Andreas Kreisel

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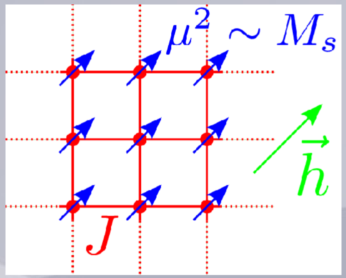
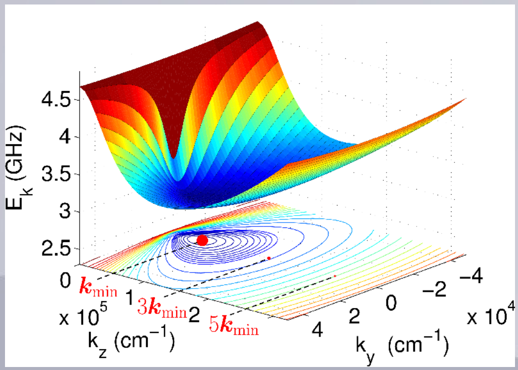
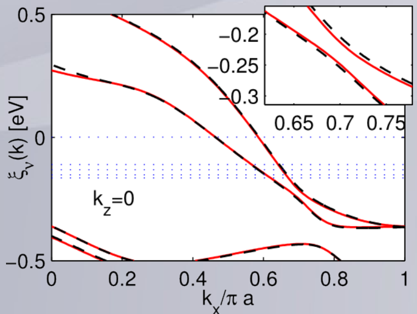
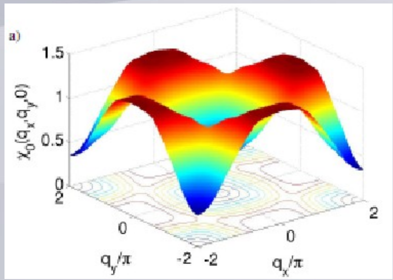
- **Bosons**: Spin-waves and BEC in thin-film ferromagnets
  - spin-wave theory
  - interactions and BEC

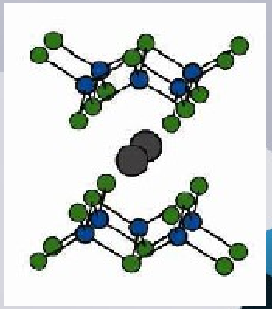




- **Fermions**: Spin fluctuation pairing and symmetry of order parameter in $K_xFe_{2-y}Se_2$
  - Fe based superconductors
  - spin-fluctuation theory
  - spin-orbit coupling







Spin-waves and BEC in thin-film ferromagnets

From textbook knowledge towards BEC of magnons

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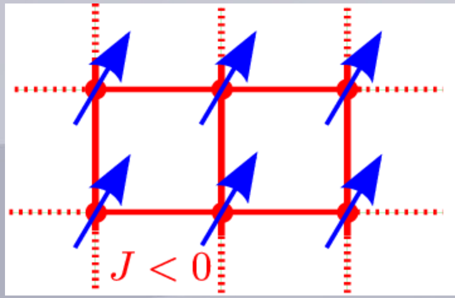
AG MAGNETISMUS TU KAISERSLAUTERN

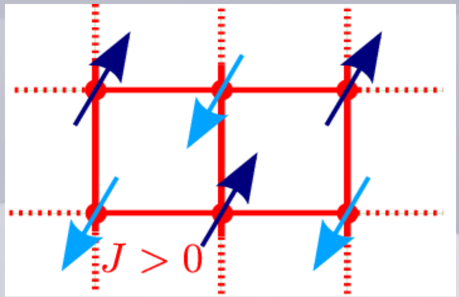
European Physical Journal B **71**, 59 (2009)
Rev. Sci. Instrum. **81**, 073902 (2010)
European Physical Journal B **78**, 429 (2010)
Phys. Rev. B **85**, 054422 (2012)
Phys. Rev. B **86**, 134403 (2012)

1. Introduction: Spin-wave theory

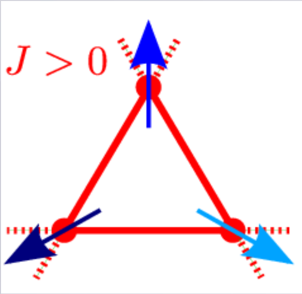
- Heisenberg model $$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$
- determine ordered classical groundstate
  - ferromagnet
    classical groundstate=quantum groundstate



  - anti-ferromagnet
    (2 sublattices, Néel groundstate)
    AK, Hasselmann, Kopietz, ('07)
    AK, Sauli, Hasselmann, Kopietz, ('08)



  - triangular anti-ferromagnet
    (3 sublattices, frustration)
    Chernychev, Zhitomirsky ('09)
    Veillette *et al.* ('05)
    AK, *et al.* ('11)



