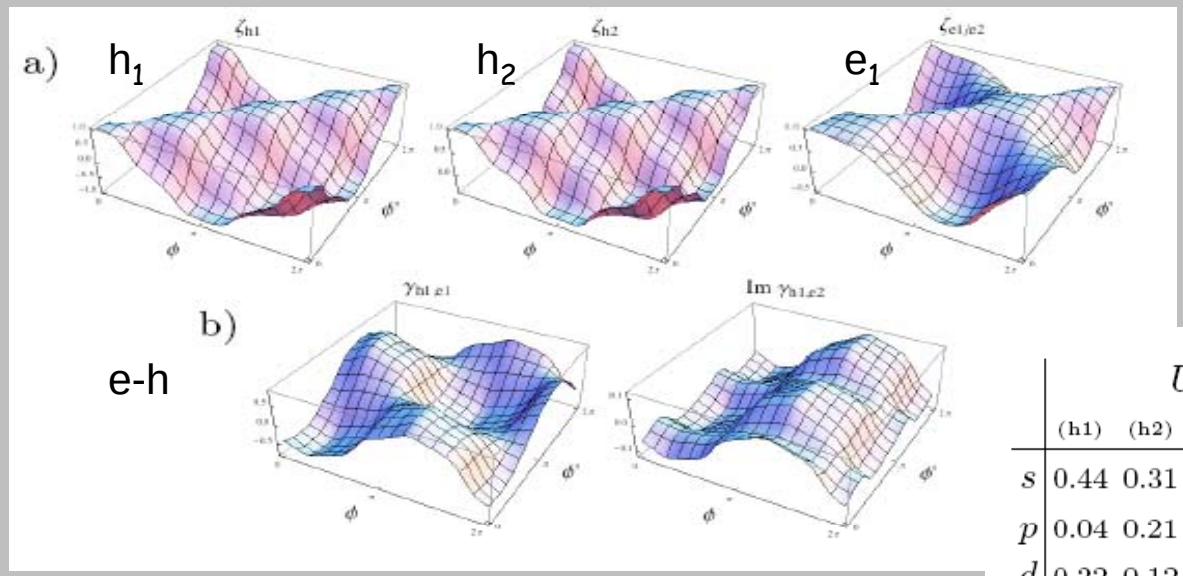
$\Gamma_{\alpha,\beta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q}) \rightarrow$ U, W, G_1, G_2

U, W, G_1, G_2 are *all* possible flavor conserving/mixing vertices

Interactions in FeAs II

V. Cvetkovic and ZT, PRB **80**, 024512 (2009); arXiv/0808.3742

vertices change significantly around Fermi surface:



k-space "Josephson" terms:

$$G_2 c^\dagger c^\dagger dd + h.c.$$

All interaction vertices @ FS: interband, intraband, mixed (typical sizes U, $W \gg G_1$, G_2)

	U				W				G_1	G_2
	(h1)	(h2)	(e1)	(e2)	(h1,e1)	(h1,e2)	(h2,e1)	(h2,e2)	(h1,e1)	(h1,e1)
s	0.44	0.31	0.35	0.35	0.21	0.25	0.27	0.29	0.14	0.14
p	0.04	0.21	0.17	0.20	0.22	0.21	0.22	0.22	0.01	0.01
d	0.22	0.12	0.09	0.10	0.11	0.13	0.09	0.11	0.03	0.02

Effective vertex at the FS:

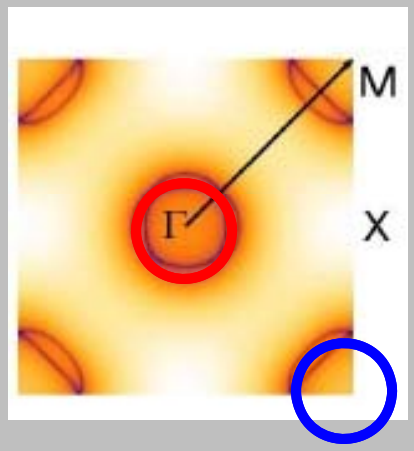
$$\Gamma_{\alpha,\beta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q}) \;\; (\mathbf{k},\mathbf{k}' \in \text{ FS}) \;\longrightarrow\; V_s + V_p p_4(\varphi) p_4(\varphi') + V_d d_4(\varphi) d_4(\varphi')$$

