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

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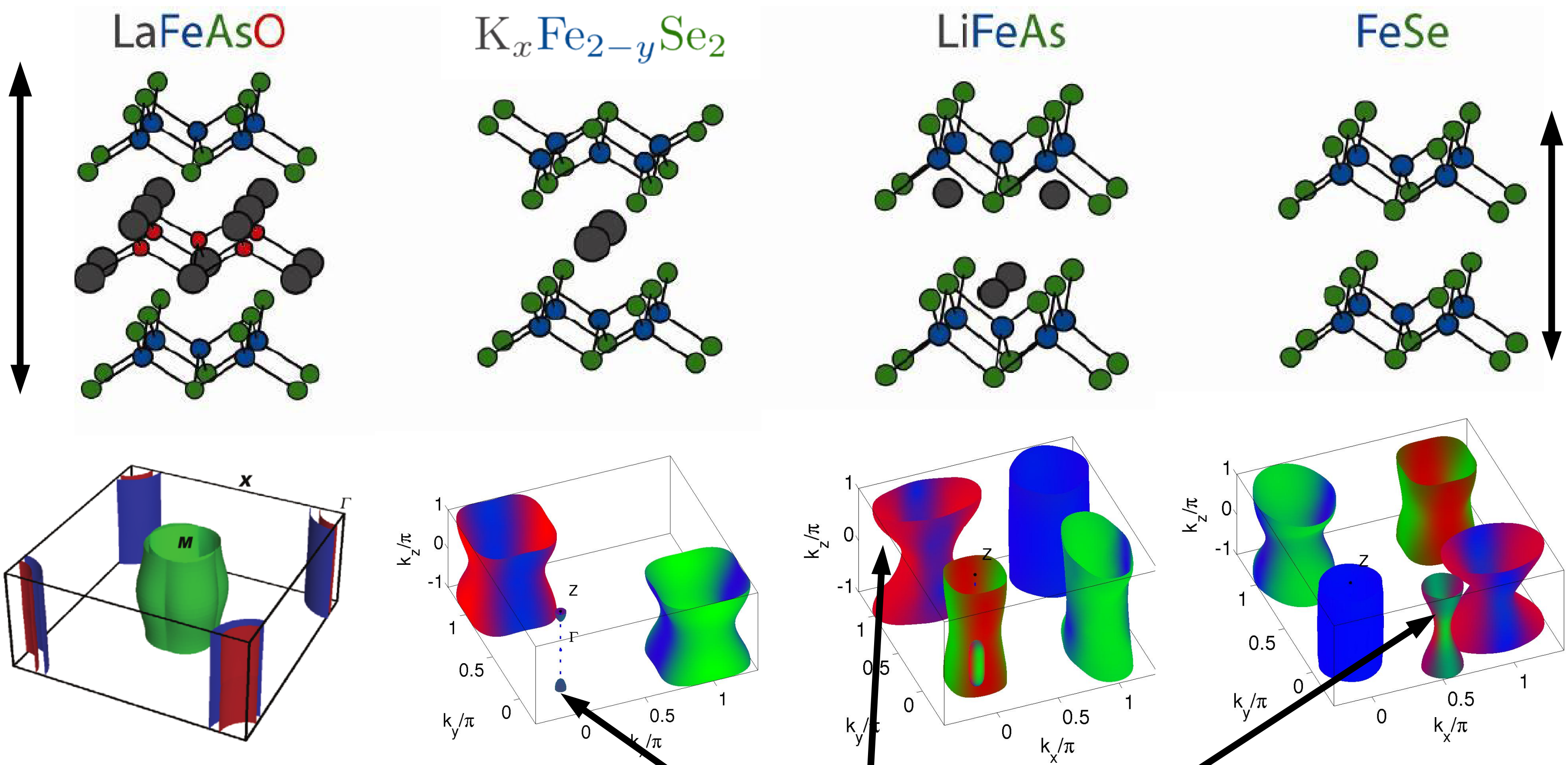
Motivation: Fe based superconductors: 2D vs. 3D

- Materials

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

$$H = H_0 + \bar{U} \sum_{i,\ell} n_{i\ell\uparrow} n_{i\ell\downarrow} + \bar{U}' \sum_{i,\ell'<\ell} n_{i\ell} n_{i\ell'}$$
$$+ \bar{J} \sum_{i,\ell'<\ell} \sum_{\sigma,\sigma'} c_{i\ell\sigma}^\dagger c_{i\ell'\sigma'}^\dagger c_{i\ell\sigma'} c_{i\ell'\sigma} + \bar{J}' \sum_{i,\ell'\neq\ell} c_{i\ell\uparrow}^\dagger c_{i\ell\downarrow}^\dagger c_{i\ell'\downarrow} c_{i\ell'\uparrow}$$

