Iron pnictides superconductors (discovered in March 08)

View of the electronic structure with photoemission (ARPES)

Véronique Brouet
Laboratoire de Physique des Solides d’Orsay
Outline

- Why study these systems?
  => High temperature superconductivity (up to 56K)
  => Exotic superconducting pairing, possibly involving magnetic fluctuations.

- A complicated electronic structure, unusual in the context of correlated systems
  => 5 Fe bands near the Fermi level, giving rise to small hole and electron pockets
  => Angle-resolved photoemission allows to map the dispersion of the different bands

- ARPES study of superconducting and magnetic properties
  => Different superconducting gaps for the different bands
  => Reconstruction of the Fermi Surface in the magnetic state, compared with nesting properties of the Fermi Surface.
The discovery of iron pnictides superconductors

LaO$_{1-x}$F$_x$FeAs

BaFe$_2$As$_2$

Doping
K instead of Ba => hole doping
Co instead of Fe => electron doping

Tc up to 56K (march 2008)

=> Origin of superconductivity ? Relationship with magnetism ?
=> Relationship with other high temperature superconductors, like cuprates ?
Origin of the superconducting pairing?

• Electron-phonon coupling seems to be too weak ($\lambda=0.2$) to induce superconductivity at such high temperatures.

• Could superconductivity be mediated by spin fluctuations?

Proposal:
Unconventional superconductivity mediated by spin fluctuations.
=> extended s-wave pairing with a sign reversal between hole and electrons sheets.

The undoped compound is a compensated semi-metal with small hole and electron FS pockets

The main orbitals at the Fermi level: Fe d_{XZ} and d_{YZ}

5 Fe 3d orbitals filled by 6 electrons

The undoped compound is a compensated semi-metal with small hole and electron FS pockets.

The main orbitals at the Fermi level: Fe $d_{xz}$ and $d_{yz}$.

The undoped compound is a compensated semi-metal with small hole and electron FS pockets.

The main orbitals at the Fermi level: Fe $d_{xz}$ and $d_{yz}$.