1. Spin wave theory

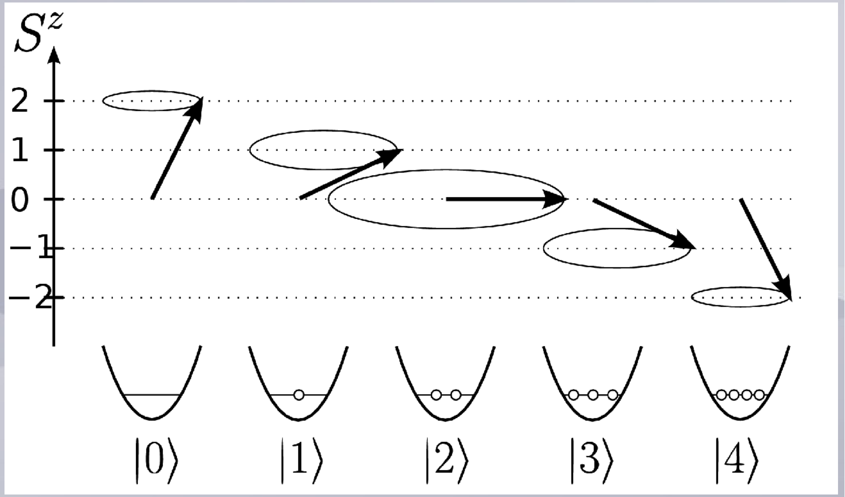
- expand in terms of bosons (1/S expansion), Holstein-Primakoff transformation

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$\hat{S}^z = S - \hat{n} \qquad \hat{n} = \hat{b}^\dagger \hat{b} \qquad \left[\hat{b}, \hat{b}^\dagger\right] = 1$$

$$\hat{S}^+ = \sqrt{2S}\sqrt{1 - \frac{\hat{n}}{2S}}\,\hat{b}$$

$$\hat{S}^- = \sqrt{2S}\,\hat{b}^\dagger\sqrt{1 - \frac{\hat{n}}{2S}} \qquad \sqrt{1 - \frac{\hat{n}}{2S}} = 1 - \frac{\hat{n}}{4S} + \mathcal{O}(\frac{1}{S^2})$$



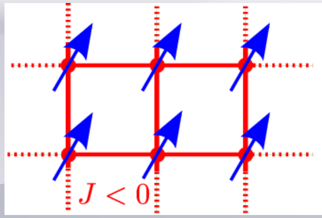
Holstein, Primakoff, Phys. Rev. **58**, 1098 (1940)

- determine properties of resulting interacting theory of bosons

$$H = \sum_{\vec{k}} E_{\vec{k}} b^\dagger_{\vec{k}} b_{\vec{k}} + \sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3} \Gamma^3(\vec{k}_1, \vec{k}_2, \vec{k}_3) b^\dagger_{\vec{k}_1} b_{\vec{k}_2} b_{\vec{k}_3} + \sum_{1,2,3,4} \Gamma^4(1,2;3,4) b^\dagger_1 b^\dagger_2 b_3 b_4 + \ldots$$