Kuroki *et al.* PRL (2008)

Spin fluctuation mediated pair scattering

- Susceptibility in normal state (orbital resolved)

$$\chi^0_{\ell_1\ell_2\ell_3\ell_4}(q) = -\frac{1}{2}\sum_{k,\mu\nu} M^{\mu\nu}_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{q})G^{\mu}(k+q)G^{\nu}(k).$$

- Interactions: RPA approximation

$$\chi^{\mathrm{RPA}}_{0\ell_1\ell_2\ell_3\ell_4}(q) = \frac{\chi_0}{1-U^s\chi_0} \quad \chi^{\mathrm{RPA}}_{1\ell_1\ell_2\ell_3\ell_4}(q) = \frac{\chi_0}{1+U^c\chi_0}$$

- Scattering vertex in singlet channel

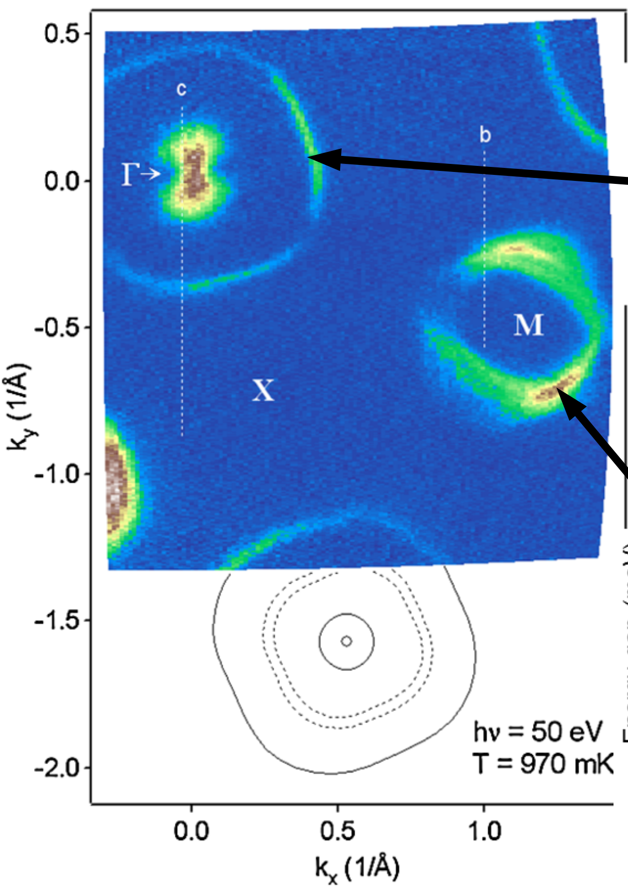
$$\Gamma_{ij}(\mathbf{k},\mathbf{k}') = \mathrm{Re}\sum_{\ell_1\ell_2\ell_3\ell_4} \tilde{M}^{ij}_{\ell_1\ell_2\ell_3\ell_4}\left[\frac{3}{2}\bar{U}^s\chi^{\mathrm{RPA}}_1(\mathbf{k}-\mathbf{k}',0)\bar{U}^s + \frac{1}{2}\bar{U}^s - \frac{1}{2}\bar{U}^c\chi^{\mathrm{RPA}}_0(\mathbf{k}-\mathbf{k}',0)\bar{U}^c + \frac{1}{2}\bar{U}^c\right]_{\ell_3\ell_4\ell_1\ell_2}$$

