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Magnetism and Superconductivity in Pnictides

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A collaboration between JOHNS HOPKINS UNIVERSITY and PRINCETON UNIVERSITY

Magnetism and Superconductivity in Pnictides

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Swing flu engag interset eciantists most in 2000

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

- LDA + RPA: Mazin, Singh et al, Kuroki et al, Scalapino et al, Schmalian et al, ...
- Weak coupling⁺⁺: Chubukov, Eremin et al, DH Lee, Vishwanath et al, Cvetkovic et al, Bernevig, Thomale 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, Hirschfeld et al, Benfatto, Castellani et al, PA Lee & Wen, Raghu, SC Zhang, et al, Nagaosa & Ng, Gor'kov et al, FC Zhang & Rice, ...



linked anti-angiogenesis to tumor growth

•Graphene, single-atom layers of carbon that have semiconductor properties. They "look like a coming revolution in electronics," Pendlebury says. Science magazine included graphene on its "Top Ten" list of breakthroughs for the year.

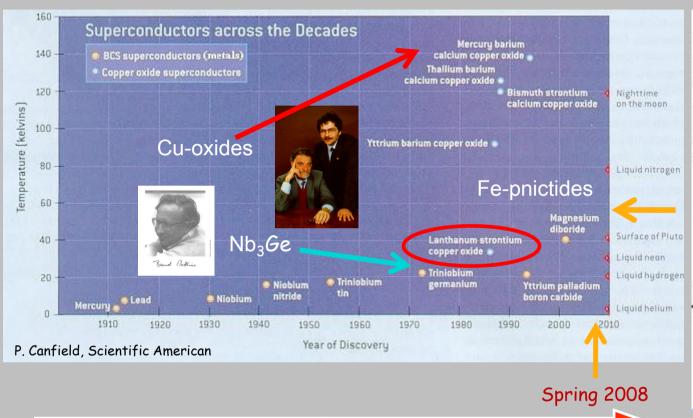
•Small RNA's, genetic materials that regulate genes in cells. They've emerged in "an astounding landscape" notes a highly-cited Nature Reviews Molecular Cell Biology survey led by V. Narry Kim of South Korea's Seoul National University. They have potential to treat diseases and reveal how genes work on a fundamental level inside cells. But not a big news item.

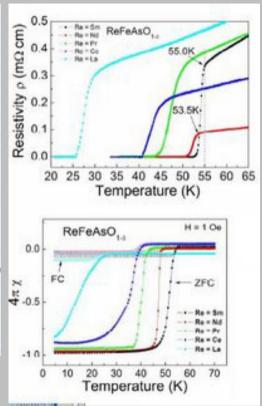
•Obesity gene, biology and diet studies. A New England Journal of Medicine report that found cutting calories, whatever their origin, mattered the most surprisingly high number of citations, considering it confirmed long-standing advice.





Superconductors \rightarrow Hg \rightarrow Nb₃Ge \rightarrow cuprates \rightarrow pnictides





time

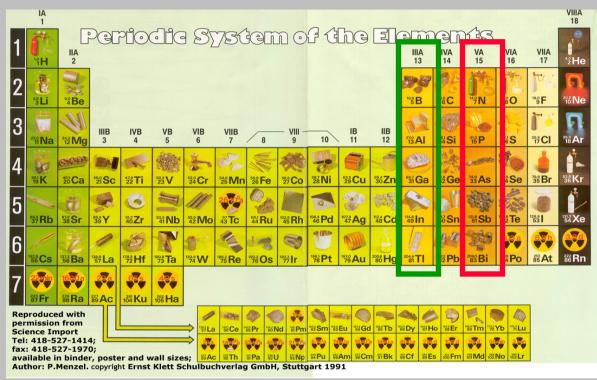






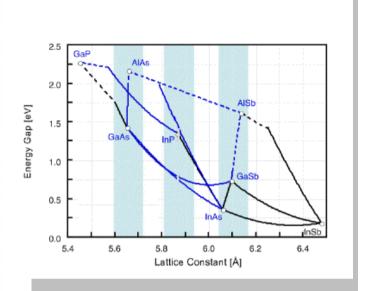
Greatest web-induced frenzy in history of condensed matter physics: 17 papers on arXiv in a single July '08 day. Comparable to the latest superstring "revolution" (Bagger-Lambert)

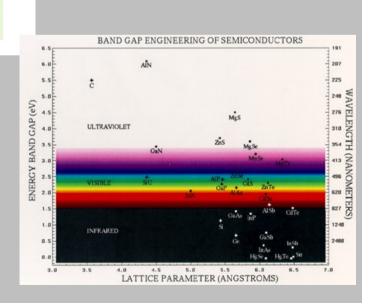
Pnictides $\pi viy \in V$ (Greek for chocking, suffocation): Semiconductors \rightarrow Semimetals \rightarrow Superconductors



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



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





ナノテクノロジーの

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)



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,

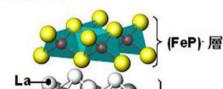
People's Republic of China arXiv:0803.3603v1 [cond-mat.supr-con] 25 Mar 2008

(Dated: March 25, 2008)

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To 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Fe²⁺イオンの3d 電子だと推定している。

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



10)+層

go Advanced search

nature

nature

International weekly journal of science

go Advanced search

Letter

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

Superconductivity at

X. H. Chen1 (#a1), T. Wu1 (#a1)

1. Hefei National Laboratory for Phys Letter

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

Since the discovery of hig from Bardeen-Cooper-Sc

been devoted to exploring A large iron isotope effect in SmFeAsO_{1-x}F_x and Ba_{1-x}K_xFe₂As₂

copper oxide supercondue R. H. Liu¹, T. Wu¹, G. Wu¹, H. Chen¹, X. F. Wang¹, Y. L. Xie¹, J. J. Ying¹, Y. J. Yan¹, Q. J. Li¹, B. C. Shi¹, W. S. Chu², Z. Y. Wu², & X. H.

superconductivity in the 1 superconductivity in the 1 sering Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China superconductivity in the 1 sering Synchrotron Radiation Facility Institute of High Energy Physics, China superconductivity in the 1 sering Synchrotron Radiation Facility Institute of High Energy Physics, China superconductivity Institute of High Energy Physics, China superconductivity Institute of High Energy Physics, China superconductivity Institute of Hi

measurements reveal a tr 3. National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei 230026, China

Accepted 5 May 2008; Published online 4 June 2008

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of science

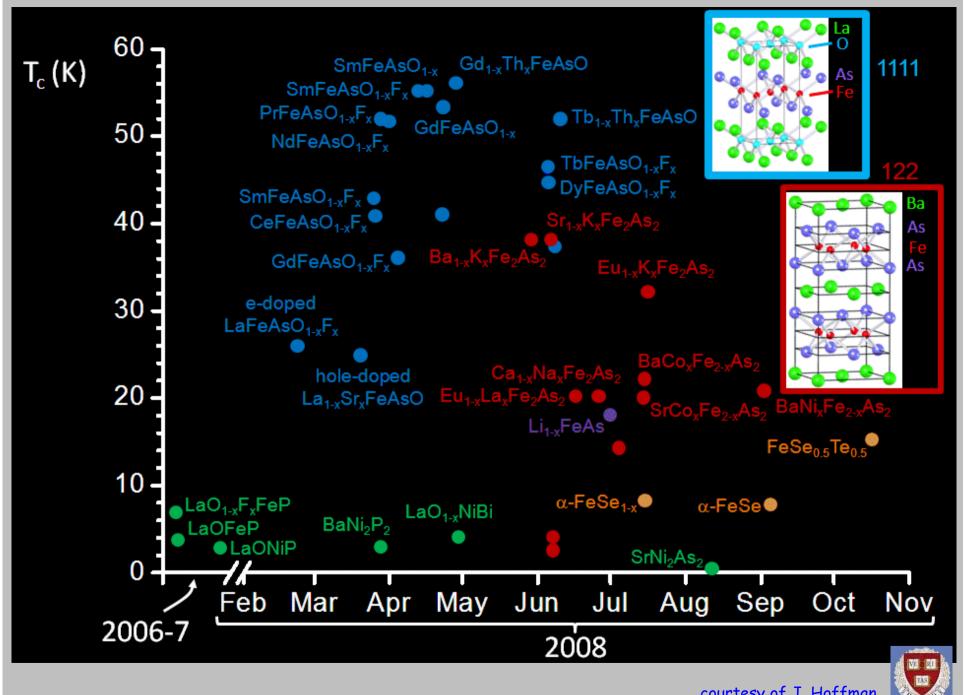
& C. L. Chien1 (#a1)

1218, USA

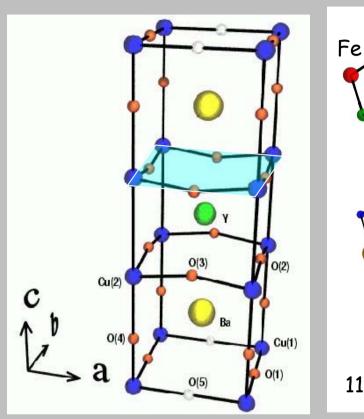
2. Heter National Laboratory for Physical Sciences at Pricroscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