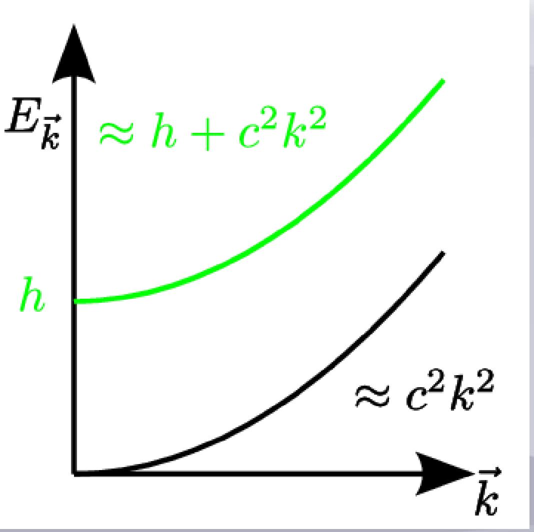
1. Spin wave theory: General results

- ferromagnet

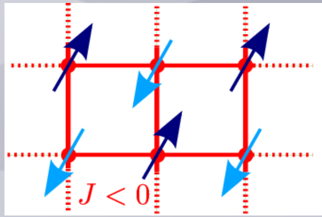


  - quadratic excitation spectrum
  - vanishing interaction vertices

$$\Gamma^4 \sim -(\vec{k}_1 \cdot \vec{k}_2 + \vec{k}_3 \cdot \vec{k}_4)$$

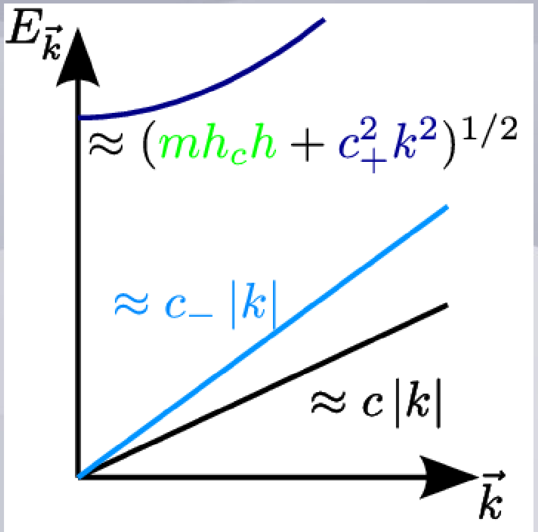


- antiferromagnet



  - linear spectrum (Goldstone mode)
  - two modes in magnetic field (2 sublattices)
  - divergent interaction vertices

$$\Gamma^4 \sim \sqrt{\frac{|\vec{k}_1||\vec{k}_2|}{|\vec{k}_3||\vec{k}_4|}} \left(1 \pm \frac{\vec{k}_1 \cdot \vec{k}_2}{|\vec{k}_1||\vec{k}_2|}\right)$$



Hasselmann, Kopietz ('06)

2.1 Spin-wave theory for thin film ferromagnets

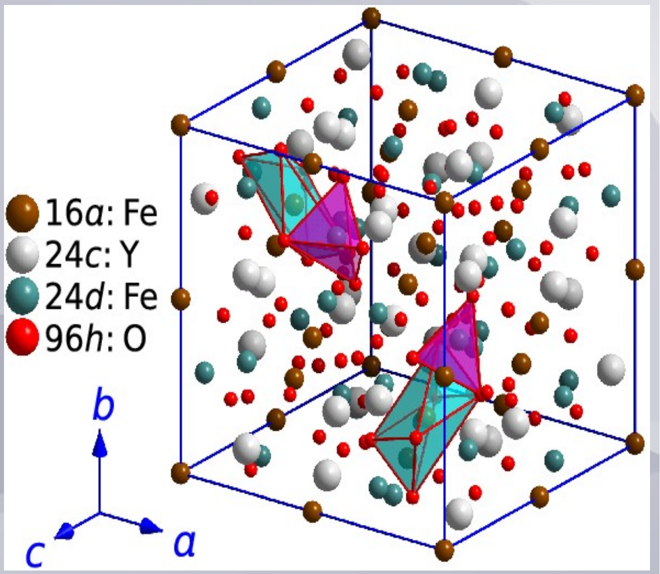
- Motivation: Experiments on YIG
  - Crystal structure:

space group: **Ia3d**
Y: 24(c) white
Fe: 24(d) green
Fe: 16(a) brown
O: 96(h) red

Gilleo *et al.* '58

Magnetic system:
40 magnetic ions in elementary cell
40 magnetic bands

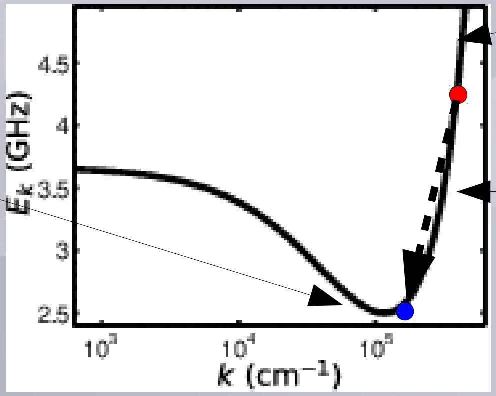
Elastic system:
160 atoms in elementary cell
3x160 phonon bands



  - low spin wave damping
  - good experimental control

Observation of the occupation number using microwave antennas or Brillouin Light Scattering (BLS)
Sandweg, AK, *et al.*, Rev. Sci. Instrum. **81**, 073902 (2010)

BEC of magnons at room temperature!
Demokritov *et al.* Nature **443**, 430 (2006)