band space

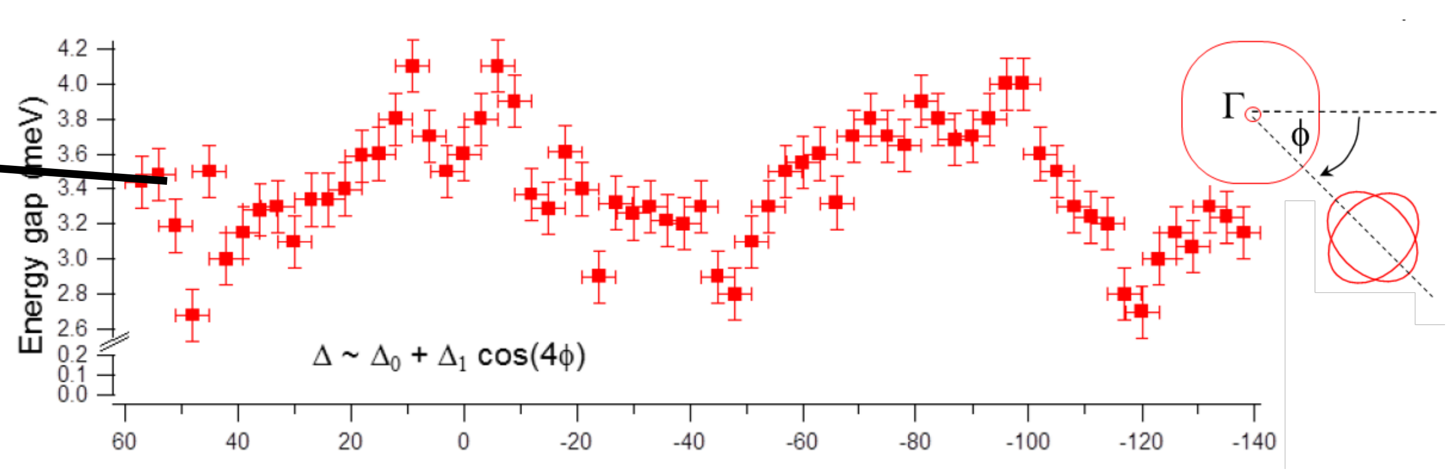
Graser *et al.* NJP (2009)

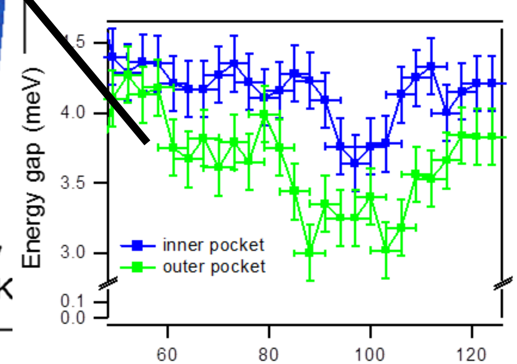
LiFeAs: Experimentally

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

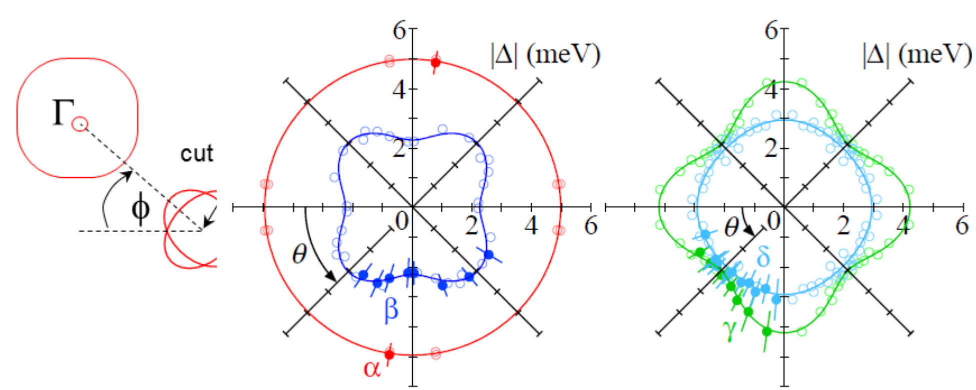


Borisenko *et al.* PRL (2010)