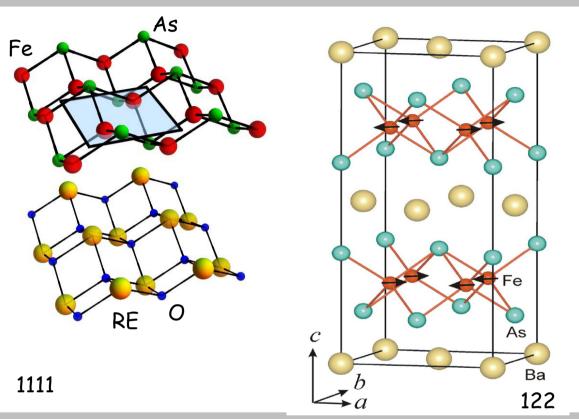
(ref. 2 (/nature/journal/v453 La-Nd, Sm and Gd) are no Chen± LaO1-xFxFeAs (ref. 3 (/nat)

high-temperature superco



Cu-oxides versus Fe-pnictides



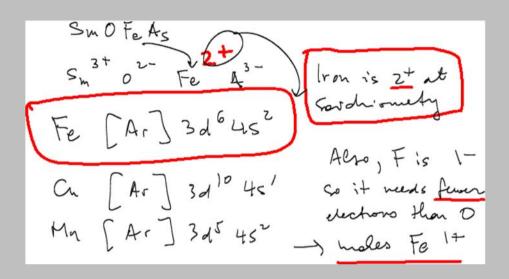


Both have d-electrons in key role (Cu vs Fe) Both are layered (CuO₂ vs FeAs) Both have AF and SC in close proximity

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)



In CuO₂ 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

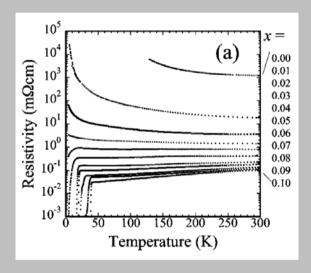
→ A multiband model is likely necessary

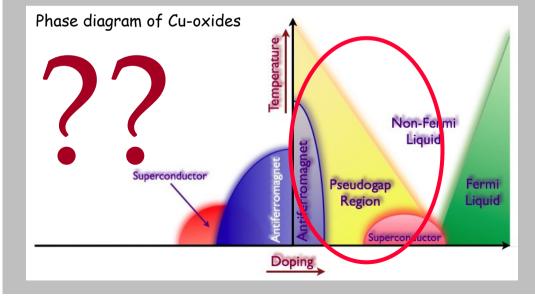
Cu-oxides: Mott Insulators -> Superconductors

In a hol

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



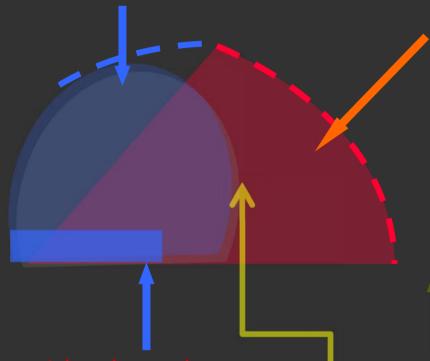


How Mott insulators turn into superconductors, particularly in the pseudogap region, remains one of great intellectual challenges of condensed matter physics

How Correlated Superconductors turn into Mott Insulators

ZT, Nature Physics **4**, 408 (2008)

Correlated superconductors have quantum (anti)vortex fluctuations



All superconductors have thermal fluctuations

Near T_c these are always phase fluctuations

BCS-Eliashberg-Migdal

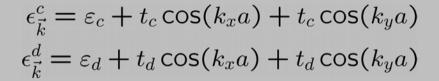
Ground state with enhanced pairing correlations but no SC!! (gauge theories, QED3, chiral SB, AdS/CMT,...

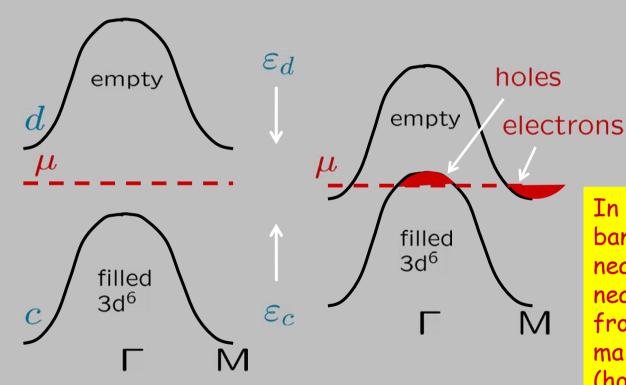
No such ground state in BCS theory (at weak coupling)!

PW Anderson, Balents, MPA Fisher, Nayak, Franz, Vafek, Melikyan, ZT, Senthil & PA Lee

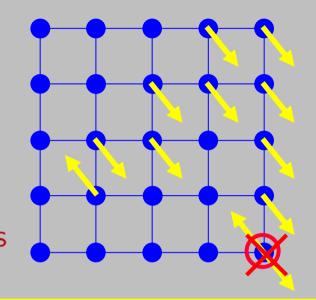
Optimal T_c in HTS is determined by quantum fluctuations

Fe-pnictides: Semimetals -> Superconductors





semiconductor → semimetal

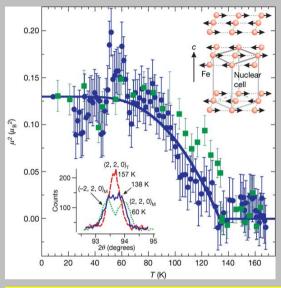


In contrast to CuO_2 , all dbands in FeAs are either nearly **empty** (electrons) or nearly **full** (holes) and far from being **half-filled**. This makes it easier for electrons (holes) to avoid each other.

→ FeAs are less correlated than CuO₂ (correlations are still important !!)

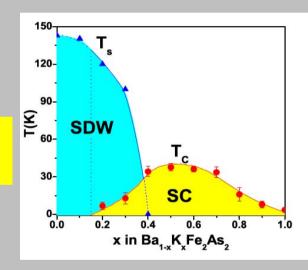
Phase diagram of Fe-pnictides

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

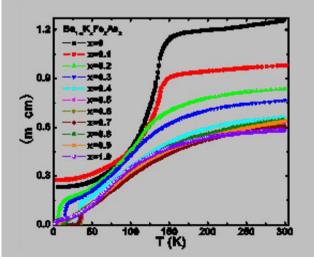


Like CuO_2 , phase diagram of FeAs has SDW (AF) in proximity to the SC state.

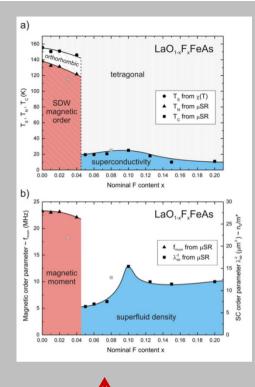
H. Chen, et al., arXiv/0807.3950

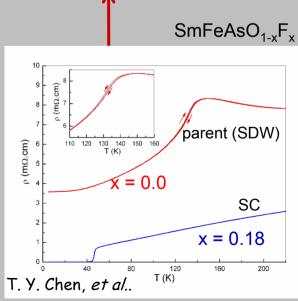


SC coexists with SDW (AF) in 122 compounds →

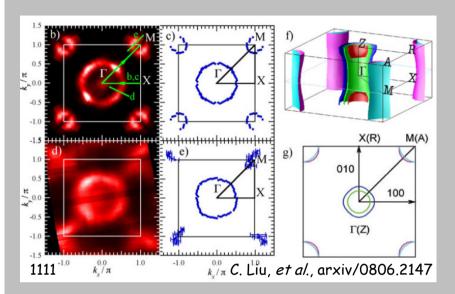


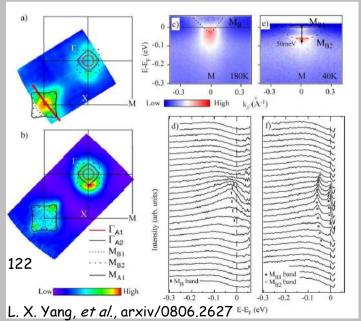
However, unlike CuO₂, all regions of FeAs phase diagram are (bad) metals!!



