SPIN FLUCTUATION MEDIATED PAIRING IN AFE_2SE_2 AND ITS CONSEQUENCES

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International workshop on recent developments in Fe-based high-temperature superconductors,
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Center for Nanophase Materials Sciences
AT OAK RIDGE NATIONAL LABORATORY

OUTLINE

AFe_2Se_2

- What is the weak-coupling prediction for the pairing state?
- What is the effect of hybridization (spin-orbit coupling)?
- Can neutron scattering distinguish different pairing states?

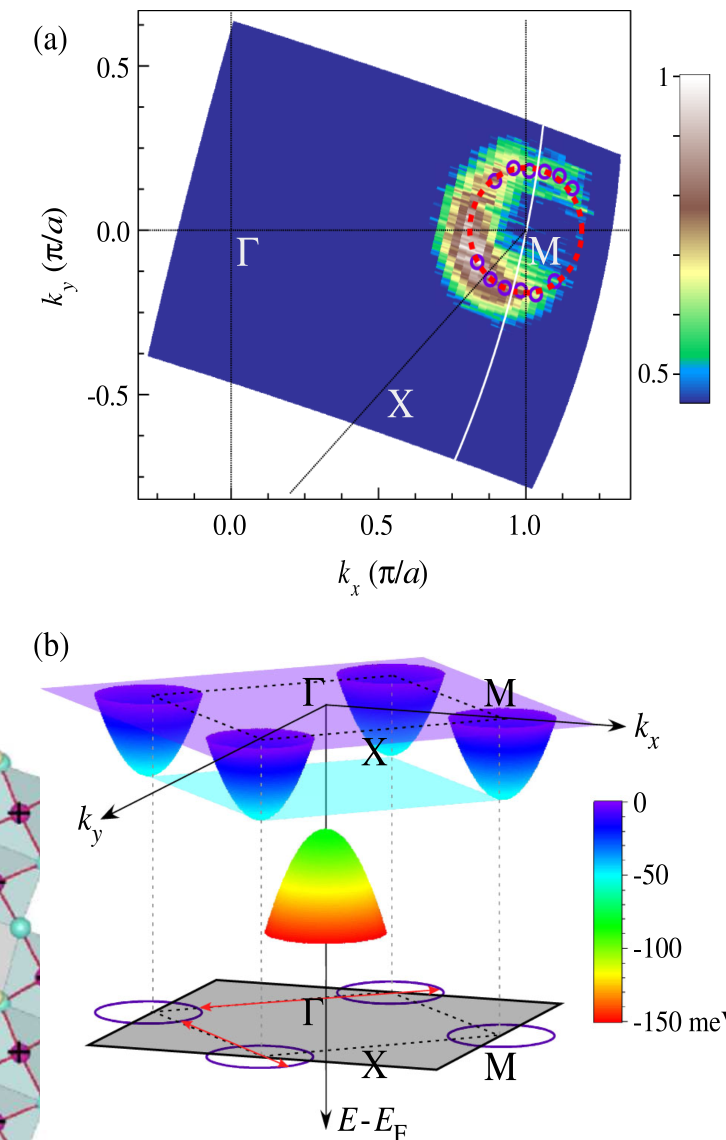
cf. M. Khodas' talk yesterday

Kreisel, Wang, Maier, Hirschfeld & Scalapino, arXiv:1308.5683

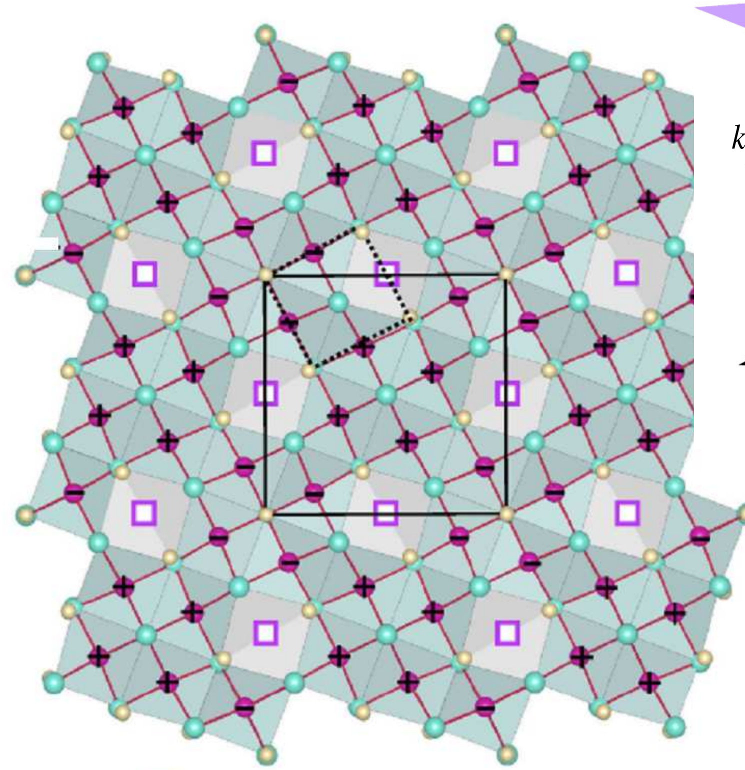
KFe_2Se_2 – Qualitatively Different?

- ARPES
  - No hole pockets, only electron pockets around M
  - Simple spin-fluctuation arguments for $s^{\pm}$ don't work
- Neutron scattering
  - 245 Fe vacancy phase
  - Insulating 2 x 2 block AF state with $\mu=3.31\mu_B$/Fe and T_N = 559 K
- STM, etc.
  - Evidence for phase separation between SC and AF phases

Qian *et al.*, PRL 2011



Bao *et al.*, CPL 2011

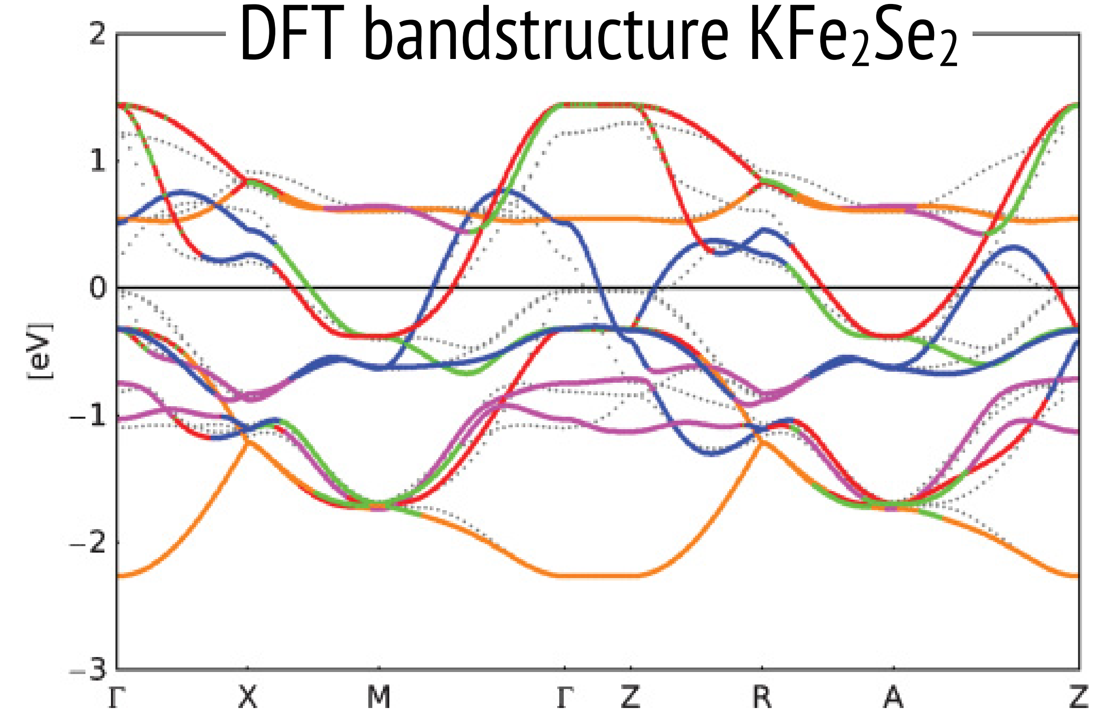


□ Fe vacancy order site

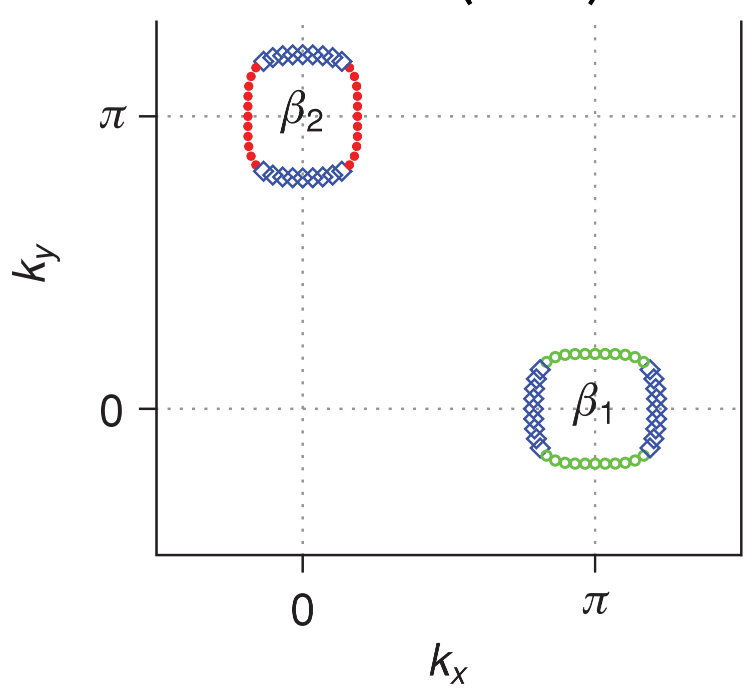
Itinerant - weak coupling - RPA approach

- Models and pairing calculations
  - DFT bandstructure calculation for KFe_2Se_2
  - 5- and 10-orbital tight-binding fits
  - Use RPA to calculate $\chi(q)$, pairing interaction $\Gamma(k,k')$ and superconducting gap $\Delta(k)$

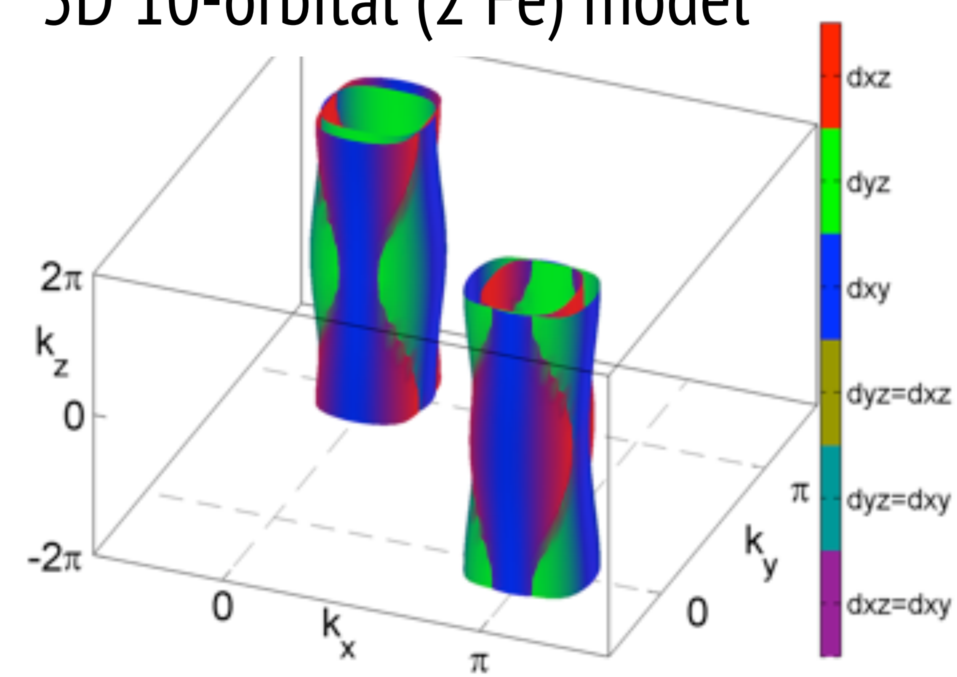
DFT bandstructure KFe_2Se_2



2D 5-orbital (1 Fe) model



3D 10-orbital (2 Fe) model



RPA Theory I

- Microscopic Hamiltonian – Multi-orbital Hubbard-Hund model

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

Multi-orbital tight-binding model obtained from fitting LDA bandstructure

Intra- and inter-orbital Coulomb interactions

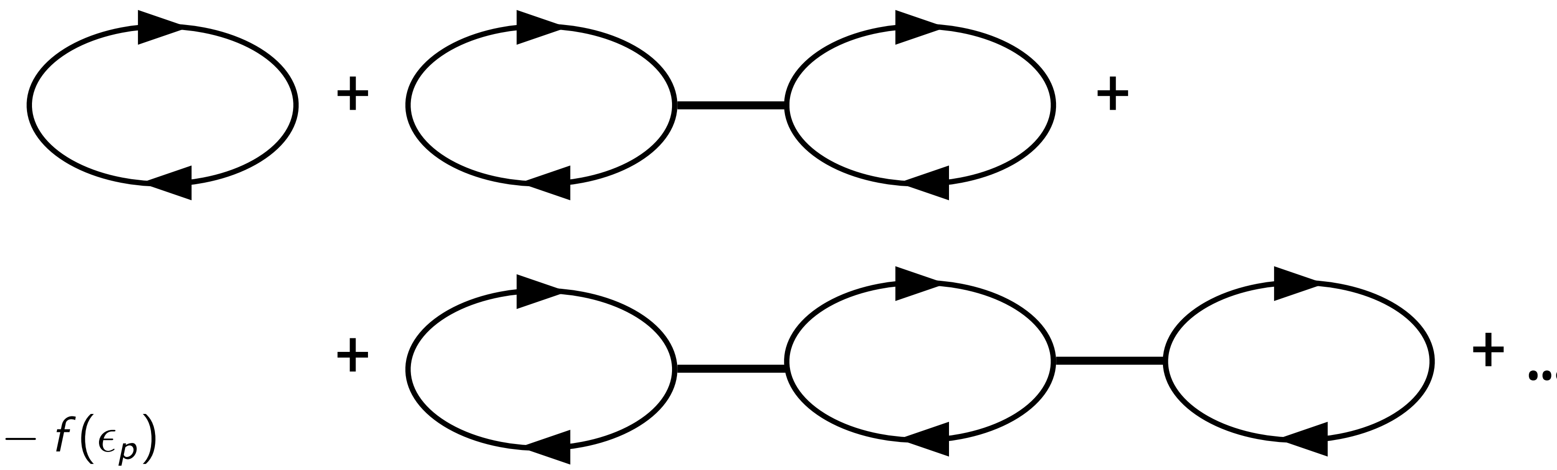
Hund's rule coupling

Pair-hopping term

– Spin rotation invariant parameters: U = U'+J+J'
– Typical values: U ~ 1 eV, U' ~ 0.5 eV, J = J' ~ 0.25 eV

