Back to the Iron age – the physics of Fe-pnictides

Andrey Chubukov

University of Wisconsin

Texas A & M, Dec. 4, 2009
The new iron age

IRON AGE (1200 - 550 B.C.E.)

Fe-Pnictides:

Binary compounds of pnictogens
A pnictogen – an element from the nitrogen group: N, P, As, Sb, Bi

RFeAsO (1111)
R = La, Nd, Sm, Pr, Gd

AFe$_2$As$_2$ (122)
A = Ba, Sr, Ca

LaOFeP
FeTe
### Fe-Superconductors, \( T_c \)

<table>
<thead>
<tr>
<th>Compound (powder &amp; single crystals)</th>
<th>( T_c )</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>LaNiOP</td>
<td>( \sim 3 ) K</td>
<td>T. Watanabe et al., Inorg. Chem. 46, 7719 (2007)</td>
</tr>
<tr>
<td>La([O_{1-x}F_x]FeAs)</td>
<td>26 K (x=0.05-0.12) 0 K</td>
<td>Y. Kamihara et al., J. Am. Chem. Soc. 130, 3296 (2008)</td>
</tr>
<tr>
<td>La([O_{1-x}Ca^{x}_{2+}]FeAs)</td>
<td>26 K (x=0.05-0.12) 0 K</td>
<td>Y. Kamihara et al., J. Am. Chem. Soc. 130, 3296 (2008)</td>
</tr>
<tr>
<td>La([O_{1-x}F_x]NiAs)</td>
<td>3.8 K (x=0.1) 2.75 K (x=0)</td>
<td>Z. Li et al., arXiv:0803.2572</td>
</tr>
<tr>
<td>(La(_{1-x}Sr_x))ONiAs</td>
<td>3.7 K (x=0.1-0.2) 2.75 K (x=0)</td>
<td>L. Fang et al., arXiv:0803.3978</td>
</tr>
<tr>
<td>(La(_{1-x}Sr_x))OFeAs</td>
<td>25 K (x=0.13)</td>
<td>H.-H. Wen et al., EPL 82, 17009 (2008)</td>
</tr>
<tr>
<td>Ce([O_{1-x}F_x]FeAs)</td>
<td>41 K (x=0.2)</td>
<td>G.F. Chen et al., PRL 100, 247002 (2008)</td>
</tr>
<tr>
<td>Pr([O_{1-x}F_x]FeAs)</td>
<td>52 K (x=0.11)</td>
<td>Z.-A. Ren et al., arXiv:0803.4283; Z.-A. Ren et al., EPL, 82 (2008)</td>
</tr>
<tr>
<td>Nd([O_{1-x}F_x]FeAs)</td>
<td>36 K (x=0.17)</td>
<td>P. Cheng et al., Science China 51(6), (2008).</td>
</tr>
<tr>
<td>Gd([O_{1-x}F_x]FeAs)</td>
<td>55 K (x=0.1-0.2)</td>
<td>Z.-A. Ren et al., Chin. Phys. Lett. 25, (2008); R.H. Liu et al., arXiv:0804.2105</td>
</tr>
</tbody>
</table>
Crystal structure

2D Fe-As layers with As above and below a square lattice formed by Fe.
Are pnictides similar to cuprates?

Parent compounds are antiferromagnets

Superconductivity emerges upon doping
TUG-OF-WAR (the rope is borrowed from cuprates)

Similar

Abrahams, Bernevig, Haule, Kivelson, Kotliar, Phillips, Sachdev, Si, Sushkov, Xu ....

Different

Carbotte, Gorkov, Hirschfeld, D-H Lee, Mazin, Scalapino, Schmalian, Tesanovic, Vishwanath ....
Cuprate high Tc superconductors

\[
\begin{array}{c}
\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4 \\
\text{La}_{2-x}\text{Sr}_x\text{CuO}_4
\end{array}
\]

Temperature (K)

Dopant Concentration \(x\)

“Normal”
Metal

Pseudogap

Mott insulator
Heisenberg antiferromagnet

metal
Fe-Pnictides

![Graph showing phase transitions in LaO$_{1-x}$F$_x$FeAs]

- $T_S$, $T_N$, $T_C$ (K)
- Nominal F content x
- Orthorhombic
- Tetragonal
- SDW magnetic order
- Superconductivity

Metal

Metal
I. Metallic behavior in the magnetic phase

![Graph showing the relationship between resistivity ($\rho$) and temperature ($T$) for BaFe$_2$As$_2$. The graph indicates a sharp increase in resistivity at a temperature $T_N$. The formula BaFe$_2$As$_2$ is also shown.](p.png)
II. Band theory calculations agree with experiments
Lebegue, Mazin et al, Singh & Du, Cvetkovic & Tesanovic…

2 hole pockets around (0,0)
2 electron pockets around (\(\pi,\pi\)) (folded BZ), or (0,\(\pi\)) and (\(\pi,0\)) (unfolded BZ)
NdFeAs(O$_{1-x}$F$_x$) (x=0.1)  
A. Kaminski et al.