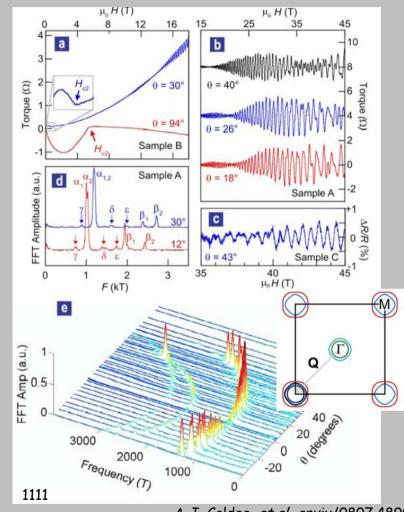


ARPES





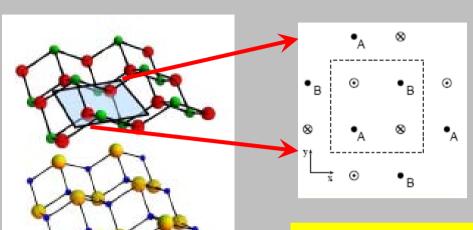
dHvA



A. I. Coldea, et al., arxiv/0807.4890

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

Minimal Model of FeAs Layers I

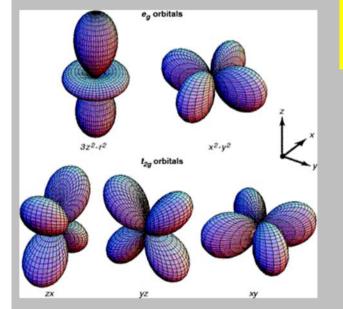


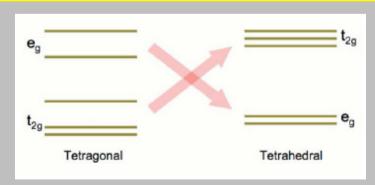
V. Cvetkovic and ZT, EPL **85**, 37002 (2009) C. Cao, P. J. Hirschfeld, and H.-P. Cheng, PRB **77**, 220506 (2008)

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

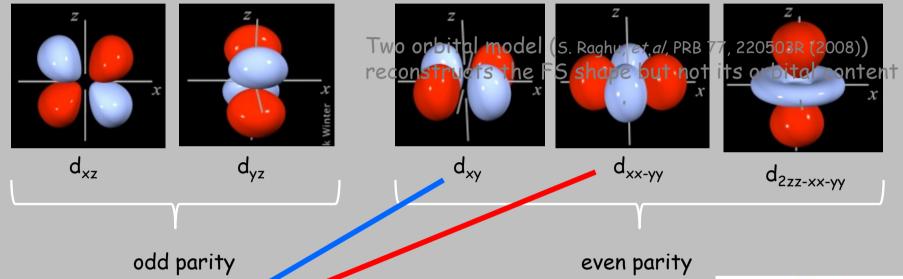




$$(5+3) \times 2 = 16 \ (\div 2)$$
 Wannier orbitals \Rightarrow "minimal" model \Rightarrow

Minimal Model of FeAs Layers II

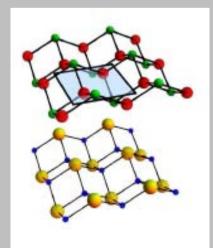
We consider an effective 2D model with 5 Fe + 3 As orbitals



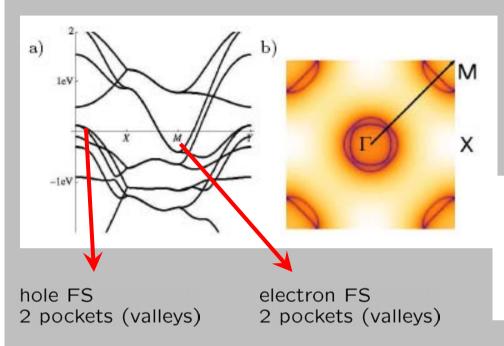
The importance of Fe 3d - As 4p hybridization:

Without pnictide atoms many hopping processes would vanish by symmetry.

These symmetries are violated by pnictide puckering.



Minimal Model of FeAs Layers III

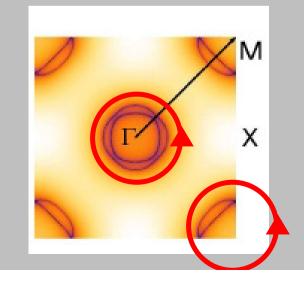


V. Cvetkovic and ZT, EPL **85**, 37002 (2009) C. Cao, P. J. Hirschfeld, and H.-P. Cheng, PRB **77**, 220506 (2008) K. Kuroki *et al*, PRL **101**, 087004 (2008)

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

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

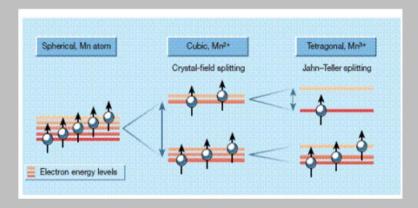
As one goes around the FS there is strong mixing of odd and even d-orbitals ⇒ no simple orbital "topology"

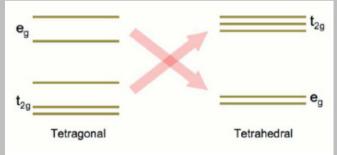


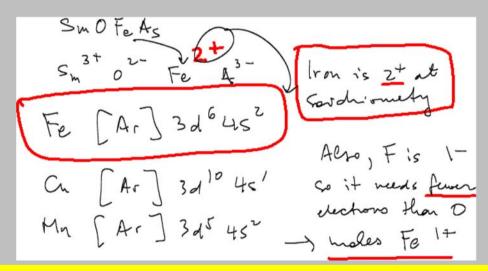
Hund's Rule Defeated (but Lurking!)

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

Y. Singh et al., arXiv/0907.4094 (MnAs)Y. Z. Zhang et al., PRB 81, 094505 (2010)





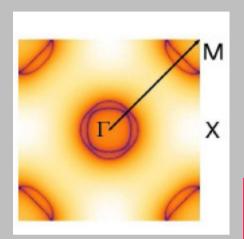


"Puckering" of FeAs planes is essential:

- i) All d-orbitals are near E_F
- ii) Large overlap with As p-orbitals below $E_F \rightarrow$ enhanced itinerancy of d electrons defeats Hund's rule and large local moment

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

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

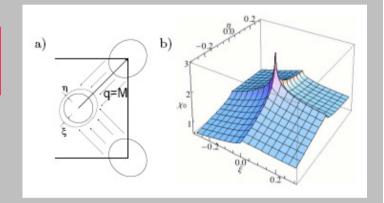


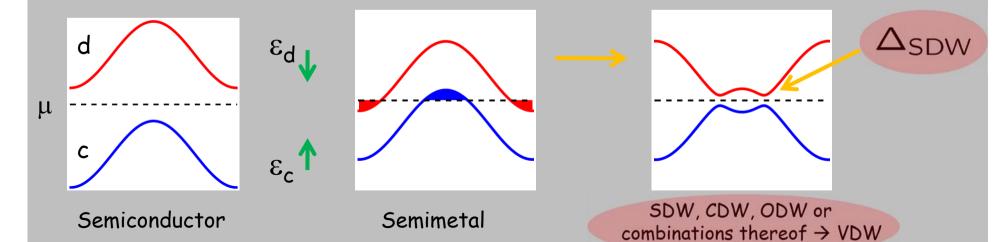
V. Cvetkovic and ZT, EPL 85, 37002 (2009)
V. Cvetkovic and ZT, PRB 80, 024512 (2009)
M. Korshunov and I. Eremin, PRB 78, 140509 (2008)

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

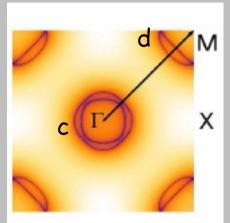
$$\chi'_0(\mathbf{q}, \omega = 0) = 2 \frac{m_e}{2\pi} \log \frac{\Lambda}{|\mathbf{q} - \mathbf{M}|},$$

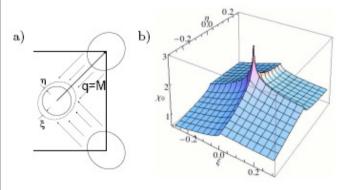
Turning on moderate interactions \rightarrow **VDW** = itinerant multiband CDW (structural), SDW (AF) and orbital orders at $\mathbf{q} = \mathbf{M} = (\pi, \pi)$





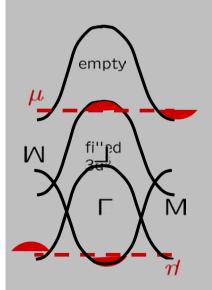
Nesting and Valley Density-Wave (VDW) in Fe-pnictides II





$$\chi'_0(\mathbf{q}, \omega = 0) = 2 \frac{m_e}{2\pi} \log \frac{\Lambda}{|\mathbf{q} - \mathbf{M}|},$$

Consider the bare-bones model for interactions:



Particle-hole transformation
$$c o h^\dagger \ , d o e \ , n_c o 1 - n_h \ , n_d o n_e$$
 $H o arepsilon_{\mathbf{k}} h^\dagger_{\mathbf{k}} h_{\mathbf{k}} + arepsilon_{\mathbf{k}} e^\dagger_{\mathbf{k}} e_{\mathbf{k}} - W n_h n_e + (\cdots)$ Negative U Hubbard model: $(h,e) \leftrightarrow (f_\uparrow,f_\downarrow)$

Many-Particle Problem in Quantum Matter

i) BCS state & Cooper indubility non-interacting Consider: A = E } = ció ció > part + + 1 2 2 V(i, i'; q) ct i+q6 ct i-q01 c i's ci6

Once quartic interaction term is present, we don't know how to solve H. except in special cases

Numerous approximate methods have been developed over decades

The quartice form of suterastion modes it difficult to solve It.

