Electronic structure of iron-based superconductors

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I. Fermi surface shrinking and the effects of electronic correlations

II. Electronic structure of bulk FeSe from ARPES and quantum oscillations
Classes of Fe-based superconductors

The common features: robust Fe/(Pn=As,P) layers where Fe atoms are tetragonally coordinated by pnictide or chalcogenide atoms.

- Tc ~ 27 K
- Tc ~ 18 K
- Tc ~ 38 K
- Tc ~ 55 K
- Tc ~ 37 K
Generic phase diagram of isoelectronic pnictides

- LaFeAsO
- BaFe\textsubscript{2}As\textsubscript{2}
- AFM
- SC
- QCP
- bandwidth
- Hund rule's coupling
- 'chemical pressure' c/a ratio
- FeSe
- 5 bands (orbitals), magnetism, structural distortions
Superconductivity develops when the nesting/magnetism is destroyed.

Different possible scenarios for nodal and nodeless superconductivity depend on orbital character.

D. Singh

Quantum oscillations map out the Fermi surface

- oscillations of the density of states in magnetic field;

\[ F = \left( \frac{\hbar}{2\pi e} \right) A(E_F) \]

- 'k-space microscopy': 0.1% IBZ; 3D map of the Fermi surface;
- bulk probe; no sensitive to surface effects like ARPES;

\[
\tilde{M} \propto \sum_{\text{extremal } A_F} \frac{F B^{\frac{1}{2}}}{m^*} \left( \frac{\partial^2 A_F}{\partial k_z^2} \right)^{\frac{1}{2}} \sum_{p=1}^{\infty} R_T R_D R_S p^{-\frac{3}{2}} \sin \left( 2\pi p \left( \frac{F}{B} - \gamma \right) \pm \frac{\pi}{4} \right)
\]
Lifshitz-Kosevich formalism (LK formula)

\[ M_{osc} \propto R_T R_D R_s R_{sc} \sin \left( \frac{2\pi F}{B} + \gamma \right) \]

- **Temperature - low temperatures**

\[ R_T = \frac{2\pi^2 p k_B T m^*/e \hbar B}{\sinh (2\pi^2 p k_B T m^*/e \hbar B)} \]

- **Finite scattering time – clean samples**

\[ R_D = \exp \left( -\frac{\pi m_b}{e B \tau} \right) \]

- **Superconducting state – random vortex lattice**

\[ R_{sc} = \exp \left[ -\pi^{\frac{3}{2}} \left( \frac{\Delta E(B)}{\hbar \omega_c} \right)^2 \left( \frac{B}{F} \right)^{\frac{1}{2}} \right] \]

- **Spin-splitting of the Fermi surface**

\[ R_S = \cos \left( \frac{\pi g m_S}{2m_e} \right) \]

- extracted parameters: orbitally averaged quasiparticle effective mass \( m^* \) (band renormalization near the Fermi energy),
- scattering times \( \tau \), spin-splitting factor \( g^* \)

Lifshitz-Kosevich formalism: The effect of electronic correlations

\[ m^*/m_b = (1 + \lambda_{el-ph})(1 + \lambda_{el-el}) \sim 1 + \lambda_{el-ph} + \lambda_{el-el} \]
Quantum oscillations in iron pnictides

- **Clean samples**: mean free path > 150 Å

- **End member compounds**: (Ba/Sr/Ca)Fe$_2$As$_2$, (Ba/Sr/Ca)Fe$_2$P$_2$, KFe$_2$As$_2$, etc

- Twinning of samples is detrimental for the observation of quantum oscillations;

Disorder induced only outside the Fe plane $\text{BaFe}_2(\text{As,P})_2$

- **Doped samples**: Co-doped or K-doped BaFe$_2$As$_2$; large upper critical fields > 60T and large randomness in the distribution of ions on the Fe sites;

- **Lighter masses** and **smaller frequencies** usually are easier to be observed than heavier masses and large frequencies;

$$\hbar \omega_c > k_B T, \quad \omega_c \tau >> 1$$

$$R_D = \exp\left(-\frac{\pi k_F}{eB\ell}\right)$$
Measurement techniques of quantum oscillations

AFM piezocantilevers micron-size crystals

\[ \tau = \mathbf{m} \times \mathbf{B}, \tau = mB \sin(\theta) \]

\[ \tau = \mu_0 (M_a H_c - M_c H_A) \]

\[ \mathcal{T} = \sum_{\text{orbits}} \frac{\partial F}{\partial \theta} \frac{V e^{5/2}}{\hbar^{1/2} \pi^2 m_e} \left( \frac{B^{3/2}}{2\pi \frac{\partial^2 A}{\partial k_{||}}} \right)^{1/2} R_T R_D R_S \sin \left( \frac{2\pi F}{B} + \phi \right) \]