Spin Fluctuation Theory of Pairing – Random phase approximation

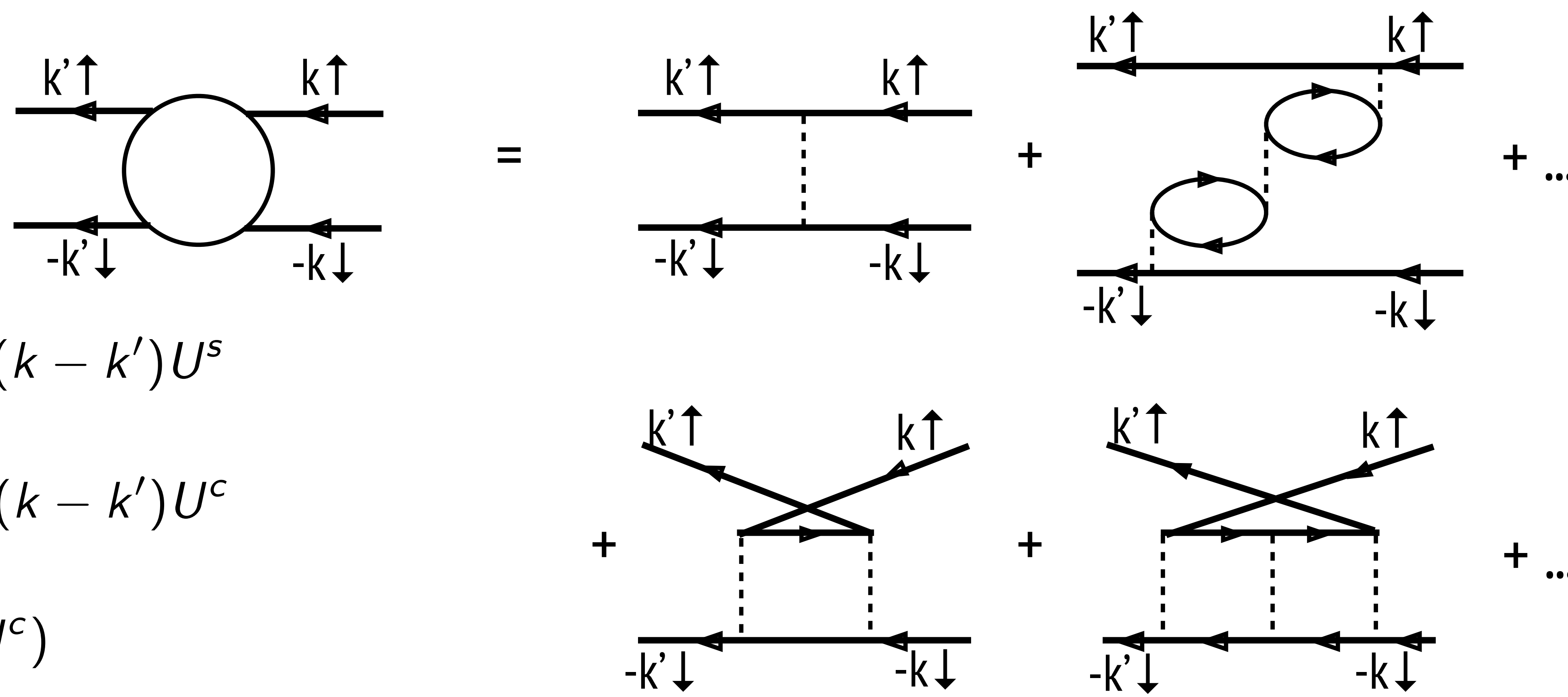
- Spin/Charge Susceptibility



$$\chi_{RPA}(q,\omega) = \frac{\chi_0(q,\omega)}{1 \pm U\chi_0(q,\omega)}$$

$$\chi_0(q,\omega) = \int \frac{d^3p}{(2\pi)^3} \frac{f(\epsilon_{p+q}) - f(\epsilon_p)}{\omega - (\epsilon_{p+q} - \epsilon_p) + i\delta}$$

- Pairing interaction Berk, Schrieffer 1966



$$\Gamma(k,k') = \frac{3}{2} U^s \chi^s_{RPA}(k-k') U^s - \frac{1}{2} U^c \chi^c_{RPA}(k-k') U^c + \frac{1}{2}(U^s + U^c)$$

... RPA Theory

- Pairing of electrons in Bloch states

$$\Gamma_{ij}(k,k') = Re \sum_{\ell_1\ell_2\ell_3\ell_4} a_{\nu_i}^{\ell_2,*}(k) a_{\nu_i}^{\ell_3,*}(-k) \Gamma_{\ell_1\ell_2\ell_3\ell_4}(k,k',\omega=0) a_{\nu_j}^{\ell_1}(k') a_{\nu_j}^{\ell_4}(-k')$$

- Pairing strength for SC gap

$$\lambda[g(k)] = -\frac{\sum_{ij} \oint_{C_i} \frac{dk_\parallel}{v_F(k)} \oint_{C_j} \frac{dk'_\parallel}{v_F(k')} g(k) \Gamma_{ik}(k,k') g(k')}{(2\pi)^2 \sum_i \oint_{C_i} \frac{dk_\parallel}{v_F(k)} [g(k)]^2}$$

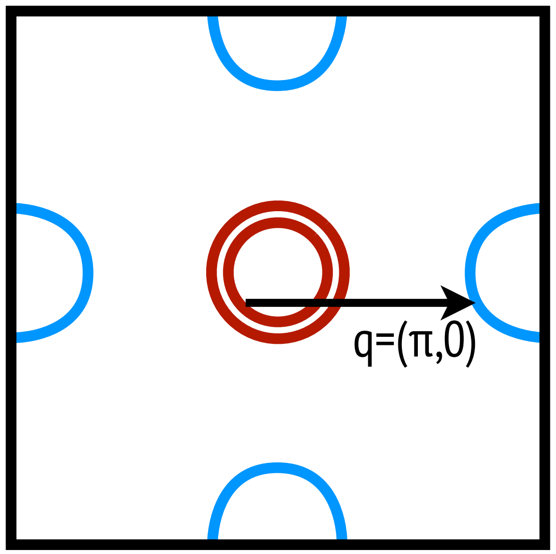
- Gap equation from stationarity

$$-\sum_j \oint_{C_j} \frac{dk'_\parallel}{2\pi} \frac{1}{2\pi v_F(k')} \Gamma_{ij}(k,k') g(k') = \lambda g(k)$$

↑

=SC gap at T=T_c

Neutron resonance within RPA



- Neutron Resonance
  - Spin susceptibility in superconducting state

$$\chi \sim GG + FF$$

  - BCS coherence factor

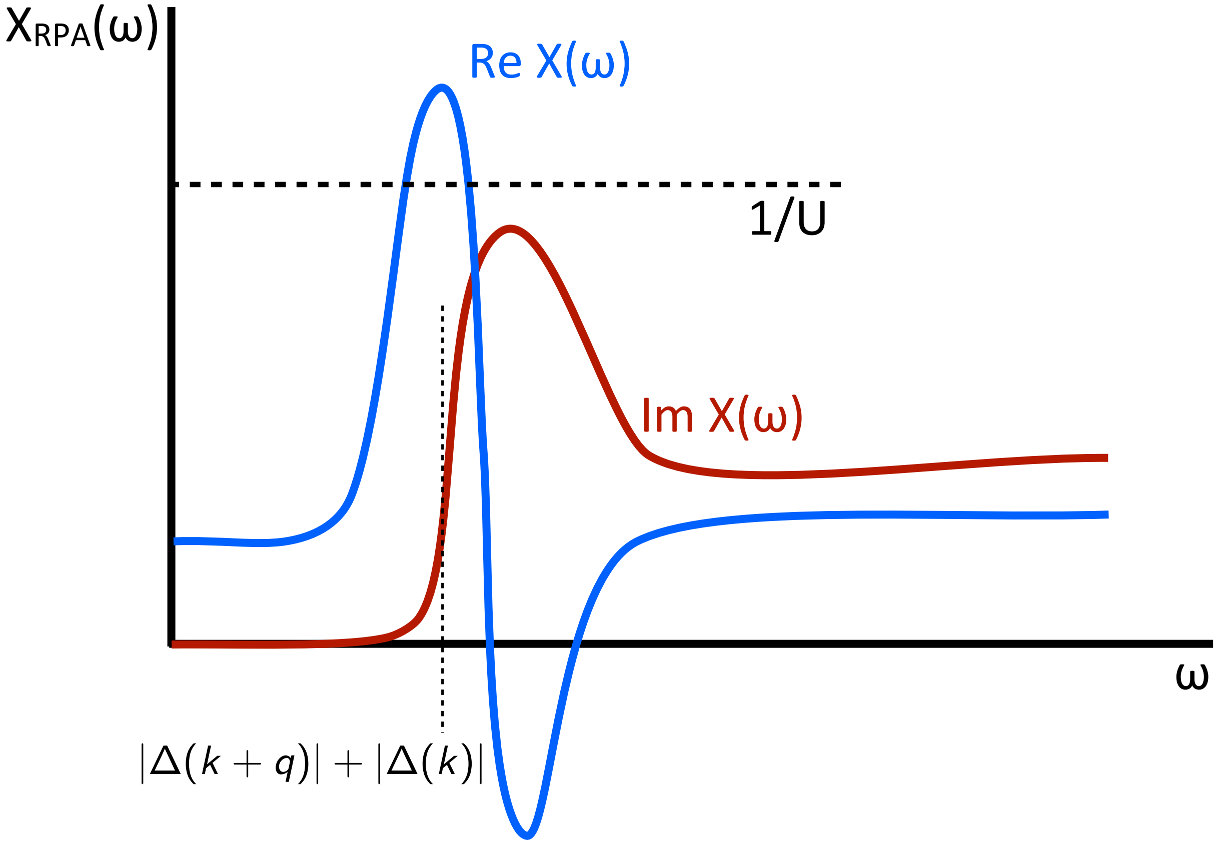
$$1 - \frac{\Delta(k+q)\Delta(k)}{E(k+q)E(k)}$$

  - Resonance in χ”(q,ω) at q when

$$\Delta(k+q)\Delta(k) < 0$$

at $\omega \lesssim |\Delta(k+q)| + |\Delta(k)|$

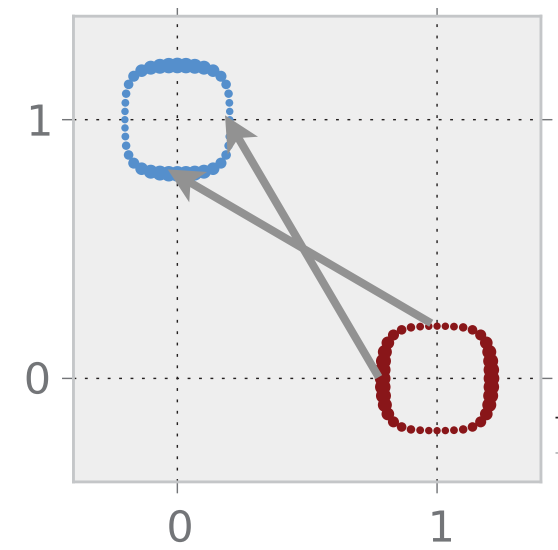
$$\chi_{RPA}(\omega) = \frac{\chi(\omega)}{1 - U\chi(\omega)}$$



Bulut & Scalapino ’93

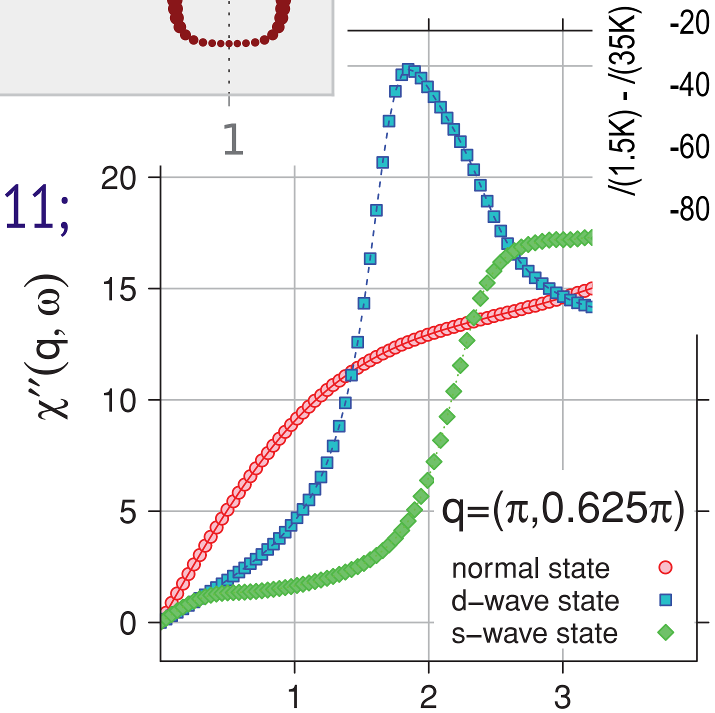
Predictions from 5-orbital (1 Fe) model

- Superconducting gap
  - Strong scattering between opposite sides of electron pockets leads to nodeless d-wave gap

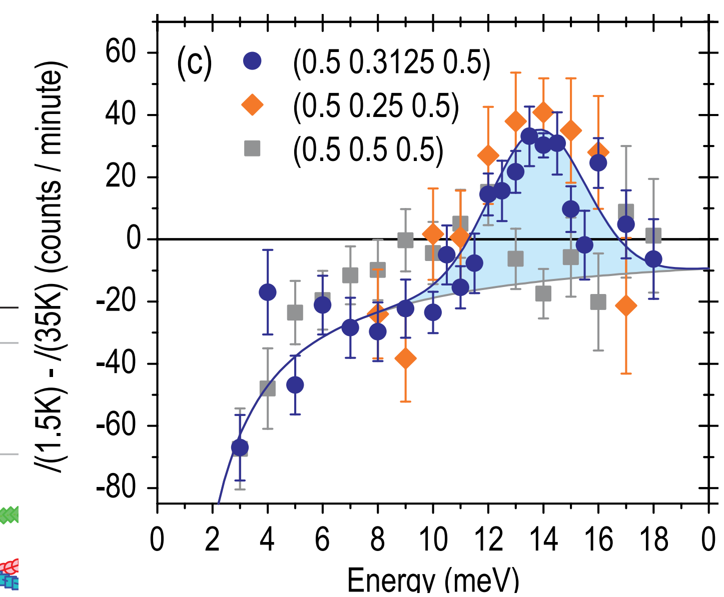


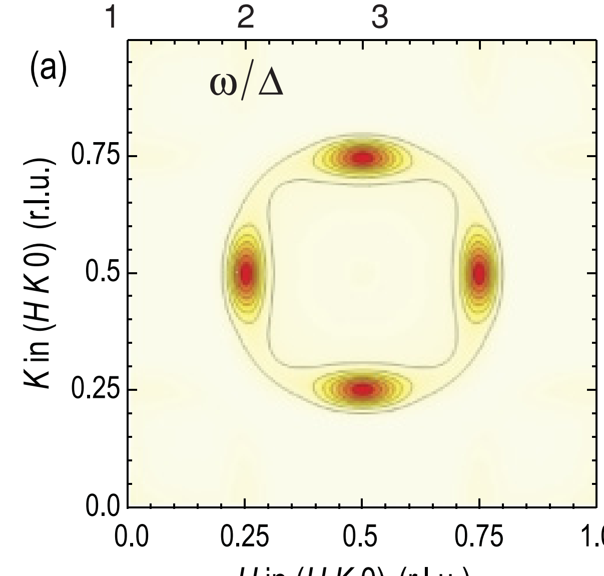
- Neutron scattering
  - Neutron resonance near Q_{res}~(π,0.5π)
  - Elliptic momentum structure
  - Resonance disperses upward in energy away from Q_{res}
  - Excellent agreement with experiments

