µSR studies of high-$T_C$ superconductivity in iron pnictides

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Superconductivity above 50 K

Metallic parent compounds!

Superconducting $T_C$

C. Hess et al., arxiv 0811.1651 (2008)
similar data: e.g. Ren et al. Chin Phys. Lett. 2008

S. Glaser, U Augsburg

Cuprates

Pnictides

Liquid Nitrogen

$\text{SmO}_{1-x}F_x\text{FeAs}$

Resistivity

Temperature(K)
General structural motif: FeAs layers with Fe square lattice


La$_{1-x}$Fe$_x$As "111"

(Sr,Ca,Ba)$_{1-x}$Fe$_{2-y}$(Co,Ni)$_y$As$_2$ "122"

X. C. Wang et al., arXiv:0806:4688

Hsu et al., arXiv:0807.2369

LiFeAs "111"

FeSe "011"
Interplanar distance may differ very much!

FeSe$_{1-x}$Te$_x$

$T_c,_{\text{max}} = 14$ K

@ 9 GPa: 36.7 K !!

S. Medvedev et al., Nature mat ‘09

(Fe$_2$P$_2$)(Sr$_4$Sc$_2$O$_6$)

$T_c,_{\text{max}} = 37$ K

H. Ogino et al., arXiv:0903.3314
Electronic band structure

- Parent compounds of FeAs superconductors are semimetals
- Crystal field splitting smaller than band width
  - All five Fe 3d bands cross $E_F$
  - Orbital degrees of freedom

LaFeAsO

La-4f
Fe-3d
Pn - p
O - 2p

Electrons
Holes

Vildosola et al., PRB 78, 064518
Fermi surface

- parent compounds of FeAs superconductors are semimetals

- crystal field splitting smaller than band width
  → all five Fe 3$d$ bands cross $E_F$
  → weak electronic correlations
  → Multi-band Fermi surface
    - Hole like at (0,0)
    - Electron-like at ($\pi$, $\pi$)

- cylindrical shape
  → nearly two-dimensional electron system

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I. I. Mazin et al., PRB 78, 085104 (2008)
Magnetism and Superconductivity

Cuprates

- Strong electronic correlations
- Local moment AFM order (1 to 2 $\mu_B$)
- Undoped cuprates are insulators!

Heavy Fermions


• Phase Diagrams of Fe-pnictides: RO$_{1-x}$F$_x$FeAs and (Sr,Ba)Fe$_{2-x}$Co$_x$As$_2$
  → electronic, magnetic and superconducting properties
  → interplay with structure, quantum criticality or phase competition

• Interplay of R and FeAs electronic system in R(O$_{1-x}$F$_x$)FeAs$_{1-y}$P$_y$
  → non-collinear order of R and Fe spin systems
  → afm and fm order of Ce sublattice

• Superconductivity in (Sr, Ba)Fe$_{2-y}$Co$_y$As$_2$ compounds
  → multi-gap sc, nodes
  → field induced magnetism

~20 Publications (Nature mat, PRL, PRB, NJP,…) on pnictides since April 2008
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In-plane Fe – Fe distance ~ 2.86 Å only, like pure Fe!

Ren et al., EPL, 83 (2008) 17002
Tetragonal to orthorhombic distortion below 156 K in LaOFeAs
**Magnetic order of LaOFeAs**

- **μSR on LaOFeAs**
  - well defined local magnetic field at muon site
  - \( \omega = \gamma_\mu B_{\text{local}} \sim \text{ordered magnetic moment} \)
  - \( \rightarrow \) commensurate AFM below 138 K

- additional change below 70 K
  - appearance of a smaller frequency
  - \( \rightarrow \) 2 muon sites

HHK et al., PRL 101, 077005 (2008)
Magnetic order of LaOFeAs

$^{57}$Fe Mössbauer spectroscopy

- well defined magnetic hyperfine field
- commensurate magnetic order below 138 K

$B_{hyp} \leftarrow 0 \sim 4.86 \text{T}$

compare with bulk iron

- ordered moment $\sim 0.3 \mu_B$
- itinerant magnet
Magnetic order of LaOFeAs

ordered moment $\sim 0.3 \, \mu_B$
proof of itinerant character

Spin density wave order = resonance on the Fermi Surface

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

M. Korshunov, I. Eremin, PRB 78, 140509(R) (2008)
Magnetic Order parameter in undoped LaOFeAs

Four band SDW theory

$U = 0.26 \text{eV}$
$J = U / 5$
$Q_{AFM} = (\pi, \pi)$

$\Delta_{SDW}(0 \text{K}) = 31 \text{ meV}$
$\Rightarrow \mu = 0.33 \mu_B$

See:
M. Korshunov and I. Eremin
arXiv:0804.1793

HHK et al., PRL08, arXiv:0805.0264
Recent neutron scattering on the same LaO$_{1-x}$F$_x$FeAs samples

