Superconductivity from repulsion in LiFeAs: novel s-wave symmetry and time-reversal symmetry breaking

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[МГУ-Январь-2014]
Superconductivity reaches the iron age

first high-temperature superconductors since the cuprates!
Iron-based superconductors

- Layered materials: transition metal (Fe) plus pnictogen (nitrogen group, such as As)

![Diagram of BaFe₂As₂ with highlighted elements]

[МГУ-Январь-2014]
Iron-based superconductors

- Layered materials: transition metal (Fe) plus pnictogen (nitrogen group, such as As)

- Rotter et al. PRL (2008)
- Kamihara et al. JACS (2008)
- Hsu et al. PNAS 2008

\[ T_c = 28K \quad (55K \text{ for Sm}) \quad T_c = 38K \quad T_c = 18K \quad T_c = 8K \]

[МГУ-Январь-2014]
Iron-based superconductors: what are the common electronic features?
Electronic-structure calculations

**LaFePO** Lebegue 2007 ($T_c=6K$)  
**LaFeAsO** Singh & Du 2008 ($T_c=26K$)

Band structures for 2 materials nearly identical!  
Hole pocket near $\Gamma$, electron pocket near $M$

[МГУ-Январь-2014]
Electronic-structure: multiorbital structure

Fe\(^{2+} \rightarrow 3d^6\)

4 holes per site – multiband structure. Chemical potential lies in the gap

All 5 Fe d-orbitals are near the Fermi level

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Comparison with other materials

Hole pockets near (0,0)
Electron pockets near ($\pi, \pi$)

La-1111

Ba-122

FeTe
courtesy of I. Mazin

[МГУ-Январь-2014]
NdFeAs(O_{1-x}F_x) (x=0.1)
A. Kaminski et al.

Hole pockets near (0,0)
Electron pockets near (\pi,\pi)

Ba_06K_04Fe_2As_2
H. Ding et al.

LaFePO
A. Coldea et al.

LiFeAs
A. Kordyuk et al
Multiorbital structure

Multiorbital and multiband physics: several d-orbitals close to $E_F$

L. Boeri, O.V. Dolgov, and A.A. Golubov,
PRL 101, 026403 (2008)

[МГУ-Январь-2014]
Iron-Pnictides: typical phase diagram

**magnetic, structural, and superconducting order**

[МГУ-Январь-2014]
Iron pnictides: structural and magnetic transitions

I) Structural Transition

II) Magnetic Transition

122/1111/111

FeTe

DFT correctly reproduces (or even predicts) correct magnetic and structural ground states, but requires magnetism as a prior condition for distortion

Transitions are simultaneous for FeTe and almost for parent 122's, but structural transition is first in 1111's and doped 122's

[МГУ-Январь-2014]
Is the physics behind superconductivity universal or model dependent?
Universality due to electron-phonon interaction? NO

Electron-phonon interaction is probably too weak

L. Boeri, O.V. Dolgov, and A.A. Golubov,
PRL 101, 026403 (2008)

\[ \lambda = 0.21 \]

\[ \lambda \lesssim 0.35, \text{ still not enough including magnetism} \]

Too small to account for $T_c \sim 50K$

L. Boeri et al., PRB 82, 020506 (2010)

Is there any universality in these systems?

[МГУ-Январь-2014]
Universality due to proximity to antiferromagnetism?
Pairing due to spin fluctuations?

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

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

\[ \Delta(k) = -\sum_{k'} \frac{V_{\text{eff}}(k-k')}{2E(k')} \Delta(k') \]

Although in some materials this may give a reasonable explanation - this is not the true origin of universality.
Universality due to initial electronic structure $\Rightarrow$ impact on the interactions

2-body Hamiltonian with intrasite interactions only!

$$H_{\text{orb}}^{\text{int}} = U \sum_i \sum_{\nu} n_{i\nu \uparrow} n_{i\nu \downarrow} + V \sum_{\nu \neq \mu, \sigma, \sigma'} n_{i\nu \sigma \uparrow} n_{i\mu \sigma'}$$

$$-J \sum_{\nu \neq \mu} S_{i\nu} \cdot S_{i\mu} + J' \sum_{\nu \neq \mu} d_{i\nu \uparrow}^\dagger d_{i\nu \downarrow}^\dagger d_{i\mu \downarrow} d_{i\mu \uparrow}$$

L. Benfatto, P. Hirschfeld, S. Graser, A. Chubukov, K. Kuroki, H. Aoki, R. Thomale, C. Honerkamp, Ch. Platt, W. Hanke, ...
Intra-band repulsion $u_4$ and pair hopping $u_3$.

Pairing interactions:

- Intra-pair hopping $(\pi,\pi)$ interaction
- Intra-band repulsion $u_4$

Toy model: one hole and one electron FSs.

