Orbital selectivity

- Fe based materials: multiband systems
electrons in some orbitals less coherent

- FeSe: nematic order, no magnetism
opportunity to study unequal states in \( d_{xz}/d_{yz} \)

Relevant for Fe based SC:
Yin, Haule, Kotliar, Nat. Mat. 10, 932 (2011)
Yi et al., Nat. Comm. 6, 7777 (2015)
Theoretical approach

- Dressed Green's function

\[ G(\vec{k}, \omega) = \frac{1}{\omega - E_{\vec{k}} - \Sigma(\vec{k}, \omega) + i0^+} \]

- Parametrization
  - true eigenenergies
  - quasiparticle weights
    - geometric mean of quasiparticle weights
      (phenomenological/measured/calculated)

\[ \tilde{G}_{\ell\ell'}(\mathbf{k}, \omega_n) = \sqrt{Z_\ell Z_{\ell'}} \sum_\mu \frac{a_\mu^\ell(\mathbf{k}) a_\mu^{\ell'}(\mathbf{k})}{i\omega_n - \tilde{E}_\mu(\mathbf{k})} \]

measured true eigenenergies

Watson, et al., PRB 94, 201107(R) (2016)
Watson, et al., PRB 90, 121111(R) (2014)
Maletz, et al., PRB 89, 220506(R) (2014)
Liu, et al., arXiv:1802.02940
Normal state properties: Spectroscopy

- Normal state QPI
  - T-matrix: no orbital selectivity $Z=1$
  - T-matrix: orbital selectivity ($Z$ as for superconductivity)

- ARPES
  - Orbitally resolved spectral function

Liu, et al., arXiv:1802.02940

A. Kostin et al., arXiv:1802.02266
Superconducting state: gap function

- Modified spin-fluctuation theory

\[ \tilde{\Gamma}_{\nu \mu}(k, k') = \text{Re} \sum_{\ell_1 \ell_2 \ell_3 \ell_4} \sqrt{Z_{\ell_1}} \sqrt{Z_{\ell_4}} a_{\nu}^{\ell_1, *}(k) a_{\nu}^{\ell_4, *}(-k) \tilde{\Gamma}_{\ell_1 \ell_2 \ell_3 \ell_4}(k, k') \sqrt{Z_{\ell_2}} \sqrt{Z_{\ell_3}} a_{\mu}^{\ell_2}(k') a_{\mu}^{\ell_3}(-k') \]

- Solve linearized gap equation

\[ -\sum_{\mu} \int_{\text{FS}_\mu} dS' \frac{\tilde{\Gamma}_{\nu \mu}(k, k') g_i(k')}{V_G |v_{F\mu}(k')|} = \lambda_i g_i(k) \]

Quasiparticle weights (same trends found in microscopic calculations)

![Images with data points and graphs](image)

Picture challenged: Kang, Fernandes, Chubukov arXiv:1802.01048
Talk: B14.00007

But: different orbital content on the hole-pocket

Strong splitting required!
Static spin fluctuations

- Use parametrization of Green's function

\[ \tilde{\chi}_{\ell_1 \ell_2 \ell_3 \ell_4}^0 (q) = \sqrt{Z_{\ell_1} Z_{\ell_2} Z_{\ell_3} Z_{\ell_4}} \chi_{\ell_1 \ell_2 \ell_3 \ell_4}^0 (q), \]

Strong renormalization of \( d_{xy} \): suppression of \((\pi,\pi)\) weight
Spin fluctuations: Inelastic neutron scattering


Band structure with reduced coherence
Magnetic penetration depth

- Penetration depth from tight binding model

\[ \frac{1}{\lambda_i^2} = \frac{4\pi e^2}{c^2 \hbar^2} \sum_{k,\nu} \left( \frac{d\tilde{E}_{\nu}(k)}{dk_i} \right) \left( \frac{d\tilde{E}_{\nu}(k)}{dk_i} \right) \left| \Delta_k \right|^2 - \frac{d\left| \Delta_k \right|}{dk_i} \left| \Delta_k \right| \tilde{E}_{\nu}(k) \right) \times \frac{\tilde{Z}_{\nu}(k)}{E_{\nu,k}^2} \left( \frac{1}{E_{\nu,k}} \tanh\left( \frac{E_{\nu,k}}{2k_B T} \right) - \frac{1}{2k_B T} \text{sech}\left( \frac{E_{\nu,k}}{2k_B T} \right)^2 \right) \]


P. Biswas, et al. (in preparation)
Summary

- Phenomenological, but microscopic approach: including low-energy renormalizations

\[ \tilde{G}_{\ell\ell'}(k, \omega_n) = \sqrt{Z_\ell Z_{\ell'}} \sum_{\mu} \frac{a_\mu^\ell(k) a_\mu^{\ell'*}(k)}{i\omega_n - \tilde{E}_\mu(k)} \]

- Consequences
  - Anisotropic quasiparticle scattering in FeSe
  - Pairing: modified spin-fluctuation theory (stabilization of s-wave pairing, anisotropic order parameter for FeSe)
  - Magnetism, spin-fluctuation spectrum: suppression of \((\pi, \pi)\) spectral weight, prediction for INS on detwinned FeSe
  - Penetration depth: anisotropies (elongated vortices), magnitude fixed by parameters

- Microscopic calculation of \(\sqrt{Z_\ell}\)

E14.00006 : Orbitally Resolved Quasiparticle Weight Renormalization Factors in Fe-based Superconductors
Tue 9:24, 304B
ARPES on FeSe


Orbitally resolved spectral function
A. Kreisel, et al.

Liu, et al., arXiv:1802.02940