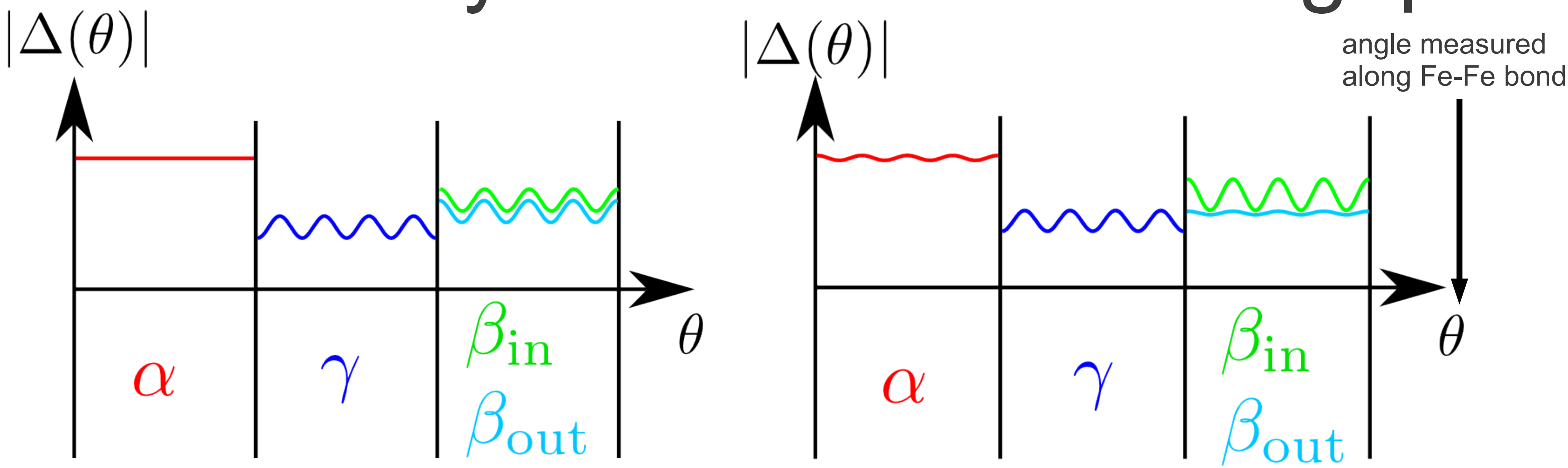


Borisenko *et al.* Symmetry (2012)



Umezawa *et al.* PRL (2012)

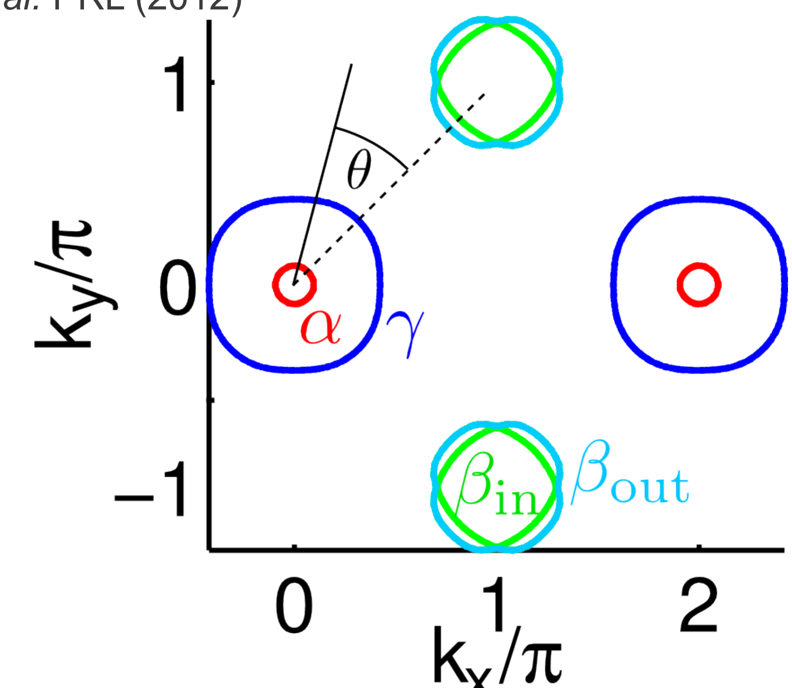
Summary: ARPES results for gap



Borisenko *et al.* Symmetry (2012)

Umezawa *et al.* PRL (2012)

- α pocket: large isotropic gap
- β pockets: “in-phase” gap
- γ pocket: minimum along Fe bond (θ=0)

