Spin fluctuation pairing and symmetry of order parameter in $K_xFe_{2-y}Se_2$

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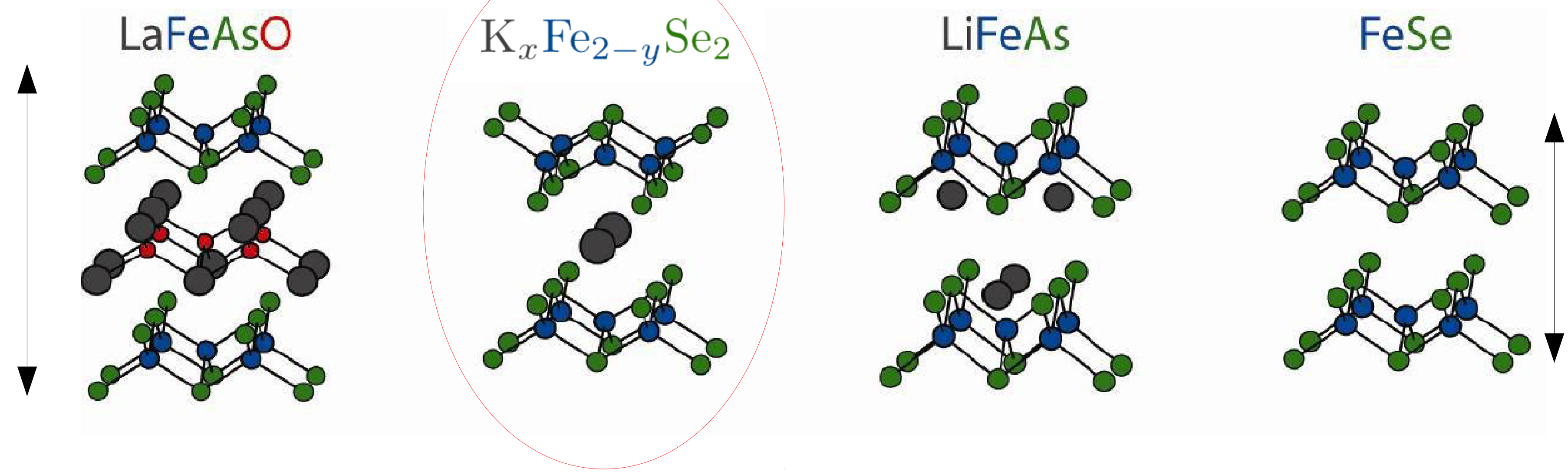
A.1 Fe based superconductors: Materials

