Physics of iron-based high-$T_c$ superconductors

Y. Matsuda

Department of Physics
Kyoto University, Kyoto, Japan
Physics of iron-based high-\(T_c\) superconductors

1) Why are Fe-based superconductors important?

2) Mechanism of superconductivity
   
   Similarities and differences between cuprates and Fe-pnictides

3) Quantum critical point and non-Fermi liquid properties

4) BCS-BEC crossover in FeSe
1) Why are Fe-based superconductors important?

2) Mechanism of superconductivity
   Similarities and differences between cuprates and Fe-pnictides

3) Quantum critical point and non-Fermi liquid properties

4) BCS-BEC crossover in FeSe
Hosono’s group was not looking for superconductor, but trying to create new kind of transparent semiconductors for flat-panel display.

LaFePO  \( T_c = 4 \text{ K} \)
LaFeP(O,F)  \( T_c = 7 \text{ K} \)
LaFeAs(O,F)  \( T_c = 26 \text{ K} \)
SmFeAs(O,F)  \( T_c = 56 \text{ K} \)
FeSe  \( T_c = 65 \text{ K} \) (110 K??)
Are iron-pnictides an Electron-Phonon Superconductor?

Attractive electron-phonon interactions

Cooper pair

Electron-phonon coupling

\[ T_c \sim \omega_D e^{-\frac{1}{\lambda}} \]

\( \omega_D \sim 200 \text{ K} \)

\( \lambda \sim 0.2 \)

Comparable to the conventional metals

Electron-phonon coupling is not sufficient to explain superconductivity in the whole family of Fe-As based superconductors
A new class of high temperature superconductors

They knocked the cuprates off their pedestal as a unique class of high temperature superconductors.
A new family of unconventional superconductors

**Iron pnictide (Fe)**

- Weakly localized $3d$-electrons

**Cuprate (Cu)**

- Strongly localized $3d$-electrons

**Heavy fermion compound (Ce, U)**

- Very strongly localized $4f, 5f$ electrons

**Weak correlation**

**Strong correlation**
Fe-based high-$T_c$ superconductors

42622 (32522)

Ca

Al

O

$(\text{A}_4\text{M}_2\text{O}_6)$ Fe$_2$As$_2$

$T_c(\text{max})=47\text{K}$

$(\text{A}_4\text{M}_2\text{O}_6)$ Fe$_2$As$_2$

$T_c(\text{max})=55\text{K}$

$\text{Ln FeAsO}$

$T_c(\text{max})=38\text{K}$

$\text{BaFe}_2\text{As}_2$

$T_c=18\text{ K}$

$\text{LiFeAs}$

$T_c=8\text{ K}$

$\text{FeSe}$

$\text{Zhu et al.}(2009)$

$\text{Y. Kamihara et al.}(2008)$

$\text{M. Rotter et al.}(2008)$

$\text{X.C.Wang et al.}(2008)$

$\text{F.C.Hsu et al.}(2008)$

Well separated electron and hole sheets

$T_c=110\text{ K}$
1) Why are Fe-based superconductors important?

2) Mechanism of superconductivity
   Similarities and differences between cuprates and Fe-pnictides

3) Quantum critical point and non-Fermi liquid properties

4) BCS-BEC crossover in FeSe
Comparison and contrast between cuprates and pnictides

Phase diagram

Cuprates

Fe-pnictides

In layered 2D metals, interactions decay more slowly and hence are stronger

P. Coleman, Science 327, 969 (2010)

Enhanced fluctuations \(\rightarrow\) suppression of magnetic order

Superconductivity in 2D planes

Similarities and differences between cuprates and pnictides
Similarities and differences between cuprates and pnictides

Superconductivity occurs in the vicinity of magnetic order.

In Fe-pnictides, structural ($T_s$) and AFM transition ($T_N$) lines follow closely each other.
Similarities and differences between cuprates and pnictides

**Cuprates**

- Parent compound
- Cu3d
- O2p
- Cu3d
- U : Coulomb $\sim 8\text{eV}$
- W : Band width $\sim 3\text{eV}$
- Strong electron-electron correlation
- Mott insulator

**Fe-pnictides**

- Parent compound
- Cu3d
- O2p
- Cu3d
- U : Coulomb $\sim 8\text{eV}$
- W : Band width $\sim 3\text{eV}$
- Intermediate correlation
- Spin density wave (SDW) metal