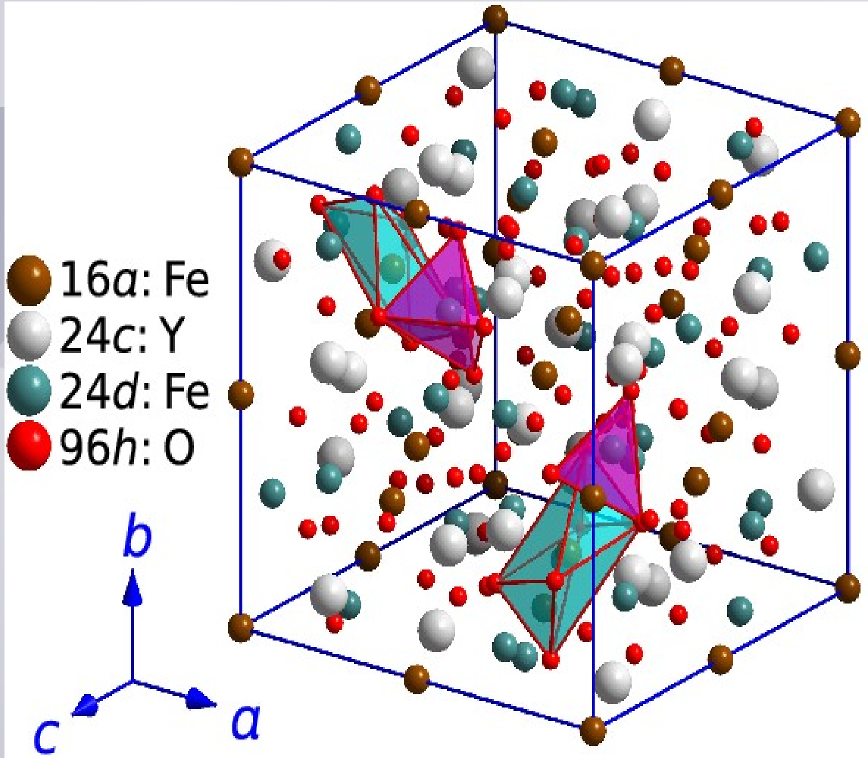


Parametric pumping of magnons at high k-vectors creates magnetic excitations

Question:
Time evolution of magnons: Non-equilibrium physics of interacting quasiparticles

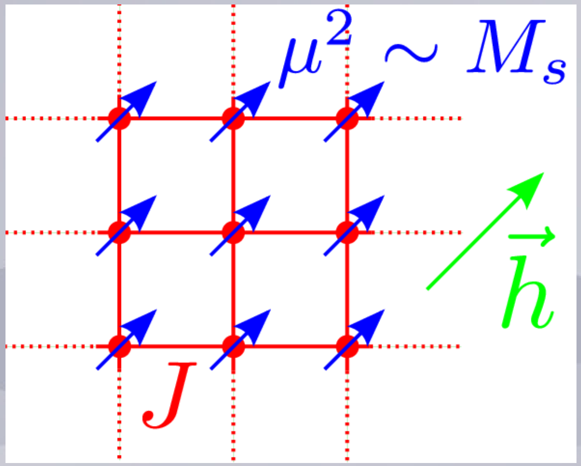
2.1 Simplifications to relevant physical properties

crystal structure of YIG



AK, Sauli, Bartosch, Kopietz ('09)

microscopic Hamiltonian



quantum spin S ferromagnet

Zeeman term

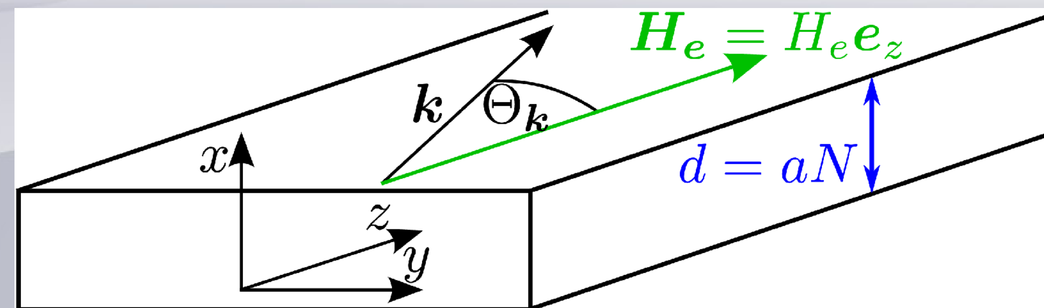
dipole-dipole interactions

$$\hat{H}_{\rm mag} = -\frac{1}{2}\sum_{ij} J_{ij}\mathsf{S}_i\cdot\mathsf{S}_j - h\sum_i S_i^z$$

$$-\frac{1}{2}\sum_i\sum_{j\neq i}\frac{\mu^2}{|\mathsf{r}_{ij}|^3}\left[3(\mathsf{S}_i\cdot\hat{\mathsf{r}}_{ij})(\mathsf{S}_j\cdot\hat{\mathsf{r}}_{ij}) - \mathsf{S}_i\cdot\mathsf{S}_j\right]$$

2.2 Linear spin-wave theory

- Geometry (thin film)



- Numerical approach
  - Ewald summation technique
  - Diagonalization of 2N x 2N matrix

$$H_2 = \begin{pmatrix} A_{\vec{k}} & B_{\vec{k}} \\ B^*_{-\vec{k}} & -A^T_{-\vec{k}} \end{pmatrix}$$