- Materials

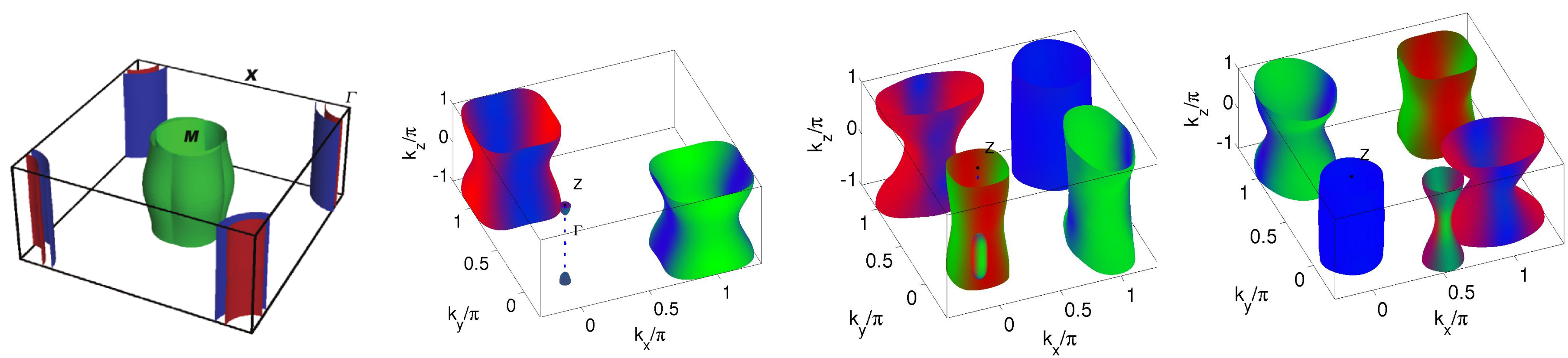
Crystal structure



	LaFeAsO	$K_xFe_{2-y}Se_2$	LiFeAs	FeSe
Tc	28 K (55 K for Sm)	38 K	18 K	8 K

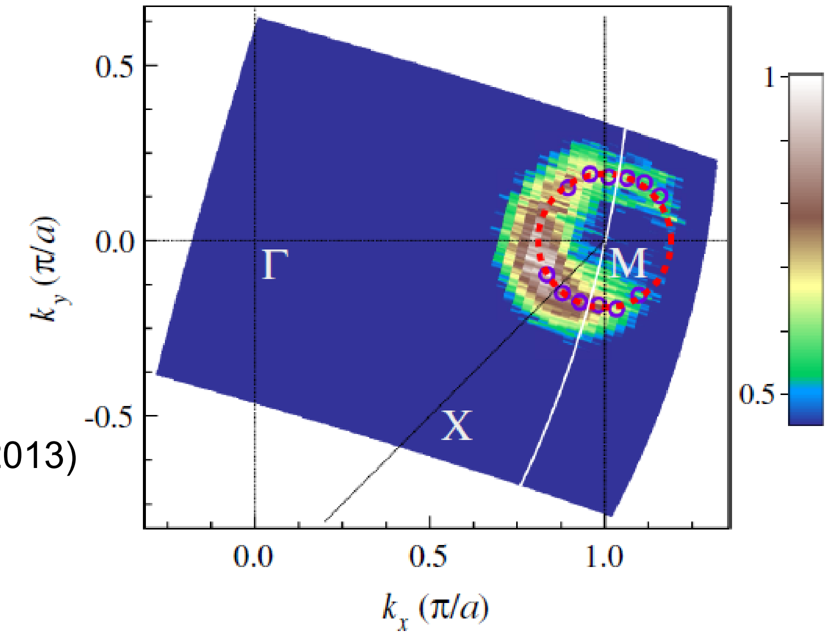
I4/mmm

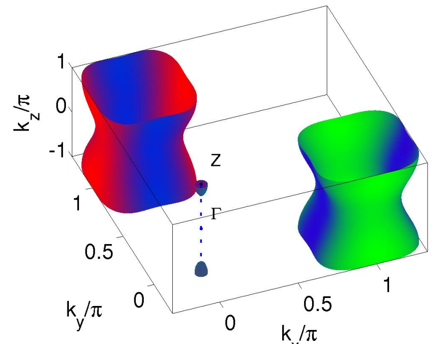
Fermi surface (DFT)

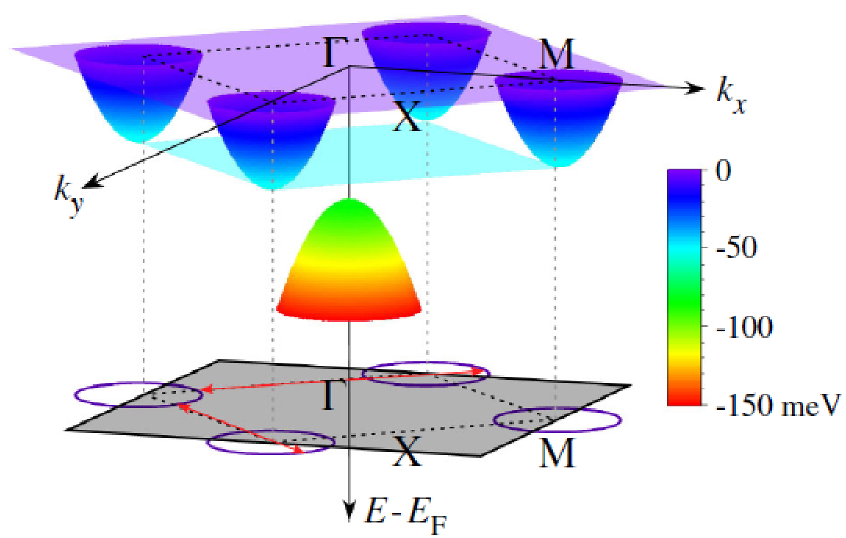


B.1 $K_xFe_{2-y}Se_2$

- 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)

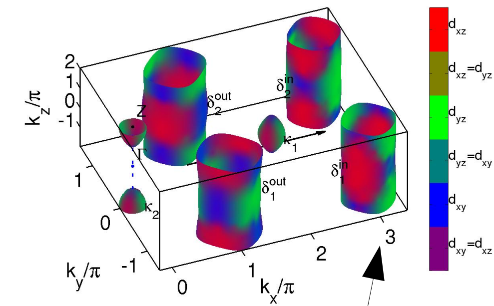






Quian *et al.* PRL (2011)

B.2 Model

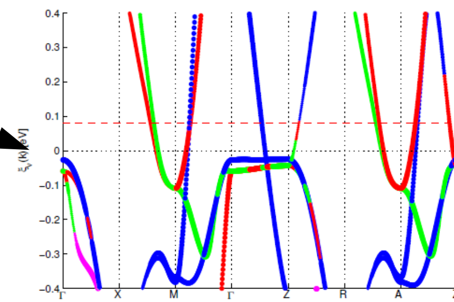


- 10 orbital tight binding band structure
  - DFT: Wien2K with *I4/mmm* for K-122
  - fully localized Wannier functions