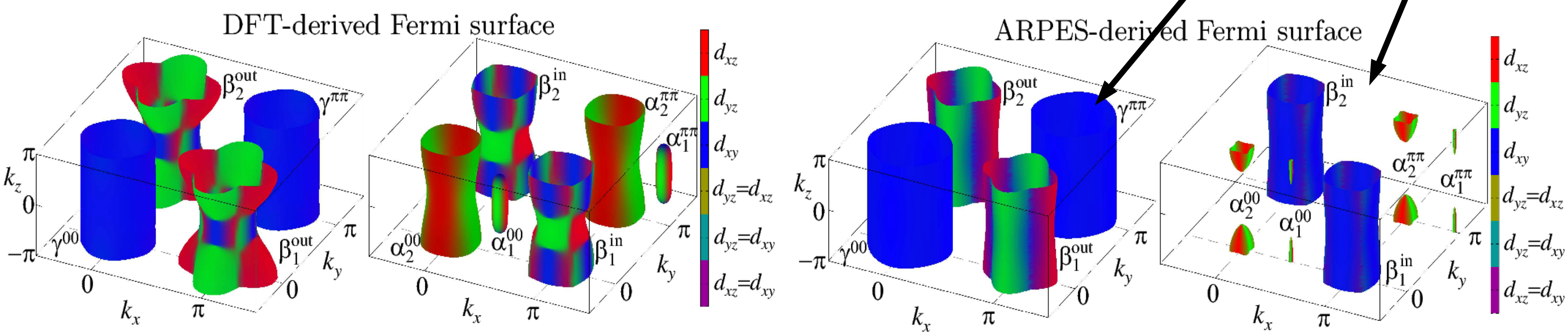


LiFeAs: Theoretically

- Fermi surface less nested than in other iron SC
  naïve: weak instability from spin-fluctuation theory
- Deviations between ARPES and DFT derived Fermi surface

"outer" sheets

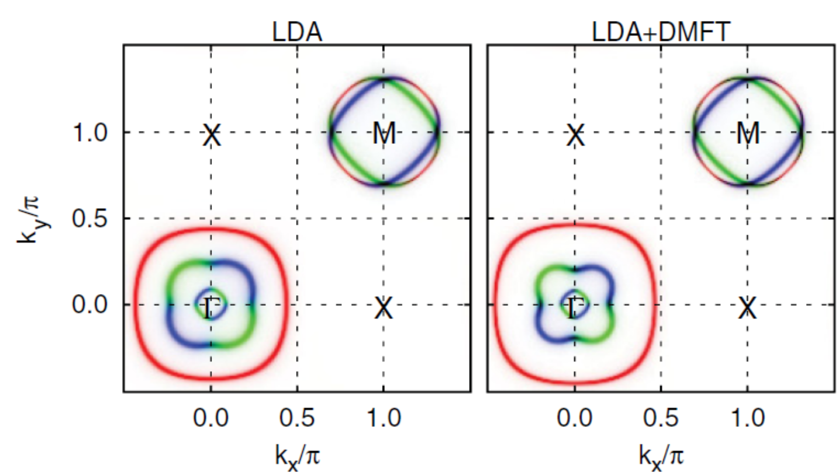
"inner" sheets



- 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)

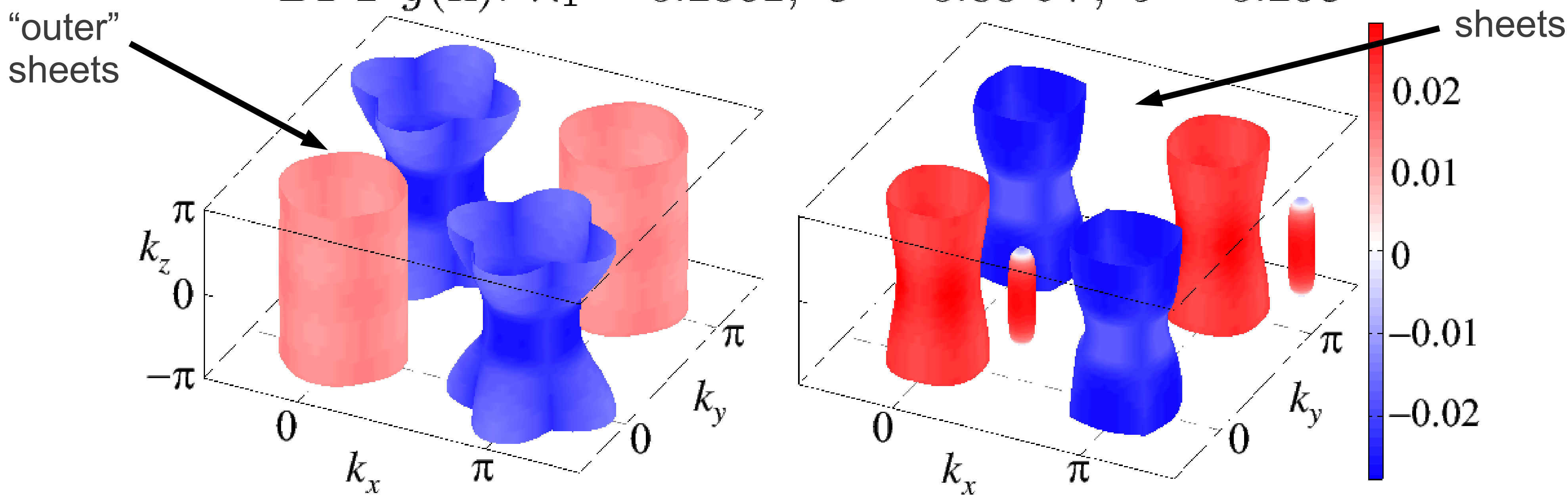
Spin-fluctuation pairing: DFT derived model