- Analytic approaches
  - Approximation for lowest mode
  - Bogoliubov transformation

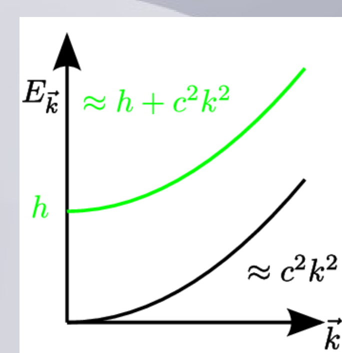
structure factor

$$E_{\vec{k}} = \sqrt{[h + \rho_{\text{ex}}\vec{k}^2 + \Delta(1 - f_{\vec{k}})\sin^2\Theta_{\vec{k}}][h + \rho_{\text{ex}}\vec{k}^2 + \Delta f_{\vec{k}}]}$$

$$\Delta = 4\pi\mu M_S$$

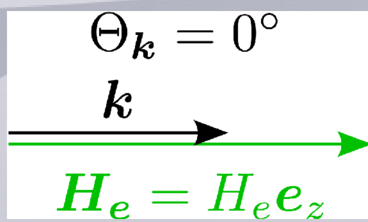
  - No dipolar interaction: known result

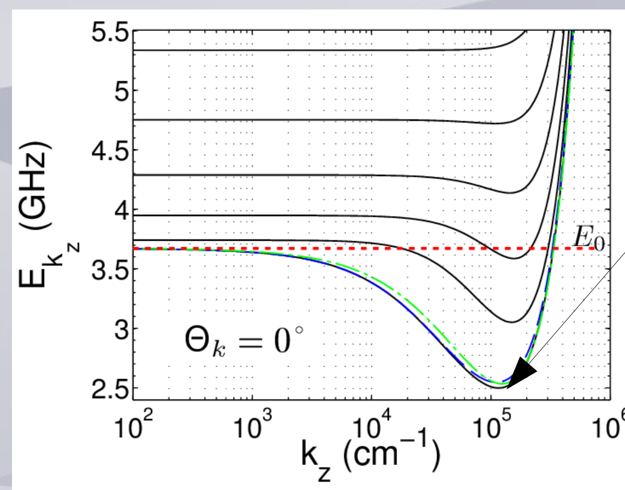
$$E_{\vec{k}} = h + \rho_{\text{ex}}\vec{k}^2 \qquad \Delta = 0$$



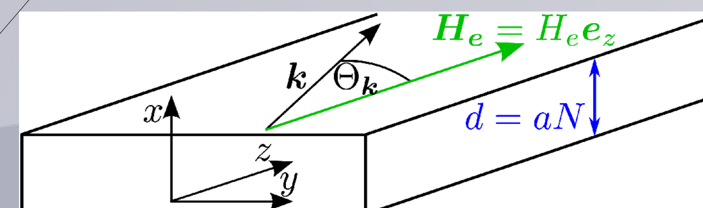
2.3 Results for magnon spectra

- Parallel mode





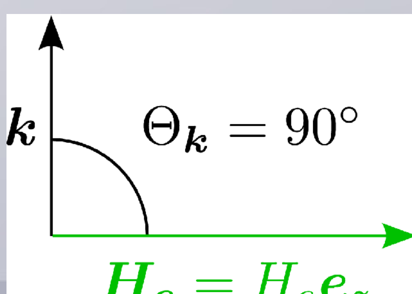
Minimum for BEC
Demokritov *et al.*
Nature ('06)

