Superconductivity in strongly coupled multi-band systems

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Iron-pnictide materials

- New high-temperature superconductors
  - discovery: LaFeAsO_{1-x}F_x (February 2008)
  - highest $T_c \approx 55K$ … SmFeAsO_{1-x}F_x

- Features
  - 4 types: 1111, 122, 111, 11
  - Fe-As layers
  - parent compounds: AF metals
  - structural transition
  - SC upon doping
  - multiple electron bands
Electron correlations

- **Fermiology**
  - two hole pockets near Γ-point
  - two electron pockets near M-points
  - orbital content:
    - Fe $d$-orbitals ($xz$, $yz$, $xy$, $x^2-y^2$, $z^2$)
    - hybridize with As $p$-orbitals (x,y)

- **Fermi surface nesting**
  - AF at $k=(\pi,0)$
  - $s$-wave SC: $k=(\pi,0)$
  - $d$-wave SC: $k=(\pi,\pi)$

- **Coulomb interactions**
- **Coupling to the lattice**
Phase diagram

- **Anti-ferromagnet (AF)**
  - SDW at (\(\pi,0\)) + multi-band FS
  - small Fe magnetic moment 0.3-0.9 \(\mu_B\)
  - orthorhombic lattice structure

- **Superconductor (SC)**
  - fully gapped, \(s\)-wave
  - pseudogap?
Theories of pnictides

- Itinerant electron picture
  - undoped parent compound is a metal
  - SDW has small magnetic moment despite $S=2$ of Iron
  - electrons are not localized
  - start from a Fermi liquid, look for SDW and SC instability
  - challenge: SC is beyond mean-field

- Localized electron picture
  - electron correlations are appreciable (Drude weight...)
  - approximate pnictides with Mott insulators
  - look for short-range spin and pairing correlations
  - disadvantage: forget about metallic behavior and quasiparticles
  - advantage: amenable to mean-field treatment of SC
Both itinerant and localized approached assume that pairing and magnetism originate from the same physics (Coulomb repulsion).

Problem in itinerant picture:
- natural description of Fermi liquid and SDW states (exciton condensates from repulsive interactions)
- SC has to defeat repulsive forces
  … does not happen at short length-scales, mean-field useless
- state-of-art: functional RG

“Solution” in localized electron picture:
- doped anti-ferromagnet
- motion of isolated holes leaves trail of frustrated spins
- frustration is avoided by pairing, there is kinetic energy gain
- qualitatively captured by slave-boson theories
Microscopic model

2-band $t$-$J$ model:

$$H = - \sum_{ij} \left( t_{ij}^{\alpha\beta} c_{i\alpha\sigma}^{\dagger} c_{j\beta\sigma} + h.c. \right) - \mu \sum_{\sigma} c_{i\alpha\sigma}^{\dagger} c_{i\alpha\sigma} + \sum J_{ij}^{\alpha\beta} \left( \vec{S}_{i\alpha} \cdot \vec{S}_{j\beta} - \frac{1}{4} n_{i\alpha} n_{j\beta} \right)$$

$$\sum_{\sigma} c_{i\alpha\sigma}^{\dagger} c_{i\alpha\sigma} \leq 1$$

$$\vec{S}_{i\alpha} = c_{i\alpha\nu}^{\dagger} \vec{\sigma}_{\nu\nu'} c_{i\alpha\nu'}$$

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Slave boson approach

- Introduce doping (electron or hole)
- Obtain superconductivity from spin-exchange