- Pairing strength by solution of linearized gap equation $-\frac{1}{V_G}\sum_j \int_{\mathrm{FS}_j} \Gamma_{ij}(\mathbf{k},\mathbf{k}')\frac{g_\alpha(\mathbf{k}')}{|v_{\mathrm{F}j}(\mathbf{k}')|} = \lambda_\alpha g_\alpha(\mathbf{k})$

  Sampling on 3D Fermi surface

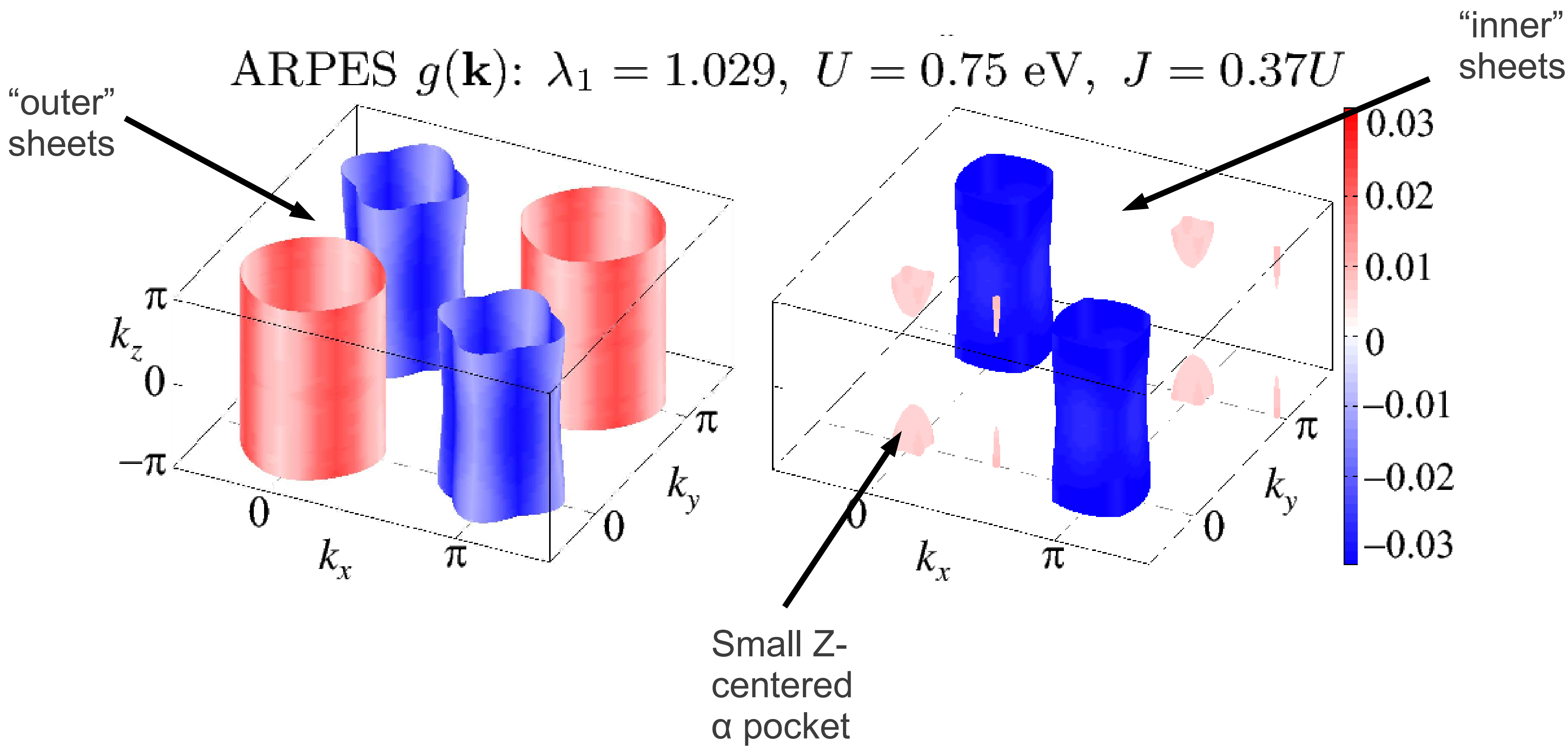
- s+/- wave for interactions close to the instability