**Stripe SDW order**
Similarities and differences between cuprates and pnictides

Cuprates

One hole band
One orbital
\( x^2-y^2 \)

Well separated hole and electron bands
Mainly three orbitals
\( xz+yz \), \( xy \), \( 3z^2-r^2 \)

Fe-pnictides

\( \text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta} \)

\( \text{BaFe}_2\text{As}_2 \)

**d-wave superconductivity in cuprates**

**s-wave**

\[ k_x \]
\[ k_y \]

![s-wave diagram](image)

**d-wave**

\[ k_x \]
\[ k_y \]

![d-wave diagram](image)

**V(q): pairing interaction**

**V(q) is negative and constant**

( attractive )

**V(q) is positive and peaks at** \( q = Q \)

\[ V_{kp} \approx \frac{3}{2} U^2 \chi (k - p) \]

\[ \chi (q) \sim \delta (q - Q) \]

Coulomb Magnetic fluctuation

Exchange of boson (spin fluctuations) between two fermions (electrons)

AF Brillouin zone

**V(q): pairing interaction**

**V(q) is negative and constant**

( attractive )

**V(q) is positive and peaks at** \( q = Q \)

\[ V_{kp} \approx \frac{3}{2} U^2 \chi (k - p) \]

\[ \chi (q) \sim \delta (q - Q) \]

Coulomb Magnetic fluctuation

Exchange of boson (spin fluctuations) between two fermions (electrons)

AF Brillouin zone
\[ \Delta(k) = -\sum_p V_{kp} \frac{\tanh(\varepsilon_p/2T)}{2\varepsilon_p} \Delta(p) \]

\[ \varepsilon_p = \sqrt{\Delta_p^2 + \xi_p^2} \]

**Gap equation**

\[ \Delta(k) = \Delta \]

\[ \Delta = -\sum_p V_{kp} \frac{\tanh(\varepsilon_p/2T)}{\varepsilon_p} \Delta > 0 \]

\[ V_{kp} = V < 0 \]

\[ V(r) \sim -\delta(r) \]

**Coulomb Magnetic fluctuation**

\[ V_{kp} \approx \frac{3}{2} U^2 \chi(k - p) \chi(q) \sim \delta(q - Q) \]

\[ Q = (\pi, \pi) \]

\[ \Delta(k) \sim -\sum U^2 \delta(k - p + Q) \frac{\tanh(\varepsilon_p/2T)}{2\varepsilon_p} \Delta(p) \]

\[ = -U^2 \frac{p \tanh(\varepsilon_p+Q/2T)}{2\varepsilon_p+Q} \Delta(k + Q) \]

\[ \Delta(k+Q)\Delta(k) < 0 \quad \text{sign change} \]

\[ V(x, y) \sim \cos \pi(x + y) + \cos \pi(x - y) \]
$d$-wave superconductivity in cuprates

$s$-wave

\[ k_x \]
\[ k_y \]

$d$-wave

\[ k_x \]
\[ k_y \]

\[ Q = (\pi, \pi) \]

Node

AF Brillouin zone

\[ \Delta(k + Q)\Delta(k) < 0 \quad \text{sign change} \]

\[ V(r) \sim -\delta(r) \]

\[ V(x, y) \sim \cos \pi(x + y) + \cos \pi(x - y) \]

Real space

repulsive

attractive

\[ y \]

\[ x \]
Iron pnictides: candidate for the SC state

- Pairing due to purely repulsive electronic interaction (enhanced by spin fluctuations)

\[ V > 0 \]

Spin fluctuations between the same orbitals

cf. \textit{d}-wave cuprate

A. V. Chubkov et al., PRB 80, 140515(R) (2009).
S. Graser et al., NJP 11, 025016 (2009).
H. Ikeda, PRB 81, 054502 (2010).
F. Wang et al., PRL 102, 047005 (2009).
Iron pnictides: candidate for the SC state

- Pairing due to attractive interaction caused by charge/orbital fluctuations.

\[ V < 0 \]

Orbital fluctuations (Quadrupole fluctuation)

Charge fluctuations between different orbitals

charge up
charge down

Occupation number of each orbit at each Fe site fluctuates

F. Kruger et al., PRB 79, 054504 (2009).
Y. Yanagi et al., PRB 81, 054518 (2010).
Iron pnictides: candidate for the SC state

AF and AFM transition (T_N) lines follow closely each other

Ferro-orbital ordering

Iron pnictides: candidate for the SC state

Spin fluctuation or orbital fluctuation?