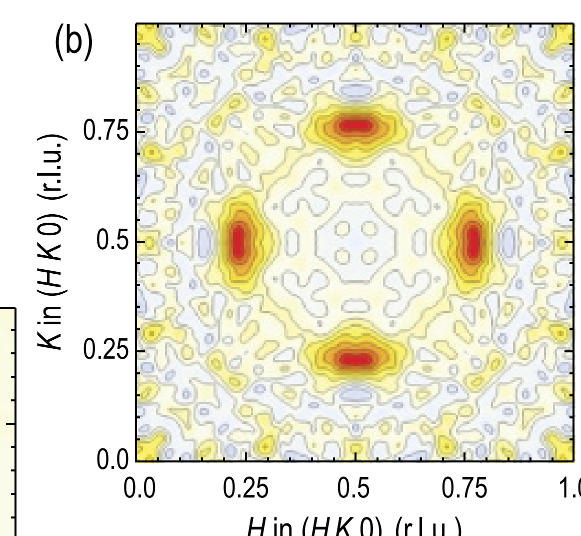
Maier et al., PRB 2011; ibid 2012



Park et al., PRL 2011







Friemel et al., PRB 2012

122 symmetry and d-wave gap nodes

PHYSICAL REVIEW B **84**, 024529 (2011)

Symmetry analysis of possible superconducting states in $K_xFe_ySe_2$ superconductors

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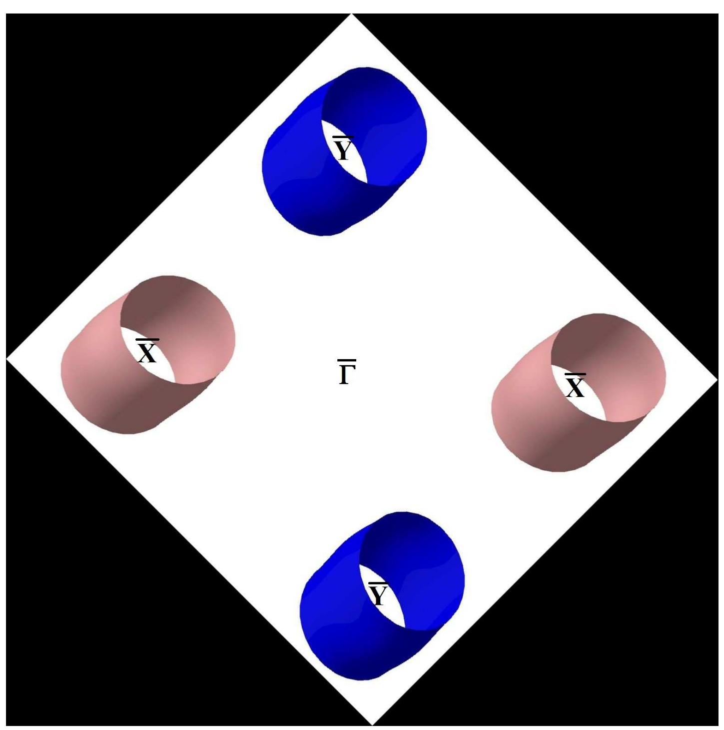
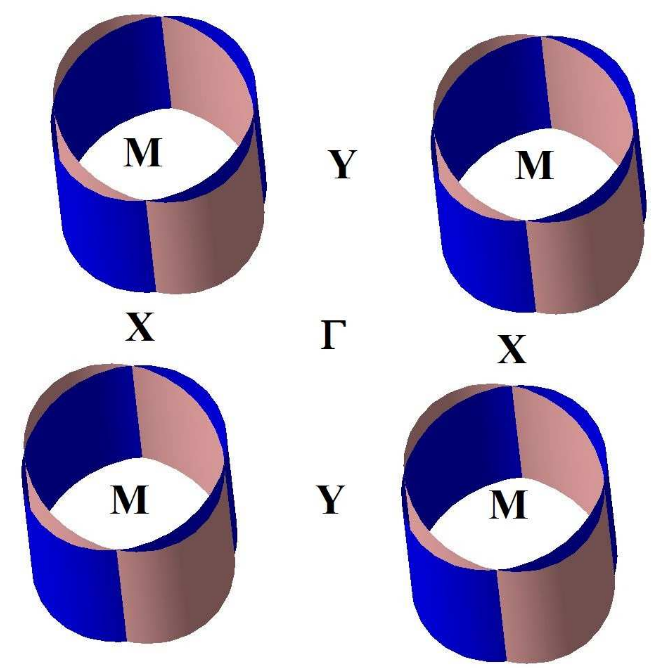
(Received 4 May 2011; revised manuscript received 8 June 2011; published 25 July 2011)