Fermi surface
n=6.25
$K_{0.8}Fe_{1.7}Se_2$

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

no hole pocket



- Hubbard-Hund Hamiltonian

extended Hubbard model

$$H_{\rm int} = \bar{U}\sum_{i,\ell} n_{i\ell\uparrow}n_{i\ell\downarrow} + \bar{U}'\sum_{i,\ell'<\ell} n_{i\ell}n_{i\ell'}$$

pair hopping

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

exchange
interaction

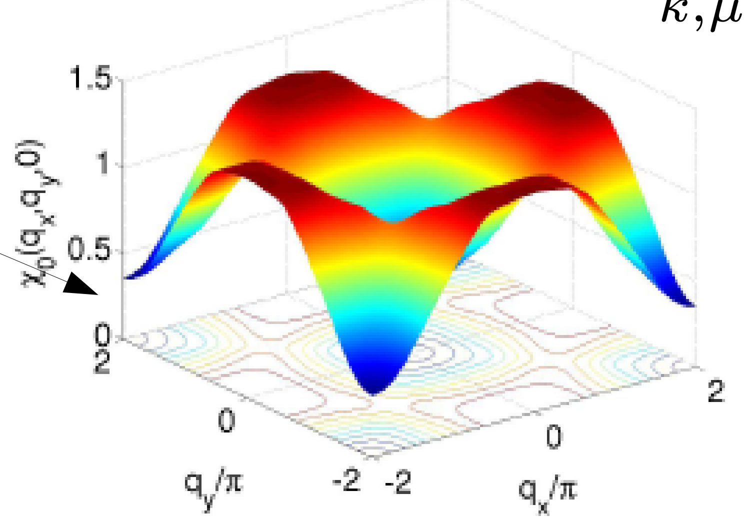
Kuroki *et al.* PRL (2008)

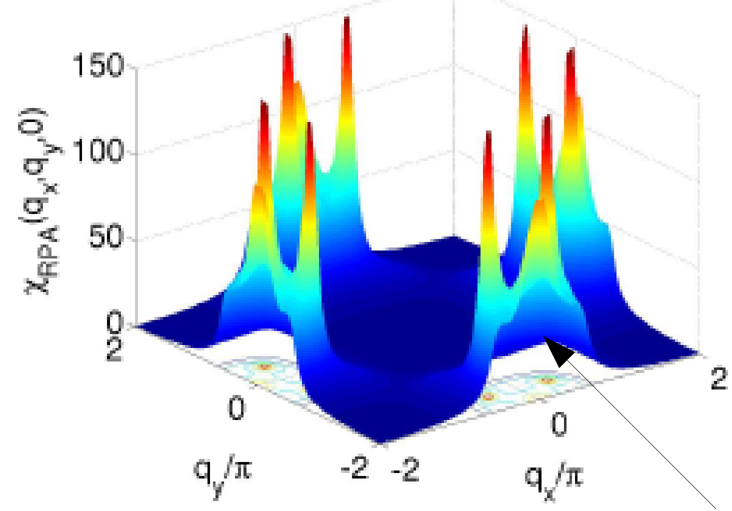
B.3 Fluctuation exchange mediated pair scattering

- Susceptibility in normal state (orbital resolved)

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

periodic with 1 Fe zone





peaked at Q=(1.65,0.35)π

- Interactions: RPA approximation spin and charge susceptibilities

$$\chi_0^{\rm RPA}(q) = \frac{\underline{\chi}^0(q)}{1 - U^s\underline{\chi}^0(q)} \qquad \chi_1^{\rm RPA}(q) = \frac{\underline{\chi}^0(q)}{1 + U^c\underline{\chi}^0(q)}$$

