Magnetism and superconductivity in iron-pnictides superconductors: a status report

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Outline

- Iron pnictide superconductors: families and phase diagrams
- Magneto-structural coupling
- Superconducting gap structure and pairing mechanism
- Coexistence between Spin Density Wave and Superconductivity
2008: discovery

Iron-Based Layered Superconductor La[O_{1-x}F_x]FeAs (x = 0.05–0.12) with $T_c = 26$ K

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dopage électrons
Structure and families

Common building block:
Fe square lattice
FeAs plane except FeSe

$T_{c,\text{max}} = 55K$
### Pnictides

**Pnictogen**

(P, As)

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- **Exception:** FeSe...
Tc vs time

A new route to high Tc superconductivity?
Electron correlations?

Comparison between kinetic energy from optics and from band structure calculations

- Iron-pnictides further away from Mott insulator than cuprates (DMFT…)
- Ab-initio calculations (DFT) predict magnetism (but not the correct Fe moment) and gross features of band structure


Phase diagrams and families

1111

CeO_{1-x}F_xFeAs

- close proximity of SC phase with magnetism (heavy fermions, cuprates)
- coexistence (or not) between magnetism and superconductivity
- magnetic and structural transitions


122

Crystal structure BaFe$_2$As$_2$

- Square plane of Fe ($d^6$)
- As alternating above and below Fe planes
- FeAs$_4$ tetrahedra
- Ba blocking layer

- FeAs plane: 2 Fe/cell
- BZ sometimes defined with 1 Fe/cell (extended BZ)
A multi-orbital system

Minimal two-orbital model: $d_{xz}, d_{yz}$

Hole and electron Fermi surfaces
5 orbital models

3D Fermi surfaces

DFT calculations
Mazin, Physica C 469, 614 (2009)

- Up to 5 Fe derived bands cross the Fermi level:
  3 hole-like and 2 electron-like
- As derived bands are 2eV below Fermi level
- relatively 2D electronic structure

- physics is governed by Fe orbitals
- importance of Fe-As-Fe hopping
- orbital physics: Hund coupling

Orbital content of Fermi surfaces
Fermi surfaces

Cuprates: 1 FS

Pnictides: multiple FS


Liu et al. Nature Phys. 2010
the x parameter: tuning magnetism and superconductivity

Different ways of tuning magnetism and SC

- Hole, electron, isovalent doping
- pressure
- doping in the FeAs plane is not detrimental to Tc

the x parameter: tuning magnetism and superconductivity

- "universal" $T_c$ (e) phase diagram in overdoped Ba-122
- $T_c$ is correlated with $T_{N/S}$ in underdoped Ba-122
- electronic parameter: FS topology?
What is controlling $T_c$?

- Fe-As-Fe bond angle controls bandwidth and nesting
- Sensitivity of the band structure and calculated Fe moment with As position

$T_c$ is max for perfect tetrahedra: « magic » angle at 109°
x: structural tuning

K (hole) doping vs pressure

- pressure and hole doping have a similar effect on bond angle (chemical vs physical pressure)
- $T_c$ is max around « magic » angle (but uncertainty in pressure dependance of $T_c$)
x parameter in BaFe$_2$As$_2$ (122)

Co doping vs pressure

- No clear structural trends between Co and pressure
- x is not just structural tuning
Phase diagram of $\text{Ba(Fe}_{1-x}\text{Co}_x\text{)}_2\text{As}_2$


- Relatively large and good quality single crystals
- Homogeneous Co doping (no segregation)
- Fine control of Co
Transport in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$


Electron doping: Co$^{3+}$ replaces Fe$^{2+}$
Electron doping in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$

ARPES: hole band sinks below $E_F$.