Hole pockets near (0,0)  

Electron pockets near (π,π)  

Ba$_{06}$K$_{04}$Fe$_2$As$_2$  
H. Ding et al.

D. Evtushinsky et al

LaFeOP  
A. Coldea et al,
Itinerant approach

Magnetism
The system remains a metal the magnetic phase
Magnetic order

$\pi, 0$ or $(0, \pi)$ in the unfolded BZ

$(\pi, \pi)$ in the folded BZ
Itinerant description: magnetism comes from nesting

Dong et al, Korshunov & Eremin, Raghu et al., K. Kuroki et al, ...
Nesting is a boost for an SDW antiferromagnetism

\[ \chi_0(Q) = \int \frac{d\omega d\varepsilon_k}{\omega^2 + \varepsilon_k^2} = \log \frac{E_F}{T} \]

\[ \chi(Q) = \frac{\chi_0(Q)}{1 - U \chi_0(Q)} \]

For a perfect nesting, AFM instability occurs already at small U

M. Rice (for Cr), V. Cvetkovic and Z. Tesanovic, …

(\pi,\pi) in the folded BZ
Questions

1. The actual order is 

$(\pi,\pi)$ folded BZ

$Q_1 = (\pi,0)$

$Q_2 = (0,\pi)$

$S = S_1 e^{iQ_1r} + S_2 e^{iQ_2r}$

2. Why the system remains a metal?
1. Selection of a magnetic order

Introduce two SDW order parameters $W_1$ with $Q_1 = (0, \pi)$, $W_2$ with $Q_2 = (\pi, 0)$.

Either $W_1 = 0$, (0,$\pi$) state

Or $W_2 = 0$, ($\pi$,0) state

$E_{gr} = F(W_1^2 + W_2^2)$

$E_{gr} = F(W_1^2 + W_2^2) + a V (W_1)^2 (W_2)^2$, $a > 0$

$O(6)$ symmetry
2. Metallicity

- Borisenko et al
- Zhou et al

Zhou et al

Bo

**Doubly degenerate**

```
E_k
```

```
E_F
```

```
(0,0)
```
Superconductivity

Itinerant approach
Electron-phonon interaction is too weak

$$\lambda = 0.21 \quad \lambda = 0.44 \text{ for Al}$$

Too small to account for $T_c = 50K$

$$\alpha^2 F(\omega) = \frac{1}{N(0)} \sum_{nmk} \delta(\epsilon_{nk}) \delta(\epsilon_{mk+q}) \times$$
$$\times \sum_{\nu q} |g_{\nu nk mq + q}|^2 \delta(\omega - \omega_{\nu q})$$

$$\lambda(\omega) = 2 \int_0^\omega d\Omega \alpha^2 F(\Omega)/\Omega$$
How about using the “analogy” with the cuprates and assume that the pairing is mediated by spin fluctuations peaked at \((\pi, \pi)\)

\[
\Delta (\theta) = \Delta_0 \left( \cos k_x - \cos k_y \right)
\]

Cuprates

\[
\Delta (\theta) = \Delta_0 \left( \cos k_x + \cos k_y \right)
\]

sign-changing extended s-wave gap

Mazin et al, Kuroki et al....
Experiments
Some experiments are consistent with no-nodal $s^{+-}$ gap
1. Photoemission in 1111 and 122 FeAs

NdFeAsO$_{1-x}$F$_x$

T. Kondo et al., arXiv:0807.0815

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

D. Evtushinsky et al

Almost angle-independent gap
2. Neutron scattering – resonance peak below 2D

\[ \text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2 \]

Theory: need \( \Delta_{k+\pi} = -\Delta_k \)

The “plus-minus” gap is the best candidate

- Eremin & Korshunov
- Scalapino & Maier
3. Penetration depth behavior in 1111 and 122 FeAs

SmOFeAs

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

$\Delta \lambda (\AA)$

$\Delta F (\text{Hz})$

Carrington et al

"Exponential" behavior at low T
(or, at least, a very flat behavior)

Y. Matsuda

$\text{Ba}_{0.46}\text{K}_{0.56}\text{Fe}_2\text{As}_2$
Other experiments, however, indicate that the gap may have nodes
1. NMR and Knight shift in 1111 FeAs

Knight shift

NMR relaxation rate

Matano et al

Non-exponential behavior!
2. The behavior of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$, $T_c = 30\text{K}$

Y. Matsuda et al
Back to simple reasoning

There is a problem: how to get rid of an intra-band Hubbard repulsion?