Hartree-Fock mean-field theory is not trivial

* Hartree-Food approximation: ctctcc -> ctctcc + ctctcc Hautree

a symmetry of A!

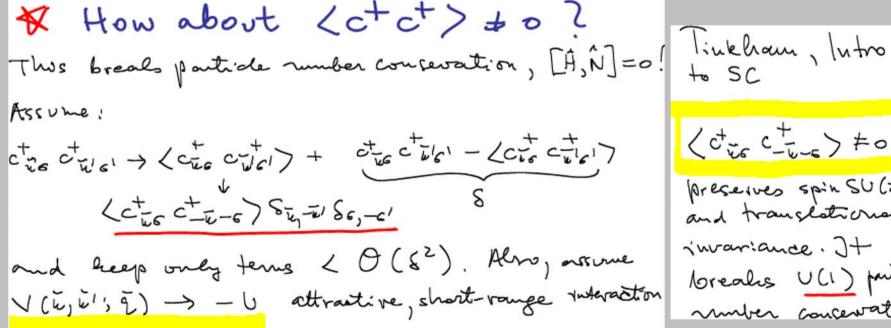
Quantum Phase Transitions

For example: (ctie ci+Q-67 +0 =) SDW ... many other Symmetry breaking stoles.

We can assume any form of the ground state, irrespective of whether it obeys the symmetries of H. As long as such Hartree-Fock state is determined self-consistently to have the lowest energy

We have the true ground state

CDW breaks translational (lattice) invariance; SDW does the same plus, spin SU(2) symmetry. All such states are allowed and can be the ground state with a suitable interaction.



(ctic c-t-=> +0 preserves spin SU(2) and translational invariance. It breaks U(1) puticle number concevation

Hartree-Fock-BCS State

Ground state of H_{BCS} is the famous BCS wavefunction

where
$$\Delta = U \sum_{\vec{u}} \langle C_{-\vec{u}-6} C_{\vec{u}6} \rangle$$
 self-consistency $|\phi_0\rangle = \prod_{k} \left(u_k + v_k c_{k\uparrow}^+ c_{-k\downarrow}^+\right) |0\rangle$

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

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

Ground state of H_{BCS} , $|\phi_0\rangle$ is a superconductor !!

Hamiltonian for new Bogoliubov-deGennes (BdG) spinors: $[c^{\dagger}_{\uparrow}(\mathbf{r}) \; ; \; c_{\downarrow}(\mathbf{r})]$

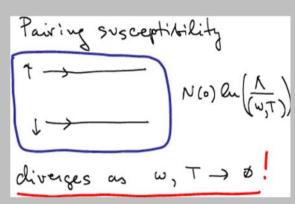
$$\mathcal{H}_{BdG} = \begin{pmatrix} \frac{(\mathbf{p} - (e/c)\mathbf{A})^2}{2m} - \epsilon_F & \Delta \\ \Delta^* & \epsilon_F - \frac{(\mathbf{p} + (e/c)\mathbf{A})^2}{2m} \end{pmatrix}$$

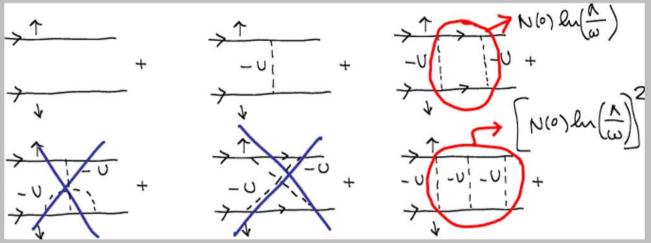
BdG quasiparticle spectrum:

$$E_{\mathbf{k}} = \pm \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$$

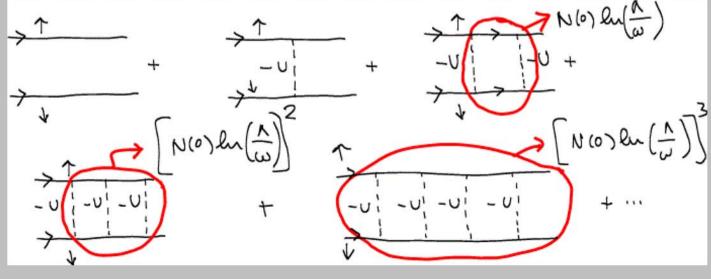
Cooper Instability

Origin of Cooper instability and BCS ground state is repeated scattering of two electrons (p-p channel)





Keep only the most divergent diagrams at any given order in perturbation theory:

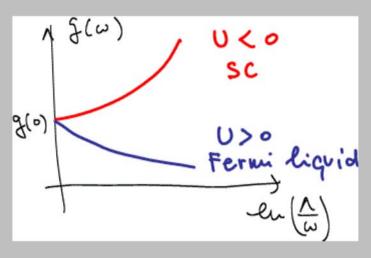


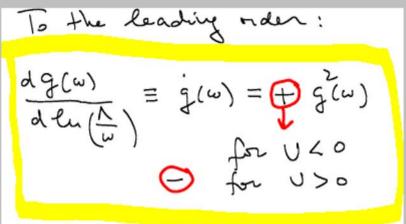
This is like having a new dimensionless suberaction $g(\omega)$ = $N(0)U\ln\left(\frac{\Lambda}{\omega}\right)$

Poor-woman Renormalization Group (RG)

This is like having a new dimensionless suberaction
$$g(\omega)$$

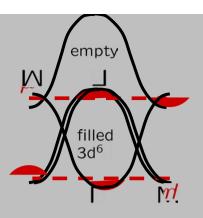
$$g(\omega) = N(0) \cup \ln\left(\frac{\Lambda}{\omega}\right)$$





So, attractive pairing interaction (U < 0) grows as ω , T \rightarrow 0 !!

For repulsive U > 0, the interaction \rightarrow 0 and becomes irrelevant as ω ,T \rightarrow 0 \rightarrow Fermi liquid (normal) ground state



Fictitious "Superconductor" → VDW in Fe-pnictides

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

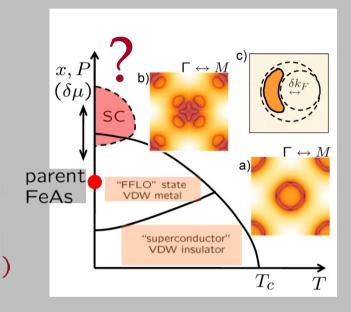
Negative U Hubbard model: $(h, e) \leftrightarrow (f_{\uparrow}, f_{\downarrow})$

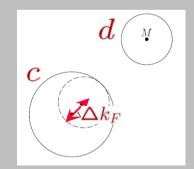
$$\rightarrow H = \sum_{\sigma} \varepsilon_{\mathbf{k}} f_{\mathbf{k},\sigma}^{\dagger} f_{\mathbf{k},\sigma} - W n_{f\uparrow} n_{f\downarrow} + (\cdots)$$

Ground state is a "superconductor":

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

insulating VDW (SDW/ODW/CDW) at $\mathbf{M}=(\pi,\pi)$





Generically, the c and d bands are different:

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

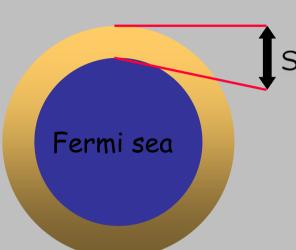
⇒ "Fulde-Ferrell-Larkin-Ovchinikov", "breached pairing" states

⇒ metallic (incommensurate?) VDW (SDW/ODW/CDW)

What about real superconductivity?



Pairing Gap Δ - Coastline of the Fermi Sea



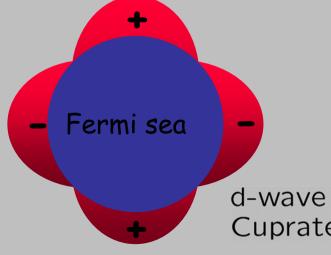
Superconducting gap Δ

Parting the waves of the Fermi Sea



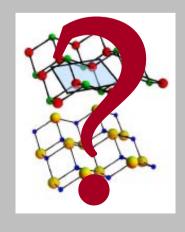
s-wave (isotropic) Conventional SC (Nb, Pb, Al, \cdots) $T_c < 25$ K

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



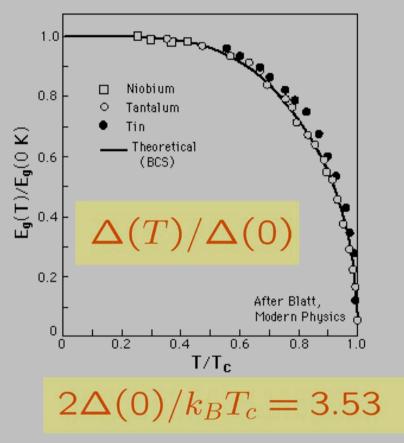
New REOFeAs SC $T_c \sim 57 \text{ K}$



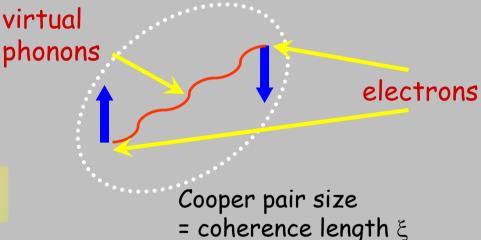


Cuprate SC $T_c \sim$ 160K

What can Δ tell us about superconducting state?



