Pairing strength and gap functions in multiband superconductors: 3D effects

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Motivation: Fe based superconductors: 2D vs. 3D

• Materials

LaFeAsO

$K_x Fe_{2-y} Se_2$

LiFeAs

FeSe

Crystal structure

Fermi surface (DFT)

Cao et al. PRB (2008)

Maier et al. PRB (2011)

Wang et al. (in preparation)

Tomic et al. (in preparation)

2D Fermi surface

Deviations from 2D Fermi surface
Method

- Tight binding model
  - Wannier projection of DFT results
  - Fit to experimental band structure (ARPES)

\[ H_0 = \frac{1}{N} \sum_{ij} \sum_{\ell_1, \ell_2 = 1}^{10} t_{ij}^{\ell_1 \ell_2} c_{i \ell_1}^\dagger c_{i \ell_2} \]

- Hubbard-Hund Hamiltonian

\[ H = H_0 + \bar{U} \sum_{i, \ell} n_{i \ell \uparrow} n_{i \ell \downarrow} + \bar{U}' \sum_{i, \ell' < \ell} n_{i \ell} n_{i \ell'} \]

\[ + \bar{J} \sum_{i, \ell' < \ell} \sum_{\sigma, \sigma'} c_{i \ell \sigma}^\dagger c_{i \ell' \sigma'} c_{i \ell' \sigma} c_{i \ell \sigma} + \bar{J}' \sum_{i, \ell' \neq \ell} c_{i \ell \uparrow}^\dagger c_{i \ell \downarrow}^\dagger c_{i \ell' \downarrow} c_{i \ell' \uparrow} \]

Kuroki et al. PRL (2008)
Spin fluctuation mediated pair scattering

- Susceptibility in normal state (orbital resolved)
  \[ \chi_{\ell_1 \ell_2 \ell_3 \ell_4}^0(q) = -\frac{1}{2} \sum_{k, \mu \nu} M_{\ell_1 \ell_2 \ell_3 \ell_4}^{\mu \nu}(k, q) G^{\mu}(k + q) G^{\nu}(k). \]

- Interactions: RPA approximation
  \[ \chi_{\ell_1 \ell_2 \ell_3 \ell_4}^{RPA}(q) = \frac{\chi_0}{1 - U^s \chi_0} \]
  \[ \chi_{\ell_1 \ell_2 \ell_3 \ell_4}^{RPA}(q) = \frac{\chi_0}{1 + U^c \chi_0} \]

- Scattering vertex in singlet channel
  \[ \Gamma_{ij}(k, k') = \text{Re} \sum_{\ell_1 \ell_2 \ell_3 \ell_4} \tilde{M}_{\ell_1 \ell_2 \ell_3 \ell_4}^{ij} \left[ \frac{3}{2} U^s \chi_{1}^{RPA}(k - k', 0) U^s \right. \]
  \[ + \frac{1}{2} U^s - \frac{1}{2} U^c \chi_{0}^{RPA}(k - k', 0) U^c + \frac{1}{2} U^c \left. \right] \ell_3 \ell_4 \ell_1 \ell_2 \]

Graser et al. NJP (2009)
LiFeAs: Experimentally

- High quality samples available with Tc~18K
- Nonpolar surfaces, ideal to apply surface spectroscopy to measure band structure and superconducting gap

Borisenko et al. PRL (2010)
Borisenko et al. Symmetry (2012)
Umezawa et al. PRL (2012)
Summary: ARPES results for gap

- $\alpha$ pocket: large isotropic gap
- $\beta$ pockets: “in-phase” gap
- $\gamma$ pocket: minimum along Fe bond ($\theta=0$)

Borisenko et al. Symmetry (2012)

Umezawa et al. PRL (2012)
LiFeAs: Theoretically

- Fermi surface less nested than in other iron SC naïve: weak instability from spin-fluctuation theory
- Deviations between ARPES and DFT derived Fermi surface
- More correlated than other Fe based SC e.g. 122
  - Hole pockets shrink
  - Electron pockets unchanged

Yin et al. Nat. Mater (2011)  
Ferber et al. PRB (2012)

