ARPES Results of '122' Iron-based Superconductors

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OUTLINES

1. Angle-Resolved PhotoEmission Spectroscopy (ARPES)

2. Crystal structure of "122" system

3. Experimental results

4. Theoretical results

5. Conclusions
ARPES

• based on Photoelectric Effect (Hertz 1887, Einstein 1905)

• powerful technique to measure the electronic structure directly (Energy vs. Momentum)

ARPES

- incidence of monochromatic photons
- photoelectrons with different energy and momentum

Crystal Structure

FIG. 2: Crystal structure of $AFe_2As_2$ ($A=\text{Ba, Sr, Ca}$).


- The parent compounds undergo a tetragonal to orthorhombic structural transition together with a magnetic transition
Experiments: BaFe$_2$As$_2$

- below $T_{SDW}$
- two enclosed hole-like pockets around the zone center
- four petal-like electron-like pockets below $T_{SDW}$
- an electron-like pocket around zone corner

M. Yi, et al, PRB, 80, 174510 (2009)
Experiments: BaFe$_2$As$_2$


- Nesting: replica of $\Gamma$-centred hole-like band (grey)
- electron-like band (grey)
- interaction of these two bands opens a gap and forms the blades (red)
Experiments: SrFe$_2$As$_2$


Normal state ($T = 230$ K)

- High $T$, only two hole-like pockets at zone center and one electron-like pocket at zone corner.
- Low $T$, $\beta$ band split into two bands $\beta_1$, $\beta_2$. And the petal-like pockets appear, but hole-like.
Experiments: CaFe$_2$As$_2$

- two hole-like pockets around zone center and one electron-like pocket around zone corner

Experiments: CaFe$_2$As$_2$

• z component of momentum is identified by the incident energy of photon.

• the bands around Γ point is more 3D than the bands around M point.

my results

- Five-orbital model + MFA

\[ H_0 = \sum_{k, \sigma} \sum_{\alpha, \beta} (\xi_{\alpha\beta}(k) + \epsilon_{\alpha} \delta_{\alpha\beta}) d_{\alpha\sigma}^\dagger(k) d_{\beta\sigma}(k) \]

\[ H_{\text{int}} = U \sum_{1,\alpha} n_{1,\alpha,\uparrow} n_{1,\alpha,\downarrow} + (U' - J/2) \sum_{1,\alpha < \beta} n_{1,\alpha} n_{1,\beta} \]

\[ -2J \sum_{1,\alpha < \beta} S_{1,\alpha} \cdot S_{1,\beta}. \]
my results
Conclusions

• two hole-like enclosed pockets and four petal-like pockets around zone center
• one electron-like enclosed pocket and four petal-like pickets around zone corner
• more 3D than cuprates
• MFA of 5-orbital model gives consistent results with experiments
• F. Ma, et al, arXiv:0806.3526v2
• M. Yi, et al, PRB, 80, 174510 (2009)
• Y. Zhang, et al, PRL, 102, 127003 (2009)
• C. Liu, et al, PRL, 102, 167004 (2009)