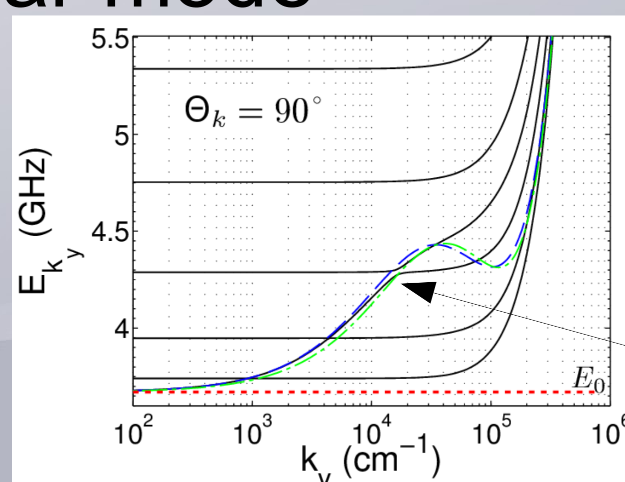


$$d = 400a \approx 0.5\mu\mathrm{m}$$
$$N = 400$$
$$H_e = 700 \text{ Oe}$$

$$E_0 = \sqrt{h(h + 4\pi\mu M_s)}$$

- Perpendicular mode

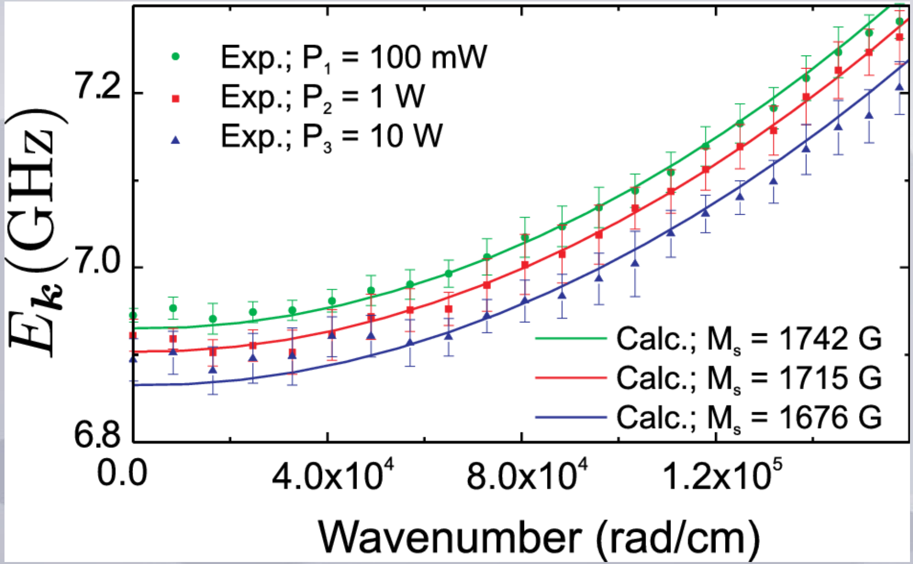




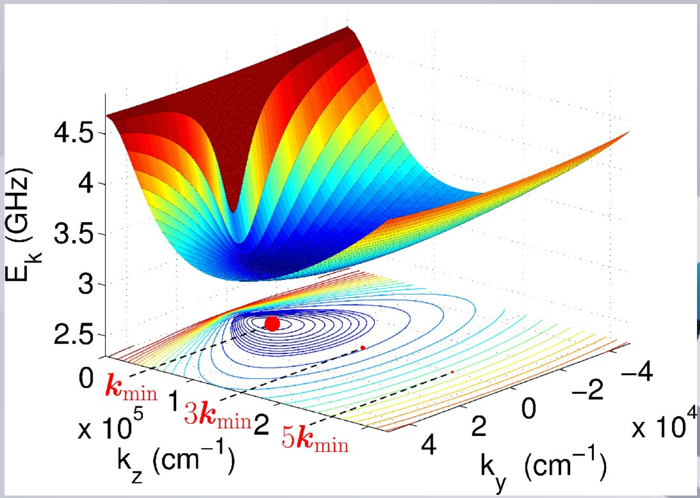
Hybridization:
surface mode

2.4 Comparison to experiments

- Excitation and detection of spinwaves using Brillouin light scattering spectroscopy (BLS) $\Theta_{\vec{k}} = 90^\circ$



- Side questions
  - excitation efficiency for “parametric pumping”
    Serga, AK, *et al.* ('12)
  - Time-dependent spin-wave theory
    Rückriegel, AK, Kopietz ('12)
  - intrinsic Damping Chernychev ('12)

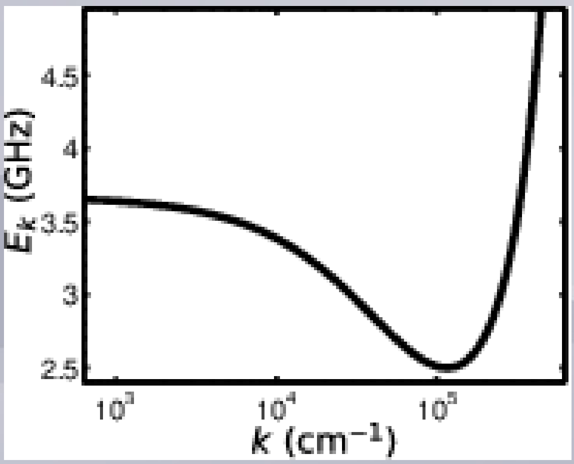


2.5 BEC at finite momentum

- Hamiltonian (after removing time dependence)

$$H_2 = \sum_{\vec{k}} \epsilon_{\vec{k}} b^\dagger_{\vec{k}} b_{\vec{k}} + \frac{1}{2}\sum \left(\gamma b^\dagger b^\dagger + \gamma^* bb\right)$$