FRG calculation: Platt et al. PRB (2011)
Spin-fluctuation pairing: DFT derived model

- Pairing strength by solution of linearized gap equation

\[ \frac{1}{V_G} \sum_j \int_{FS_j} \Gamma_{ij}(\mathbf{k}, \mathbf{k}') \frac{g_\alpha(\mathbf{k}')}{|v_{Fj}(\mathbf{k}')|} = \lambda_\alpha g_\alpha(\mathbf{k}) \]

- s+/- wave for interactions close to the instability

DFT \( g(\mathbf{k}) \): \( \lambda_1 = 0.2361 \), \( U = 0.88 \) eV, \( J = 0.25U \)
Gapfunction: ARPES fitted tight binding model

- s+/− wave for interactions close to instability

\[ \text{ARPES } g(k): \lambda_1 = 1.029, \ U = 0.75 \text{ eV}, \ J = 0.37U \]
## Comparison to experiments

<table>
<thead>
<tr>
<th></th>
<th>DFT model</th>
<th>ARPES derived model</th>
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<tbody>
<tr>
<td><strong>Fermi surface</strong></td>
<td><img src="RedCross" alt="X" /></td>
<td><img src="GreenCheck" alt="Check" /> (fit)</td>
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<tr>
<td>(correlations?)</td>
<td></td>
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<tr>
<td><strong>Superconducting gap</strong></td>
<td>s +/-</td>
<td>s +/-</td>
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<tr>
<td><strong>α pockets: large, isotropic</strong></td>
<td><img src="GreenCheck" alt="Check" /></td>
<td><img src="RedCross" alt="X" /></td>
</tr>
<tr>
<td><strong>β pockets: intermediate size</strong></td>
<td><img src="GreenCheck" alt="Check" /></td>
<td><img src="GreenCheck" alt="Check" /></td>
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<tr>
<td><strong>“out of phase” oscillation</strong></td>
<td><img src="RedCross" alt="X" /></td>
<td><img src="GreenCheck" alt="Check" /> (at some $k_z$)</td>
</tr>
<tr>
<td><strong>γ pockets: intermediate size</strong></td>
<td><img src="GreenCheck" alt="Check" /></td>
<td><img src="GreenCheck" alt="Check" /></td>
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<tr>
<td><strong>maxima of oscillation along Fe-Fe direction</strong></td>
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- **Experiment: ARPES**
  - $α$
  - $γ$
  - $β_{in}$
  - $β_{out}$

- **Spin-fluctuation theory: DFT model**
  - $α$
  - $γ$
  - $β_{in}$
  - $β_{out}$

- **Spin-fluctuation theory: ARPES derived model**
  - $α$
  - $γ$
  - $β_{in}$
  - $β_{out}$
Conclusions

- Spin fluctuation pairing including 3D scattering
  - Fermi surface in LiFeAs less nested, but sign-changing s-wave gap
  - Gap magnitudes and phases mainly in agreement with results from ARPES experiments
  - ARPES fitted tight binding model: way to include effects of correlations

- Acknowledgments
\( \text{K}_x \text{Fe}_{2-y} \text{Se}_2 \)

- Experimentally
  - Different phases
    - 245 vacancy phase
    - Pure SC phases
      \( \text{K}_{0.6} \text{Fe}_2 \text{Se}_2, \text{K}_{0.3} \text{Fe}_2 \text{Se}_2 \)?
  - Absence of hole pocket?
  - Evidence for fully gapped SC state
    - Specific heat
    - ARPES
    - Spin-lattice relaxation in NMR

Ye et al. PRL (2011)
Ying et al. JACS (2013)
Zeng et al. (2011)
Mou et al. (2011)
Ma et al. (2011)
Quian et al. PRL (2011)
$K_xFe_{2-y}Se_2$: Spin-fluctuation pairing

- DFT calculation for KFe$_2$Se$_2$
- 5-orbital tight binding fit
- Suppression of hole pockets by adjustment of nearest neighbor hoppings \textit{Maier et al. PRB (2011)}
- Leading instability: d-wave (robust in parameter space)
- Small pockets around Z-point: small density of states: Might not been seen in experiments