Cuprates

- Hubbard repulsion cancels out, only d-wave, $(\pi,\pi)$ interaction matters

Pnictides

- Intra-band repulsion does not cancel and has to be overtaken by a $(\pi,\pi)$ interaction
The two-band nested Fermi liquid with intra-band and inter-band interactions

\[ \epsilon_p^c = E_F - \frac{p^2}{2m}, \quad \epsilon_p^{f+Q} = \frac{(p + Q)^2}{2m} - E_F \]

\[
H = U_1^{(0)} \sum \left[ c_{p_3 \sigma}^\dagger f_{p_4 \sigma'}^\dagger f_{p_2 \sigma'} c_{p_1 \sigma} + U_2^{(0)} \sum f_{p_3 \sigma}^\dagger c_{p_4 \sigma'}^\dagger f_{p_2 \sigma'} c_{p_1 \sigma} \right] \\
+ \frac{U_3^{(0)}}{2} \sum \left[ f_{p_3 \sigma}^\dagger f_{p_4 \sigma'} c_{p_2 \sigma'} c_{p_1 \sigma} + h.c \right] \\
+ \frac{U_4^{(0)}}{2} \sum f_{p_3 \sigma}^\dagger f_{p_4 \sigma'} f_{p_2 \sigma'} f_{p_1 \sigma} \\
+ \frac{U_5^{(0)}}{2} \sum c_{p_3 \sigma}^\dagger c_{p_4 \sigma'} c_{p_2 \sigma'} c_{p_1 \sigma}
\]

\[ u_i^{(0)} = U_i^{(0)} N_0 \quad \quad N_0 = m/(2\pi) = \text{density of states in 2D} \]

Intra-band repulsion \( u_4 = u_5 \)

Pair hopping \((\pi,\pi)\) interaction

Inter-band forward and “back-scattering”
Let's see how pair hoping and intra-band repulsion compete

1. Spin density wave
   \[ \chi^{SDW} = \frac{(\chi^{SDW})_0}{1 - (\Gamma^{SDW})_0 \Pi_{sdw}} \]
   \[ \Pi_{sdw} \propto \log \frac{E_F}{T} \]
   \[ \Gamma^{SDW}_0 = u_3 + u_1 > 0, \]
   The system surely favors an SDW instability

2. S+ superconductivity
   \[ \chi^{SC}_{s+} = \frac{(\chi^{SC}_{s+})_0}{1 - (\Gamma^{SC}_{s+})_0 \Pi_{sc}} \]
   \[ \Pi_{sc} \propto \log \frac{E_F}{T} \]
   \[ (\Gamma^{SC}_{s+})_0 = u_3 - u_4, \]
   If intra-band repulsion \( (u_4) \) is stronger than the pair hopping \( (u_3) \), the pairing interaction is repulsive

Orbital model -> band model: \( u_4 > u_3 \)
SDW magnetism, but no superconductivity
Two ways to go beyond this level of consideration and obtain superconductivity

Maxim Vavilov
Anton Vorontsov
Ilya Eremin

Dmitry Efremov, Maxim Korshunov
I. Explore nesting AND the smallness of the pockets

The terms in the Hamiltonian are bare interactions, at energies comparable to a fermionic bandwidth

We, however, need interactions at energies smaller than the Fermi energy [we have $\log E_F/T$]

$E_F \sim 0.1 \text{ eV}$  $W \sim 2 \text{ eV}$

Couplings flow due to renormalizations by particle-particle and particle-hole bubbles
We know this story for conventional (phonon) superconductors

\[ \omega_D \quad \text{E}_F \sim W \]

Coulomb repulsion is renormalized down by the renormalization in the particle-particle channel (McMillan-Tolmachev renormalization)

If only Cooper channel is involved, this cannot change a repulsion into an attraction

\[ u_4 - u_3 = \frac{(u_4 - u_3)_0}{1 + (u_4 - u_3)_0 \log W/E} \]