Chicken or the egg?
S-- or S++?

1. Phase sensitive test
2. NMR
3. Neutron scattering
4. Quasi-particle interference
5. Impurity effect

No conclusive experimental evidence so far
1) Why are Fe-based superconductors important?

2) Mechanism of superconductivity
   Similarities and differences between cuprates and Fe-pnictides

3) Quantum critical point and non-Fermi liquid properties

4) BCS-BEC crossover in FeSe
Quantum Critical Point (QCP)

\[ \xi \propto |g - g_c|^\nu \]

Quantum time scale

\[ \xi_T \propto \xi^z \]

Thermal time scale

\[ \xi_T < L_T \]

QP excitations are well defined

\[ \xi_T > L_T \]

Physical properties are seriously influenced by QCP at \( g = g_c \).

Control parameter \( g \)

(Quantum critical point)

\( g \): pressure, chemical substitution, magnetic field

S. Sachdev, Quantum Phase Transitions

Ordinary phase transition – driven by thermal fluctuations

Quantum phase transition – driven by zero temperature quantum fluctuations associated with Heisenberg’s Uncertainty Principle
Quantum Critical Point (QCP)

Control parameter $g$ (Quantum critical point)

$g$: pressure, chemical substitution, magnetic field

S. Sachdev, Quantum Phase Transitions

Does the QCP lie beneath the SC dome?

1. Mechanism of superconductivity
2. non-Fermi liquid properties
Superconductivity in BaFe$_2$As$_2$ systems

**Parent compound**
BaFe$_2$As$_2$
(AF Metal)

- **Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2**
  - $T_c^{\text{opt}} \approx 24$ K
  - electron-doping

- **K$_x$Fe$_{2-y}$Se$_2**
  - $T_c^{\text{opt}} \approx 31$ K
  - hole-doping

- **(Ba$_{1-x}$K$_x$)Fe$_2$As$_2**
  - $T_c^{\text{opt}} \approx 38$ K
  - hole-doping
Superconductivity in BaFe$_2$As$_2$ systems

**Parent compound**
BaFe$_2$As$_2$ (AF Metal)

$K_x$Fe$_{2-y}$Se$_2$ ($T_c^{opt} \sim 31$ K)

$Ba(Fe_{1-x}Co_x)_2$As$_2$ ($T_c^{opt} \sim 38$ K)

$(Ba_{1-x}K_x)Fe_2$As$_2$

$BaFe_2(As_{1-x}P_x)_2$

isovalent ($T_c^{opt} \sim 30$ K)

hole-doping

electron-doping

Ground state can be tuned without doping carriers
Doping evolution of the transport property

\[ \rho_{xx}(T) \propto T^\alpha \]

\( \alpha \) 1.0 1.2 1.4 1.6 1.8 2.0

\( T \) 0 50 100 150

\( x \) 0.2 0.4 0.6

SDW \( \rightarrow \) SC

Quantum critical region??

Non-FL

FL

S. Kasahara et al., PRB 81, 184519 (10)

T-linear resistivity at \( x=0.33 \) just beyond SDW end point (\( x_c=0.3 \))

Hallmark of non-Fermi liquid

See also

S. Sachdev and B. Keimer, Physics Today (11)

\( T^2 \)-dependence at \( x=0.71 \)

Fermi-liquid behavior

BaFe\(_2\)(As\(_{1-x}\)P\(_x\))\(_2\)
**Effective mass** $m^\ast$ is strongly enhanced at $x=0.3$

Doping evolution of the superfluid density in BaFe$_2$(As$_{1-x}$P$_x$)$_2$

\[ \lambda_L^{-2}(0) = \frac{\mu_0 n_s e^2}{m^*} \]

Striking enhancement of $\lambda_L^{-2}(0)$ on approaching $x=0.3$ from either side. The data represents the behavior at the zero temperature limit.

QCP at $x=0.3$

Magnetic force microscopy
Y. Kamhot et al.

K. Hashimoto, Y.M. et al. Science ('12)

Al coating
Nodal slope
Microwave cavity
1. The QCP is the origin of the non-Fermi liquid behavior above $T_c$.
2. Microscopic coexistence of superconductivity and SDW.
3. The quantum critical fluctuations help to enhance the high-$T_c$ superconductivity.

1) Why are Fe-based superconductors important?

2) Mechanism of superconductivity
   Similarities and differences between cuprates and Fe-pnictides

3) Quantum critical point and non-Fermi liquid properties

4) BCS-BEC crossover in FeSe
If you ask a student

What do
Neutron star
metals
nuclei
atoms
have in common?