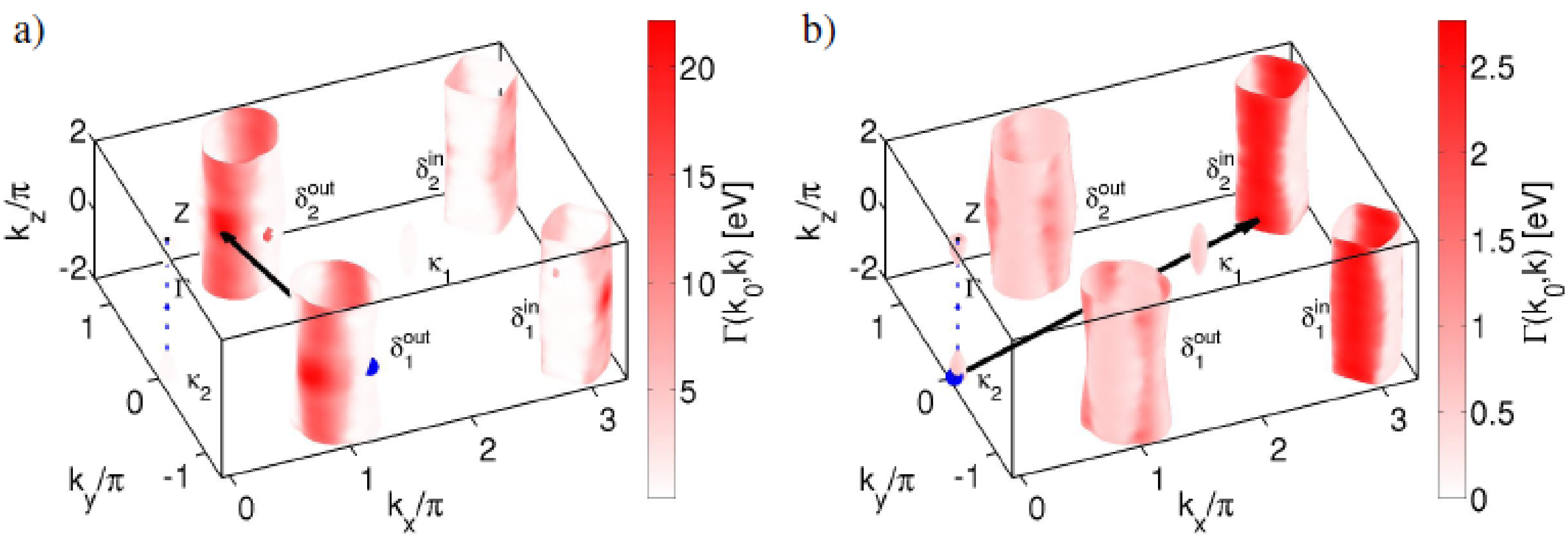
B.4 Spin fluctuation mediated pair scattering

- Scattering vertex in singlet channel

$$\Gamma_{ij}(\mathsf{k},\mathsf{k}') = \mathrm{Re} \sum_{\ell_1\ell_2\ell_3\ell_4} \tilde{M}^{ij}_{\ell_1\ell_2\ell_3\ell_4} \left[\frac{3}{2}\bar{U}^s \chi_1^{\mathrm{RPA}}(\mathsf{k}-\mathsf{k}',0)\bar{U}^s + \frac{1}{2}\bar{U}^s - \frac{1}{2}\bar{U}^c \chi_0^{\mathrm{RPA}}(\mathsf{k}-\mathsf{k}',0)\bar{U}^c + \frac{1}{2}\bar{U}^c\right]_{\ell_1\ell_2\ell_3\ell_4}$$

band space

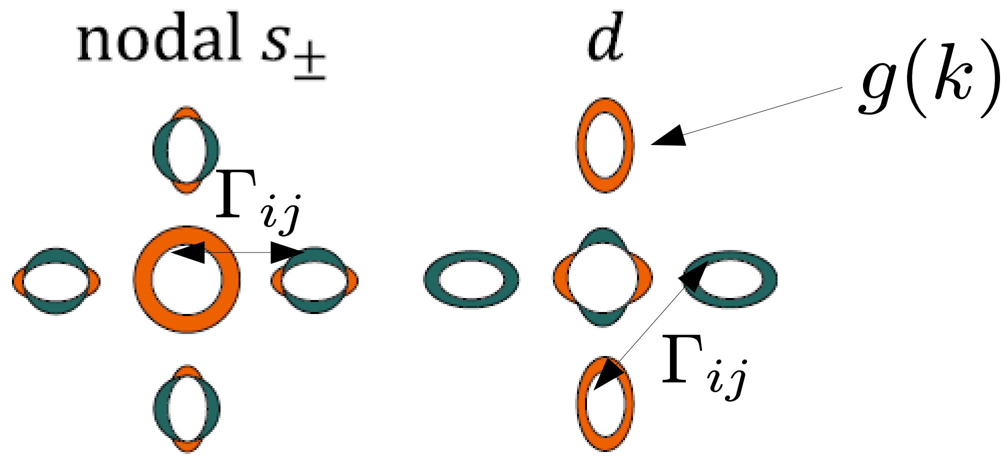
Graser *et al.* NJP (2009)