In our case, there are renormalizations in both particle-particle AND particle hole channel. This implies that we need to construct parquet RG to analyze the system flow between W and \( E_F \)

(H. Shultz, Dzyaloshinskii & Yakovenko)
The pair hopping term is pushed up by the density-density interaction $u_1$ responsible for a SDW order.
One-loop parquet RG

\[ \dot{u}_1 = u_1^2 + u_3^2 \]
\[ \dot{u}_2 = 2u_2(u_1 - u_2) \]
\[ \dot{u}_3 = 2u_3(2u_1 - u_2 - u_4) \]
\[ \dot{u}_4 = -u_3^2 - u_4^2 \]

The fixed point: the pair hopping term \( u_3 \) is the largest

\[ u_1 = -u_4 = -u_5 = \frac{|u_3|}{\sqrt{5}}, \quad u_2 \propto |u_3|^{1/3} \]
In the process of RG flow, the interaction in the extended s-wave channel becomes attractive.

Perfect nesting – SDW wins

Non-perfect nesting – SDW vertex remains the strongest, but the SDW instability is cut, and a node-less s+ SC wins.
However,

Parquet RG stops at $E \sim E_F$

$$u_0L_{\text{max}} = u_0 \log \frac{W}{E_F}$$

A sign-changing, nodeless s+ gap does not emerge

No s+ pairing?

$$\Delta (\theta) = \Delta_0 (\cos k_x + \cos k_y)$$
II. Let’s include momentum-dependent part of the pair hopping

The idea: if the gap averages to zero along either hole or electron FSs, or both, the effect of intra-pocket repulsion will be eliminated, at least partly

\[ u_3(q - q')c_q^\dagger c_{-q}^\dagger f_{q'}f_{-q'} \]

\[ u_3(p) = u_3 + 2 \tilde{u}_3 \cos \frac{p_x}{2} \cos \frac{p_y}{2} + \tilde{u}_3 (\cos p_x + \cos p_y) + ... \]

The expansion in the size of a Femi pocket

\[ \Delta(q) = \Delta_0 (\cos q_x + \cos q_y) + \Delta_1 \cos \frac{q_x}{2} \cos \frac{q_y}{2} + \Delta_2 (\cos q_x - \cos q_y) + ... \]

a plus-minus gap
an s-wave gap with nodes on electron FSs
a d-wave gap with nodes on all FSs
\[ u_3(p) = u_3 + 2 \tilde{u}_3 \cos \frac{p_x}{2} \cos \frac{p_y}{2} \quad \Delta(q) = \Delta_0 (\cos q_x + \cos q_y) + \Delta_1 \cos \frac{q_x}{2} \cos \frac{q_y}{2} \]

\[ \Delta_h(q) = \Delta_h \quad \Delta_e(q) = \Delta_e + \sqrt{2} \tilde{\Delta}_e \cos 2\phi \]

Solve three coupled BCS equations for the gaps:

\[(1 + u_4 L)^2 - u_3^2 L^2 = \tilde{u}_3^2 (1 + u_4 L) L^2 \]

\[ L = \ln(2e^\gamma \Lambda / \pi T_c), \quad \Lambda \sim E_F \]

When \( \tilde{u}_3 \) is zero, the solution \( L > 0 \) exists only for \( u_3 > u_4 \)

When \( \tilde{u}_3 \) is non-zero, the solution exists for arbitrary \( u_3 / u_4 \)

and has nodes for \( u_3 > u_4 \)
s+ gap with the nodes on electron FS

\[ \Delta_e(q) = \Delta_e + \sqrt{2}\tilde{\Delta}_e \cos 2\phi \]

Gap symmetry does not change!

Less SDW fluctuations

Underdoped 1111, 122 FeAs

LaFeOP, BaFe$_2$(As$_{1-x}$P$_x$)$_2$

Overdoped 1111, 122 FeAs
Conclusions:

Fe-pnictides are itinerant systems, no evidence for Mott physics

Magnetism is of SDW type, the system remains a metal

Superconductivity is the result of the interplay between intra-pocket repulsion and the pair hopping.

If the tendency towards SDW is strong, pair hopping increases in the RG flow, and the system develops an $s^{+-}$ gap without nodes, once SDW order is eliminated by doping.

If the tendency towards SDW is weaker, intra-pocket repulsion remains the strongest. The system still becomes an $s^{+-}$ superconductor, but the gap has nodes along the two electron Fermi surfaces.
THANK YOU