“When fermions become bosons: Pairing in ultracold gases”
Carlos Sa de Melo, Physics Today (2008)

Undergraduates

They are made of fermions, i.e. neutrons, protons, quarks and electrons.

Graduates

These fermions may exhibit a collective and macroscopic properties called superfluidity, in which a large number of particles can flow coherently without any friction or dissipation of heat.
Critical Temperature

Type of Matter

- Neutron stars
- Nuclear matter
- Superconductors
- Helium-3
- Cold atoms

Color superconductivity (neutron star)

Superconductivity (Metal)

BEC (Ultracold atom)
BCS-BEC crossover

- **BCS**
  - cooperative Cooper pairing
  - strongly interacting pairs
  - pair size \( \sim k_F^{-1} \)

- **BEC**
  - tightly bound molecules
  - pair size \( \ll k_F^{-1} \)

Conventional superconductors
\[
\frac{\Delta}{\epsilon_F} \sim 10^{-3} - 10^{-4}
\]
High-\(T_c\) cuprates
\[
\frac{\Delta}{\epsilon_F} \sim 10^{-2} - 10^{-3}
\]
Large magnetoresistance, $S_{dH} (0) \sim 80$ mW cm$^{-1}$ ($300K$), $\Delta r (0) \sim 5-6$ A.

D. Böhm et al., PRB (2013).

Dr/\rho(0) \approx (w_{ch} \theta_{ch})(w_{ce} \theta_{ce}) \sim 0.5-2$ mW cm$^{-1}$ ($300K$), $\Delta r(0) \sim 200-800$.

An ideal platform for the research of Fe-based superconductors.


SK. et al., JPS fall meeting (2013).

F.-C. Hsu et al., PNAS 105, 14262 (2008).

$T_c = 9$ K (30 K under pressure)
FeSe: High temperature superconductor

- Only electron pockets

ARPES

S. Tan et al., Nature Mater. (13).

Meissner effect

\[ T_c \text{ up to } 65 \text{ K} \]

Z. Zhang et al., Science Bulletin (15)

Resistivity

\[ T_c > 100 \text{ K} \]

J-F. Ge et al.
Nature Mat. (14)

- High-\( T_c \) superconductivity in monolayer FeSe

Small residual resistivity, large $RRR$, huge MR effect

Extremely small level of impurities and defects (1/2000 sites)
Fermi surface of bulk FeSe

Quantum oscillations

Terashima, Y.M. et al., PRB (2014)


1 hole + 1 electron
(+ 1 very small electron, \( \alpha \)-branch)

<table>
<thead>
<tr>
<th>Branch</th>
<th>( F ) (kT)</th>
<th>( m^*/m_e )</th>
<th>( A ) (%BZ)</th>
<th>( k_F ) (Å(^{-1}))</th>
<th>( E_F ) (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha )</td>
<td>0.06</td>
<td>1.9(2)</td>
<td>0.20</td>
<td>0.043</td>
<td>3.5</td>
</tr>
<tr>
<td>( \beta )</td>
<td>0.20</td>
<td>4.5(5)</td>
<td>0.69</td>
<td>0.078</td>
<td>5.1</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>0.57</td>
<td>7.0(7)</td>
<td>2.0</td>
<td>0.13</td>
<td>9.4</td>
</tr>
<tr>
<td>( \delta )</td>
<td>0.67</td>
<td>4.8(5)</td>
<td>2.3</td>
<td>0.14</td>
<td>16</td>
</tr>
</tbody>
</table>


\( \checkmark \) Extremely small Fermi surface & Fermi energy
Fermi energy comparable to the SC gap

**Electron-like**

- $E_{\text{electron}}$

**Hole-like**

- $E_{\text{ホール}}$

$B = 12$ T

Extremely small Fermi energy

A possible BCS-BEC crossover regime $\varepsilon_F \sim \Delta$

Never realized in any other superconductors!

cf.) Cold atoms
Extremely small Fermi energy

**Quasi-particle interference (STM)**

FeSe  \( \Delta \sim 3 \text{ meV} \)

Electron-pocket: \( \varepsilon_F \sim 2-3 \text{ meV} \)

\( \Delta/\varepsilon_F \sim 1 \)

Hole-pocket: \( \varepsilon_F \sim 10 \text{ meV} \)

\( \Delta/\varepsilon_F \sim 0.3 \)