d-wave in unfolded zone develops nodes after folding



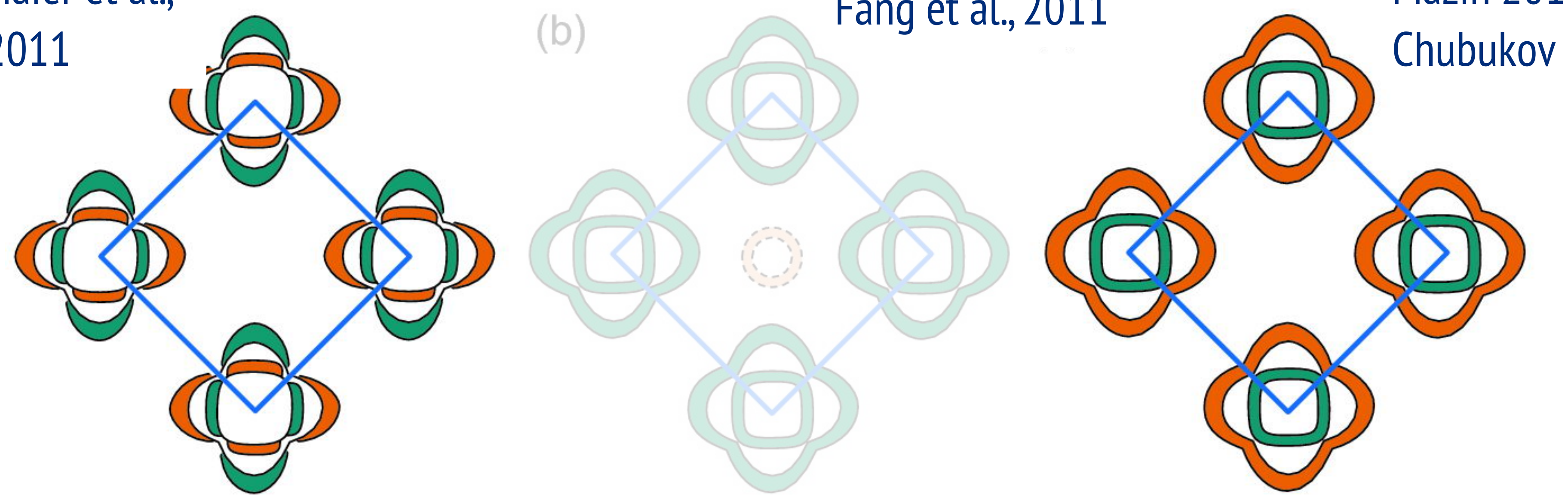


Possible gap structures

Fang et al., Maier et al., Saito et al., 2011

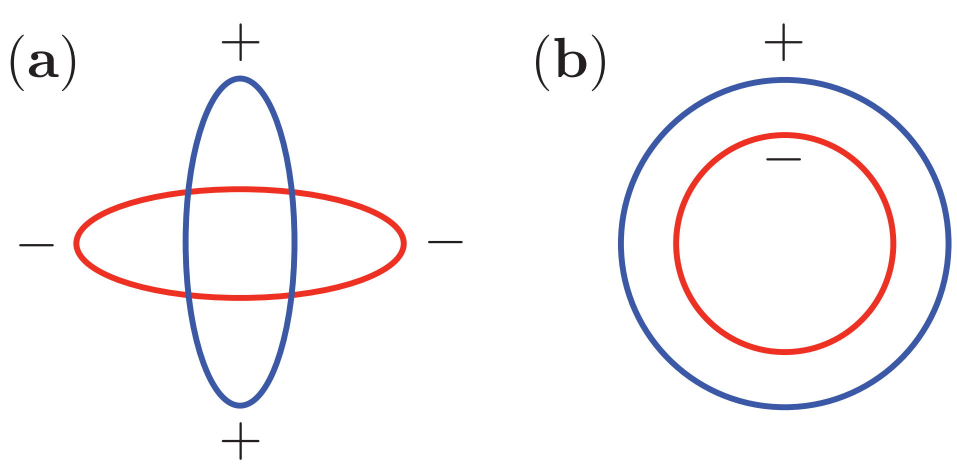
Fang et al., 2011

Mazin 2011, Khodas & Chubukov 2011

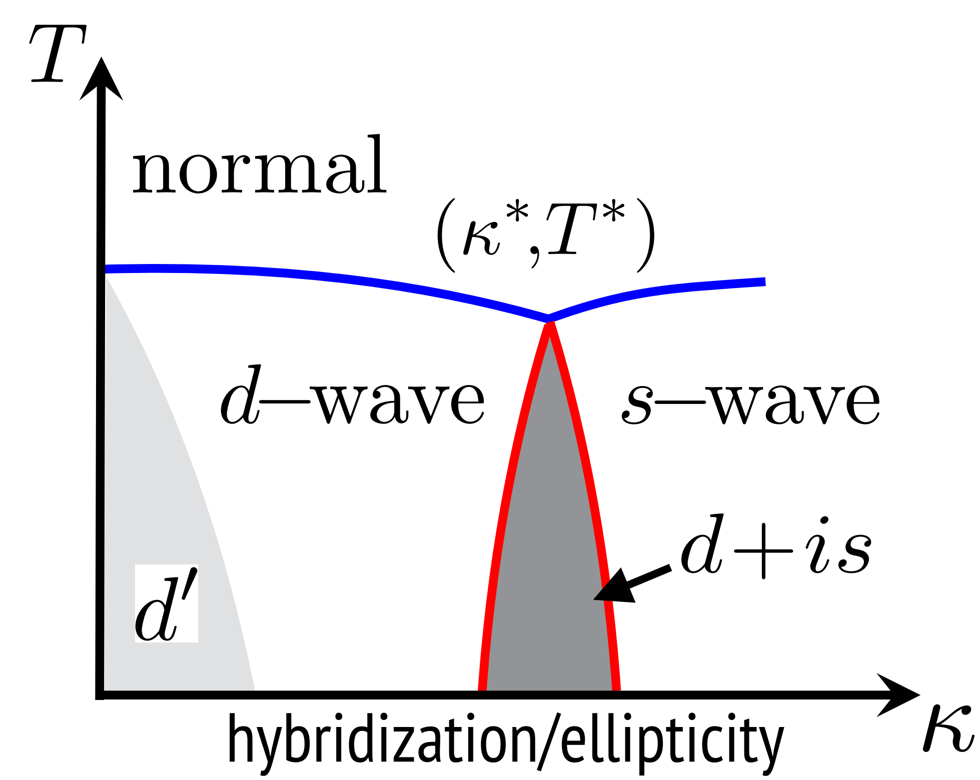


quasi-nodeless d   incipient $s^{\pm}$ bonding – antibonding $s^{\pm}$

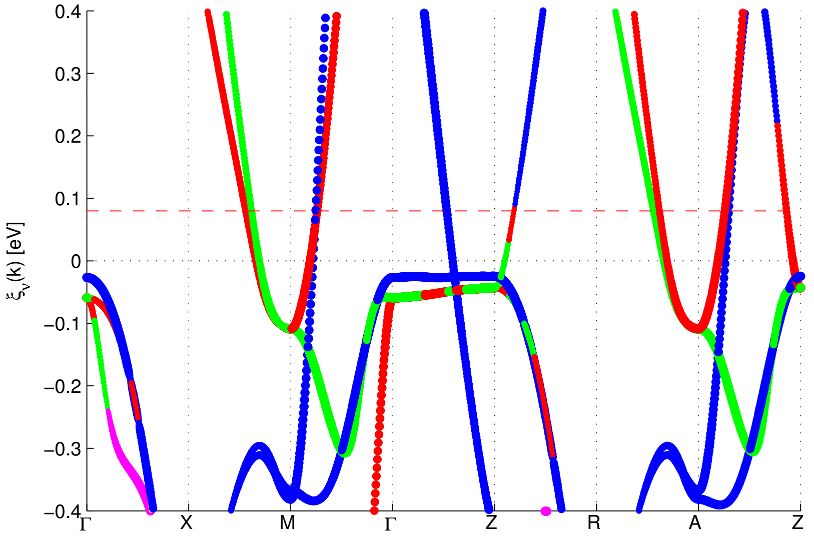
Hirschfeld, Kurshunov & Mazin '11



Khodas & Chubukov , PRL 2012

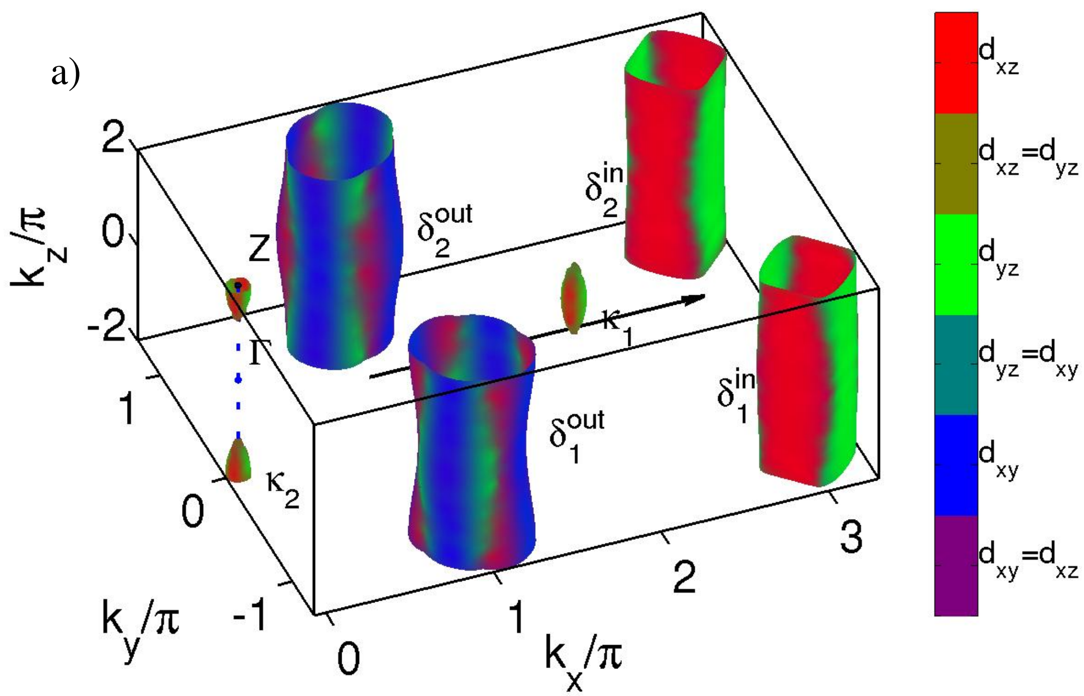


RPA calculation for 10-orbital (2 Fe) TB model

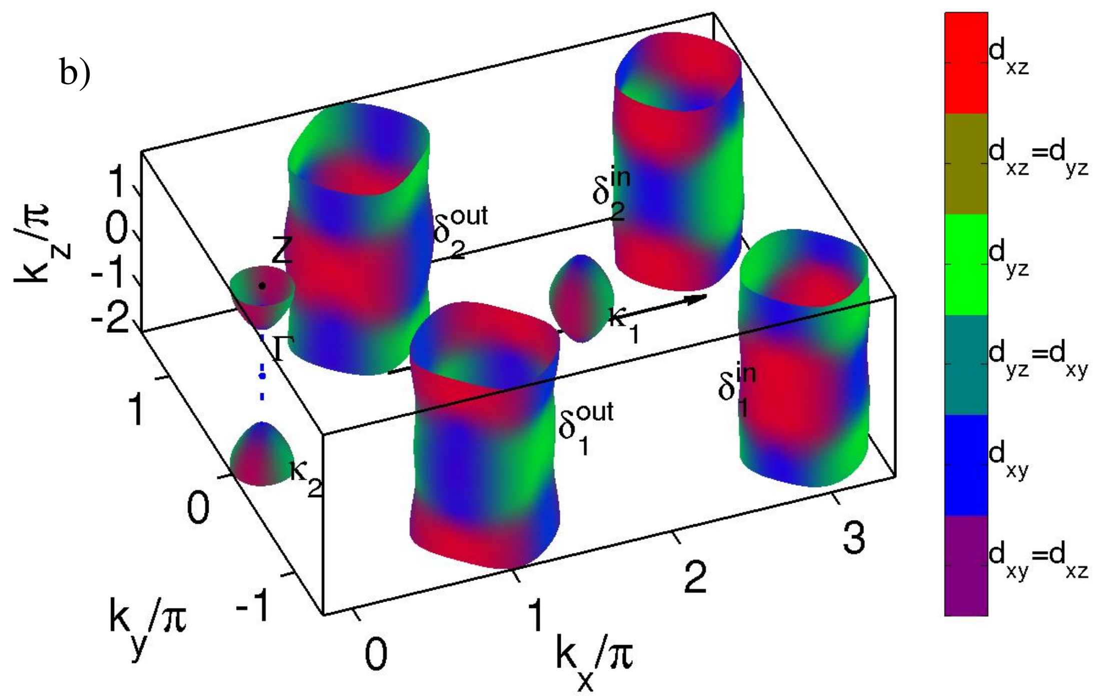


Wannier TB fit of non-relativistic WIEN2k bandstructure

$$H_0 = \sum_{\sigma} \sum_{ij} \sum_{\ell\ell'} t_{ij}^{\ell\ell'} c_{i\ell\sigma}^{\dagger} c_{j\ell'\sigma}$$



x = 0.12 electrons/Fe
$K_{0.8}Fe_{1.7}Se_2$



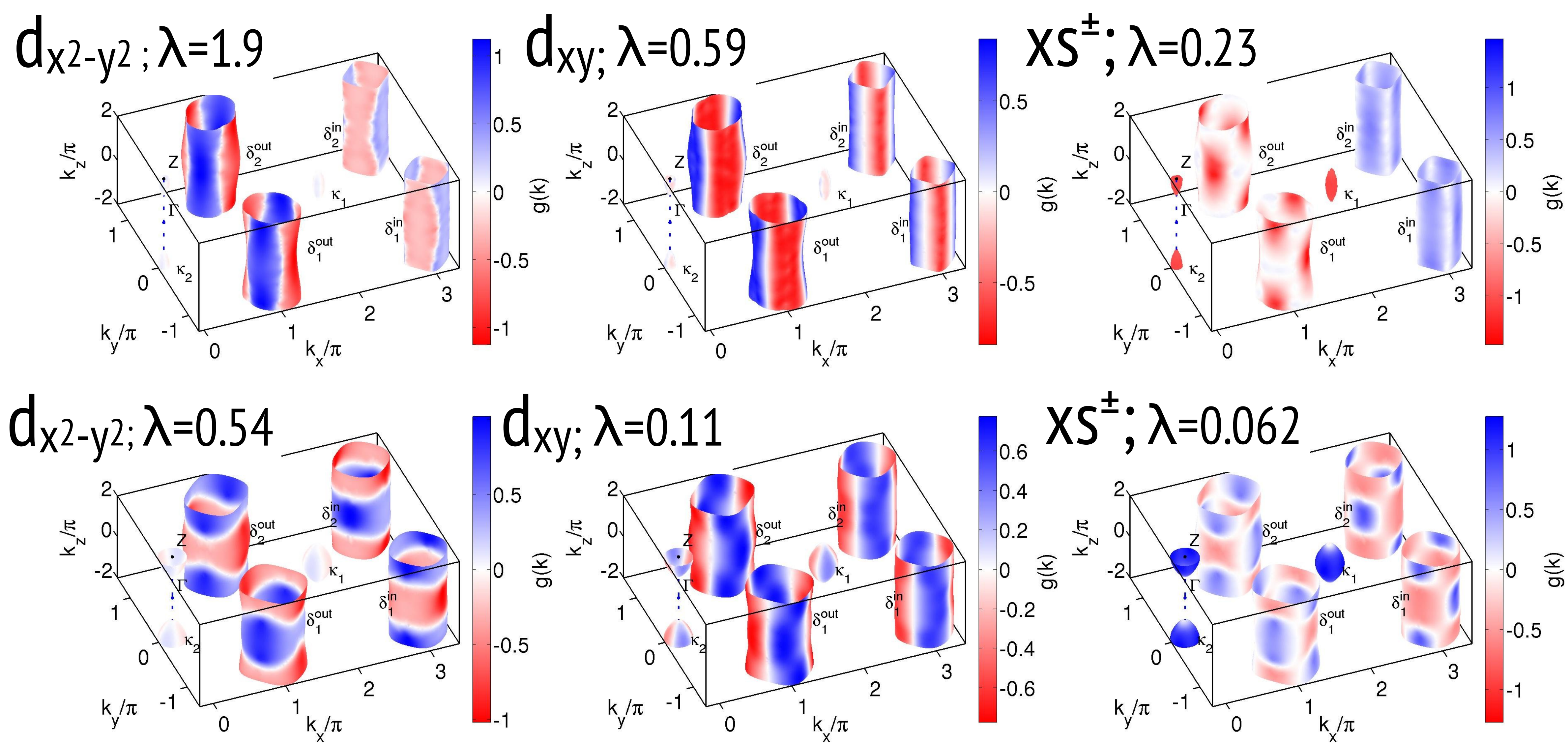
x = 0.25 electrons/Fe
$K_{0.85}Fe_{1.7}Se_2$

Kreisel, Wang, Maier, Hirschfeld & Scalapino, arXiv:1308.5683

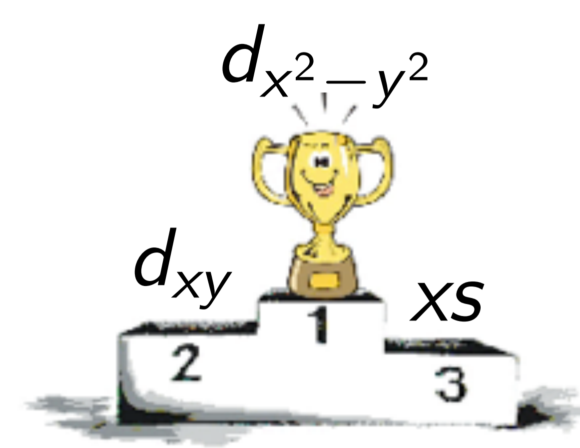
Leading gap structures:

x=0.12

x=0.25

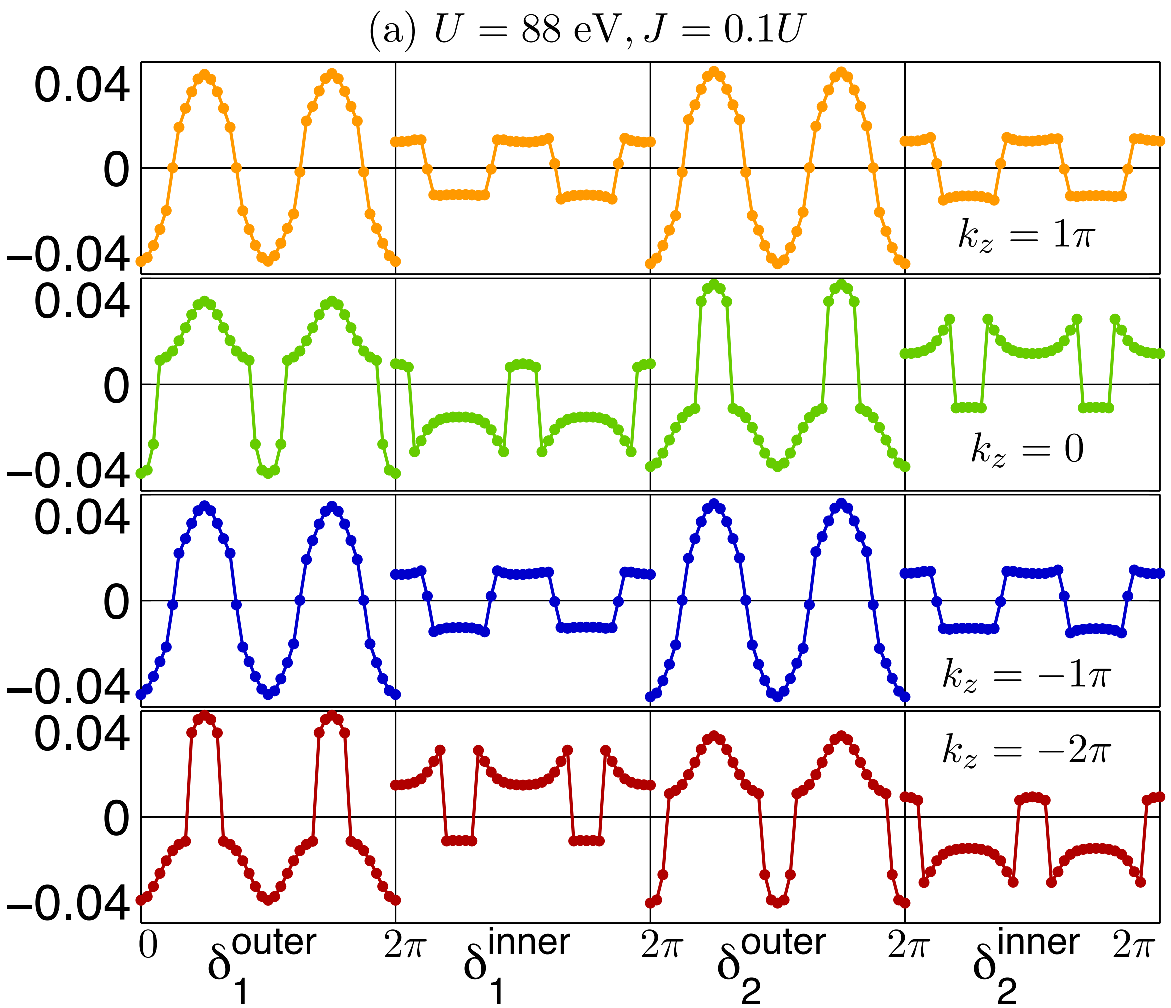


> $d_{x^2-y^2}$ leading, with xs bonding-antibonding subdominant

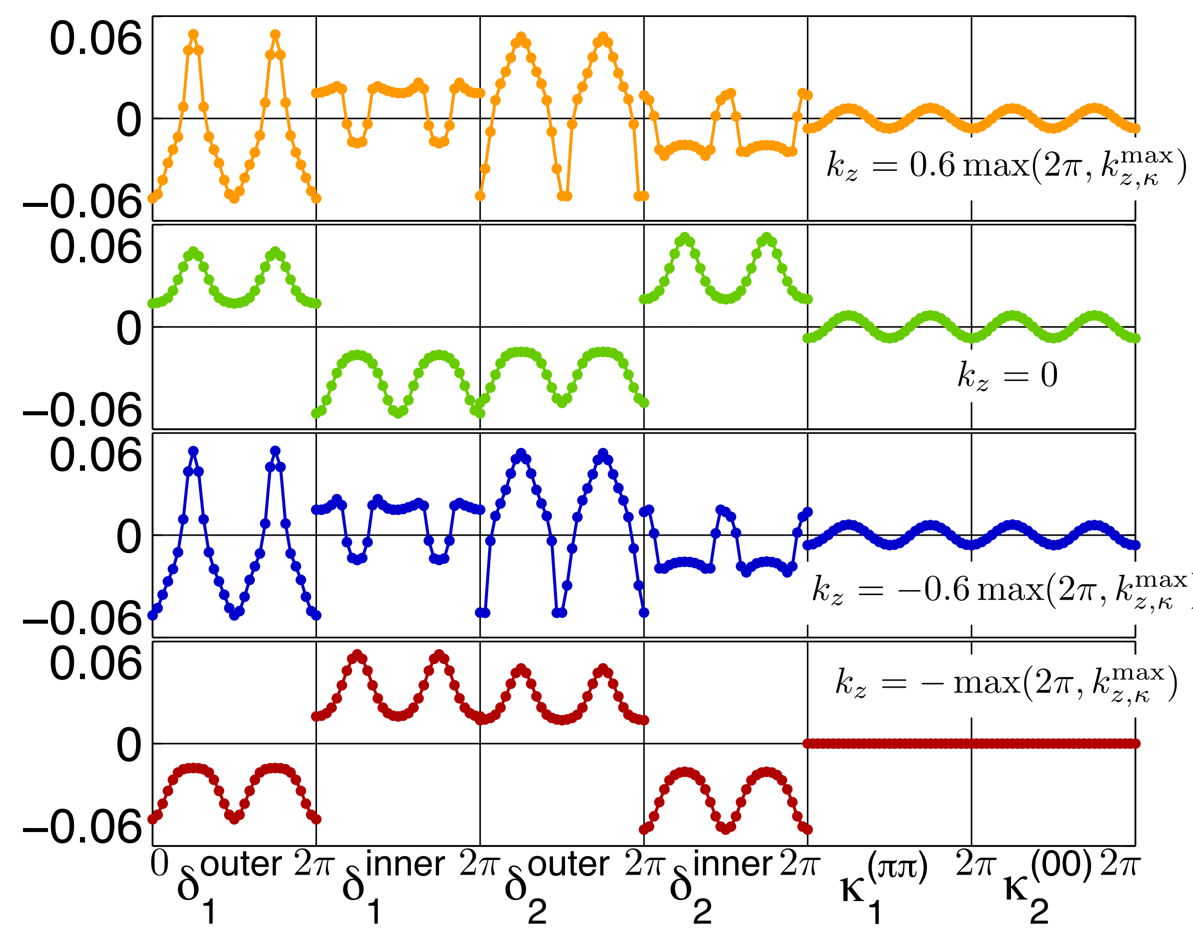


d-wave has quasi-nodes

<n>=6.12; $d_{x^2-y^2}$-wave



<n>=6.25; $d_{x^2-y^2}$-wave



– "Nodal thickness" infinitely small

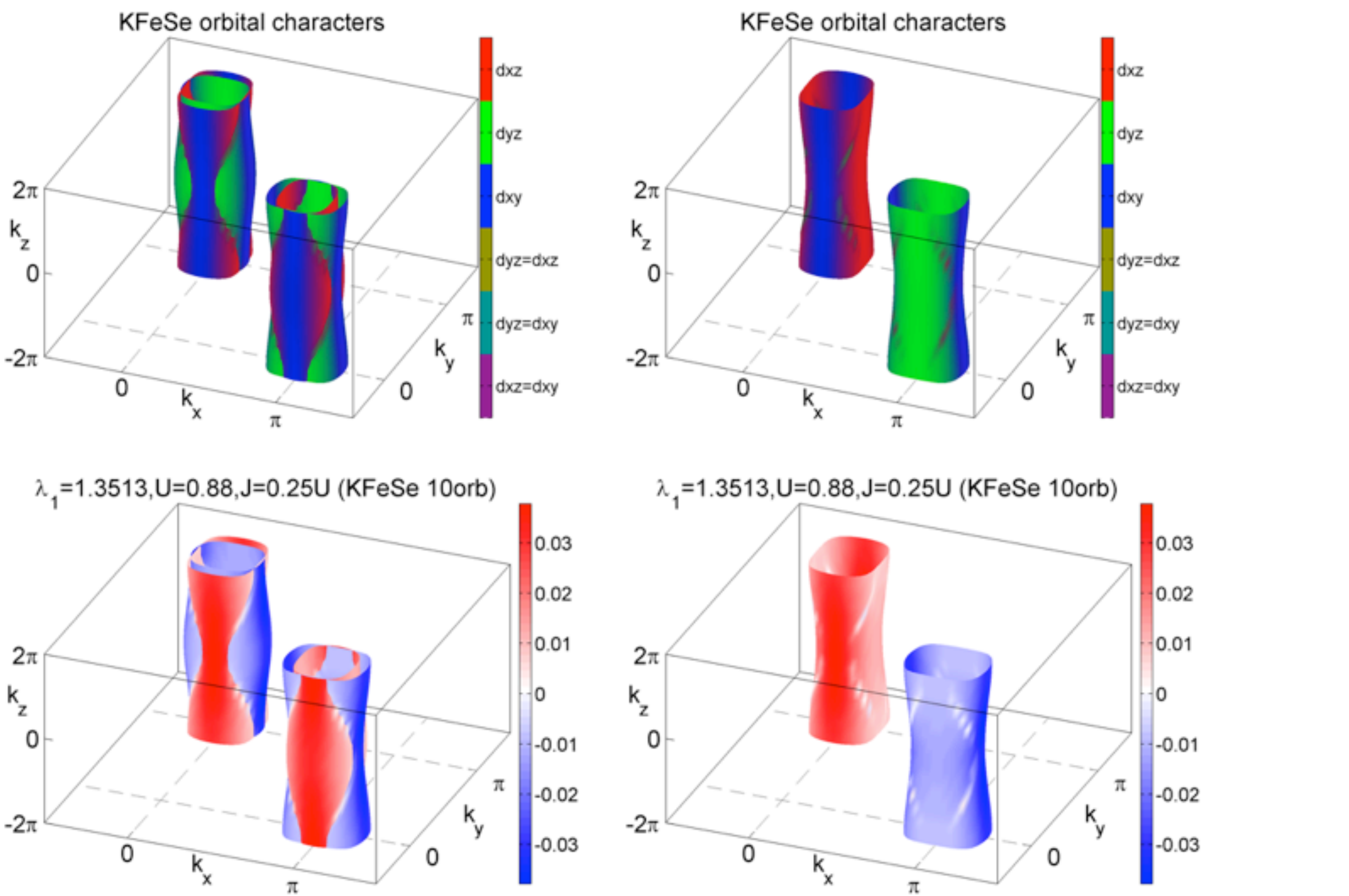
– Nodes on Z-pocket - inconsistent with ARPES?

M. Xu *et al.*, PRB 2012

Absence of hybridization - unfolding

<n>=6.12

unfolding Q=(π,π,π)



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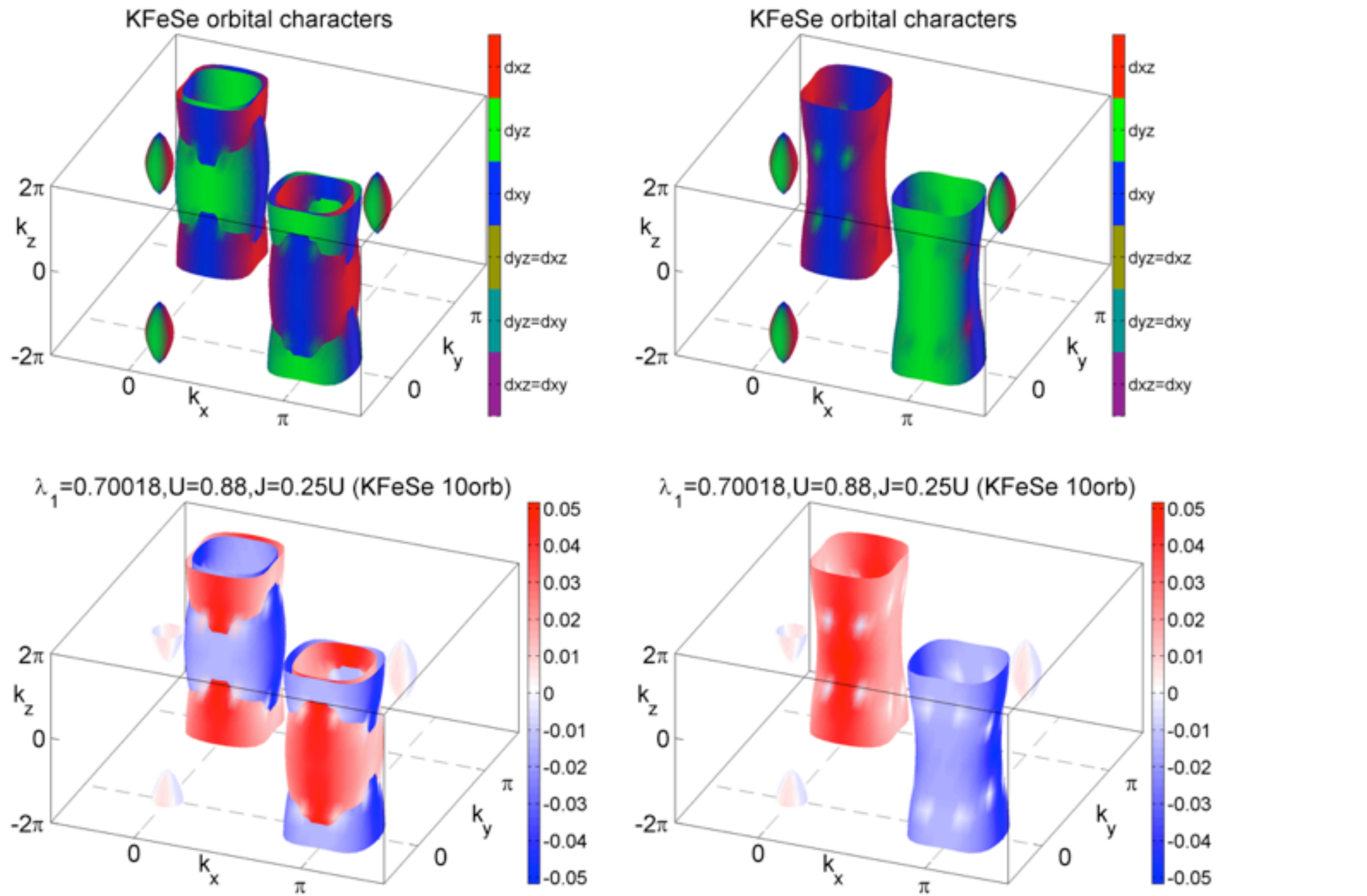
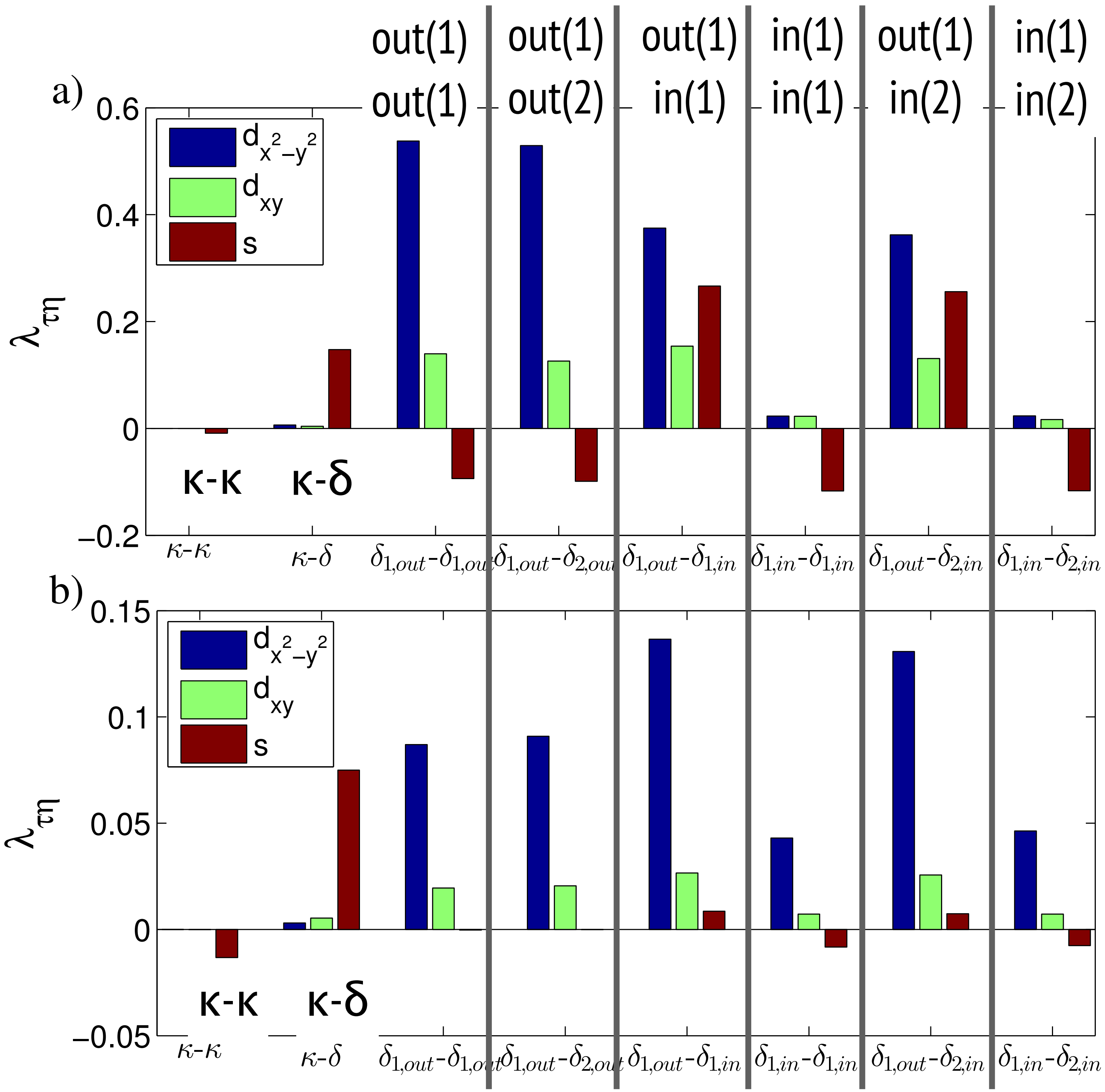
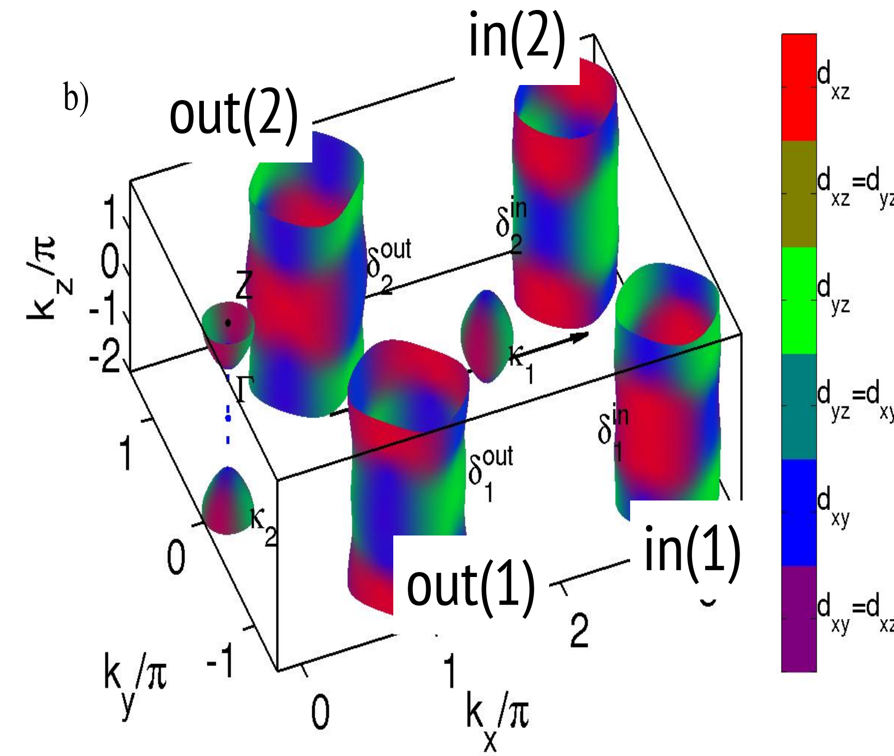


Why is the d-wave favored?