Hall effect: increase in electron-like carrier

fair agreement between Hall and ARPES (Luttinger theorem): rigid band picture
BaFe$_2$As$_2$ : magnetic transition

- transition second (Ba-122) or first (Ca-122) order
- stripe-like AF order: in-plane magnetic anisotropy

itinerant magnetism, not Mott magnetism

Neutron diffraction: new Bragg peaks below 135K

Wilson et al. PRB 79, 184519 (2009)
Huang et PRL 2008
Spin Density Wave transition

transport

magnetization

specific heat

itinerant magnet: SDW transition

SDW and Fermi surface nesting

- approximate Fermi surface nesting $Q_{SDW}$ between holes and electrons pockets
- enhancement of susceptibility at $Q_{SDW}=(\pi,\pi)$: instability
- DFT correctly predicts magnetism but over-estimate magnetic moment

k-space susceptibility

r-space


Mazin et al. PRL 2008
Fermi surface reconstruction in the SDW state

- Backfolding of the band
- Spin density wave gap at $E_F$ (anticrossing)

- Perfect nesting: insulator
- Imperfect nesting: SDW metal

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**perfect nesting**

$m = m_x = m_y$

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**ellipticity**

$m \neq m_x \neq m_y$

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hole FS: circular
electron FS: elliptic

Fermi surface reconstruction

- imperfect nesting: residual Fermi surfaces
- Not all the bands are clearly resolved
- SDW gaps unclear
- More than simple band folding?

Fermi surface reconstruction: quantum oscillations (SdH)

- very small FS area in the SDW phase (1.7%, 0.7% et 0.3% de ZB para): FS reconstruction
- one FS is isotropic and the other 2 anisotropic (cigar-shaped: Dirac point)
Spin density wave gaps

![Optical Conductivity Graph](image)

**Optical Conductivity**
- **BaFe$_2$As$_2**
- Conductivity vs. Wavenumber ($\Omega^{-1} \text{cm}^2$)
- Data points for different temperatures: 5K, 100K, 125K, 130K, 135K, 140K, 150K

![Raman Scattering Graph](image)

**Raman Scattering**
- Raman Response (arb. units)
- Raman Shift (cm$^{-1}$)
- Data points for different temperatures: 230K, 150K, 130K, 30K

**Cr Alloys**
- **Cr alloys**
- Conductivity vs. Frequency (cm$^{-1}$)
- Data for various concentrations

**References**

**Observations**
- Opening of SDW gaps consistent with band folding
- Residual Drude weight in the SDW state: incomplete gap

*Further details and discussion can be found in the references.*
Magneto-structural transition

- first order in (Ca,Sr)-112 but second order in Ba-122
- orthorhombic distortion is less than 0.5%
- Spin driven structural transition?
Splitting of the transition in $\text{Ba(Fe}_{1-x}\text{Co}_x\text{)}_2\text{As}_2$

- magnetic and structural transitions split upon Co doping
- not observed in all systems (disorder?)
- fluctuating magnetic domains?
Splitting of the transition in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$

**magnetization**

**transport**

**neutrons**
Spin-lattice coupling

- phonon splitting much larger than expected from lattice distortion alone
- strong spin-phonon coupling: modulation of the exchange constant by atomic motion
- linear relation between lattice distortion, phonon splitting and magnetic moment

Anisotropic transport

transport in mechanically detwinned crystals

- very large transport anisotropy at low temperature
- extremely strong sensitivity of properties to stress above $T_S$: nematic susceptibility

Nematic order?

transport in mechanically detwinned crystals

anisotropy (or nematic susceptibility?) is maximum around onset of SC order

strong in-plane anisotropy of the electronic properties

optical conductivity

strong reduction of Drude weight along b-direction only


Nakajima et al. PNAS 108, 12238 (2011)
Nematic order?

- no anisotropy above Ts for Ca122 and Sr122
- first order vs second order transition
- nematic phase above T_s is not generic
- Fluctuating magnetic domain

small stress induced large shift of T_{S,N}
Orbital dependent band splitting

ARPES on detwinned crystals

- $C_4$ symmetry is broken
- splitting larger than expected from structural distorsion
- orbital degrees of freedom may play a role in the magneto-structural transition

Yi et al. PNAS 108, 6878 (2011)
Magneto-structural coupling

what is the driving force behind the M/S transition? a chicken and egg problem

1. **Magnetic driven structural distortion**: magnetic fluctuations drive the distortion via magneto-elastic coupling or via Ising nematic fluctuations that break $C_4$ symmetry above $T_S (\varphi=m_1,m_2)$ (‘nemato-elastic’ coupling)


2. **Orbital ordering**: difference in $d_{xz}$ and $d_{yz}$ occupation drives both magnetic and structural transitions (Kügel-Khomskii)

Superconducting state

AC Josephson effect: charge 2e

NMR: spin-singlet


Teresaki et al. JPSJ 78, 13701 (2008)