Low temperatures \((0.3 \text{ K} < T < 4 \text{ K})\), high magnetic fields \((0 < B < 55 \text{ T})\), rotation in field \((-90^\circ < \theta < 90^\circ)\);

Capacitive levers mm-size crystals (Sebastian)

Transport measurements to de-twin crystals (Terashima)

BaFe2As2
I. Fermi surface shrinking and the effects of electronic correlations - LaFePO
Superconducting order parameter with line nodes in LaFePO

- Clean superconductor with no structural transition. Superfluid density shows linear dependence down to 100 mK suggesting the presence of nodes in the symmetry of the superconducting gap;

\[ \Delta \lambda \sim T \]

J. Analytis et al., arXiv:0810.5368

J. Fletcher, et. al., PRL 102, 147001 (2009)
de Haas-van Alphen effect in LaFePO

- high $B$: normal state; oscillations periodic in inverse field, de Haas-van Alphen effect.
- $\tau \sim B^2$ - characteristic to a paramagnet;
- a simple corrugation of the Fermi cylinder leads to a beat pattern in the magnetization.

The de Haas-van Alphen effect in LaFePO

\[ F = \frac{\hbar}{2\pi e} A(E_F) \]

Different frequencies correspond to extremal areas of the Fermi surface perpendicular to the applied magnetic field for a particular orientation;

Fermi surface warping and Yamaji angle

At Yamaji angles all Fermi surface cross sections have equal areas; their magnetization contributions interfere constructively=peak effect.

\[ F(\theta) = F(0) / \cos \theta \]

Quasi-two dimensional cylinder;

\[ \Delta F_\alpha / F_\alpha \approx 4\%; \]

\[ \Delta F_\beta / F_\beta \approx 23\%; \]

dHvA data versus band structure calculations

- electronic branches show similar dispersion to the experimental $\alpha$ and $\beta$ pockets;
- no experimental branch matches the weak dispersion due to the 3D hole pocket;
Band shifting and charge balance

Electron bands shifted by $\Delta E=+85$ meV (band 5), $+30$ meV (band 4); hole bands all shifted by $\Delta E=-53$ meV; Charge imbalance $\sim0.034$ el/fu; $\sim1.7\%$ oxygen deficiency in LaFePO.
Shrinking of the Fermi surface in LaFePO

Experimental observation of upward shift of the electron bands and of a downward shift of the hole band may be evidence of dominance of interband scattering (nesting);

L. Ortenzi et al., PRL 103, 046404 (2009).
Shrinking of the Fermi surface in LaFePO

Shifts proportional to interband coupling $V$

Larger coupling $\rightarrow$ shrinks FS, increases mass, increases $T_c$

L. Ortenzi, E. Cappelluti, L. Benfatto, L. Pietronero (PRL 09)

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L. Ortenzi et al., PRL 103, 046404 (2009).
Shrinking of the Fermi surface pockets

SDW/able instability in the iron pnictide tends to shrink both the electron and hole pockets. Antiferromagnetically driven electronic correlations.


<table>
<thead>
<tr>
<th>Process</th>
<th>Dual processes</th>
<th>Two ways of decoupling</th>
<th>Implication</th>
<th>Cuprate</th>
<th>Iron pnictide</th>
</tr>
</thead>
<tbody>
<tr>
<td>SDW/SC</td>
<td>$V_{c_{k+Q},c_{k-Q},c_{k-Q},c_{k}}$</td>
<td>$-V_{S_{k}}S_{k-Q}$ or $V_{D_{k-Q}}A_{k}$</td>
<td>$\langle\Delta_{k}\rangle\langle\Delta_{k-Q}\rangle&lt;0$ (*$)$</td>
<td>$Q=(\pi,\pi)$, both $\cos k_x+\cos k_y$ and $\cos k_x-\cos k_y$ satisfy (*$)$</td>
<td>$Q=(\pi,0)/(0,\pi)$, both $\cos k_x\cos k_y$ and $\sin k_x\sin k_y$ satisfy (*$)$</td>
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<tr>
<td></td>
<td>$V_{c_{k+Q},c_{k-Q},c_{k-Q},c_{k}}$</td>
<td>$\Delta_{k}=c_{k+Q}^{\dagger}c_{k-Q}$</td>
<td>$\delta n_{k}\delta n_{k-Q}&lt;0$</td>
<td>$C_{4v}$ breaking</td>
<td>Shrinking of all pockets. See Figs. 5(c) and 5(d)</td>
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<td></td>
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<td>$D_{2d}$</td>
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I. Fermi surface shrinking and the effects of electronic correlations – LiFeP and LiFeAs
Quantum oscillations in the superconducting LiFeP and LiFeAs