Partial contributions to $\lambda = \sum_{\tau\eta} \lambda_{\tau\eta}$





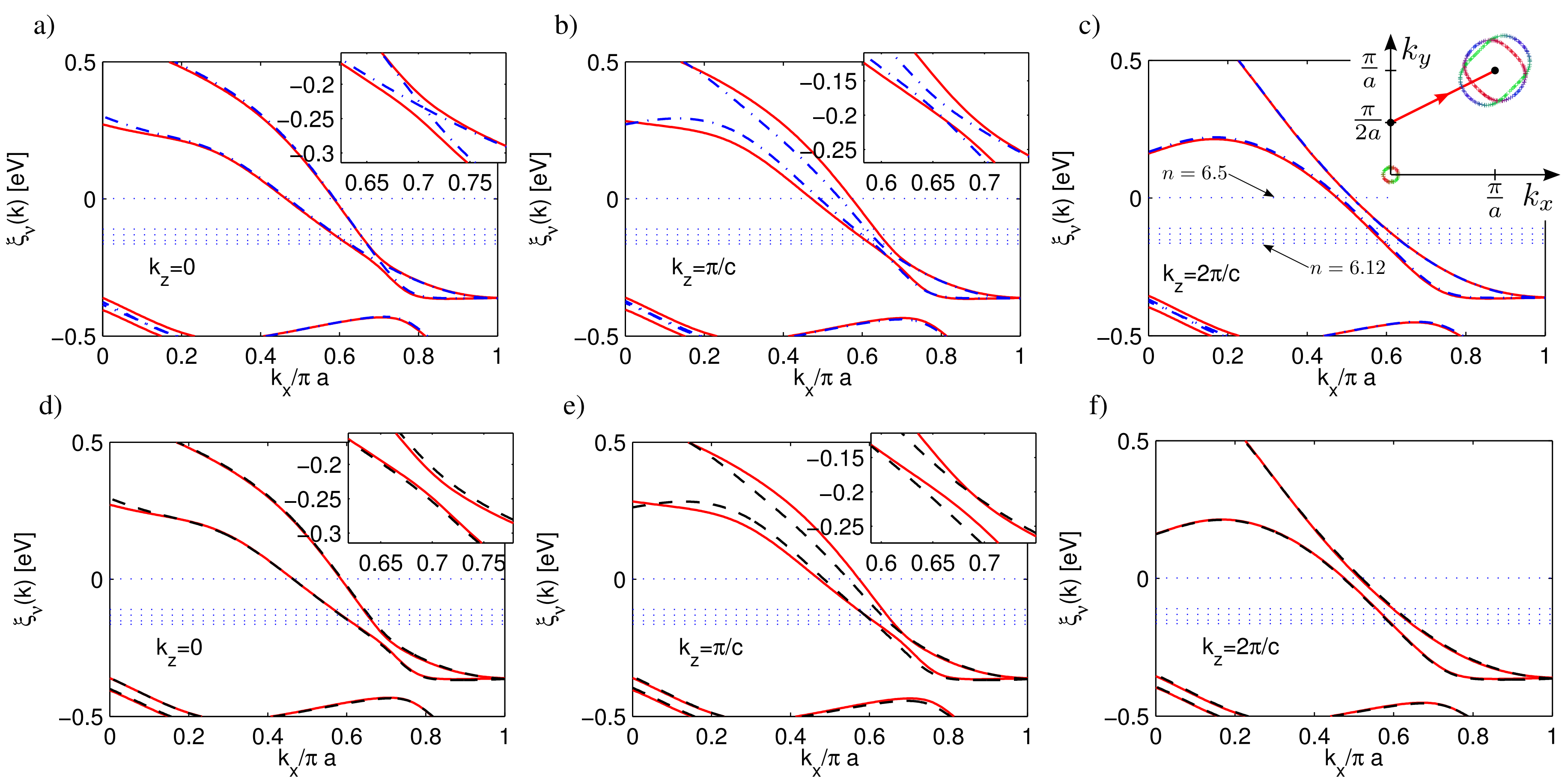
> Significant scattering between inner pockets and between outer pockets favors d-wave

Effect of band hybridization

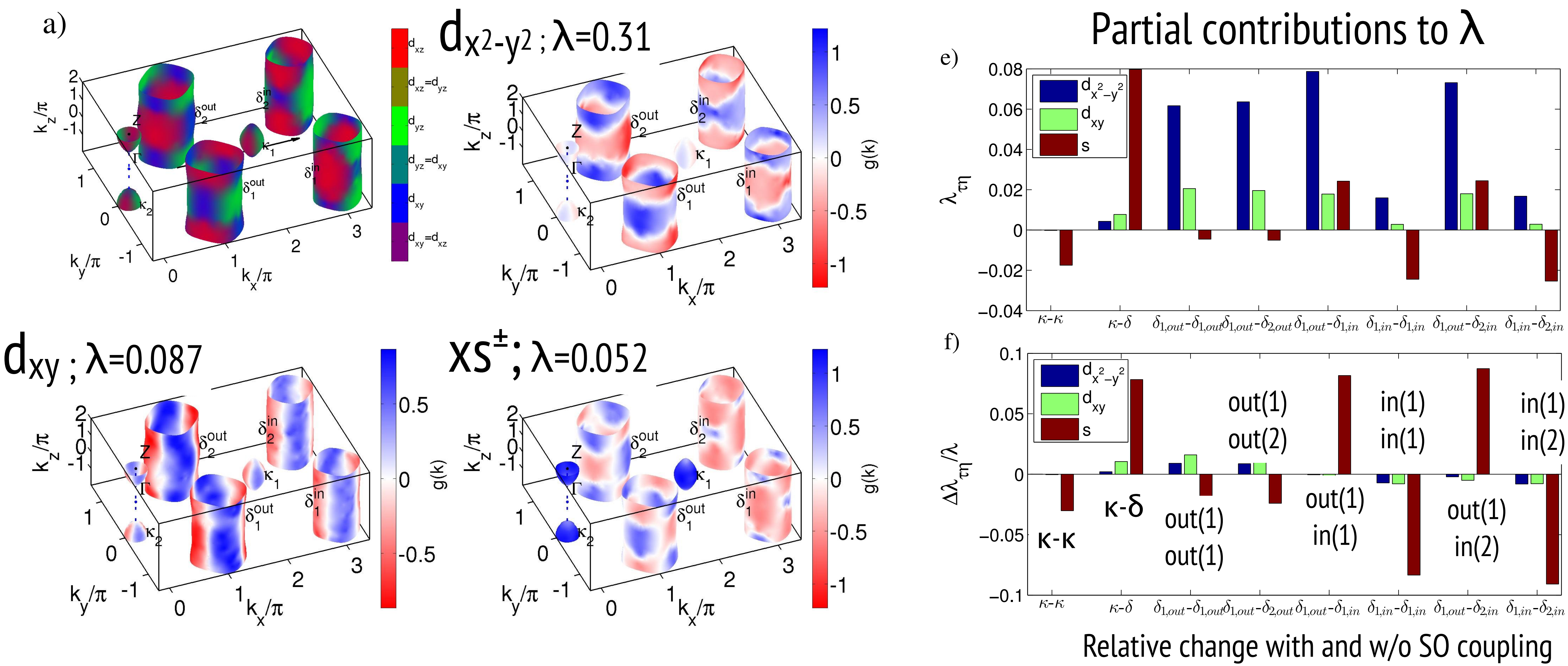
- Consider spin-orbit coupling on Fe d-orbitals

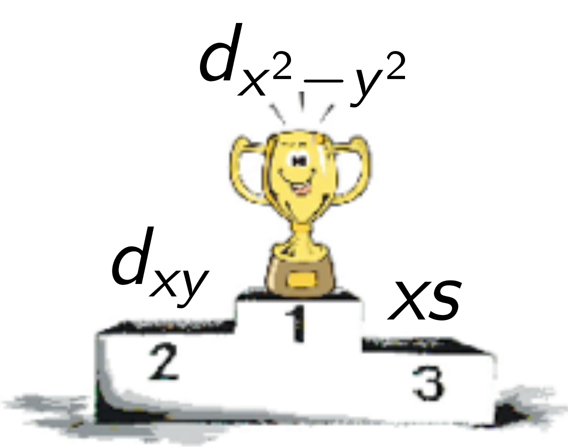
$$H_{\mathrm{SO}} = \lambda_{\mathrm{Fe}}^{3d} \sum_i \sum_{\alpha=x,y,z} L_i^\alpha S_i^\alpha$$

  - Project eigenstates onto majority spin component (and re-normalize)
  - Bands calculated with λ = 0.05 eV describes DFT bands with SO well