DFT $g(\mathbf{k})$: $\lambda_1 = 0.2361,\ U = 0.88$ eV, $J = 0.25U$



Gapfunction: ARPES fitted tight binding model

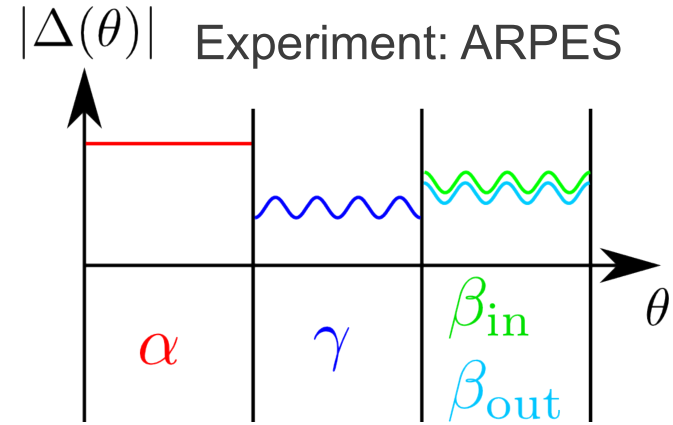
- s+/- wave for interactions close to instability



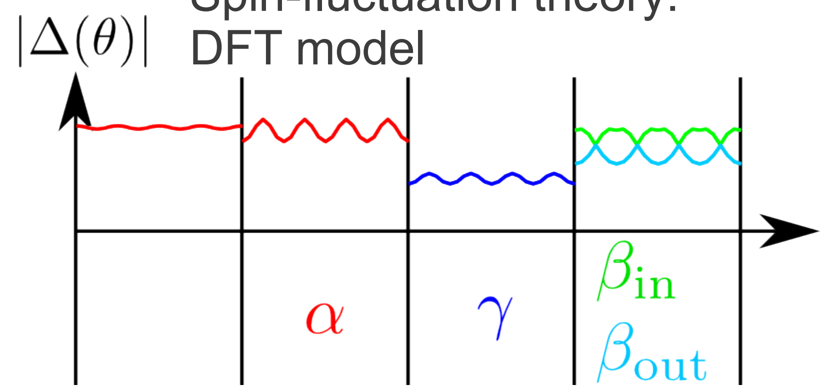
Comparison to experiments

	DFT model	ARPES derived model
Fermi surface	✗ (correlations?)	✓ (fit)
Superconducting gap	s +/-	s +/-
α pockets: large, isotropic	✓	✗
β pockets: intermediate size	✓	✓
"out of phase" oscillation	✗	✓ (at some k_z)
γ pockets: intermediate size	✓	✓
maxima of oscillation along Fe-Fe direction	✓	✓