- electron = holon + spinon

- constraint at each site and orbital:
- hole doping:

\[ c_\sigma = b^\dagger f_\sigma \]

\[ b^\dagger b + f_\sigma^\dagger f_\sigma = 1 \]

\[ \delta = \langle b^\dagger b \rangle \]

\[
H = - \sum \left( t_{ij}^{\alpha\beta} f_{i\alpha\sigma}^\dagger b_{i\alpha} b_{j\beta}^\dagger f_{j\beta\sigma} + h.c. \right) - \mu \sum_\sigma f_{i\alpha\sigma}^\dagger f_{i\beta\sigma} - \sum \frac{J_{ij}^{\alpha\beta}}{2} B_{ij,\alpha\beta}^\dagger B_{ij,\alpha\beta}
\]

\[
B_{ij,\alpha\beta}^\dagger = (f_{i\alpha\uparrow}^\dagger f_{j\beta\downarrow}^\dagger - f_{i\alpha\downarrow}^\dagger f_{j\beta\uparrow}^\dagger)
\]
Mean-field theory

Mean-field order parameters:

$$\Delta_{ij}^{\alpha\beta} = \langle B_{ij}^{\alpha\beta} \rangle$$

Neglect fluctuations about the mean-field

- Hamiltonian becomes quadratic for spinons
- diagonalize \(\Rightarrow\) Bogoliubov - de Gennes quasiparticles
- Obtain BdG spectrum: \(\pm E_{\alpha'k}(\Delta)\)

Free energy density for non-interacting BdG quasiparticles:

$$\mathcal{F} = \sum \frac{J_{ij}^{\alpha\beta}}{2} |\Delta_{ij}^{\alpha\beta}|^2 - \int \frac{d^2k}{4\pi^2} \left[ E_{1k}(\Delta) + E_{2k}(\Delta) - E_{1k}(0) - E_{2k}(0) \right]$$
Symmetries

- Minimize free energy density with respect to order parameters
  1) fix chemical potential, ignore constraints
  2) fix average spinon density $n = \langle f^\dagger f \rangle$, enforce $n + \delta = 1$

- Eight microscopic order parameters:
  $\Delta_{x}^{11}, \Delta_{y}^{11}, \Delta_{x+y}^{11}, \Delta_{x-y}^{11}, \Delta_{x}^{22}, \Delta_{y}^{22}, \Delta_{x+y}^{22}, \Delta_{x-y}^{22}$

- Reorganize by point-group symmetry: $D_{4h}$

\[
\begin{align*}
  s_{x^2+y^2}^{A_{1g}} &= \frac{1}{4} \left( \Delta_{x}^{\alpha\beta} + \Delta_{y}^{\alpha\beta} \right) \tau_{\alpha\beta}^0, \\
  d_{x^2-y^2}^{A_{1g}} &= \frac{1}{4} \left( \Delta_{x}^{\alpha\beta} - \Delta_{y}^{\alpha\beta} \right) \tau_{\alpha\beta}^z, \\
  s_{x^2y^2}^{A_{1g}} &= \frac{1}{4} \left( \Delta_{x+y}^{\alpha\beta} + \Delta_{x-y}^{\alpha\beta} \right) \tau_{\alpha\beta}^0, \\
  d_{xy}^{A_{2g}} &= \frac{1}{4} \left( \Delta_{x+y}^{\alpha\beta} - \Delta_{x-y}^{\alpha\beta} \right) \tau_{\alpha\beta}^z, \\
  s_{x^2+y^2}^{B_{1g}} &= \frac{1}{4} \left( \Delta_{x}^{\alpha\beta} + \Delta_{y}^{\alpha\beta} \right) \tau_{\alpha\beta}^z, \\
  d_{x^2-y^2}^{B_{1g}} &= \frac{1}{4} \left( \Delta_{x}^{\alpha\beta} - \Delta_{y}^{\alpha\beta} \right) \tau_{\alpha\beta}^0, \\
  s_{x^2y^2}^{B_{1g}} &= \frac{1}{4} \left( \Delta_{x+y}^{\alpha\beta} + \Delta_{x-y}^{\alpha\beta} \right) \tau_{\alpha\beta}^z, \\
  d_{xy}^{B_{2g}} &= \frac{1}{4} \left( \Delta_{x+y}^{\alpha\beta} - \Delta_{x-y}^{\alpha\beta} \right) \tau_{\alpha\beta}^0.
\end{align*}
\]
Symmetries