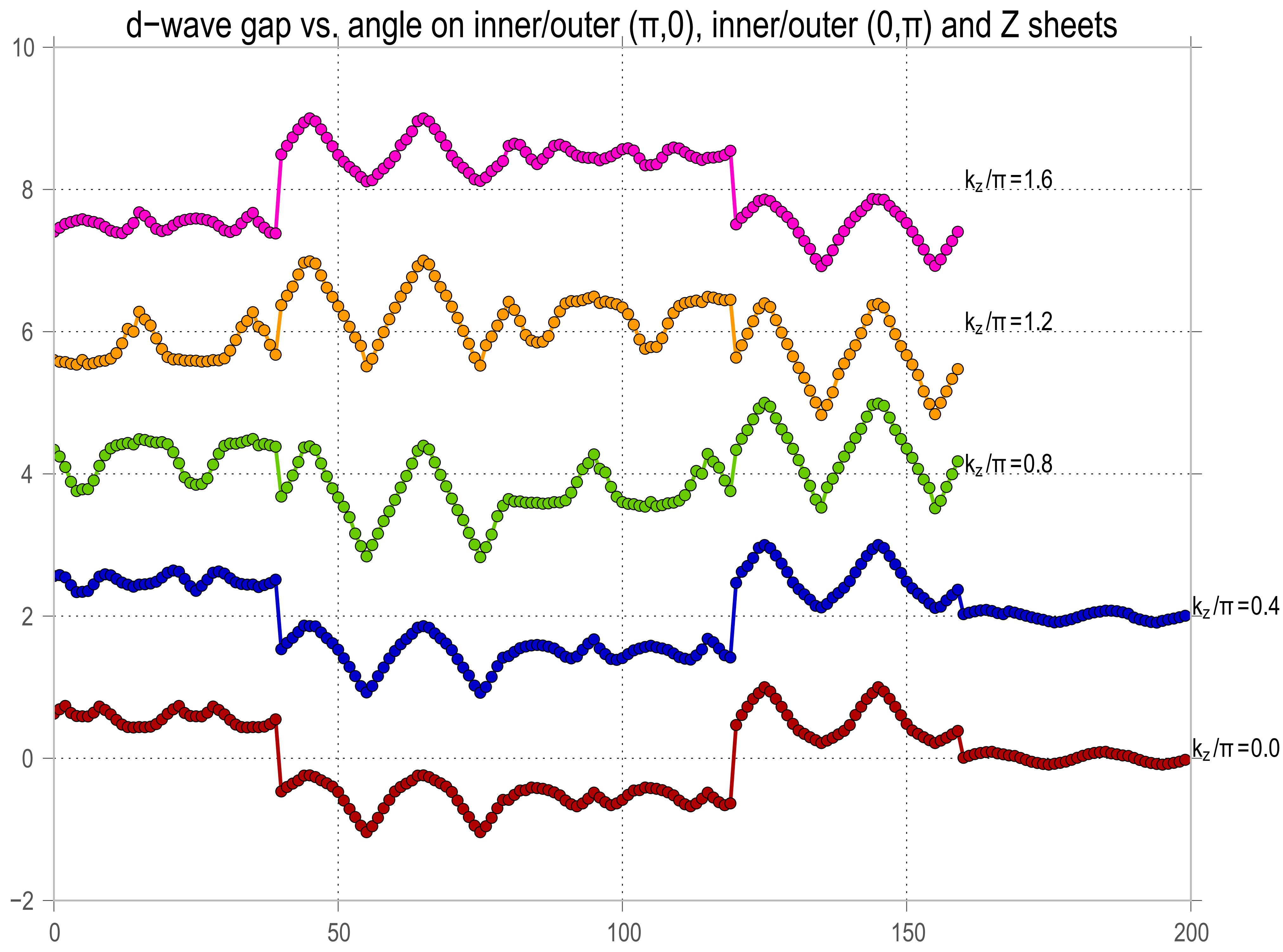
Leading pairing states with SO coupling





> Enhanced interpocket scattering stabilizes bonding-antibonding s-wave state

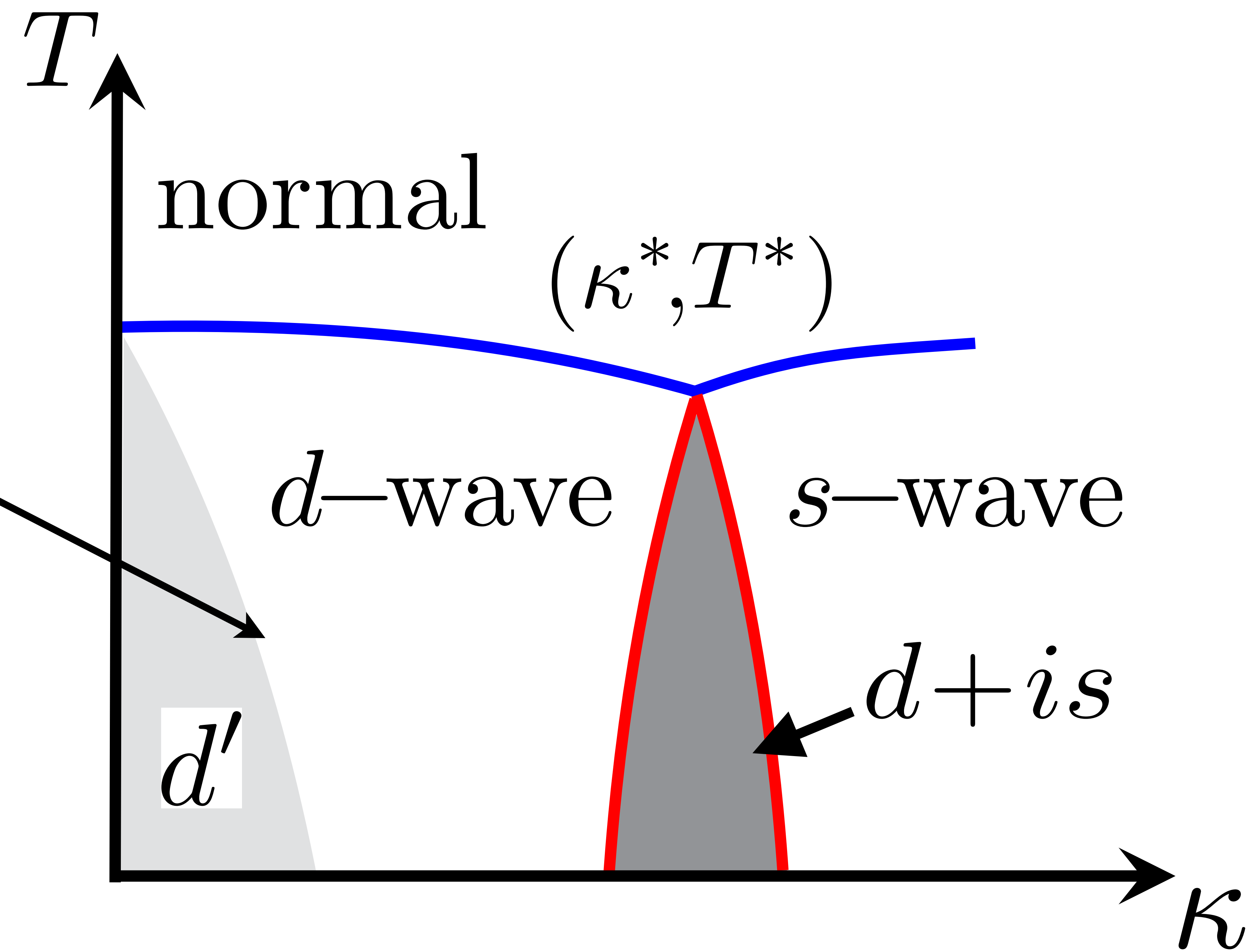
Angular structure of d-wave gap



Summary: Pairing state in KFe_2Se_2

Spin-fluctuation theory

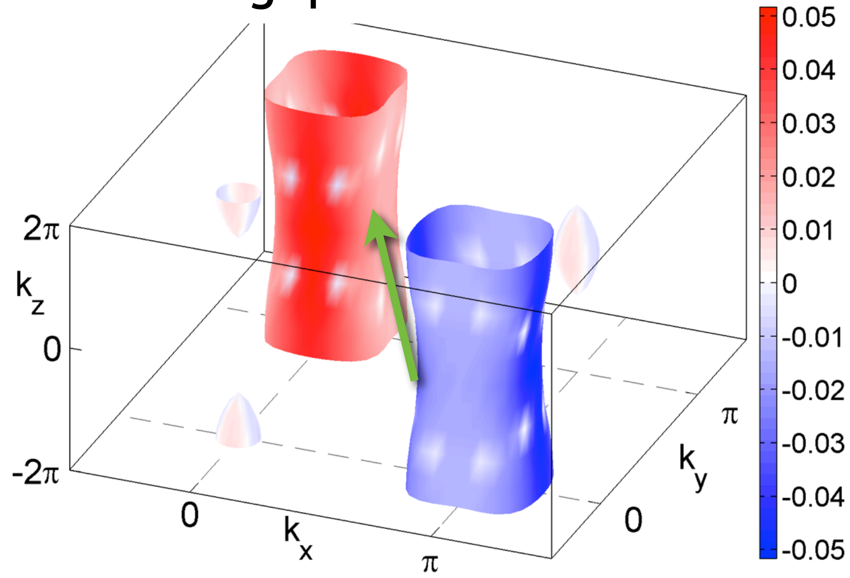
$$\kappa_{\text{eff}} \simeq \frac{\delta\xi}{\langle \frac{\Delta\xi_{\mathbf{k}}}{v_F(\mathbf{k})k_F(\mathbf{k})} \rangle} \approx 0.1 - 0.3$$



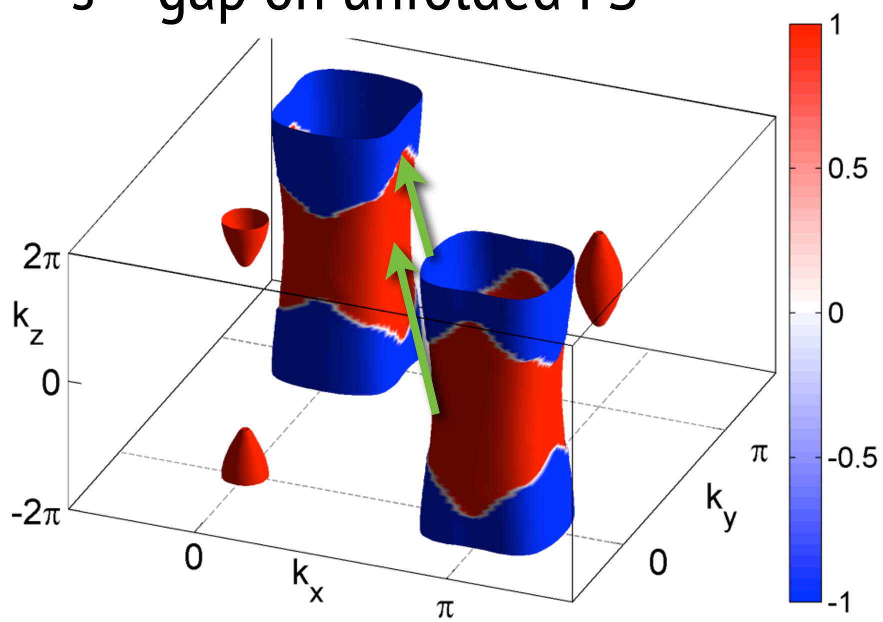
Khodas and Chubukov, PRL '12

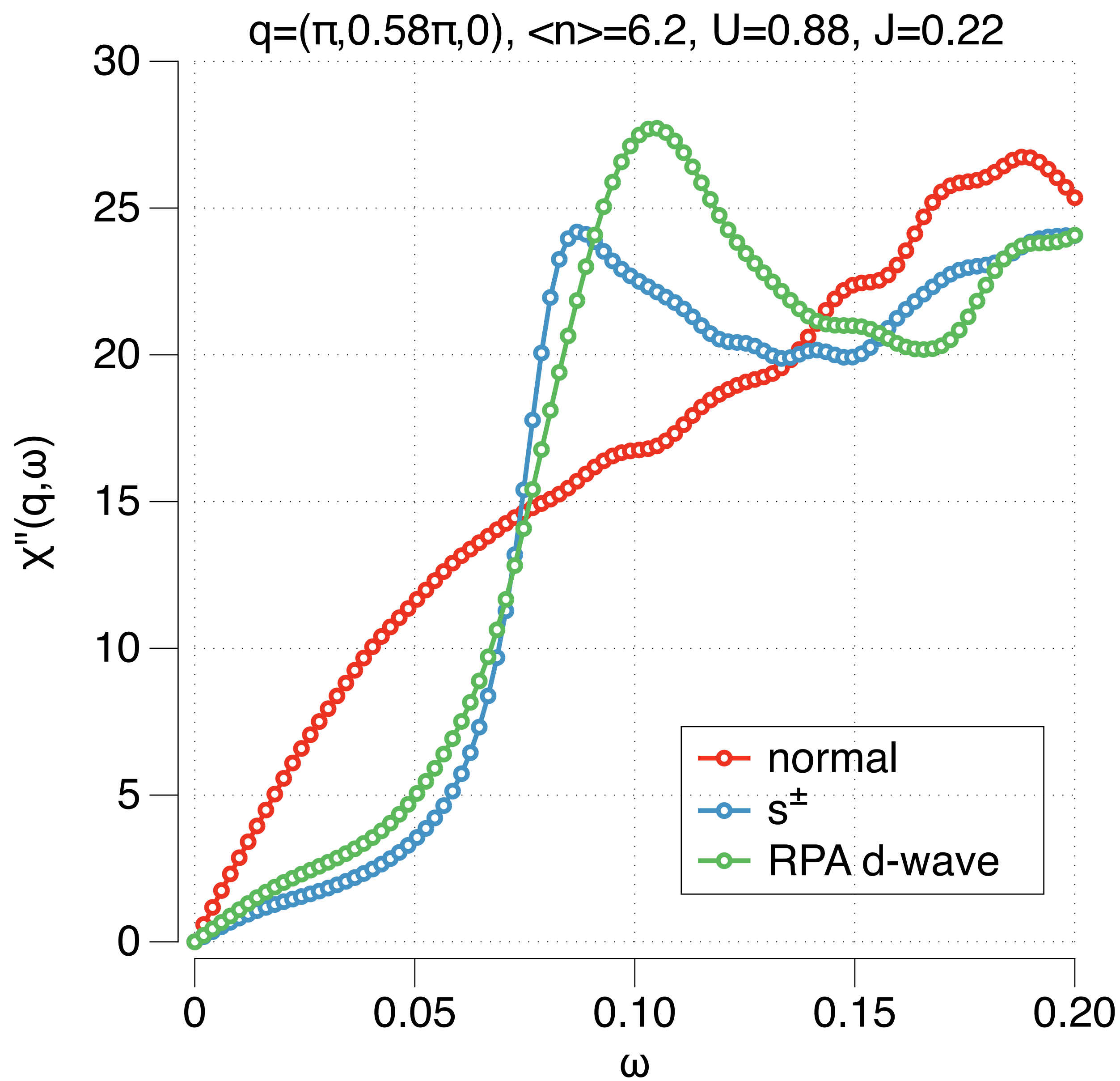
Neutron scattering - electron doped system - no SO coupling

d-wave gap on unfolded FS



s+- gap on unfolded FS

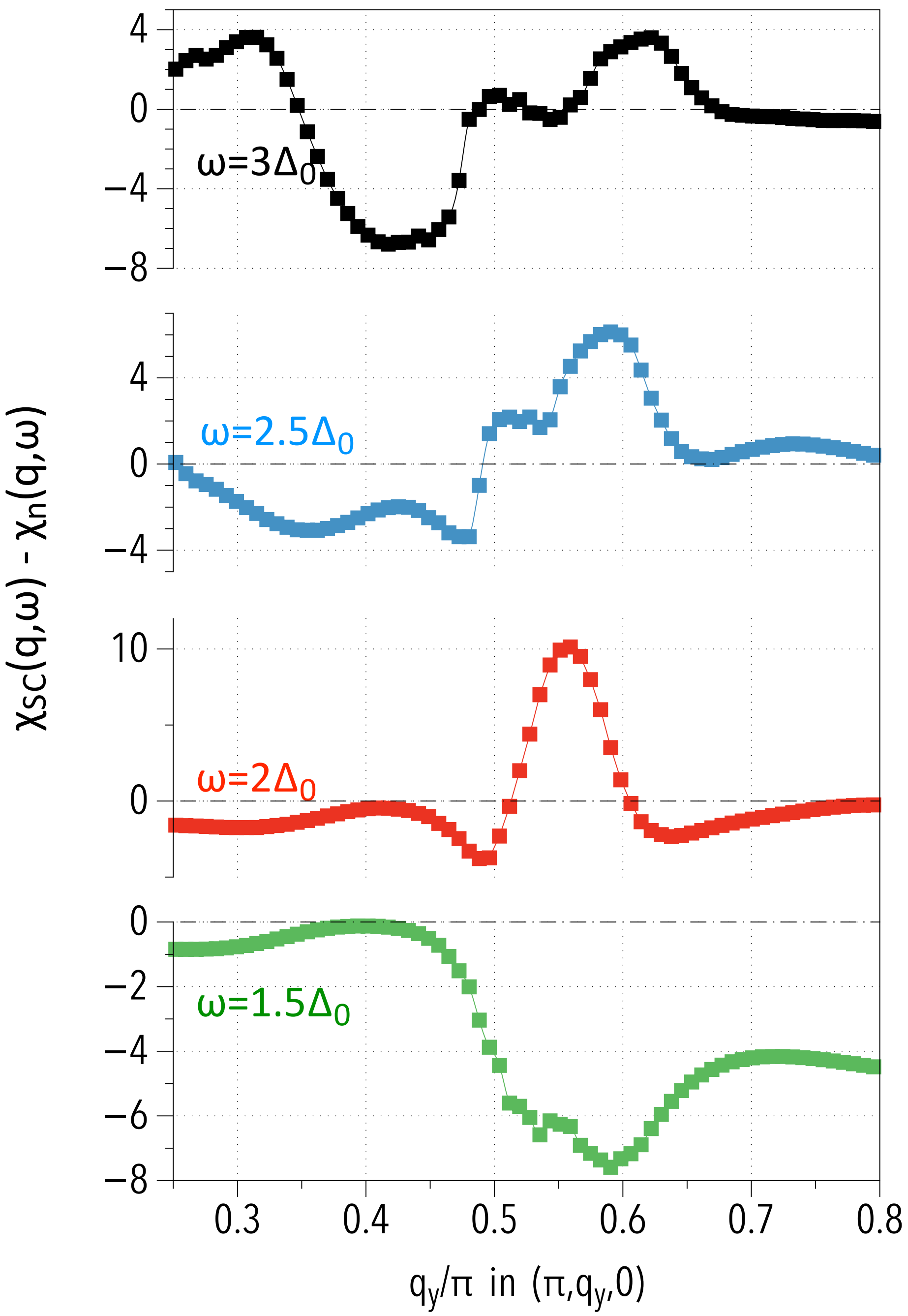




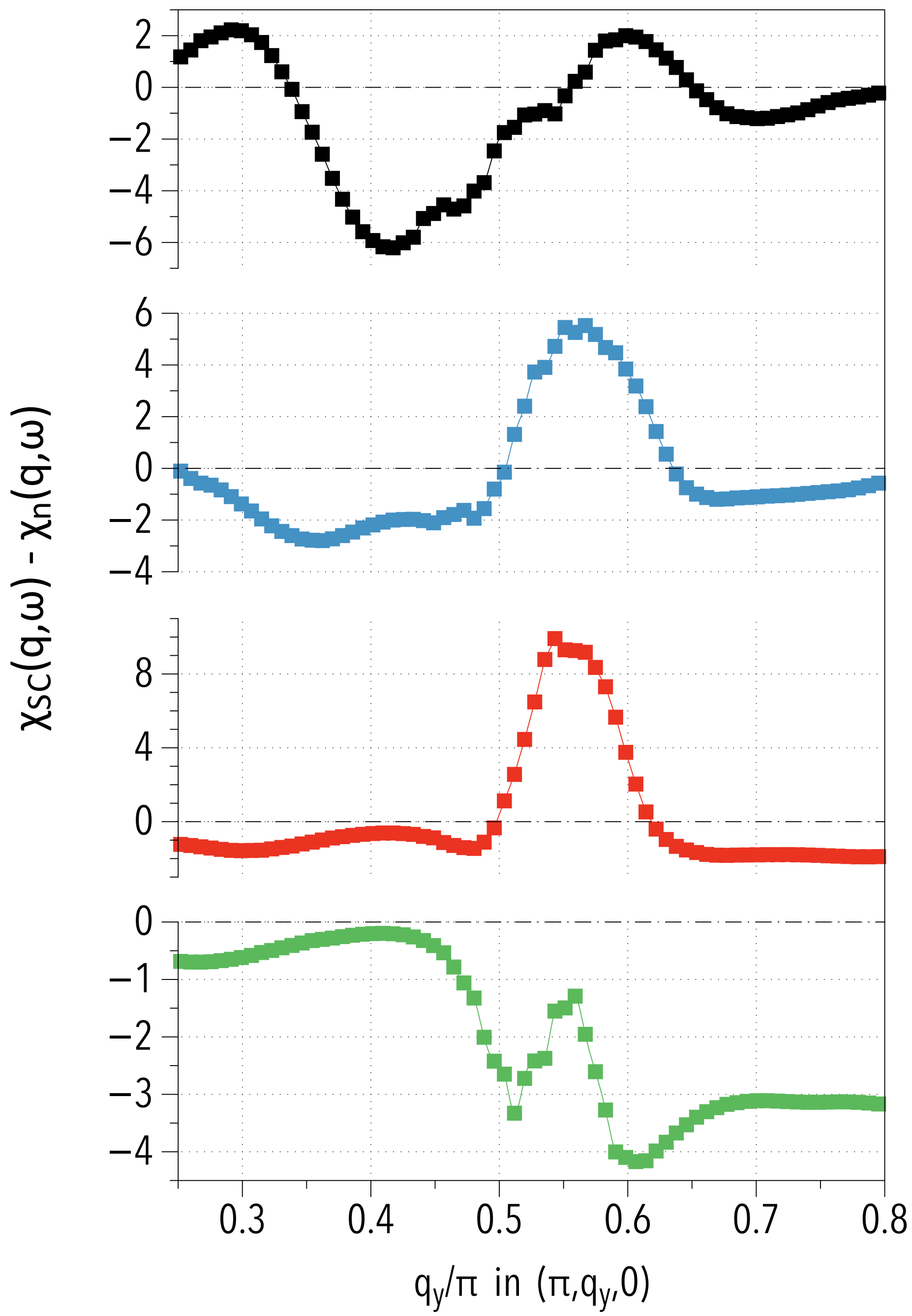
– Resonance for d-wave and $s^{\pm}$ gap, $s^{\pm}$ weaker