LiFeP nodal superconductor $T_C \sim 4K$

LiFeAs nodeless superconductor $T_C \sim 18K$

Quantum oscillations in LiFeAs and LiFeP

Torque shows quantum oscillations in LiFeP and LiFeAs above $H_{c2}$. There are 5 different frequencies for LiFeP and 3 different frequencies observed for LiFeAs.
Quantum oscillations in LiFeAs and LiFeP

For LiFeP, small shifts of the band energies: +20 meV and +45 meV for band 4 and 5 (electron) and −65, −80, 18 meV for bands 1, 2 and 3 (hole) bring the observations and calculations into almost perfect agreement. These shifts shrink both the electron and hole FSs and likely originate from many body corrections to the DFT bandstructure.

**Fermi surface parameters in LiFeAs and LiFeP**

<table>
<thead>
<tr>
<th>LiFeP</th>
<th>DFT calc.</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orbit</td>
<td>$F(T)$</td>
<td>$m_b$</td>
</tr>
<tr>
<td>$1_a$</td>
<td>557</td>
<td>-0.44</td>
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<td>$2_a$</td>
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<td>$4_a$</td>
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<td>$5_a$</td>
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<td>3142</td>
<td>+0.83</td>
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<td>Orbit</td>
<td>$F(T)$</td>
<td>$m_b$</td>
</tr>
<tr>
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<td>$4_b$</td>
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<td>$5_a$</td>
<td>1584</td>
<td>+1.54</td>
</tr>
<tr>
<td>$5_b$</td>
<td>2942</td>
<td>+1.02</td>
</tr>
</tbody>
</table>


PRL 108, 047002 (2012)
The effect of correlations on the Fermi surface manifests itself mainly in a shrinking of the middle hole pocket, and, in order to preserve the electron count, an increase of the outer hole pocket size.

I. Fermi surface shrinking and the effects of electronic correlations – BaFe2(As,P)
Effect of chemical pressure: P/As substitution

W. Xie, PRB 79, 115128 (2009)  
S. Kasahara et al., PRB 81, 134422 (2010)
Evolution of Fermi surface in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

oscillations observed for materials with $T_c = 0 - 25$ K; $T_{\text{max}} = 30$ K for $x = 0.33$;

H. Shishido et al. AIC, PRL 104, 057008 (2010)
Spin fluctuations in BaFe$_2$(As$_{1-x}$P$_x$)$_2$

$\rho = \rho_0 + AT\alpha$

S. Kasahara et al., PRB 81, 184519 (2010)

Antiferromagnetic spin fluctuations close to QCP

$1/T_1T \sim 1/(T+\theta)$


H. Shishido et al., AIC, PRL 104, 057008 (2010)
Moderate mass enhancement in LaFePO

The effective masses between 1.7-2.1 $m_e$ for both electrons and holes; moderate mass enhancement for the electronic bands;
Heavier quasiparticles in LiFeAs

Heavy effective masses in LiFeAs for the electron bands as compared to other iron pnictides; band masses 1-1.5 me and electron-phonon coupling ~0.25;

\[
m^*/m_b = (1 + \lambda_{el-ph})(1 + \lambda_{el-el}) \sim 1 + \lambda_{el-ph} + \lambda_{el-el}
\]
Correlations in iron pnictides

The strength of electronic correlations. Electronic bands in clean superconductors

Nodal superconductors

Fully gapped superconductor

\[ \lambda_e = m^*/m_b - (1 + \lambda_{e-ph}) \]

\[ T_c (K) \]

PRL 108, 047002 (2012); PRL 101, 216402 (08); PRL 104, 057008 (2010);
Summary of quantum oscillation in iron-based superconductors

- Quantum oscillations in iron pnictides are in broad agreement with band structure.

- Fermi surface shrinking for superconducting compounds as compared with band structure calculations; local correlations or partially from long-range spin fluctuations?

- Mass enhancement in the clean and nodal superconductors correlates with the increase in $T_c$ for isoelectronic system like $\text{BaFe}_2(\text{P}_{1-x}\text{As}_x)_2$ and $\text{LiFeAs}$ and $\text{LiFeP}$; electronic correlations are important (quantum critical point ?).

PRL 101, 216402 (08); PRL 103, 026404 (09), PRL 103, 076401 (2009); PRL 104, 057008 (2010);
Electronic structure of bulk FeSe from ARPES and quantum oscillations
Unusual high $T_c$ in a mono-layer of FeSe
ARPES and pressure effects

Medvedev et al 2010

Bendele et al 2012: magnetic state at low pressure
Superconductivity and structural transition in FeSe

M. Watson et al., Oxford (2014)