- Symmetry classes
  - $A_{1g}$ .... symmetric under all transformations
  - $B_{1g}$ .... sign-change under 90° rotation and reflection through diag.
  - $B_{2g}$ .... the same as above, but rotated by 45°
  - $A_{2g}$ .... higher orbital harmonic (g-wave)

- Orbital harmonics
  - $s_{x^2+y^2}$ .... $\cos(k_x) + \cos(k_y)$
  - $s_{x^2 y^2}$ .... $\cos(k_x)\cos(k_y)$
  - $d_{x^2-y^2}$ .... $\cos(k_x) - \cos(k_y)$
  - $d_{xy}$ .... $\sin(k_x)\sin(k_y)$

- Symmetries are fundamental.
  Orbital harmonics mix by fluctuations.
Order Parameter

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Phase diagram

| A1: $d_{xy}^{B_{2g}} \pm i\left(s_{x^2y^2}^{A_{1g}} - d_{x^2-y^2}^{A_{1g}}\right)$ | A2: $d_{xy}^{B_{2g}}, s_{x^2y^2}^{A_{1g}}, s_{x^2+y^2}^{A_{1g}}, d_{x^2-y^2}^{A_{1g}}$
|---|---|
| B1: $s_{x^2y^2}^{A_{1g}} - d_{x^2-y^2}^{A_{1g}}$ | B2: $s_{x^2+y^2}^{A_{1g}} \pm i\left(s_{x^2y^2}^{A_{1g}} - d_{x^2-y^2}^{A_{1g}}\right)$
| C1: $s_{x^2y^2}^{A_{1g}} \pm i\left(s_{x^2y^2}^{B_{1g}} - d_{x^2-y^2}^{B_{1g}}\right)$ | C2: $s_{x^2+y^2}^{A_{1g}} \pm i\left(d_{x^2-y^2}^{B_{1g}} - s_{x^2y^2}^{B_{1g}}\right)$

Superconductivity in strongly coupled multi-band systems
Phases

- $A \ldots A_{1g} + iB_{2g} \Rightarrow$ broken time-reversal symmetry $(J_1 < J_2)$
- $B \ldots A_{1g} (s-d) = \text{sign-changing extended } s\text{-wave } (s^\pm) (J_1 \sim J_2)$
- $C \ldots A_{1g} + iB_{1g} \Rightarrow$ broken time-reversal symmetry $(J_1 >> J_2)$

Coexisting symmetry classes $\Rightarrow$ time-reversal symmetry breaking follows from Landau-Ginzburg theory:
W-C. Lee, S-C. Zhang and C. Wu, PRL 102, 217002 (2009)

Coexisting orbital harmonics $\Rightarrow$ relative minus sign
inter-band pair tunneling & pairing despite repulsive Coulomb interactions
Critical temperature

Superconductivity in strongly coupled multi-band systems
Fixed density: $\delta = 0.5$

$A_{1g} : s_{x^2+y^2}$

$A_{1g} : d_{x^2-y^2}$

$A_{1g} : s_{x^2+y^2}$

$B_{2g} : d_{xy}$

Free energy density

$\mu$
**Strongly coupled multi-band superconductivity**

- Orbital degrees of freedom + symmetries
  - multi-component order parameter...
  - multiple superconducting states?
  - translational, rotational & time-reversal symmetry breaking?
  - vortex core structure?

- Quasiparticles
  - fully gapped, nodal, or coexisting quasiparticle Fermi surfaces?
  - breached or “FFLO” superconductor?
  - can affect vortex lattice structure
  - affects vortex dynamics (is there a “pseudogap” state?)
Conclusions

- What if pnictides were Mott insulators...
  - 2-band t-J model
  - low magnetic moment from spin frustration
  - superconductivity from spin-exchange

- Tractable by slave-boson mean-field theory
  - classification of states by symmetries and orbital content
  - T=0 phase diagram

- Is there a tractable effective theory for pnictides which contains:
  - metallic SDW with low magnetic moment
  - superconductors created by Coulomb interactions
  - structural transitions (coupling to phonons)?