Electron-phonon coupling too weak to explain $T_c > 10K$

Gap structure and spin fluctuation pairing

- weak electron-phonon coupling
- proximity of AF order suggests spin fluctuation pairing

\[ \Gamma_s(k, k') = \frac{3}{2} U^2 \frac{\chi_0(q)}{1 - U \chi_0(q)} \]

singlet repulsive interaction (Stoner-Hubbard)

\[ \Delta_k = -\sum_{k'} \Gamma_s(k, k') \frac{\Delta_{k'}^s}{2E_{k'}} \tanh \frac{E_{k'}^s}{2T}, \]

solution allowed if \( \Delta \) changes sign

**In cuprates**: susceptibility is peaked at \( Q=(\pi,\pi) \)

**In pnictides**: susceptibility is peaked at \( Q=(\pi,0) \)

\[ \Delta_i = \sum_j \Lambda_{ij} \Delta_j F(\Delta_j, T) \]

**alternative model**: orbital fluctuations theory predicts s^{++}

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Gap structure and spin fluctuation pairing

- weak electron-phonon coupling
- proximity of AF order suggests spin fluctuation pairing

\[ \Gamma_s(k, k') = \frac{3}{2} U^2 \frac{\chi_0(q)}{1 - U\chi_0(q)} \]

... singlet repulsive interaction (Stoner-Hubbard)

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Pairing interaction for cuprates
(Monte Carlo and 3rd order perturbation theory)
Repulsive!

Pairing interaction is attractive for specific regions in real space

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Gap symmetry vs gap structure

- spin fluctuation pairing naturally leads to $s^\pm$ symmetry in pnictide
- Coulomb interband interaction is responsible for both SDW and SC phase
- gap symmetry does not tell much about presence of nodes

\[ s_{++} \quad s_{\pm} \]

\[ \text{nodal } s_{\pm} \quad d \]

same symmetry but different gap structure!

- possible source of anisotropy around FS: orbital content, intraband interaction, FS topology
- crucial role of nesting properties

Multiple gaps in optimally-doped K-Ba122

$T_c = 37K$

FS dependent pairing strength ($3.5 - 7 k_B T_c$)

Multiple gaps in optimally-doped Co-Ba122

\( T_c = 25 \text{K} \)

**STM**

- at least 2 gaps around electron and hole pockets
- up to three different gaps have been reported

**ARPES**

**Raman**

\[
\frac{2\Delta_e}{k_B T_c} \approx 4 \quad \frac{2\Delta_h}{k_B T_c} \approx 6
\]

Terashima et al. PNAS 106, 7330 (2009)  
Specific Heat in Co-Ba122

- significantly smaller gaps: one smaller than BCS weak coupling ratio one bigger
- role of anisotropy?
London penetration depth in Co-Ba122

- significantly smaller gaps: one smaller than BCS weak coupling ratio one bigger
- fit must be done self-consistently: one cannot assume two independent BCS T dependences
- different techniques may be sensitive to different FS (effective mass, Fermi velocity….)

Probing the phase - Cuprates: reminder

tricristal experiment

Half-Integer Flux Quantum Effect

cristal orientations: \( \pi \) ring

YBCO single crystal

Tsuei et al. Rev. Mod. Phys. 72, 969 (2000)
Neutron resonance in Co-Ba122

$T_c=25K$

**Spin excitation spectrum in SC state**

- collective spin excitation below $2\Delta$ at $Q_{AF}$
- fingerprint of a sign changing gap and residual AF fluctuations
- observed in various families (11, 122, 1111...) and other SC: cuprates; heavy fermions...
- no truly conclusive phase sensitive test up to now (phase shift in Josephson loops, qp interferences...)

*Isonov et al. Nature Phys. 6, 178 (2010)*
Gap anisotropy in Co-Ba122

ARPES sees isotropic and large gaps

• Surface vs bulk issue?
• ARPES resolution?