B.5 Gap equation

- Decompose gap function into magnitude and dimensionless symmetry function

$$\Delta_k = \Delta g(k)$$

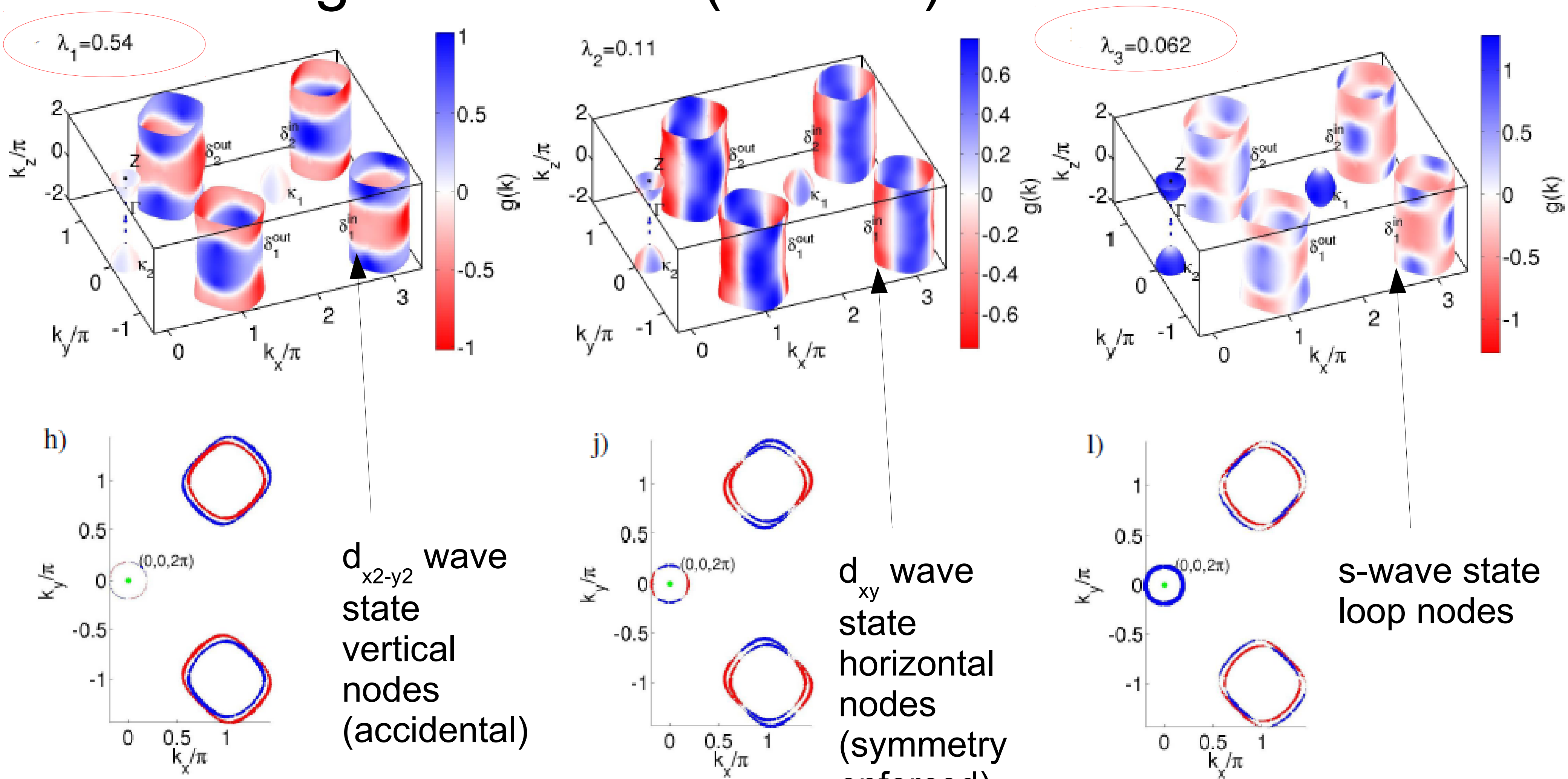


- Pairing strength functional
- variation leads to eigenvalue equation

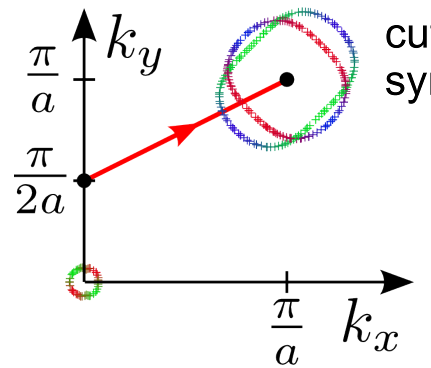
$$\lambda_\alpha g_\alpha(k) = -\sum_i \oint_{C_j} \frac{dk'}{(2\pi)^2 v_F(k')} \Gamma_{ij}(k,k') g_\alpha(k')$$

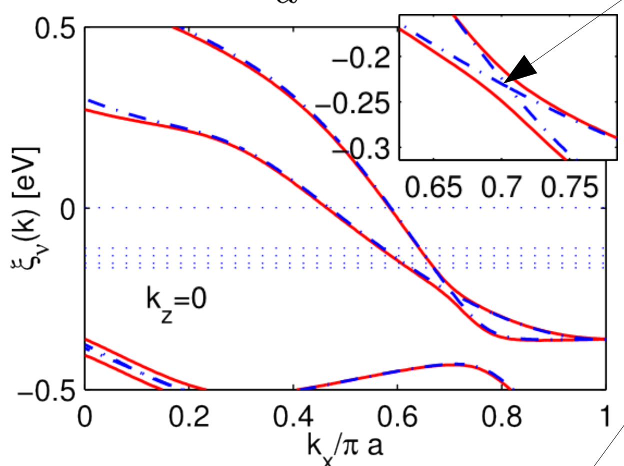
B.5 Gap function (3D calculation)