V_s, V_p, and V_d are C_4 version of s-, p- and d-wave coupling constants

$G_2 c^\dagger c^\dagger dd$ These "Josephson" terms do not appear in fictitious superconductor analogy → **Could they cause real SC ?**

Hierarchy of Energy Scales U, W >> G_1, G_2
→ Unified Model of Valley Density-Wave (VDW)

Unified model N = 4 → SU(4)XSU(4)
V. Cvetkovic and ZT, arXiv/0808.3742



$$H_0 = \sum_{\mathbf{k},\sigma} \xi^{(0)}_{\mathbf{k}} [\sum_\alpha h^{(\alpha)\dagger}_{\mathbf{k}} h^{(\alpha)}_{\mathbf{k}} + \sum_\beta e^{(\beta)\dagger}_{\mathbf{k}} e^{(\beta)}_{\mathbf{k}}]$$

All e and h bands are identical $\Rightarrow$ H_0 has SU(8) internal symmetry

Orbital flavor-conserving vertices (U, W) reduce this to U(4)×U(4):

	T_S (K)	T_N (K)	m_{ord} (μ_B)
LaFeAsO	155	137	0.36
CeFeAsO	155	140	0.83
PrFeAsO	153	127	0.48
NdFeAsO	150	141	0.9
CaFeAsF	134	114	0.49
SrFeAsF	175	120	
$CaFe_2As_2$	173	173	0.8
$SrFe_2As_2$	220	220	0.94-1.0
$BaFe_2As_2$	140	140	0.9

$$H_{\text{int}} \to U^{(h)} \sum_{\alpha\alpha'\sigma\sigma'} h^{(\alpha)\dagger}_{\sigma} h^{(\alpha')\dagger}_{\sigma'} h^{(\alpha')}_{\sigma'} h^{(\alpha)}_{\sigma} + U^{(e)} \sum_{\beta\beta'\sigma\sigma'} e^{(\beta)\dagger}_{\sigma} e^{(\beta')\dagger}_{\sigma'} e^{(\beta')}_{\sigma'} e^{(\beta)}_{\sigma} + 2W \sum_{\alpha\beta\sigma\sigma'} e^{(\beta)\dagger}_{\sigma'} h^{(\alpha)\dagger}_{\sigma} h^{(\alpha)}_{\sigma} e^{(\beta)}_{\sigma'}$$

$U(4)\times U(4)$ symmetry is reasonable since U and W do not vary much in different (e, h) channels

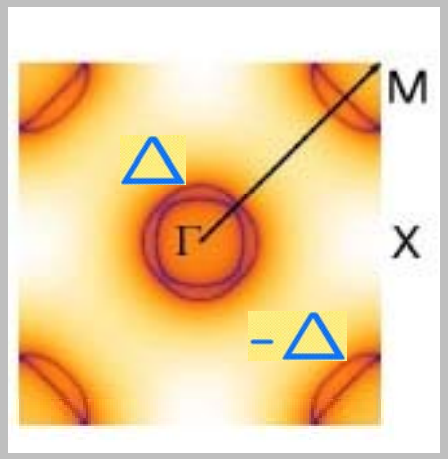
	(h1)	(h2)	(e1)	(e2)	(h1,e1)	(h1,e2)	(h2,e1)	(h2,e2)	(h1,e1)	(h1,e1)
s	0.44	0.31	0.35	0.35	0.21	0.25	0.27	0.29	0.14	0.14
p	0.04	0.21	0.17	0.20	0.22	0.21	0.22	0.22	0.01	0.01
d	0.22	0.12	0.09	0.10	0.11	0.13	0.09	0.11	0.03	0.02