$s^{+-}$ superconductivity, BCS theory

$$(\Gamma_{SC}^{s^{+-}}) = u_3 - u_4,$$

need $(\Gamma_{SC}^{s^{+-}}) > 0$

If the intra-pocket repulsion ($u_4$) is stronger than the pair hopping ($u_3$), the pairing interaction is repulsive.

In general, intra-pocket interaction should be the largest ($u_4$ is Coulomb repulsion at a small momentum transfer).

Intra-orbital interactions are bigger than the interorbital ones.

fRG and/or one-loop RG is extremely important

\( u_{ee} \) and \( u_{he} \) are bare interactions at energies of a bandwidth

For SC we need interactions at energies smaller than the Fermi energy

\[ E_F \sim 0.1 \text{ eV} \quad \text{W }\sim 3-4 \text{ eV} \]

Couplings flow due to renormalizations in particle-particle and particle-hole channels
One-loop parquet RG

\[ u_1 = u_1^2 + u_3^2 \]
\[ u_2 = 2u_2(u_1 - u_2) \]
\[ u_3 = 2u_3(2u_1 - u_2 - u_4) \]
\[ u_4 = -u_3^2 - u_4^2 \]

Intra-band repulsion \( u_4 \)

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

Inter-band density-density and exchange interaction

(H. Shultz, Dzyaloshinskii & Yakovenko, Rice, Honerkamp...)

SDW

\[ u_3 \text{ is pushed up by } u_1, \text{ which gives rise to SDW} \]

If the tendency towards SDW is strong, \( u_3 \) becomes larger than \( u_4 \), leading to an attraction in \( s^+ \)-superconducting channel
Tests for pairing symmetry ($s^{+-}$)

\[ \Delta_h = -\Delta_e \]

[МГУ-Январь-2014]
ARPES: Symmetry of the superconducting gap

- nearly isotropic gap in ARPES

\[ \text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2 \]
H. Ding et al., EPL (2008)

\[ \text{NdFeAsO}_{1-x}\text{F}_x \]

[МГУ-Январь-2014]
Nodal gap: the behavior of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$, $T_c = 30K$

Y. Matsuda et al

Consistent with line nodes
Extension for the realistic model

- convert the model into band basis,

- fit the interactions by the lowest angular harmonics, and extracted parameters $u_{eh}, u_{ee}$, etc.

- solve and analyze the gap equations for moderate and large hole and electron dopings

- for a bare interaction and for interaction dressed by the higher order bubble and ladder diagrams (spin fluctuations)

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**Multiorbital physics is missing** ⇒ **Origin of the gap anisotropy**

1. importance of orbital character on Fermi sheets
2. scattering between $\beta_1$ and $\beta_2$ sheets
3. intraband Coulomb repulsion

See also: Chubukov et al 2009, Thomale et al 2009, 2011 (band picture), Kemper et al 2010, P. Hirschfeld et al. (orbital picture)
Pairing vertex in multiband (multiorbital) systems

S-wave pairing

\[ \Gamma(k, p) = \sum_{n,m} \Gamma_{n,m} \psi_n(k) \psi_m(p) \]

\[ \psi_{n,m}(\pm k_x, \pm k_y) = \psi_{n,m}(\pm k_y, \pm k_x) \]

Near \( k=0 \),

\[ \psi_n(k) = A_n + B_n \cos 4 \varphi + C_n \cos 8 \varphi + \ldots \]

\( \varphi \) along hole FS

Near \( p=(\pi,0) \),

\[ \psi_n(p) = (\tilde{A}_n + \tilde{B}_n \cos 4 \theta + \tilde{C}_n \cos 8 \theta + \ldots) \]

\[ \pm (D_n \cos 2 \theta + E_n \cos 6 \theta + \ldots) \]

\( \theta \) along electron FS

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Leading harmonics in the superconducting s-wave gap

\[ \psi_n^r (k) = A_n + B_n \cos 4\psi + C_n \cos 8\psi + \ldots \Rightarrow A_n \]

\[ \psi_n^p (p) = \tilde{A}_n + \tilde{B}_n \cos 4\theta + \tilde{C}_n \cos 8\theta + \ldots \]
\[ \pm (\tilde{D}_n \cos 2\theta + \tilde{E}_n \cos 6\theta + \ldots) \Rightarrow \tilde{A}_n \pm \tilde{D}_n \cos 2\theta \]

Near hole FSs
Near electron FSs

Effective interactions dependent on the angles along electron FSs

\[ \Gamma_{h,h} (k, p) = u_{h,h}, \quad \Gamma_{e,h} (k, p) = u_{e,h} \left( 1 \pm 2 \alpha \cos 2\theta \right), \]

\[ \Delta_h (q) = \Delta_h, \quad \Delta_{e,1,2} (q) = \Delta_e \pm \Delta \cos 2\theta \]

Depending on the ratio the gap is just anisotropic or nodal

[МГУ-Январь-2014]
Leading harmonics in the superconducting s-wave gap

combination of magnetic fluctuations and angle-dependence of the interaction between hole and electron pockets
⇒ attraction in s-wave channel for all electron and hole dopings.