parallel pumping



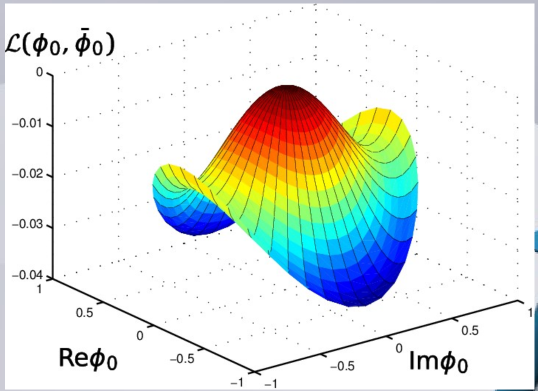
- new features for YIG system
  - condensate at finite wave-vectors

$$\phi_k = \delta_{k,k_{\mathrm{min}}}\phi_0$$

  - possible 2 condensates $\epsilon_{\vec{k}} = \epsilon_{-\vec{k}}$

$$\phi_k = \delta_{k,k_{\mathrm{min}}}\phi_0^+ + \delta_{k,-k_{\mathrm{min}}}\phi_0^-$$

  - explicitly symmetry breaking term



Napoleons hat potential

Hick, Sauli, AK, Kopietz ('10)

2.5 Gross-Pitaevskii equation

- two component BEC does not solve GPE

$$\phi^\sigma_{\mathsf{k}} = \delta_{\mathsf{k},\mathsf{q}}\psi^\sigma_n + \delta_{\mathsf{k},-\mathsf{q}}\psi^\sigma_n$$

- interactions provoke condensation at integer multiples of $\vec{k}_{\min}$

$$\phi^\sigma_{\mathsf{k}} = \sqrt{N}\sum_{n=-\infty}^{\infty}\delta_{\mathsf{k},n\mathsf{q}}\psi^\sigma_n$$

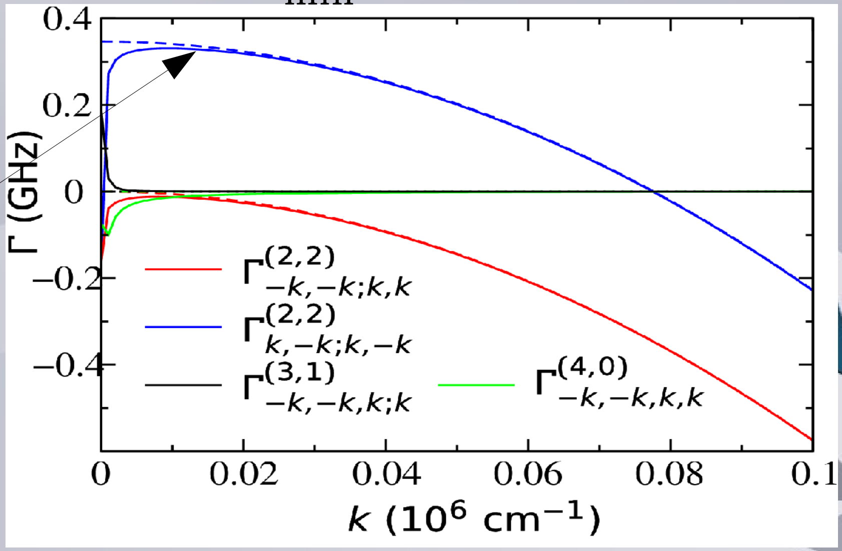
- condensate density

$$\begin{aligned}\rho(\mathsf{r}) &= |\phi^a(\mathsf{r})|^2 \\ &= 4\sum_n|\psi_n|^2\cos^2(n\mathsf{q}\cdot\mathsf{r})\end{aligned}$$

- Interaction vertices from analytical approach

$$H_4 \sim \Gamma^{(2,2)}b^\dagger b^\dagger bb + \Gamma^{(3,1)}b^\dagger bbb + \mathrm{h.c.}$$