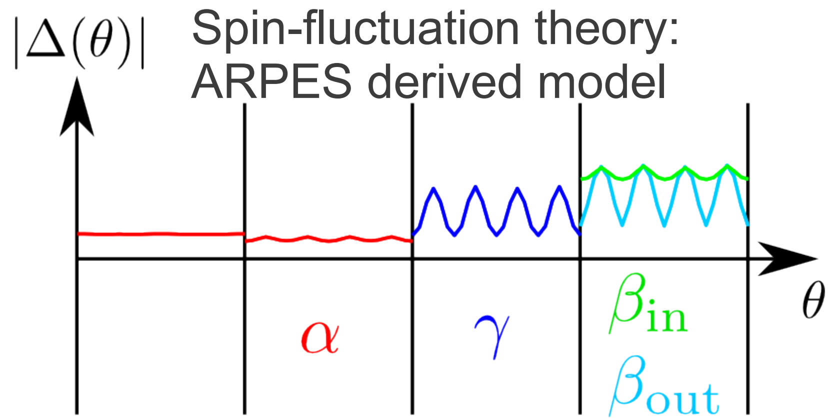
Experiment: ARPES



Spin-fluctuation theory: DFT model



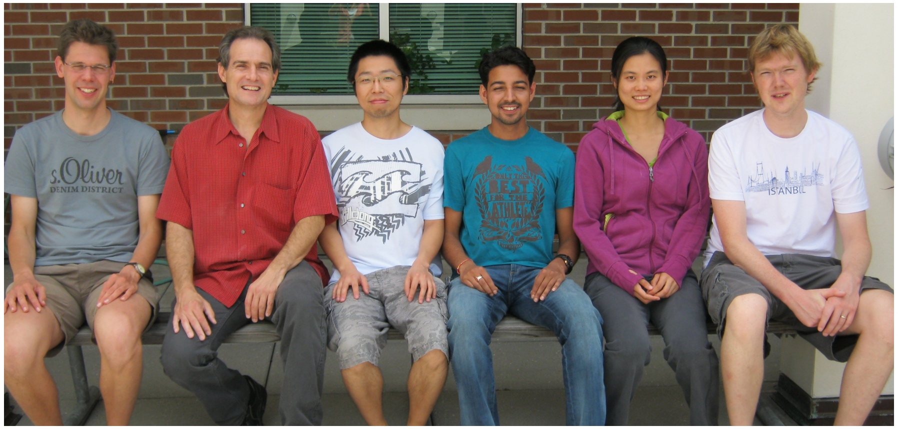
Spin-fluctuation theory: ARPES derived model



Conclusions

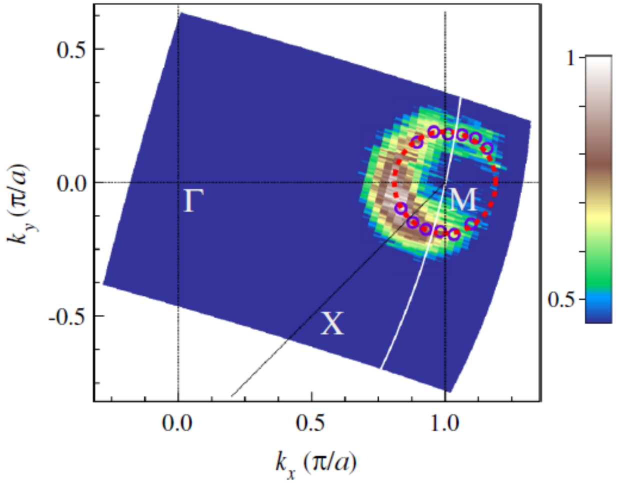
- Spin fluctuation pairing including 3D scattering
  - Fermi surface in LiFeAs less nested, but sign-changing s-wave gap
  - Gap magnitudes and phases mainly in agreement with results from ARPES experiments
  - ARPES fitted tight binding model: way to include effects of correlations
- Acknowledgments

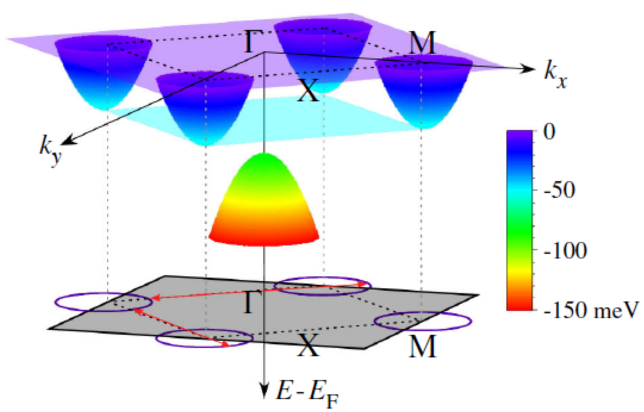


$K_xFe_{2-y}Se_2$

- Experimentally
  - Different phases
    - 245 vacancy phase   Ye *et al.* PRL (2011)
    - Pure SC phases $K_{0.6}Fe_2Se_2$, $K_{0.3}Fe_2Se_2$?   Ying *et al.* JACS (2013)
  - Absence of hole pocket?
  - Evidence for fully gapped SC state
    - Specific heat   Zeng *et al.* (2011)
    - ARPES   Mou *et al.* (2011)
    - Spin-lattice relaxation in NMR   Ma *et al.* (2011)





Quian *et al.* PRL (2011)

$K_xFe_{2-y}Se_2$:Spin-fluctuation pairing

- DFT calculation for KFe_2Se_2
- 5-orbital tight binding fit
- Suppression of hole pockets by adjustment of nearest neighbor hoppings 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