Qureshi et al., arXiv:1002.4326)

→ ordered moment $\sim 0.63 \mu_B$!
Doping electrons or holes: $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$

**ARPES on s-xtals**: Liu et al.; arXiv:0806.3453

Fe ($3d^6$) $\rightarrow$ Co ($3d^7$)

= Electron doping

or

$\text{Ba}^{2+} \rightarrow \text{K}^+$

= Hole doping

$\rightarrow$ Nesting condition on Fermi surface destroyed
Magnetism of lightly doped La(O$_{1-x}$F$_x$)FeAs

H. Luetkens et al., Nature Materials 2009
Magnetism in lightly doped La(O$_{1-x}$F$_x$)FeAs

- Weak reduction of $T_N$ and low temp order parameter for $0 \leq x \leq 0.04$

SDW magnetism correlated with orthorhombic distortion at higher temperature!
SDW magnetism in \( \text{SrFe}_2\text{As}_2 \)

- \( \mu \text{SR} \) similar to \( \text{LaOFeAs} \)
- two signals same intensity ratio
- \( \sim 2 \) times larger frequency

\( \rightarrow \) 2 times larger ordered moment (crf. Mössbauer, ns)
Structural and magnetic order parameter

- 1st order transitions!
- identical temperature dependence of both order parameters

\[ T_N = T_S \]

Structure and magnetism are driven by the same Fermi surface instability

Jesche et al., PRB’08, arXiv:0807.0632
Comparison of “1111” and “122”

- Temperature dependence of the magnetic order parameter:
  - “1111” family → second order magnetic phase transition
  - “122” family → first order magnetic phase transition
How can we measure the superfluid density $n_s / m^*$?

via the magnetic penetration depth $\lambda$

$n_s / m^*$ is proportional to $1/ \lambda^2$

• measure $\lambda$ in vortex state of type II superconductor via field profile $p(B)$

→ transverse field $\mu$SR, NMR

In powder of anisotropic superconductors

$P(B)$ shows Gaussian shape

$$\left\langle \Delta B^2 \right\rangle \propto \lambda_{ab}^{-4}$$
μSR on superconducting La(O_{1-x}F_x)FeAs

Gaussian relaxation $\sigma_{sc} \sim 1/\lambda^2 \sim n_s / m^* = \text{sc order parameter}$

The fundamental parameter of a superconductor is the gap $\Delta(k)$.

- **s-wave**: isotropic gap
- **d-wave**: nodes in $k$-space where gap vanishes

→ Influence on stiffness of superconducting state
Magnetic penetration depth in $La(O_{1-x}F_x)FeAs$

H. Luetkens, HHK et al, PRL08

Temperature dependence of the relaxation rate $\sigma \propto n_s/m^*$

- Only weak temperature dependence below $T_C / 3$ : s-wave ?

Magnetic field dependence of TF-$\mu$SR relaxation rate

- Strong field dependence: d-wave ?
- No, extended $s_+$-wave
- multi-band Fermi surface with two different gaps
Fe pnictides are semimetals with itinerant magnetism

suppress magnetism by doping charge carriers, impurities or small changes of the Fermi surface (e.g. by high pressure)

→ superconductivity!
Pressure and chemical pressure


C. Wang et al., EPL 86, 47002 (2009)
Order Parameters in La(O$_{1-x}$F$_x$)FeAs

- no indications of quantum criticality in LaO$_{1-x}$F$_x$FeAs

H. Luetkens et al., Nature Materials 2009
Phase Diagrams of $\text{CeFeAsO}_{1-x}\text{F}_x$ and $\text{SmFeAsO}_{1-x}\text{F}_x$

Drew et al., Nature Materials 2009

(crf. E. Baggio-Saitovich talk Tuesday)

No continuous transition between AFM and Superconductivity in the orthorhombic phase !!
Phase diagram of Co doped $\text{BaFe}_2\text{As}_2$

Single crystal neutron study: similar separation of structural and magnetic transition

Lester et al., PRB 2009
- Phonon DOS too small for $T_C$ above 1K

- AFM spin fluctuations result in attractive interaction in case of phase change only:
  - d-wave sc in cuprates
  - $S_{+-}$ symmetry in pnictides (Mazin et al., PRL08):

  $\rightarrow$ Full gap on each Fermi pocket
  $\rightarrow$ Phase change from scattering between hole and electron pocket

But:

d-wave and spin-triplet p-wave sc also discussed!
Competition of SDW and SC order

Important: Existence of nesting condition between electron and hole pockets

Two-band model:
Hole and electron pockets with different size and ellipticity

Vavilov et al., PRB 2010
Classification of Fe-based SC

Uemura plot:

- Conventional superconductors have low $T_C$ and high superfluid density
- Unconventional superconductors have relatively low superfluid density ("dilute superfluid")

\[ k_B T_F = \hbar \pi c_{int} \frac{n_S}{m^*} \propto c_{int} \sigma_{SC} \]


Magnetic Rare earth ions in $\text{RO}_{1-x}\text{F}_x\text{FeAs}$

Replace La with magnetic rare earth
$\rightarrow T_C$ doubles!