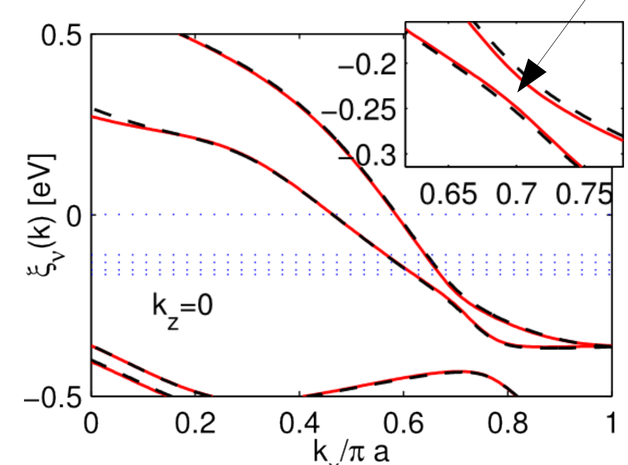
- leading instabilities (n=6.25)



C.1 Hybridization in $K_xFe_{2-y}Se_2$





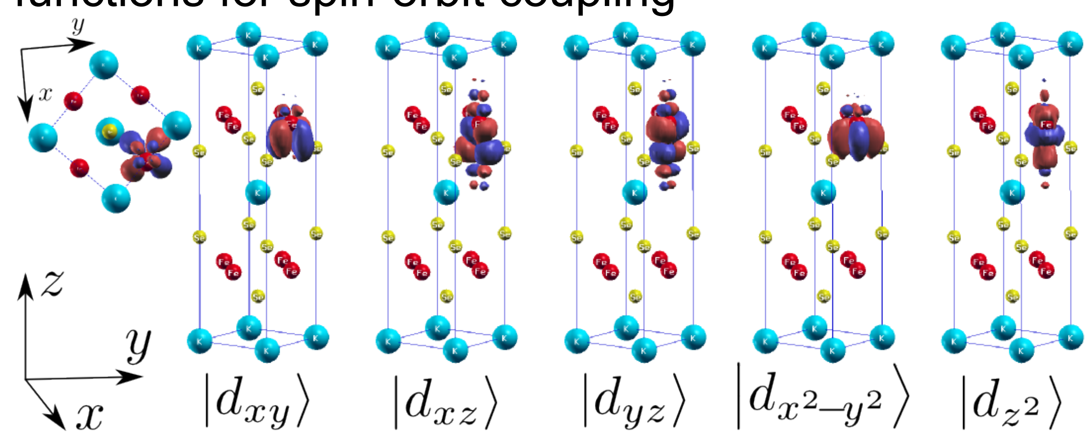


- Origin of hybridization
  - DFT (blue, dash dotted): *I4/mmm* space group (tiny!)
  - DFT + spin-orbit coupling (red)
  - tight-binding + spin-orbit (black, dashed)

$$H_{\rm SO} = \lambda^{3d}_{\rm Fe} \sum_i \sum_{\alpha=x,y,z} L_i^\alpha S_i^\alpha$$

Friedel ('64)