Finally, flavor-mixing vertices $G_{1,2}(\ll U, W)$ have the highest symmetry that physics will allow:

$$(\ldots) \to 2G_1 \sum_{\alpha\beta\sigma\sigma'} (\sigma\sigma') e^{(\beta)\dagger}_{\sigma} h^{(\alpha)\dagger}_{-\sigma} h^{(\alpha)}_{-\sigma'} e^{(\beta)}_{\sigma'} + G_2 \sum_{\alpha\alpha'\beta\beta'\sigma\sigma'} (\sigma\sigma') h^{(\alpha)}_{-\sigma} e^{(\beta)}_{\sigma} h^{(\alpha')}_{-\sigma'} e^{(\beta')}_{\sigma'} \epsilon^{\alpha\alpha'} \epsilon^{\beta\beta'} + h.c.$$

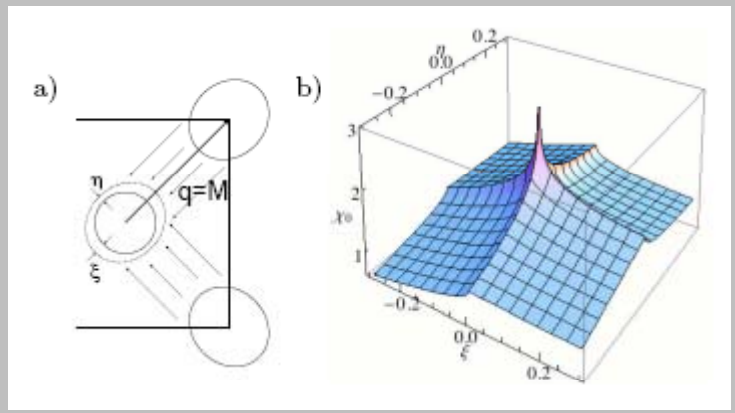
VDW in Fe-pnictides is a (nearly) highly symmetric combination: SDW/CDW/ODW

Valley Density-Wave (VDW) and SC in FeAs I



If hole (Γ) and electron bands (M) are identical
$\Rightarrow$ perfect nesting at $\mathbf{q} = \mathbf{M}$

$$\chi_0'(\mathbf{q}, \omega = 0) = 2\frac{m_e}{2\pi}\log\frac{\Lambda}{|\mathbf{q} - \mathbf{M}|},$$



Outcome: combined SDW/CDW/ODW and structural orders at **q = M → VDW**

VDW ←→ SC

$$G_2 c^\dagger c^\dagger d d$$

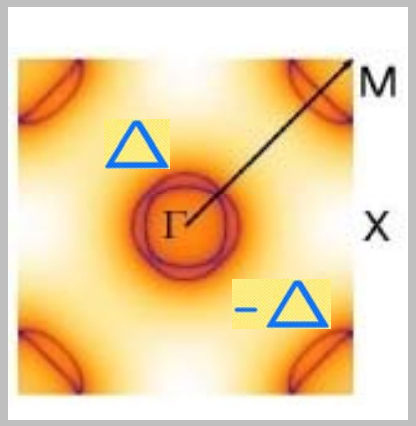
"Josephson" terms in k-space break U(4)XU(4) symmetry to U(1)XSU(2) and play key role in SC → **it's all in the (⋯)**

Near VDW transition VDW fluctuations enhance interband "Josephson" repulsion.
→ SC state with Δ (holes) and -Δ (electrons).

$$G_2 > \sqrt{U_c U_d} \quad ?$$

Valley Density-Wave (VDW) and SC in FeAs II

V. Stanev, J. Kang, ZT, PRB **78**, 184509 (2008)



The condition for interband SC is actually milder:

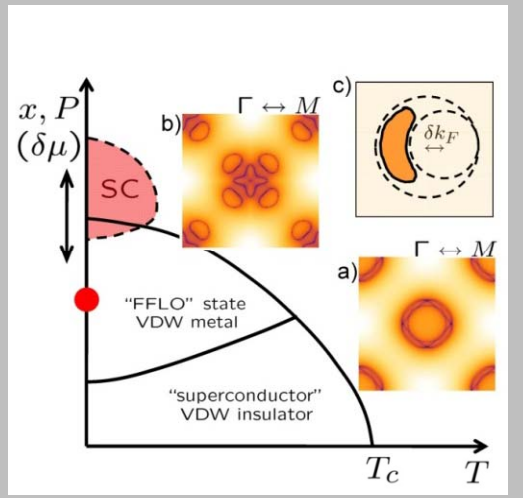
$$G_2 < \sqrt{U_c U_d} \quad \text{but} \quad G_2^\star > \sqrt{U_c^\star U_d^\star}$$

$$U_{c,d}^\star = \frac{U_{c,d}}{1 + U_{c,d} \log(\omega_{C2}/\omega_{C1})}$$

ω_{C1} (ω_{C2}) - Inter (intra) band energy scales

RG calculations indicate, near a VDW state:

G_2 grows, while $U_{c(d)}$ is suppressed



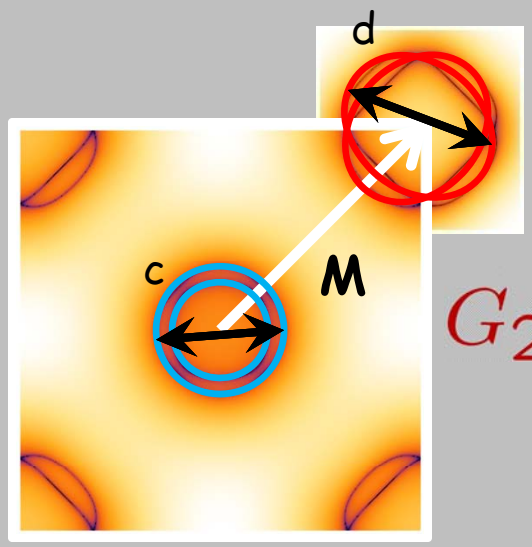
V. Cvetkovic and ZT, arXiv/0804.4678; A. V. Chubukov *et al*, PRB **78**, 134512 (2008)

In Fe-pnictides interband superconductivity (s' or s+- state) is a strong possibility (perhaps with little help from phonons)

I. I. Mazin *et al.*, PRL **101**, 057003 (2008); M. Parish, J. Hu, and B. A. Bernevig, PRB **78**, 144514 (2008)

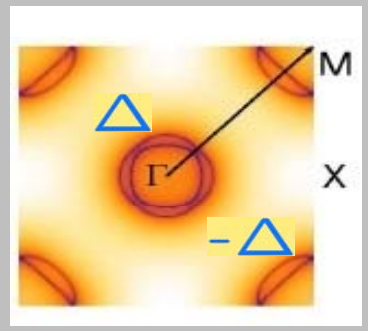
Two Kinds of Interband Superconductivity

V. Stanev, J. Kang, ZT, PRB **78**, 184509 (2008)
ZT, Physics **2**, 60 (2009)

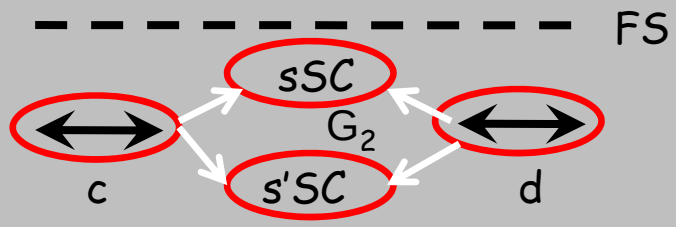


Interband pairing acts like Josephson coupling in k-space.
If G_2 is repulsive → antibound Cooper pairs (s'SC)

$$G_2 c^\dagger c^\dagger d d$$



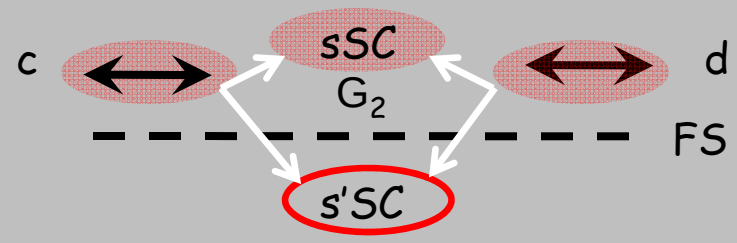
Type-A interband SC:



$(c_\uparrow c_\downarrow \ , \ d_\uparrow d_\downarrow) \quad \rightarrow \Psi_c \ , \Psi_d$

intraband Cooper pairing further enhanced by G_2

Type-B (intrinsic) interband SC:



$(c_\uparrow c_\downarrow - d_\uparrow d_\downarrow)$

intrinsic interband Cooper pairs !

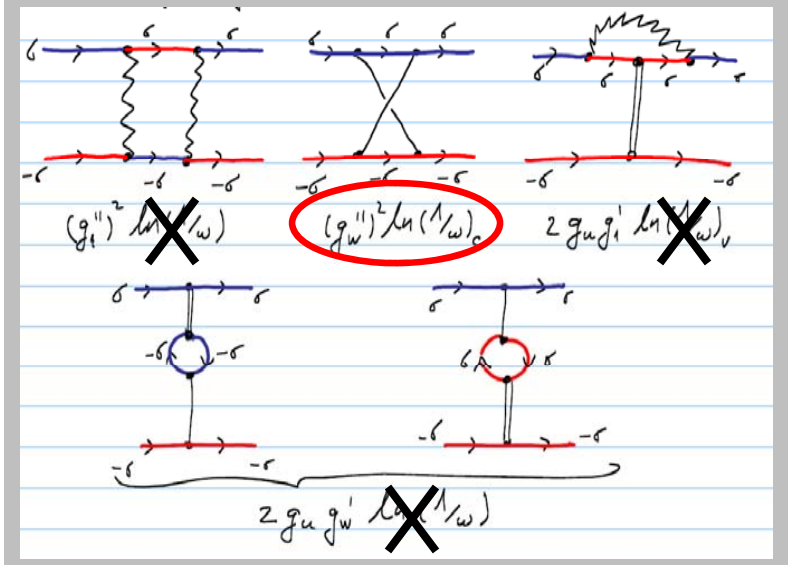
Single SC order parameter $\Psi_{s'}$!!

Interactions in FeAs III

Unified model N = 2 → SU(2)XSU(2)
V. Cvetkovic and ZT, arXiv/0808.3742

Effective interaction at the Fermi surface:
$\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \Gamma_{\alpha,\beta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q}) f^{\dagger}_{\mathbf{k}+\mathbf{q},\alpha} f^{\dagger}_{\mathbf{k}'-\mathbf{q},\beta} f_{\mathbf{k}',\delta} f_{\mathbf{k},\gamma} \quad \rightarrow \quad \boxed{U, W, G_1, G_2}$

$$
\begin{aligned}
g_U(\omega) &= g_U - g_U^2 \ln\left(\frac{\Lambda}{\omega}\right)_{pp} - g_2^2 \ln\left(\frac{\Lambda}{\omega}\right)_{pp}, \\
g_2(\omega) &= g_2 - 2g_2 g_U \ln\left(\frac{\Lambda}{\omega}\right)_{pp} + 2g_2 g'_W \ln\left(\frac{\Lambda}{\omega}\right)^{c}_{ph} + \\
&\quad 2g_2 g''_W \ln\left(\frac{\Lambda}{\omega}\right)^{v}_{ph} - 2g_2 g''_1 \ln\left(\frac{\Lambda}{\omega}\right)_{ph}, \\
g'_W(\omega) &= g'_W + (g'_W)^2 \ln\left(\frac{\Lambda}{\omega}\right)_{ph} + g_2^2 \ln\left(\frac{\Lambda}{\omega}\right)_{ph}, \\
g''_W(\omega) &= g''_W + (g''_W)^2 \ln\left(\frac{\Lambda}{\omega}\right)_{ph}, \\
g'_1(\omega) &= g'_1 - 2g'_1 g''_1 \ln\left(\frac{\Lambda}{\omega}\right)_{ph} + 2g'_1 g''_W ln\left(\frac{\Lambda}{\omega}\right)^{v}_{ph}, \\
g''_1(\omega) &= g''_1 - (g'_1)^2 \ln\left(\frac{\Lambda}{\omega}\right)_{ph} - (g''_1)^2 \ln\left(\frac{\Lambda}{\omega}\right)_{ph} - \\
&\quad g_2^2 \ln\left(\frac{\Lambda}{\omega}\right)_{ph} + 2g''_1 g''_W \ln\left(\frac{\Lambda}{\omega}\right)^{v}_{ph}, \qquad (15)
\end{aligned}
$$