Structure: different ion size
$\rightarrow$ more favorable bond angles

regular FeAs tetrahedron has highest $T_C$

Magnetic interaction between rare earth ions and FeAs electronic system?

- Collinear Heisenberg interaction impossible due to frustration for planar Fe-SDW order
- Non-collinear Heisenberg interaction possible

$\rightarrow$ Non-collinear order of rare earth below $T_{SDW}$!

ROFeAs (R = La, Pr, Ce, Sm)

**ZF-μSR:**

- Zero Field Muon Spin Rotation
  - Static magnetic order below $T_N$
  - 100% magnetic volume fraction
  - Commensurate magnetic structure

- $T$-dependence of $\mu$SR frequency
  - Second order transition at $T_N(\text{Fe})$
  - $T_N(\text{R}) \sim 4$ K
  - Why is CeOFeAs different?

**Moessbauer:**

- Moessbauer spectroscopy
  - All compounds have the same ordered Fe moment!

- Neutron scattering: 0.25 – 0.8 $\mu_B$?
Ce magnetization above $T_{N}^{Ce}$

- Ce-magnetization in molecular field of the Fe sublattice
  - Contributes to same Bragg peaks as the Fe order
  - Additional field at the muon site proportional to the Ce magnetization

- Quantitative analysis
  - Curie-like term to the $\mu$SR frequency
  - calculation of thermal population of Ce crystal electric field (CEF) levels

\[ f(T) = f_0 \left[ 1 - \left( \frac{T}{T_N} \right)^\alpha \right]^\gamma \cdot \left[ 1 + \frac{\tilde{C}}{T - \Theta} \right] \]

Fe sublattice magnetization  Curie-like Ce magnetization

Interplay of Rare Earth and FeAs electronic systems

- LDA band structure
  - CeOFeAs
  - PrOCeAs

- Strong hybridization between Fe and Ce states
- CeOFeP is a moderate heavy fermion system

- Pr states shifted 2 eV downwards

L. Pourovskii et al., EPL 84 37006 (2008)

Gap Anisotropy in $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, $T_c = 32$ K

blades instead of barrels
$\rightarrow$ correlation effect?

Coupling strength $2 \Delta/k_B T_c$

$\sim 7$

$\sim 2.5$

D.V. Evtushinsky et al., PRB 09, arXiv: 0809.4455

Similar results see eg. Ding et al EPL 2008
\[ \frac{1}{\lambda^2(0)} = I_1 + I_2 = \frac{e^2}{2\pi \epsilon_0 c^2 h L_c} \left[ \int_{\text{inner } \Gamma} v_F(k) \, dk + \int_{\text{outer } \Gamma} v_F(k) \, dk + \int_{\text{X-pocket}} v_F(k) \, dk + \int_{\text{blades}} v_F(k) \, dk \right] \]

calculated from ARPES
measured by $\mu$SR

D.V. Evtushinsky et al., NJP 09 in print
R. Khasanov, PRL 09, in print
Multiband Superconductivity

**Ba$_{1-x}$K$_x$Fe$_2$As$_2**


**FeSe$_{1-x}$Te$_x**

- M. Bendele et al., PRB 81, 224520 (2010).

**SrFe$_{2-x}$Co$_x$As$_2**


**RbFe$_2$As$_2**

- Z. Shermadini et al., arXiv:1005.3989

**BaFe$_{2-x}$Co$_x$As$_2**

• From spin density wave magnetism to superconductivity in LaO$_{1-x}$F$_x$FeAs
  Unconventional metal in normal state
  SDW strongly coupled to orthorhombic phase
  reduced moment ~ 0.3 - 0.6 $\mu_B$
  1st order transition to superconductivity
  Superfluid density finite at $x=0.05$

• RO$_{1-x}$F$_x$FeAs and ROFeAs$_{1-x}$P$_x$
  no SC in orthorhombic phase for $R=$Ce,Sm
  independent R order below ~ 4-12 K
  non-collinear magnetic interaction
  between Ce and FeAs electronic systems

• Intermetallic (Sr,Ba)$_{1-x}$K$_x$Fe$_2$As$_2$
  Strong coupling of structural and magnetic order parameter
  Phase coexistence/separation
  under doping (and high pressure)
  Two gap values on different FS sheets