Conventional superconductors

\( \Delta/\varepsilon_F \sim 10^{-3} - 10^{-5} \)

High-\( T_c \) cuprates

\( \Delta/\varepsilon_F \sim 10^{-2} - 10^{-3} \)

A possible BCS-BEC crossover regime \( \varepsilon_F \sim \Delta \)

Never realized in any other superconductors!

cf.) Cold atoms

Extremely small Fermi energy

Spatially-modulated SC gap

$T \sim 1.5$ K

Gap $(2\Delta)$ map

Topograph

$100 \text{ nm} \times 100 \text{ nm}, +20 \text{ mV}/100 \text{ pA}$

SC gap is modulated at $q \sim 2k_F$. ‘Friedel oscillations’

Observable only in the system with very small $k_F$

T. Hanaguri et al, in preparation
Extremely small Fermi energy

Vortex lattices in FeSe

\[ \frac{dI}{dV}(E_F) \]

\( T \sim 1.5 \text{ K} \)

500 nm \( \times \) 500 nm, +10 mV/0.1 nA

0.1 T

0.25 T

0.5 T

1 T

Extremely small Fermi energy

Vortex-core spectroscopy

\[ \frac{\Delta^2}{\varepsilon_F} \]

\[ \frac{dI}{dV} \]

\[ T \sim 0.4 \text{ K}, \ B = 0.1 \ T \]

- No zero-bias conductance peak at the core center

- Vortex core is in the quantum limit

Large \[ \Delta^2/\varepsilon_F \]

\[ 50 \text{ nm} \times 50 \text{ nm}, \ +10 \text{ mV/100 pA} \]

T. Hanaguri et al, in preparation
Very strong coupling superconductivity

Superconducting-gap structure of FeSe

Multi-gap
\[ \frac{2\Delta_1}{k_B T_c} \approx 9 \]
\[ \frac{2\Delta_2}{k_B T_c} \approx 6.5 \]

See also C.-L. Song et al., Science (2011).

Positional dependence

Very strong coupling

BCS-BEC crossover
Preformed Cooper pairs and pseudogap above $T_c$

FeSe

- strongly interacting pairs
- pair size $\sim k_F^{-1}$
- $k_F \xi \sim 1$

BCS

- cooperative Cooper pairing
- pair size $\gg k_F^{-1}$
- $k_F \xi \gg 1$

BEC

- tightly bound molecules
- pair size $\ll k_F^{-1}$
- $k_F \xi \ll 1$

M. Randeria
Annu. Rev. Condens. Matter Phys (14)
Preformed Cooper pairs and pseudogap formation above $T_c$

- **Ultracold atom**: preformed pairs and pseudogap remain unclear
- **Fermi liquid behavior even in the unitary Fermi gas**
- **Cuprates**: pseudogap is observed but is unlikely to be caused by preformed pairs
- **Non-Fermi liquid behavior in the pseudogap regime**

M. Randeria
*Annu. Rev. Condens. Matter Phys* (14)
Nonlinear diamagnetic response
>> Gaussian fluctuations
Phase fluctuations

S. Kasahara, Y.M. et al. a preprint
New high-field phase in the superconducting state

New high-field phase in the superconducting state

\[ \varepsilon_F \sim \Delta \sim \mu_B H \]

Fermi ~ Gap ~ Zeeman

**B-phase**

\[ \alpha_M = \sqrt{2 \frac{H_{c2}^{\text{orb}}}{H_{c2}^P}} \approx 2 \frac{m^* \Delta}{m_0 \varepsilon_F} \]

\( \alpha_M > 1.5 \) is required in the BCS limit

\( \alpha_M \sim 5 \) in electron pocket

2.5 in hole pocket

( \( \mathbf{k}^\uparrow, -\mathbf{k} + \mathbf{q}_\downarrow \))

pairing between Zeeman split parts of the Fermi surface

\[ \Delta(\mathbf{r}) = \Delta_0 \cos(\mathbf{q} \cdot \mathbf{r}) \]

**B-phase may not be a simple FFLO phase**

Multiband system

FFLO state is not stable in the crossover regime


Summary

1) Why are Fe-based high-\(T_c\) superconductors exciting?

A new family of unconventional superconductors

2) Mechanism of superconductivity

Spin fluctuation or orbital fluctuation?

3) What lies beneath the superconducting dome?

Quantum critical point

4) FeSe

The first superconducting system in which BCS-BEC crossover is realized.