approximate with atomic wave functions for spin-orbit coupling

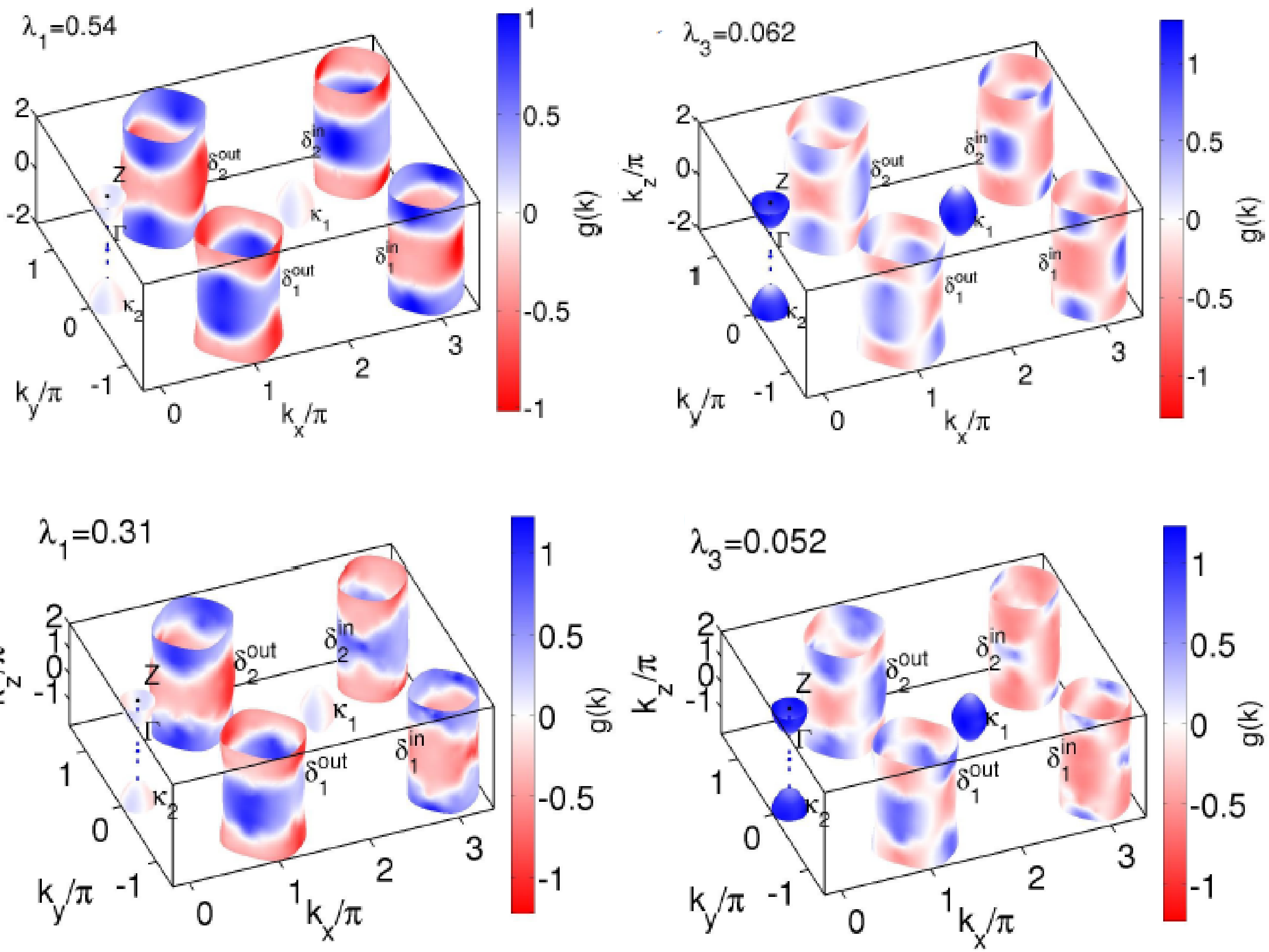


C.2 Gap function with spin-orbit coupling

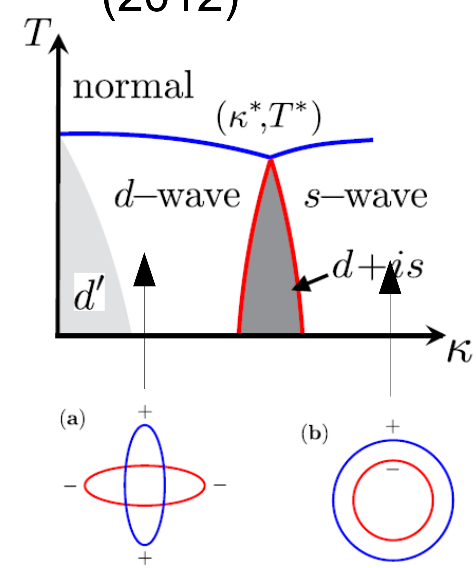
- weakening of superconducting instability
  (all symmetries)

no spin-orbit coupling

spin-orbit coupling (λ=0.05 eV)



Khodas, Chubukov PRL (2012)



$$\kappa_{\text{eff}} \simeq \frac{\delta\xi}{\langle \frac{\Delta\xi_k}{v_F(k)k_F(k)} \rangle} = \frac{\text{hybridization}}{\text{ellipticity}}$$