S+- gap with or without nodes

interaction is necessary angle-dependent, the gaps on electron FSs have cos 2θ components and may have accidental nodes

[Diagram showing S+- gap with or without nodes]
Sensitivity to the relatively small changes
Nevertheless the physics is still universal

a) isotropic $s_{+/-}$

b) nodes

c) deep minima

$s_{+/-}$ solution exists for ANY $u^2_{\text{he}}/u_{\text{hh}}$ $u_{\text{ee}}$

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Another example:

LiFeAs

[МГУ-Январь-2014]
**LiFeAs: weak-characterized electronic structure**

### Near hole FSs

**Exp STM: Allan et al**

\[ \psi_n(k) = A_n + B_n \cos 4\psi + C_n \cos 8\psi + \ldots \Rightarrow A_n \]

**Putzke et al.**

**Borisenko et al.**

*Figure taken from Wang et al. 2013*
LiFeAs: low-q fluctuations competing with incommensurate AF fluctuations

Low-q fluctuations (almost FM): Brydon et al PRB 83 (2011)

How the superconducting instability arises in this case

Subset 1: two hole pockets mainly of xz and yz character

\[ \Delta_{h1}, \Delta_{h2} \]

Subset 2: large hole pocket and two electron pockets with strong admixture of xy orbital

\[ \Delta_{h3}, \Delta_{e1,e2} = \Delta_e \pm \bar{\Delta}_e \cos 2\theta \]

The coupling between two subsets is relatively weak without taking into account spin fluctuations
Possibility for the time-reversal symmetry breaking

\textbf{s+is}

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If only the $\gamma$ – pocket and two $\beta$ – pockets are present, the gap changes sign between them.

\[
\begin{pmatrix}
\Delta_h \\
\Delta_e
\end{pmatrix} = -L
\begin{pmatrix}
U_{hh} & 2U_{he} & 2U_{he}\alpha_{he} \\
U_{he} & 2U_{ee} & 2U_{ee}\alpha_{ee} \\
2U_{he}\alpha_{he} & 4U_{ee}\alpha_{ee} & 4U_{ee}\beta_{ee}
\end{pmatrix}
\begin{pmatrix}
\Delta_h \\
\Delta_e
\end{pmatrix}
\]
Weakly coupled subsets, degeneracy of various s-wave states

$s$-wave $A$ state:
If the coupling via $\alpha - \beta$ and $\alpha - \gamma$ interactions is small, both subset are effectively uncoupled and the pairing state is $s^{+-}$ in each subset.

$s$-wave $B$ state: (conventional $s^{+-}$ state)
If $\alpha - \beta$ and $\gamma - \beta$ interactions are enhanced, both subsets are coupled and the gap changes sign between electron and hole pockets.
Weakly coupled subsets, degeneracy of various s-wave states

\[\text{МГУ-Январь-2014}\]

**s-wave C state:**
If the coupling via \(\alpha - \gamma\) interaction is larger than by \(\alpha - \beta\) interaction, the gaps changes sign between \(\alpha\) and \(\gamma\) instead of \(\alpha\) and \(\beta\) pockets

**s-wave D state:**
If the the intra-subset \(\beta - \gamma\) interaction is small, the gap changes sign between both subset I and II
Weakly coupled subsets, degeneracy of various s-wave states
Weakly coupled subsets, degeneracy of various s-wave states

**Theory**

![Graphs showing gap functions for s-wave states A, B, C, and D]

**Experiment**

![Graphs showing experimental results for A, B, and C states]

A-state matches the experimental results

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Possible time-reversal symmetry breaking

The transition from one state to another might also occur discontinuously.

Possible scenario: at some \( T < T_c \), existence of an s+is state with relative phases \( \varphi_{1,2} \neq (\pi \text{ or } 0) \) (Figure on the right).

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Superconductivity in iron-based systems

- Inter-band interaction (enhanced by spin fluctuations) ⇒ glue for the pairing for all dopings, gap structure and symmetry may change

- If both h and e pockets are present ⇒ driving force is electron-hole interaction. [SC gap has $s^\pm$ form, $d$-wave is a competitor, $s$-wave gap with accidental nodes on electron FS]

LiFeAs ⇒ orbital character may change the character of the $s$-wave state

- Novel effects due to multiorbital structure

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