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!!

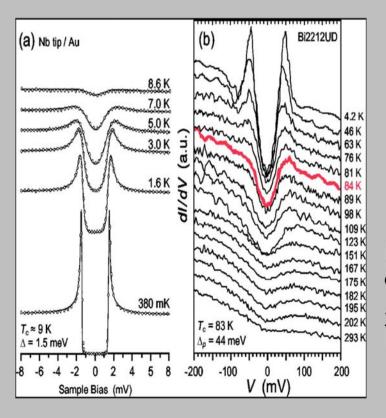


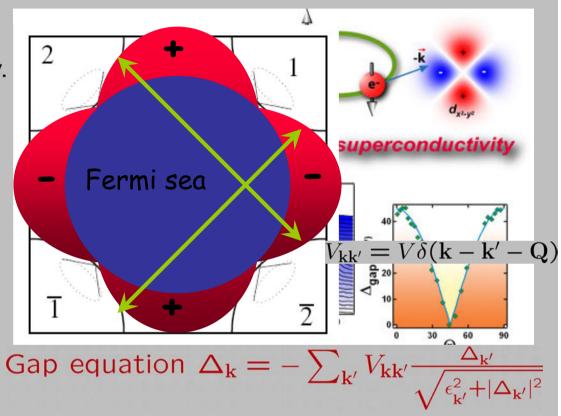
Universal BCS behavior

Standard BCS theory works well in materials like Nb, Sn or Hg. In Pb and more complex systems (Nb₃Ge) 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



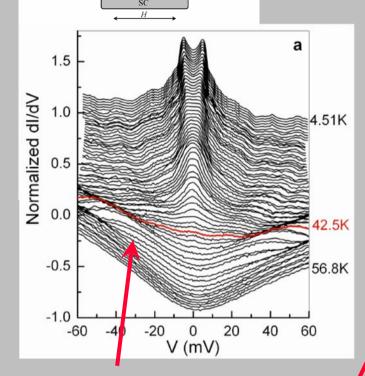


Furthermore, high temperature cuprate SCs exhibit a pseudogap behavior:

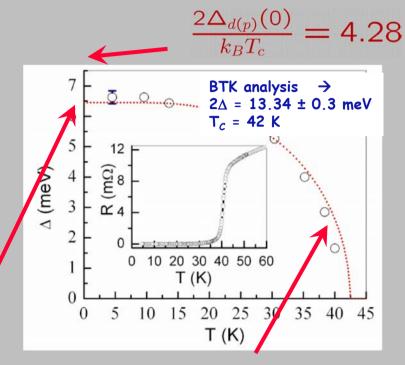
 Δ remains finite even for $T>T_c$! This reflects strong fluctuations!

Results for FeAs mostly appear inconsistent with these features

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



No pseudogap! Δ disappears at $T=T_c$ $2\Delta(0)/k_BT_c=3.68\sim3.53$

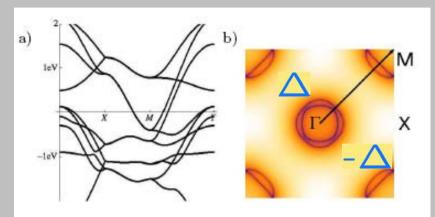


Nodeless isotropic gap! $\Delta(T)$ consistent with BCS theory (sign/phase variation still possible!)

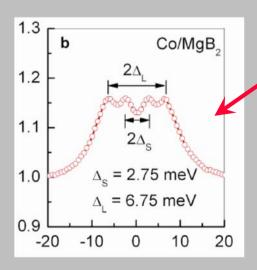
Conclusions: Nodeless superconducting gap and no pseudogap behavior. Very different from high T_c cuprate superconductors!!

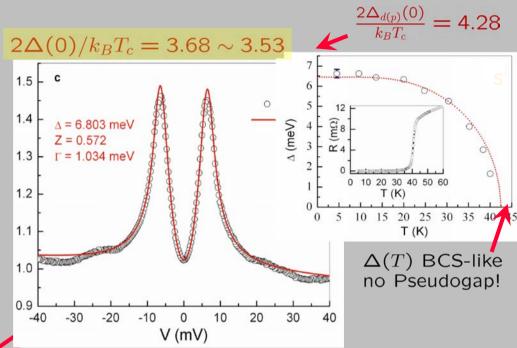
Δ in FeAs superconductors II

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



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



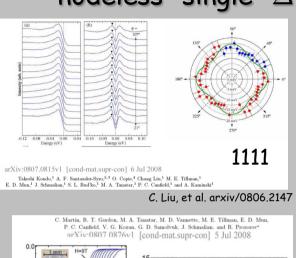


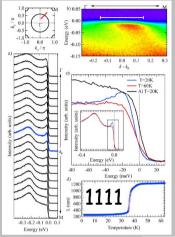
We see only a single isotropic BCS-like gap If different Fermi "lakes" had significantly different Δ we would see them

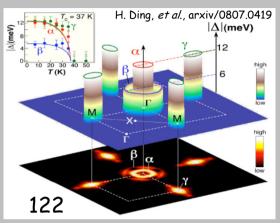
Only a "single" superconducting gap - but sign/phase could be different for holes and electrons. No pseudogap!

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, μ w, SQUID, ...): nodeless "single" Δ in 1111, "two" Δ 's in 122, nodes in lower T_c SC??



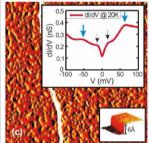


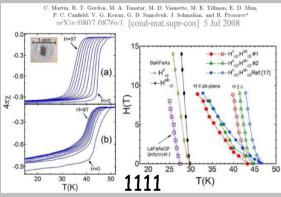


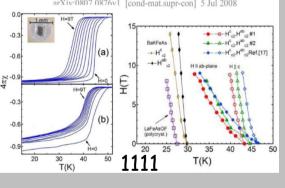
T/T

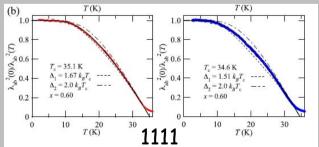
R. T. Gordon et al., arxiv/0810.2295

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



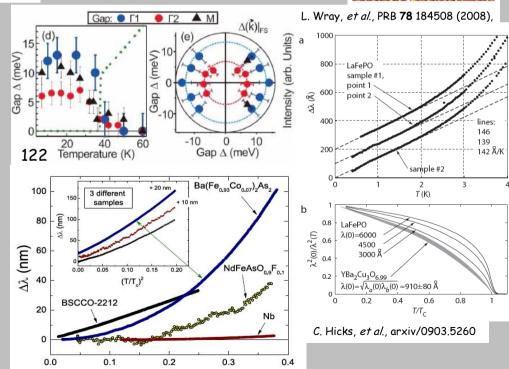






K. Hashimoto, et al., PRL 102 017002 (2009),

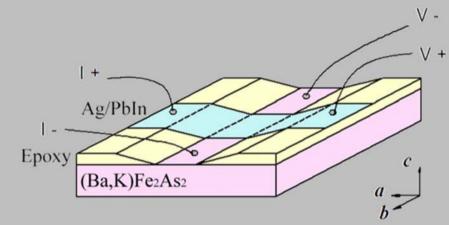
Multiband superconductivity in Fe-pnictides!?