If G_1, G_2 << U, W
→
relevant vertices: U, W, & G_2

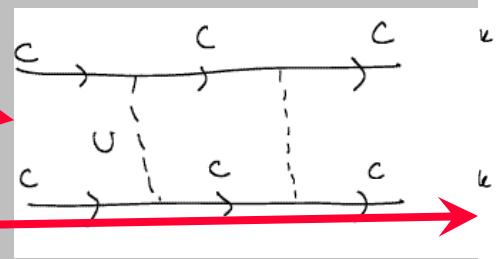
Interplay of VDW and SC in FeAs I

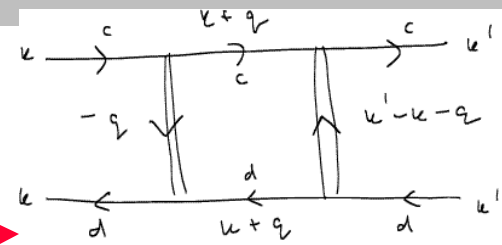
RG (near VDW):

$$\dot{U} = -U^2 - G_2^2$$

$$\dot{G}_2 = -2G_2U + 4G_2W$$

$$\dot{W} = +W^2 + G_2^2 \quad (G_1 \to 0)$$





$$\int d^2q\, G_d(k+q)\, G_c(k+q)$$

$$\boxed{\int d^2p\, G_d(p)\, G_c(p) \propto \ln \frac{\Omega}{\omega}}$$

Proximity to VDW is crucial:

$$\dot{U} \pm \dot{G}_2 = -(U \pm G_2)^2 \pm 4WG_2$$

$$\dot{W} = W^2 + G_2^2$$

If $W \to 0$ then $\dot{U} \pm \dot{G}_2 = -(U \pm G_2)^2$

SC only for $G_2 > U$!!

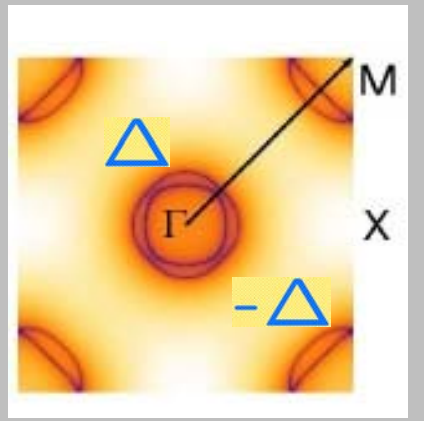
This is true interband SC since U > 0 – different from U < 0 :

$(c_\uparrow c_\downarrow - d_\uparrow d_\downarrow)$

interband Cooper pairs !