Thermal conductivity: anisotropic gap or very small gap (but no nodes)
Gap anisotropy in Co-Ba122

- Field dependence of the low temperature residual term of electronic specific heat: anisotropic gap but doping dependent!
- Optimal doping: full gaps
- Under and overdoped: significant anisotropy
Gap anisotropy in Co-Ba122


- significant anisotropy around electron pocket: $\Delta_{\text{max}} = 6-7 \Delta_{\text{min}}$
- in-plane or out of plane anisotropy
2D vs 3D Fermi surfaces

$k_z$ is tuned via incident photon energy

Note: 11 and 1111 families are more 2D

Brouet et al. PRB 80, 165115 (2009)
Directionnal thermal conductivity in Co-Ba122

- nodes on FS part with high $v_F$ along c-axis
- penetration depth shows similar behavior
- strong doping dependence
$k_z$ dependence of the gap via ARPES

$$\Delta_{sc} = \Delta_{2D} (1 + \eta \cos k_z)$$

(BaK)Fe$_2$As$_2$ (hole doped)

- Hole FS strong $k_z$ dependence (3D): c axis $\kappa_{in}$
- Electron FS weak $k_z$ dependence (2D): Raman

$k_z$ is tuned via incident photon energy
Directionnal thermal conductivity in K-Ba122

the structure of the gap is strongly doping dependent
Substitution dependence of the gap anisotropy

\( \kappa_{th} \): isovalent versus hole doping

London penetration depth: isovalent vs hole doping

- \( \text{BaFe}_2(\text{As}_{1-x}\text{P}_x) \) shows clear indication of nodes
- gap structure is not universal

Gap structure in Ba122

Interband pair interaction \[\rightarrow\] Intra and interband pair interaction

- **plus** k-dependence of interaction (nesting) + orbital dependence
- doping dependent ! fine tuning

Maier et al. PRB 79, 224510 2010
Role of orbital content

Fermi surfaces

- orbital dependent FS leads to modulation of interband interaction matrix: intra-orbital scattering dominates

- $d_{yz}/d_{xz}$ scattering between electron and hole pocket lead to $s^+$ pairing

- $d_{xy}$ scattering between electron pocket frustrates $s^+$ pairing: anisotropy

- additional hole pocket stabilizes isotropic $s^+$

Strong sensitivity to FS topology (doping, As height...)

Kuroki et al. PRB 79, 224511 (2009)
Maier et al. PRB 79, 224510 (2010)
Doping dependant gap and interband spin fluctuations

Figure 20. Schematic phase diagram of Fe-based superconductors vs. doping, with order parameter expected from 2D spin fluctuation theory plotted in one quadrant of Brillouin zone as false color on Fermi surface \[\text{[red=}+, \text{blue=}\].

\[\text{gap nodal structures to power laws in temperature } \Delta \lambda \sim T^n\] was pointed out by Gross et al. In a fully gapped system at low temperatures relative to the smallest full gap in the system an exponentially activated behavior is expected; if this gap is very small however, the penetration depth can typically be fit to a power law in \(T\) over some intermediate temperature range. Another factor complicating the interpretation is disorder; at the lowest temperatures, impurity scattering can lead to a \(T^2\) dependence. If residual densities of states at the Fermi level induce these, see Section to uio. Thus fits to low temperature power laws at low but not asymptotically low temperatures may not be completely straightforward to interpret, but do provide evidence for low-lying quasiparticle excitations. Only in the case that a true linear power law \(\Delta \lambda \sim T\) is observed may one make definitive statements about the existence of hlinei nodes.

In both the LaFePO system and in BaFe\(_2\)As\(_{1-x}\)P\(_x\) a linear \(T\) dependence of the low \(T\) penetration depth \(\Delta \lambda\) was reported. By contrast in BaFe\(_1-x\)Co\(_x\)\(_2\)As\(_2\) and BaFe\(_1-x\)Ni\(_x\)\(_2\)As\(_2\) \(\Delta \lambda\) was initially reported to vary close to \(T^2\) over most of the phase diagram; these power laws are in contrast to the activated temperature dependencies expected for an isotropic gap. While \(T^2\) is the power law one naively expects for a hdirtyi line nodal state, one may also show that in an isotropic h\(s^\pm\) upper conductor mi can create sub gaps under certain conditions depending on the ratio of intern to intraband impurity scattering. If these states are at the Fermi level, a fully gapped \(s^\pm\) state will also lead to \(\Delta \lambda \sim T^2\). Fits of the same or very similar data on these systems BaFe\(_1-x\)Co\(_x\)\(_2\)As\(_2\) and BaFe\(_1-x\)Ni\(_x\)\(_2\)As\(_2\) near optimal doping are also possible for an isotropic multigap model and at optimal doping the \(T^2\) fit is rather poor suggesting a small true gap. In this context, it is worth noting that a number of multigap fits—to penetration depth, specific heat, and other observables—in the literature violate BCS theory by taking arbitrary ratios of the gaps \(\Delta_i/T_c\) as fit parameters. Kogan et al. arXiv:1106.3712 (2011)