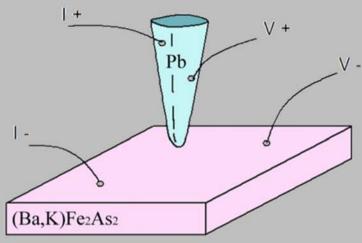


122

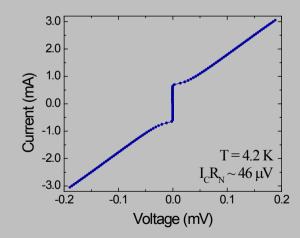
Josephson Effect Between FeAs and Pb

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

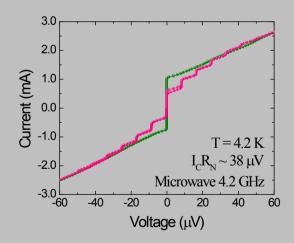




Point Contact Junction



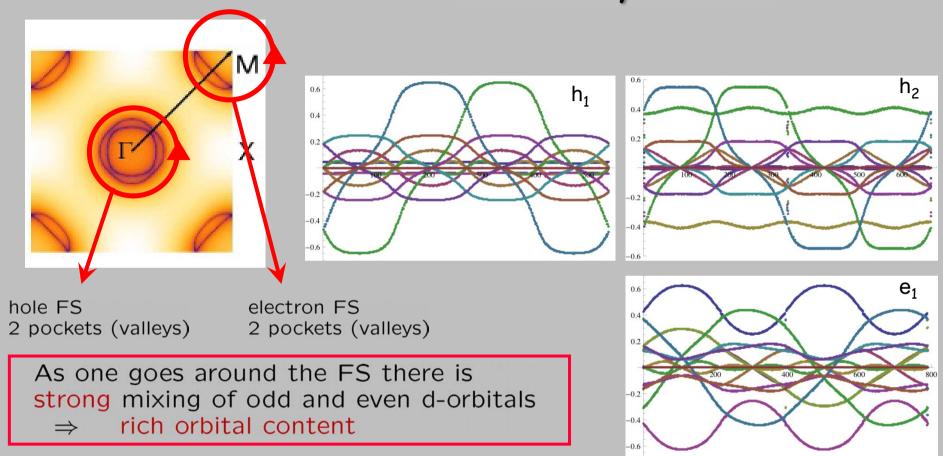
Strong indication of s-wave like SC state



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



Minimal Model of FeAs Layers IV



FeAs are different from CuO₂

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

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

Sawatzky et al discuss various interorbital interactions (\cdots)

Effective interaction at the Fermi surface:

$$\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \mathsf{\Gamma}_{lpha,eta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q}) f^{\dagger}_{\mathbf{k}+\mathbf{q},lpha} f^{\dagger}_{\mathbf{k}'-\mathbf{q},eta} f_{\mathbf{k}',\delta} f_{\mathbf{k},\gamma}$$

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

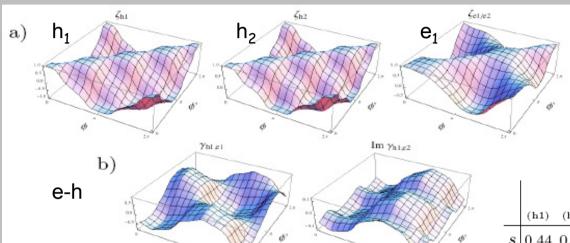
All flavor conserving (U, W) and flavor mixing (G_1, G_2) vertices

Interactions in FeAs II

vertices change significantly around Fermi surface:

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

A. V. Chubukov et al. PRB 78, 134512 (2008)



k-space "Josephson" terms:

$$\rightarrow G_2 c^{\dagger} c^{\dagger} dd + h.c.$$

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

	U				l .					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

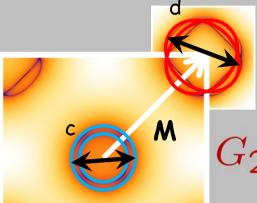
Effective vertex at the FS:

$$\Gamma_{\alpha,\beta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q})$$
 $(\mathbf{k},\mathbf{k}'\in\mathsf{FS})\to V_s+V_pp_4(\varphi)p_4(\varphi')+V_dd_4(\varphi)d_4(\varphi')$

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

Two Kinds of Interband Superconductivity

ZT, Physics 2, 60 (2009)



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

$$G_2 c^{\dagger} c^{\dagger} dd$$

X - A

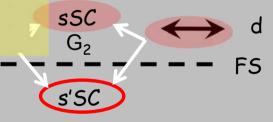
The Problem: Need

Type-A interband 5

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

trinsic) interband SC:

Most unlikely!



$$(c_\uparrow c_\downarrow \;,\; d_\uparrow d_\downarrow) \;\; o \Psi_c \;, \Psi_d$$

intraband Cooper pairing further enhanced by G_2

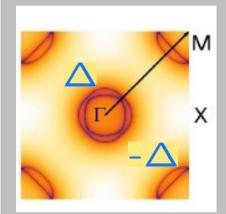
$$(c_\uparrow c_\downarrow - d_\uparrow d_\downarrow)$$

intrinsic interband Cooper pairs!

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

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

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



The condition for interband SC is actually milder:

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

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

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

 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

'FFLO" state 'superconductor

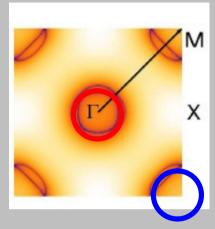
A. V. Chubukov et al, PRB 78, 134512 (2008)

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)

Hierarchy of Energy Scales U, W \Rightarrow G₁, G₂ \Rightarrow Unified Model of Valley Density-Wave (VDW)

Unified model N = $4 \rightarrow SU(4)XSU(4)$ V. Cvetkovic and ZT, PRB **80**, 024512 (2009)



$$H_0 = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}^{(0)} \left[\sum_{\alpha} h_{\mathbf{k}}^{(\alpha)\dagger} h_{\mathbf{k}}^{(\alpha)} + \sum_{\beta} e_{\mathbf{k}}^{(\beta)\dagger} e_{\mathbf{k}}^{(\beta)} \right]$$

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

Orbital flavor-conserving vertices (U, W) reduce this to $U(4) \times U(4)$:

	$T_{\rm S}\left({ m K} ight)$	$T_{N}(K)$	$m_{\mathrm{ord}} (\mu_{\mathrm{B}})$
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 ₂ As ₂	173	173	0.8
SrFe ₂ As ₂	220	220	0.94-1.0
BaFe ₂ As ₂	140	140	0.9

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

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

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

$$(2G_1 \sum_{\alpha\beta\sigma\sigma\sigma'} (\sigma\sigma') e_{\sigma}^{(\beta)\dagger} h_{-\sigma}^{(\alpha)\dagger} h_{-\sigma'}^{(\alpha)} e_{\sigma'}^{(\beta)} + G_2 \sum_{\alpha\alpha'\beta\beta'\sigma\sigma'} (\sigma\sigma') h_{-\sigma}^{(\alpha)} e_{\sigma}^{(\beta)} h_{-\sigma'}^{(\alpha)} e_{\sigma'}^{(\beta)} h_{-\sigma'}^{(\alpha)} e_{\sigma'}^{(\beta)} + h.c.$$

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

s 0.44 0.31 0.35 0.35 0.21 0.25 0.27 0.29 0.14 0.14

d 0.22 0.12 0.09 0.10 0.11 0.13 0.09 0.11 0.03 0.02

p 0.04 0.21 0.17 0.20 0.22 0.21 0.22 0.22 0.01

Interactions in FeAs III

V. Cvetkovic & ZT (RG); A. V. Chubukov, I. Eremin et al (parquet); F. Wang, H. Zhai, Y. Ran, A. Vishwanath & DH Lee (fRG)

R. Thomale, C. Platt, J. Hu, C. Honerkamp & A. Bernevig (fRG)

Effective interaction at the Fermi surface:

$$\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \Gamma_{\alpha,\beta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q}) f_{\mathbf{k}+\mathbf{q},\alpha}^{\dagger} f_{\mathbf{k}'-\mathbf{q},\beta}^{\dagger} f_{\mathbf{k}',\delta} f_{\mathbf{k},\gamma} \longrightarrow U, W, G_1, G_2$$

$$U, W, G_1, G_2$$

$$g_{U}(\omega) = g_{U} - g_{U}^{2} \ln\left(\frac{\Lambda}{\omega}\right)_{pp} - g_{2}^{2} \ln\left(\frac{\Lambda}{\omega}\right)_{pp},$$

$$g_{2}(\omega) = g_{2} - 2g_{2}g_{U} \ln\left(\frac{\Lambda}{\omega}\right)_{pp} + 2g_{2}g_{W}' \ln\left(\frac{\Lambda}{\omega}\right)_{ph}^{c} +$$

$$2g_{2}g_{W}'' \ln\left(\frac{\Lambda}{\omega}\right)_{ph}^{v} - 2g_{2}g_{1}'' \ln\left(\frac{\Lambda}{\omega}\right)_{ph},$$

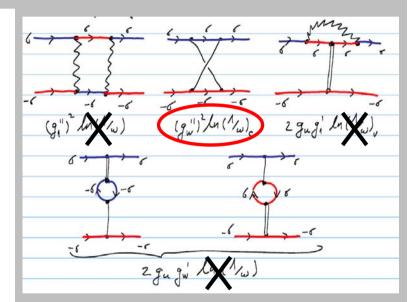
$$g_{W}'(\omega) = g_{W}'' + (g_{W}'')^{2} \ln\left(\frac{\Lambda}{\omega}\right)_{ph} + g_{2}^{2} \ln\left(\frac{\Lambda}{\omega}\right)_{ph},$$

$$g_{W}''(\omega) = g_{W}'' + (g_{W}'')^{2} \ln\left(\frac{\Lambda}{\omega}\right)_{ph},$$

$$g_{1}''(\omega) = g_{1}'' - 2g_{1}'g_{1}'' \ln\left(\frac{\Lambda}{\omega}\right)_{ph} + 2g_{1}'g_{W}'' \ln\left(\frac{\Lambda}{\omega}\right)_{ph}^{v},$$

$$g_{1}''(\omega) = g_{1}'' - (g_{1}')^{2} \ln\left(\frac{\Lambda}{\omega}\right)_{ph} - (g_{1}'')^{2} \ln\left(\frac{\Lambda}{\omega}\right)_{ph} -$$