$(c_\uparrow c_\downarrow \;,\; d_\uparrow d_\downarrow)$

intraband Cooper pairs



Interplay of VDW and SC in FeAs II

V. Cvetkovic and ZT, PRB **80**, 024512 (2009); arXiv/0808.3742

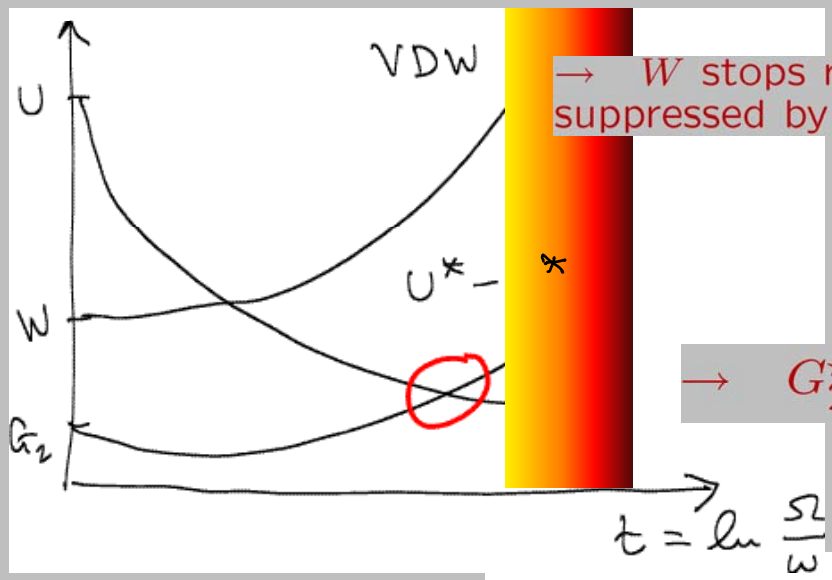
RG flows (near VDW):

$$\dot{U} = -U^2 - G_2^2$$

$$\dot{G}_2 = -2G_2U + 4G_2W$$

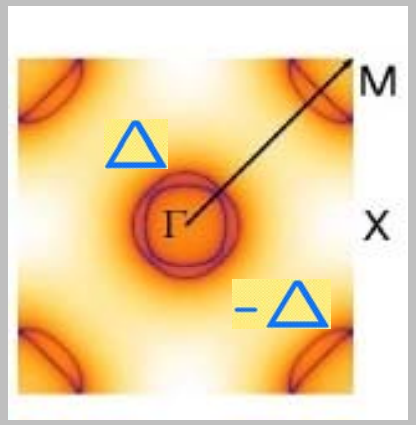
$$\dot{W} = +W^2 + G_2^2 \quad (G_1 \to 0)$$

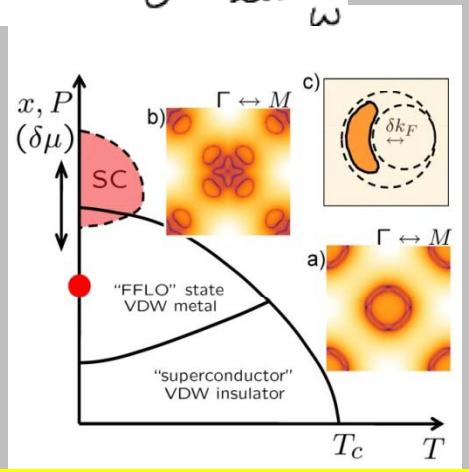
Also, A. V. Chubukov *et al*, PRB **78**, 134512 (2008)
F, Wang *et al*, PRL **102**, 047005 (2009)



→ W stops running; VDW suppressed by lack of nesting

→ $G_2^\star > \sqrt{U_c^\star U_d^\star}$





In Fe-pnictides interband superconductivity (s' or s+- state) is a strong possibility but it is a fine tuning with SDW/CDW/ODW (little help from phonons in reducing U* would not hurt)

Conclusions

- Iron pnictides are semimetals turned superconductors
- Correlations are significant, hence a SDW in parent compounds, but weaker than in cuprates
- Superconducting gap has substantial s-wave character
- Both magnetism and superconductivity are intrinsically multiband in nature – s' interband SC is a likely possibility near a nesting-driven SDW

→ new physics, beyond the "standard" model?

Zlatko Tesanovic, Johns Hopkins University
E-mail: zbt@pha.jhu.edu Web: http://www.pha.jhu.edu/~zbt