Neutron scattering - transverse momentum scans - no SO coupling

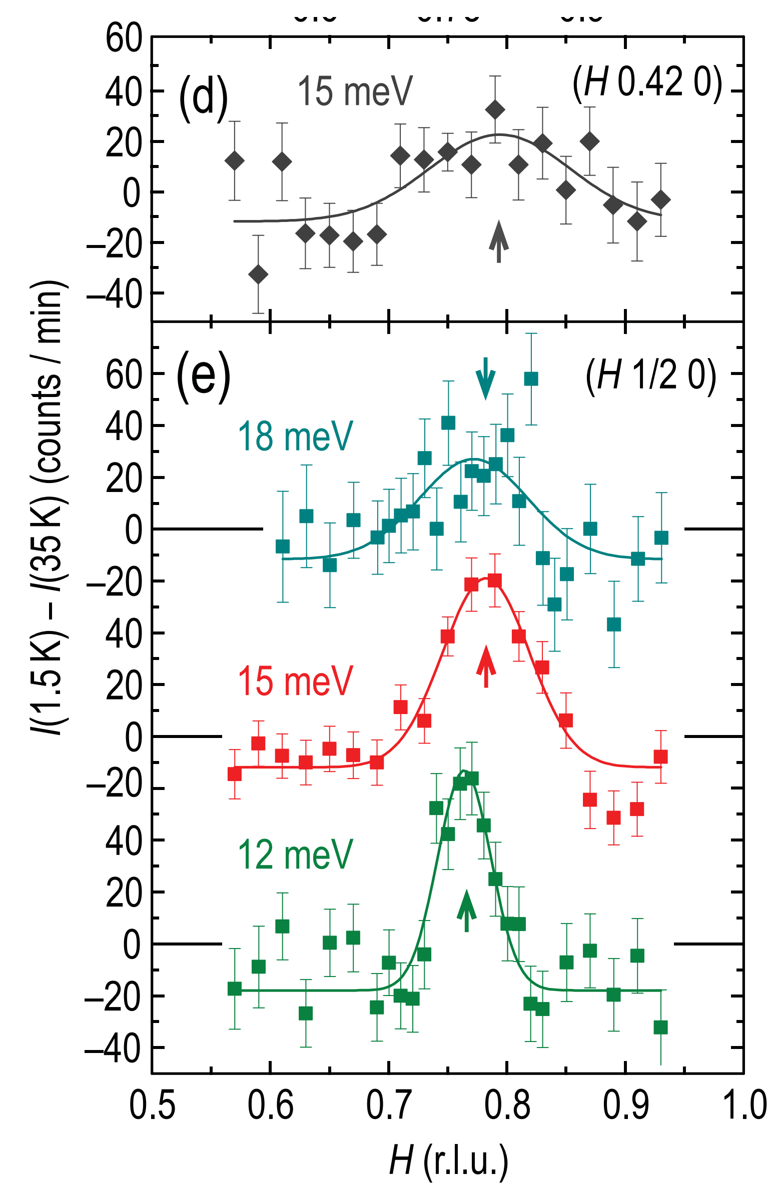
isotropic $s^{\pm}$ gap



d-wave gap



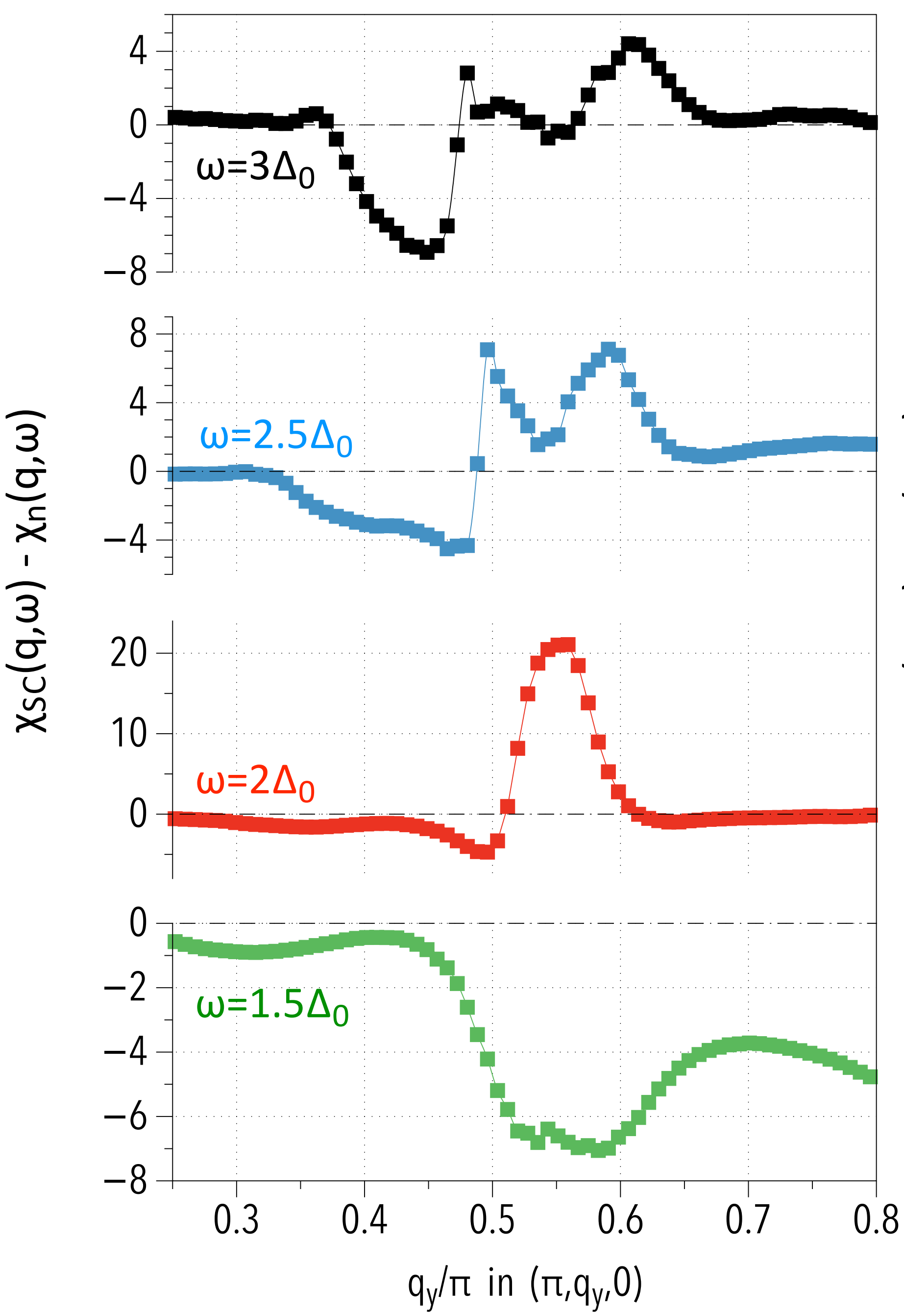
Experiment



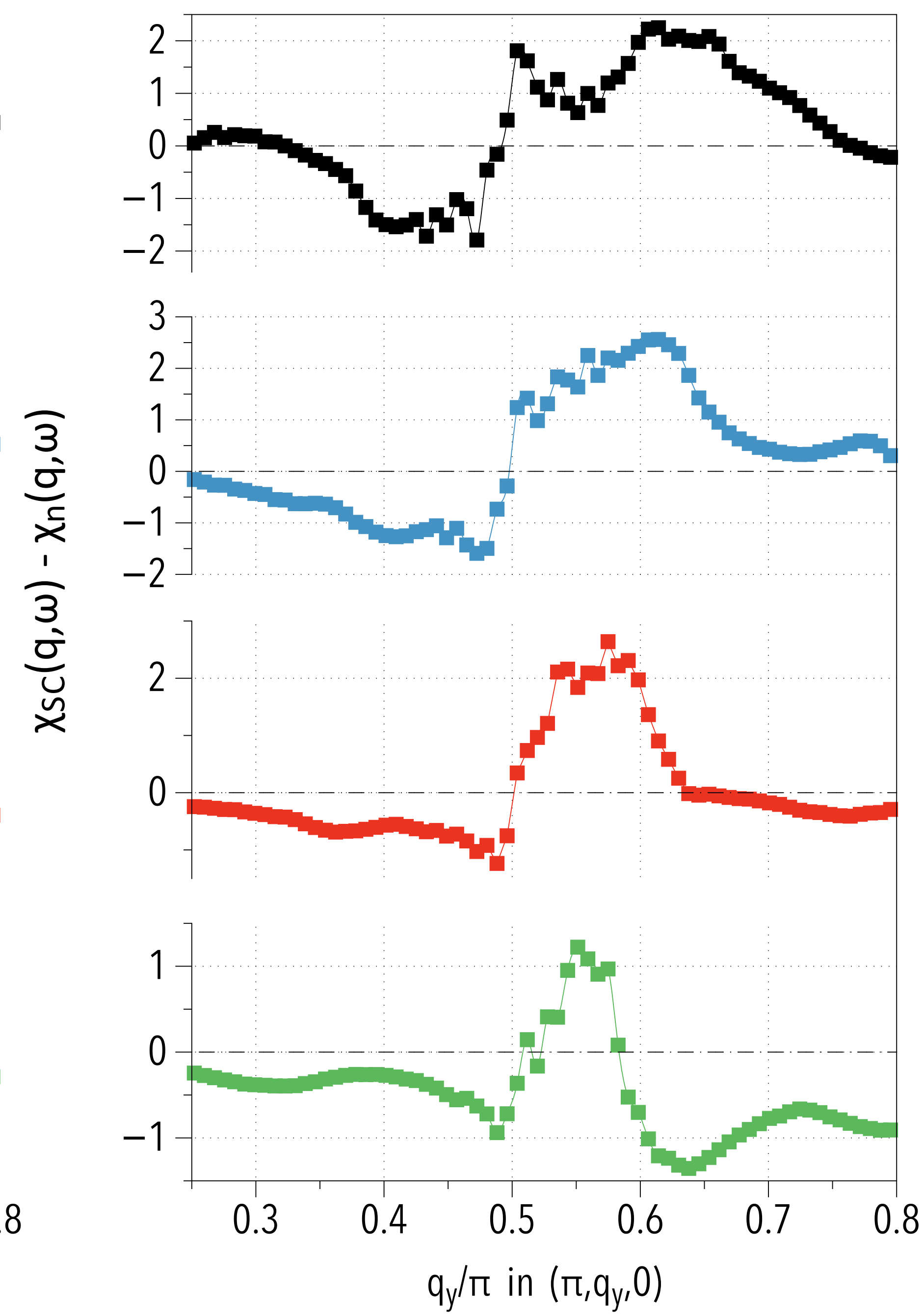
Friemel et al., PRB 2012

Neutron scattering - Transverse momentum scans - SO coupling λ=0.05

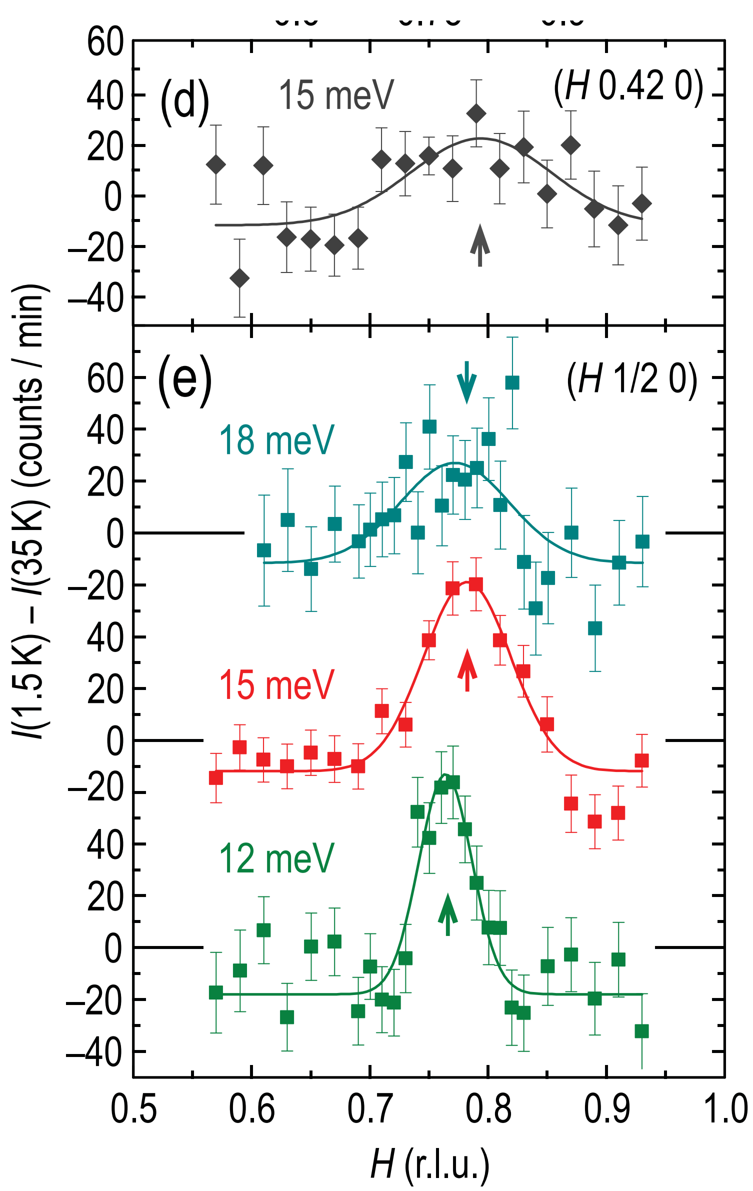
isotropic s$^{\pm}$ gap



RPA d-wave gap



Experiment



Friemel et al., PRB 2012

Summary & Conclusions

- 3D 10-orbital (2-Fe) model RPA studies of pair structure and neutron scattering response
- $d_{x^2-y^2}$ pairing state is leading, with d_{xy} and $xs^{\pm}$ subdominant
- $d_{x^2-y^2}$ gap has vertical or horizontal quasi-nodes due to negligible hybridization
- Hybridization due to SO coupling stabilizes $xs^{\pm}$, but $d_{x^2-y^2}$ still leading
- Realistic model based on DFT is in small κ_{eff} limit
- Both gaps have resonance in neutron scattering and are hard to distinguish