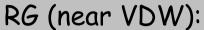
$$g_{2}^{2} \ln\left(\frac{\Lambda}{\omega}\right)_{ph} + 2g_{1}''g_{W}'' \ln\left(\frac{\Lambda}{\omega}\right)_{ph}^{v}, \tag{15}$$

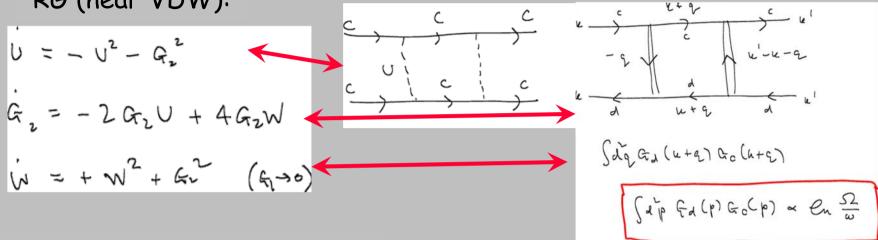


If
$$G_1$$
, $G_2 \ll U$, $W \rightarrow$

relevant vertices: U, W, & G₂

Interplay of VDW and SC in FeAs II





Proximity to VDW is crucial:

$$\dot{U} \pm \dot{G}_{2} = -\left(U \pm \dot{G}_{2}\right)^{2} \pm 4WG_{2}$$

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

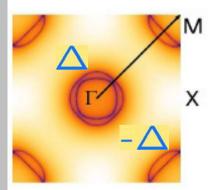
This is true interband SC since U > 0 - different from U < 0:

$$\dot{U} \pm \dot{G}_{1} = -\left(U \pm \dot{G}_{1}\right)^{2} \pm 4WG_{2} \text{ If } W \rightarrow 0 \text{ then } \dot{U} \pm \dot{G}_{2} = -(U \pm G_{2})^{2}$$

$$\dot{S} = -\left(U \pm \dot{G}_{1}\right)^{2} \pm 4WG_{2} \text{ if } W \rightarrow 0 \text{ then } \dot{U} \pm \dot{G}_{2} = -(U \pm G_{2})^{2}$$

$$(c_\uparrow c_\downarrow - d_\uparrow d_\downarrow)$$
 interband Cooper pairs !

$$(c_{\uparrow}c_{\downarrow}\ ,\ d_{\uparrow}d_{\downarrow})$$
 intraband Cooper pairs



RG Theory of Interband Mechanism of SC in FeAs

V. Cvetkovic and ZT, PRB 80, 024512 (2009)

RG flows (near SDW):

$$U = -U^{2} - G_{2}^{2}$$

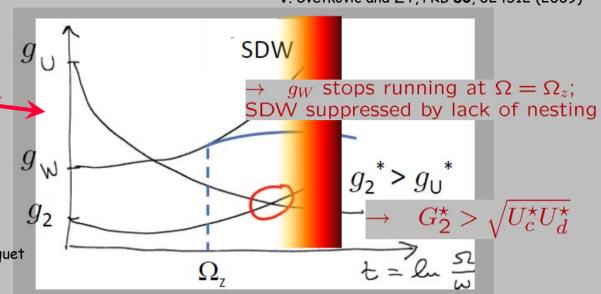
$$\dot{G}_{2} = -2G_{2}U + 4G_{2}W$$

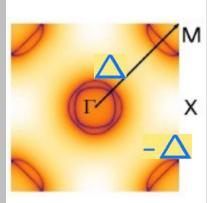
W=+W2+G2 (G>0)

A. V. Chubukov et al, PRB 78, 134512 (2008) parquet

F, Wang et al, PRL 102, 047005 (2009) fRG

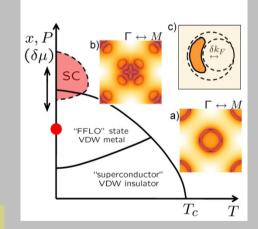
R. Thomale et al, PRB 80, 180505(R) (2009) fRG





$$G_2 < \sqrt{U_c U_d}$$

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



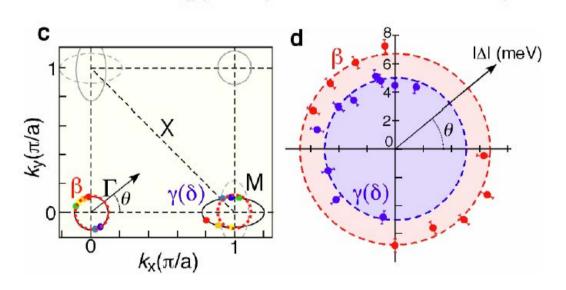
$$\rightarrow$$
 $T_c \sim \Omega_z \exp(-1/(g_2^{\star} - \sqrt{\mu_c^{\star} \mu_d^{\star}}))$

In Fe-pnictides interband superconductivity (s' or s+- state) is a strong possibility but there is some fine tuning with SDW/CDW/ODW

Correlation between SC and Nesting (ARPES)

H. Ding group (CAS Beijing & BC)

In optimally electron doped samples, quasi FS nesting between the outer (β) hole pocket and the electron pockets



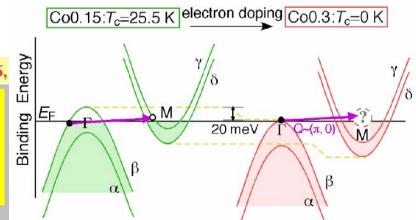
- Large SC gaps for wellnested hole and electron pockets
- SC collapses as one dopes away from near nesting
- Holds for both hole and electron doping

Strong pairing also happens to these FSs!

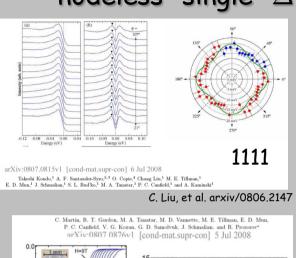
$$2\Delta/k_BT_c = 6$$
, 4.5 for β , $\gamma(\delta)$

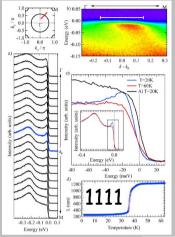
K. Terashima et al., PNAS 106,

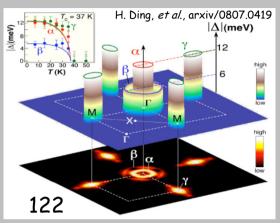
Nodeless SC correlates with degree of nesting and SC disappears as h(e) Fermi pockets are doped away.



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



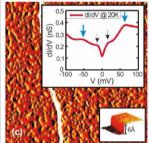


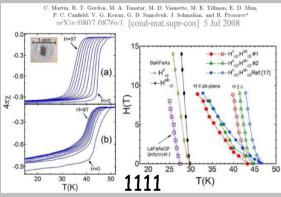


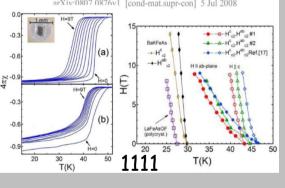
T/T

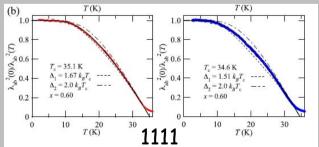
R. T. Gordon et al., arxiv/0810.2295

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



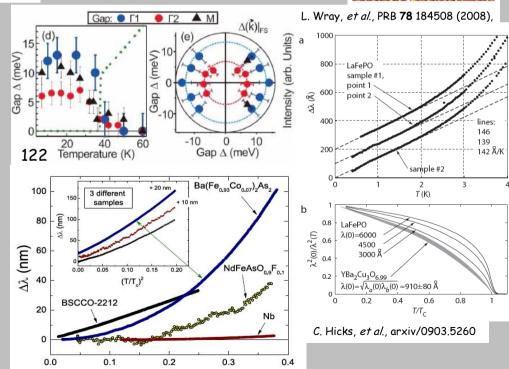






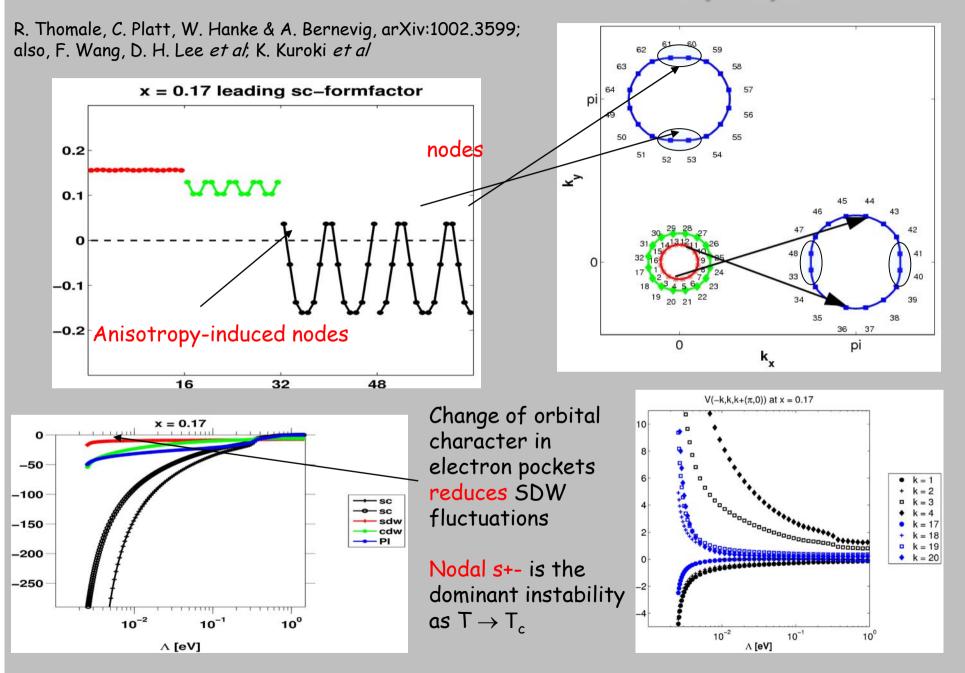
K. Hashimoto, et al., PRL 102 017002 (2009),

Multiband superconductivity in Fe-pnictides!?