=> Good nesting between hole and electron pockets

Band structure along diagonal

```
<table>
<thead>
<tr>
<th>Energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.1</td>
</tr>
<tr>
<td>-0.1</td>
</tr>
<tr>
<td>0.0</td>
</tr>
<tr>
<td>0.0</td>
</tr>
<tr>
<td>0.1</td>
</tr>
<tr>
<td>0.1</td>
</tr>
</tbody>
</table>

« holes »

« electrons »

Fermi Surface (undoped)
Origin of the superconducting pairing?

- Electron-phonon coupling seems to be too weak ($\lambda=0.2$) to induce superconductivity at such high temperatures.

- Could superconductivity be mediated by spin fluctuations?

Proposal:
Unconventional superconductivity mediated by spin fluctuations.

=> extended s-wave pairing with a sign reversal between hole and electrons sheets.

The magnetic phase is metallic with rather small magnetic moments (0.3 - 1 \( \mu_B \)) => this suggests a Spin Density Wave picture

Rotter et al., PRL 2008

De la Cruz et al., Nature 2008

The magnetic phase is metallic with rather small magnetic moments (0.3 - 1 \( \mu_B \)) => this suggests a Spin Density Wave picture
Magnetism: localized or itinerant?

Magnetic structure usually observed in iron pnictides
Consistent with nesting vector OR superexchange interactions (2nd neighbors)

Magnetic structure observed in FeSe family
NOT consistent with Fermi Surface nesting

Problems with itinerant approaches
• Systematic overestimation of the magnetic moment by ab initio calculations
• Also wrong estimation of the As position

Could the moments be much larger in fluctuating domains?

cf Mazin and Johannes, Nature Physics 2009
The superconducting temperature seems to scale with the As height!

Mizuguchi et al., cond-mat 2010
View of the electronic structure with ARPES

- How many hole and electron pockets?
- Are they well nested?

- What is the strength of electronic correlations?
- Are there analogies with cuprates?
Angle-resolved photoemission

Crystal

Electron analyser

\[ E_{\text{kin}} = h \nu - W - |E_B| \]

\[ \hbar k_\parallel = \sqrt{2mE_{\text{kin}}} \sin \theta \]

Hole pockets in Ba(Fe_{0.92}Co_{0.08})As_2
Angle-resolved photoemission

\[ E_{\text{kin}} = h\nu - W - |E_B| \]

\[ \hbar k || = \sqrt{2mE_{\text{kin}}} \sin \theta \]

CASSIOPEE beamline, SOLEIL synchrotron

Photons from:
- Synchrotrons: 10-100\,\text{eV}
- He lamp: 21\,\text{eV}
- Laser: 6-7\,\text{eV}
Angle-resolved photoemission

$E_{kin} = h\nu - W - |E_B|$

$\hbar k_\parallel = \sqrt{2mE_{kin}} \sin \theta$

Hole pockets in Ba(Fe$_{0.92}$Co$_{0.08}$)As$_2$
Some aspects of the photoemission theory

Surface:
Work function $W$, information on $k_\perp$ lost

\[ I(k, \omega) = \sum_{i,f} \frac{2\pi}{\hbar} \left| \left\langle \psi_f^N \left| \frac{e}{mc} \vec{A}.\vec{p} \right| \psi_i^N \right\rangle \right|^2 \delta(E_f^N - E_i^N - \hbar \nu) \]

Sudden approximation:
\[ \psi_f^N = \varphi_f^k \psi_f^{N-1} \]

Matrix element describing the photoemission process. May depend on $A$ and $\hbar \nu$.

Spectral function $A(k,\omega)$
Interaction effects
Measuring interaction effects

\[ I(k, \omega) = \sum_{i,f} |M_{i,f}^{k}|^2 f(\omega) A(k, \omega) \]

with \[ A(k, \omega) = -\frac{1}{\pi} \frac{\Sigma''(k, \omega)}{[\omega - E_k - \Sigma'(k, \omega)]^2 + \Sigma''(k, \omega)^2} \]

Without interactions

With interactions

=> Renormalization of the dispersion (« higher effective mass »)
=> Finite linewidth (measurable for a 2D system)
=> Reduced quasiparticle weight \( Z \), transfer of spectral weight to incoherent structures

A. Damascelli, Rev. Modern Physics 2003
Estimating the strength of electronic correlations

ARPES in Ba(Fe,Co)$_2$As$_2$ around $\Gamma$

LDA calculation for BaFe$_2$As$_2$ (M. Aichhorn et al.)
Estimating the strength of electronic correlations


=> Band structure renormalized by factor 2
This renormalization agrees well with calculations including correlation effects.

LaFeOAs - M. Aichhorn et al., PRB 2009

- The degree of correlations may change significantly between different families => $m^*/m = 2$ to $4$
- Different behaviors for bands with different orbital symmetries
Probing the symmetry of orbitals with ARPES

Fe 3d orbitals

Horizontal polarization => even orbitals
Vertical polarization => odd orbitals

A. Damascelli et al.,
Rev. Mod. Physics 2003
The inner pocket is doubly degenerated, with odd and even symmetries (probably $d_{xz}$ and $d_{yz}$).

The outer pocket is mainly even: could have strong $d_{z^2}$ character.

Zhang, Feng et al.
cond-mat 2009

S. Thirupathaia et al., B. Mansart et al.
Correlations may enhance the contribution of the $d_{z^2}$ band

Gutzwiller density functional calculations ($\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$)

Wang et al., cond-mat/0903.1385

$\Rightarrow$ Consequences for the electronic properties?
Probing 3D effects in ARPES

\[ k_\perp = \frac{\sqrt{2m}}{\hbar} \sqrt{h \nu - W + V_0} \]

Final state (free electron parabola)

Initial states

P. Hofmann
3D effects on the hole pockets

There are strong variations of the hole pockets with photon energy

Oscillations with $k_z$ periodicity

=> Significant 3D effects in this family (unlike for example in cuprates)
Evolution with electron doping: $\text{Ba(Fe}_{1-x}\text{Co}_{x})_2\text{As}_2$

**Graph:**
- X-axis: Co percentage
- Y-axis: Temperature (K)
- Co percentages: 0%, 4%, 7%, 15%, 30%
- Graphs showing evolution of holes and electrons with Co doping.

**Diagrams:**
- Co 0%
- Co 4%
- Co 7%
- Co 15%
- Co 30%

**Key Observations:**
- SDW and SC regions indicated.
- Energy (eV) vs. Co percentage for holes and electrons.
Evolution with electron doping: $\text{Ba(Fe}_{1-x}\text{Co}_x\text{)}_2\text{As}_2$

=> A rigid band filling can be applied
=> « Best » nesting between the electron and outer hole band at $k_z = 1$

V. Brouet et al., PRB 2009
Exploring the magnetic and superconducting properties with ARPES

=> Value and symmetry of the superconducting gap on the different bands?
=> Role of nesting in the formation of the magnetic state?
First determination of superconducting gaps in Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$


=> Nearly isotropic gaps
=> Same values on the hole and electron bands exhibiting the best nestings, smaller value on the other hole band
Is «nesting» important for superconductivity?

Asymmetry between hole and electron sides, as well as the disappearance of superconductivity when the hole band is filled support the importance of interband transitions.

However, in LiFeAs, nesting is completely lost, which does not weaken much superconductivity ($T_c=18K$).

Borisenko, cond-mat 2010
Is «nesting» important for magnetism?

BaFe$_2$As$_2$

Fermi Surface above $T_N$ (150K)

Fermi Surface below $T_N$ (150K)

Only small parts of the FS are remaining: «droplets» FS

M.F. Jensen, in preparation
Is «nesting» important for magnetism?

BaFe$_2$As$_2$

Fermi Surface above $T_N$ (150K)

Fermi Surface below $T_N$ (150K)

Only small parts of the FS are remaining: «droplets» FS

M.F. Jensen, in preparation
More than a simple folding

Reconstruction of the electron pockets (splitting)

150 K

20 K

Splitting due to:
- local moments?
- inequivalency between X and Y (orthorhombicity)?
Conclusions

- Renormalization of the LDA band structure by a factor 2-3
  => *moderately correlated systems*

- Three hole bands and two electron pockets
  => *one hole band probably with d_\(z^2\) character*

- Significant 3D dispersion

- Rigid-band evolution with doping - *unlike in other families of superconductors like Ba(Fe,Ru)\(_2\)As\(_2\)*

- Different superconducting gaps for the different bands

- Significant reconstruction of the electronic structure in the magnetic state.
Collaborators

Maria Fuglsang Jensen, Marino Marsi, Barbara Mansart
*LPS Orsay*

Amina Taleb-Ibrahimi, Patrick Lefèvre, François Bertran, Alessandro Nicolaou
*CASSIOPEE beamline, SOLEIL*

Dorothée Colson, Anne Forget, Florence Rullier-Albenque
*SPEC, CEA-Saclay*