Phase diagram of the gap structure in Ba122 from spin fluctuation theory

Role of disorder: optical conductivity

- subgap absorption in Co-Ba122: anisotropy or pair-breaking?
- interband impurity scattering is pair-breaking for $s^+-$
- importance of interband versus intraband impurity scattering?
SDW + SC orders

- SDW+SC: atomic coexistence (NMR, muSr...) for Co-Ba122: situation less clear in other systems
- Fe conduction electrons are involved in both orders: competition
- $s^+$ gap and incommensurability favor coexistence

NMR spectra homogeneously broadened
All Fe involved in SDW order

Laplace et al. PRB 80, 140501 (2009)
Julien et al. EPL 87, 37001 (2009)

SDW vs SC: neutron diffraction

- reduction of Fe moment below $T_c$
- SC affects SDW
- interplay/competition around the FS
- re-entrance of the tetragonal phase!

before (green triangles) and after (brown circles) the Al coating on region, we have considered the case of

\[ \Delta = \frac{\pi}{\lambda_{ab}} \]

produced using parameters that agree with the phase diagram experimental values. This theory does not take into account 180 and 270 nm to account for the quite large dispersion of the higher side of the scatter that exists within the TDR

\[ \lambda_{ab} = \frac{1}{2 \pi} \int \frac{d\omega}{2\pi} \frac{g(\omega)}{m(\omega)} \]

where

\[ \frac{\Delta_{\text{AF}}}{\Delta} = \frac{\Delta_{\text{AF}}}{\Delta_0} \]

making the result in equation (2011) 124505 within the scatter. It may also be important to

\[ \Delta_{\text{AF}} = \Delta \left( 1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2} \right) \]

with our results within the scatter. It may also be important to

\[ \Delta_{\text{AF}} = \Delta \left( 1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2} \right) \]

The solid gray line is a fit to the TDR data only of the form

\[ \lambda_{ab} = \lambda_{ab}^0 \sqrt{1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2}} \]

In inset: zoomed-in low-temperature region, we have considered the case of

\[ \lambda_{ab} = \lambda_{ab}^0 \sqrt{1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2}} \]

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\[ \lambda_{ab} = \lambda_{ab}^0 \sqrt{1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2}} \]

Thus, to perform

\[ \Delta_{\text{AF}} = \Delta \left( 1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2} \right) \]

we can now analyze

\[ \Delta_{\text{AF}} = \Delta \left( 1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2} \right) \]

antiferromagnetic fluctuations

\[ \Delta_{\text{AF}} = \Delta \left( 1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2} \right) \]

while

\[ \Delta_{\text{AF}} = \Delta \left( 1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2} \right) \]

The solid gray line is a fit to the TDR data only of the form

\[ \lambda_{ab} = \lambda_{ab}^0 \sqrt{1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2}} \]


- drastic increase of penetration depth in the coexistence regime
- drop in the superfluid density
SDW vs SC: Raman


Coexistence SDW + SC

- The $2\Delta_{\text{max}}$ component is suppressed
- At $x=0.055$ only a low energy component remains

Superconductivity is confined in k-space in both systems close to competing order
Summary

- key role of magnetic fluctuations
- interband Coulomb interaction drive both SC and SDW
- gap structure is not universal (but gap symmetry is s-wave)
- maximum $T_c$: optimum nesting without magnetism

- need to confirm s+- gap!
- is there a role for structural degrees of freedom?
The case of $\text{A}_2\text{Fe}_4\text{Se}_5$

$\text{Fe}$ vacancy peaks ($\text{A}_2\text{Fe}_4\text{Se}_5$)

absence of electron-hole nesting

$T_N=560K$ (Fe ordered vacancies)

local magnetism?

coexistence or phase separation?

$\text{J. Guo et al., Phys. Rev. B 82, 180520(R) (2010)}$


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