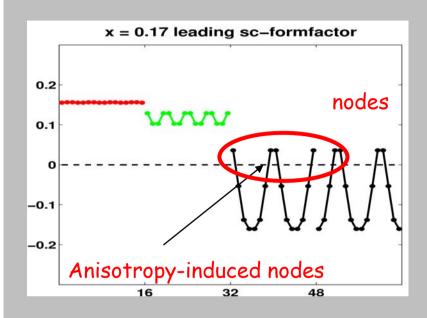
122

Nodal SC from Orbital Structure (fRG)



Accidental Gap Nodes and Zeroes in Iron-Pnictides I

V. Stanev et al., arXiv:1006.0447



These nodes are accidental and NOT protected by any symmetry - SC state is still s+- or s'. They are caused by strong orbital anisotropy of pairing interaction.

Such nodal s' states arise in various calculations (fRG, RG, etc) near $T = T_c$. But do these accidental nodes survive as $T \rightarrow 0$?

Consider interband interaction:

$$g_2(k, k') = \lambda_0 + \lambda_n \cos 4\theta$$

$$\rightarrow \Delta_e(\theta) \equiv \Delta_0 + \Delta' \cos 4\theta$$

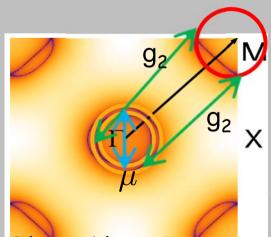
$$\Delta_{h} = -\int_{0}^{\Lambda} d\xi \int_{0}^{2\pi} \frac{d\theta}{2\pi} \frac{\tanh(E_{e}/2T)}{E_{e}} (\lambda_{0} + \lambda_{n} \cos 4\theta) \Delta_{e}$$

$$-\mu \int_{0}^{\Lambda} d\xi \frac{\tanh(E_{h}/2T)}{E_{h}} \Delta_{h}$$

$$\Delta_{0} = -\mu \int_{0}^{\Lambda} d\xi \int_{0}^{2\pi} \frac{d\theta}{2\pi} \frac{\tanh(E_{e}/2T)}{E_{e}} \Delta_{e}$$

$$-\lambda_{0} \int_{0}^{\Lambda} d\xi \frac{\tanh(E_{h}/2T)}{E_{h}} \Delta_{h}$$

$$\Delta' = -\lambda_{n} \int_{0}^{\Lambda} d\xi \frac{\tanh(E_{h}/2T)}{E_{h}} \Delta_{h} , \qquad (1)$$

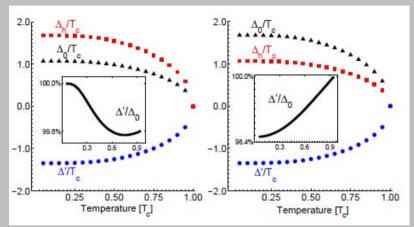


The problem: Gap equations can wipe out accidental nodes for $T \ll T_c$

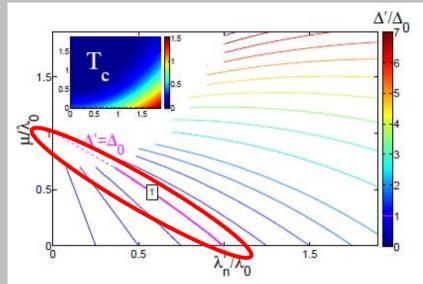
Accidental Gap Nodes and Zeroes in Iron-Pnictides II

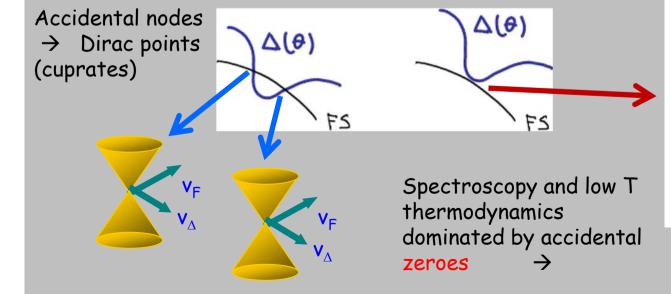
V. Stanev et al., arXiv:1006.0447

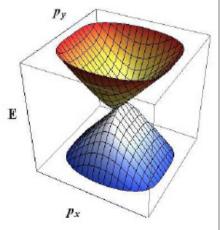
These accidental nodes appear "robust" as $T \rightarrow 0$



$$\Delta_e(\theta) \equiv \Delta_0 + \Delta' \cos 4\theta$$





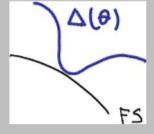


Zero-point BdG quasiparticles Δ (θ) $\sim \theta^2$

Critical "Zero-Point" Quasiparticle Scaling

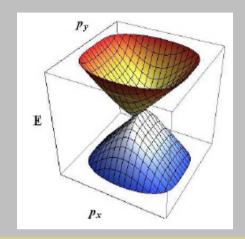
 Δ ' = Δ_0 defines a line of quantum phase transitions in (T, H) phase diagram \rightarrow Critical scaling of zero-point BdG quasiparticles

$$\mathcal{H}_{\text{BdG}} = \begin{bmatrix} \frac{\mathbf{p}^2}{2m} - \epsilon_F & \hat{\Delta}(\mathbf{r}) \\ \hat{\Delta}(\mathbf{r}) & -\frac{\mathbf{p}^2}{2m} + \epsilon_F \end{bmatrix} \approx \begin{bmatrix} v_F p_x & \frac{8\Delta_0}{p_F^2} p_y^2 \\ \frac{8\Delta_0}{p_F^2} p_y^2 & -v_F p_x \end{bmatrix}$$



$$\Rightarrow E = \pm \sqrt{(v_F p_x)^2 + (8\Delta_0 p_y^2/p_F^2)^2}$$

V. Stanev et al., arXiv:1006.0447



Spectroscopy and thermodynamics dominated by zero-point scaling ←→ Different from Dirac and Simon-Lee scaling in cuprates

$$N(E) \sim \text{Re}\left(\int d\theta \frac{E}{\sqrt{E^2 - \Delta(\theta)^2}}\right) \sqrt{E}$$

$$C(T) \approx \frac{1}{T^2} \int_0^\infty dE E^2 N(E) \frac{1}{\cosh^2(E/2T)} \propto T^{3/2}$$

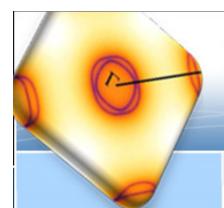
$$\chi_s(T)/\chi_n \approx \frac{1}{T} \int_0^\infty dE N(E) \frac{1}{\cosh^2(E/2T)} \propto T^{1/2}$$

$$\frac{(T_1)_n}{(T_1)_s} \approx \frac{1}{T} \int_0^\infty dE N(E)^2 \frac{1}{\cosh^2(E/2T)} \propto T$$

$$\lambda(T) = \sqrt{\frac{c^2 m}{4\pi e^2 \rho_s(T)}} \approx \lambda_0 + \lambda_1 T^{1/2}$$

At finite H new form of scaling replaces nodal Simon-Lee scaling:

$$N(E o 0,H)\sim H^{1/3+\eta}$$
 $N(0)\sim H^{1/2}$ $C(H,T)\sim TH^{1/3+\eta}$



INSTITUTE FOR QUANTUM MATTER

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Conclusions

- Iron pnictides are semimetals turned superconductors
- Correlations are significant, hence a SDW in parent compounds, but weaker than in cuprates
- Both magnetism and superconductivity are intrinsically multiband in nature – s' interband SC is a likely possibility near a nesting-driven SDW
- o Orbital anisotropy of pairing interaction can lead to anisotropic SC gap with accidental nodes/zeroes → quantum critical "zero-point" scaling replaces Dirac-SL scaling seen in cuprates
 - → new physics, beyond the "standard" model?





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