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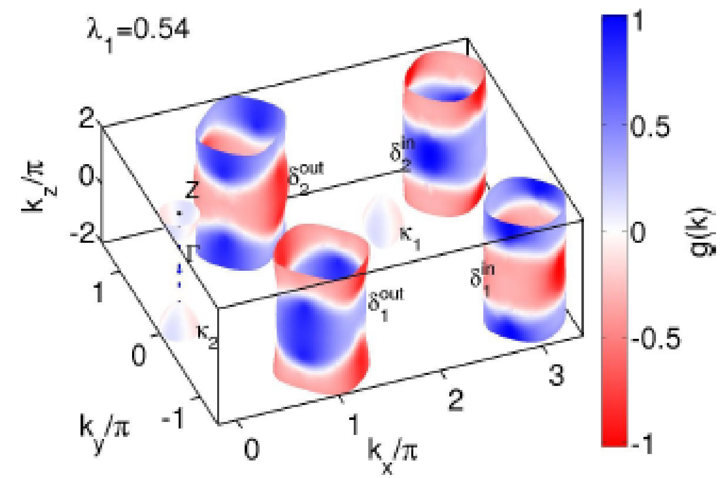
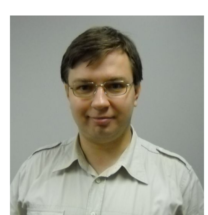
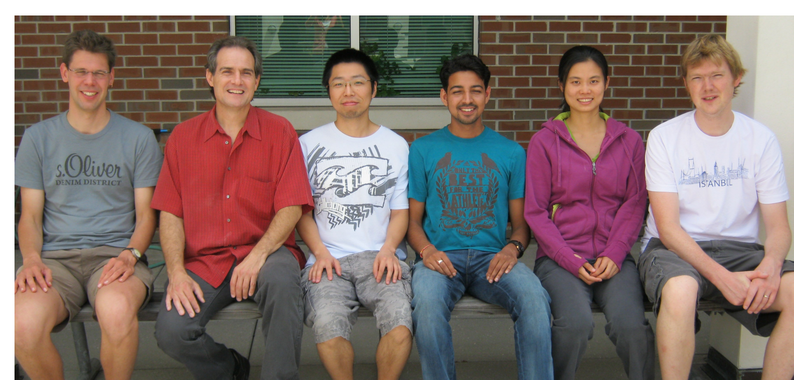
D Summary

- $K_xFe_{2-y}Se_2$ different from other Fe based SC
- missing hole-pocket makes s-wave instability less likely (spin-fluctuation theory), dominant d_{x2-y2} wave symmetry
- quasinodes (vertical or horizontal)
- small hybridization regime
  also with spin-orbit coupling
- differences to experimental results
  - small effect of Z-centered hole pockets
  - quasinodal behavior makes detection difficult
  - missing ingredients as correlations or deviations from normal-state properties due to doping / impurities



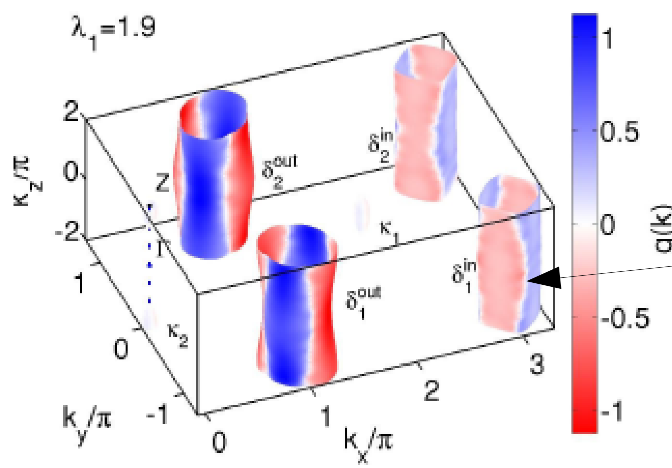
- **acknowledgements**





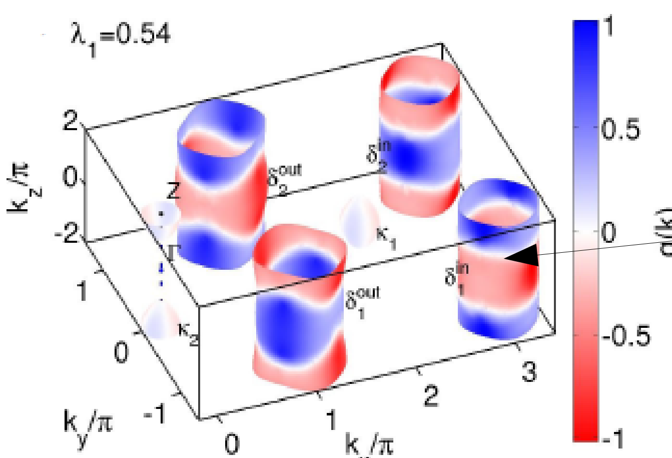
B.5 Gap function doping dependence

- underdoped case (n=6.12)



d_{x2-y2} wave state horizontal nodes (accidental)

- overdoped case (n=6.25)



d_{x2-y2} wave state vertical nodes (accidental)

C.1 Hybridization effects

- Transition from d to s-wave

Khodas, Chubukov PRL (2012)

$$\kappa_{\mathrm{eff}} \simeq \frac{\delta\xi}{\left\langle \frac{\Delta\xi_{\mathsf{k}}}{v_{\mathrm{F}}(\mathsf{k})k_{\mathrm{F}}(\mathsf{k})} \right\rangle} = \frac{\text{hybridization}}{\text{ellipticity}}$$