$k = k_{\min}$ finite size effects



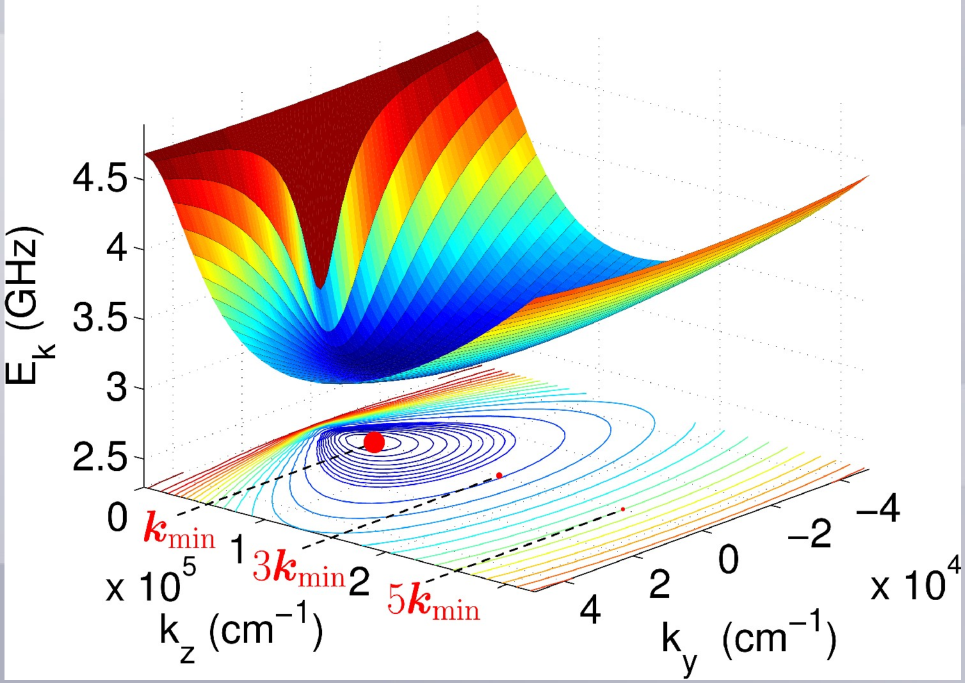
$\Gamma^{(2,2)} \sim -Jk^2$ ferromagnetic magnons

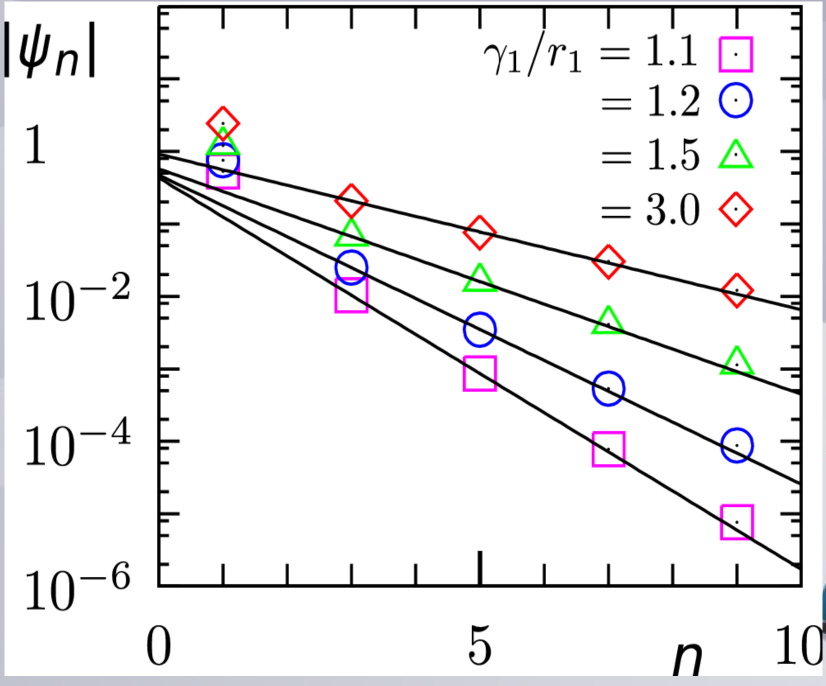
2.6 Results BEC in YIG

- discrete Gross-Pitaevskii equation

$$-(\epsilon_{n\mathrm{q}}-\mu)\psi_n^{\bar\sigma}-\gamma_n\psi_n^{\sigma} = \frac{1}{2}\sum_{n_1n_2}\sum_{\sigma_1\sigma_2}\delta_{n,n_1+n_2}V_{nn_1n_2}^{\sigma\sigma_1\sigma_2}\,\psi_{n_1}^{\sigma_1}\psi_{n_2}^{\sigma_2}$$

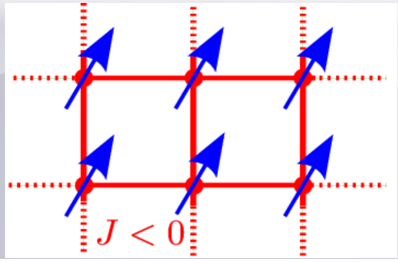
$$+\frac{1}{3!}\sum_{n_1n_2n_3}\sum_{\sigma_1\sigma_2\sigma_3}\delta_{n,n_1+n_2+n_3}U_{nn_1n_2n_3}^{\sigma\sigma_1\sigma_2\sigma_3}\,\psi_{n_1}^{\sigma_1}\psi_{n_2}^{\sigma_2}\psi_{n_3}^{\sigma_3}\,.$$

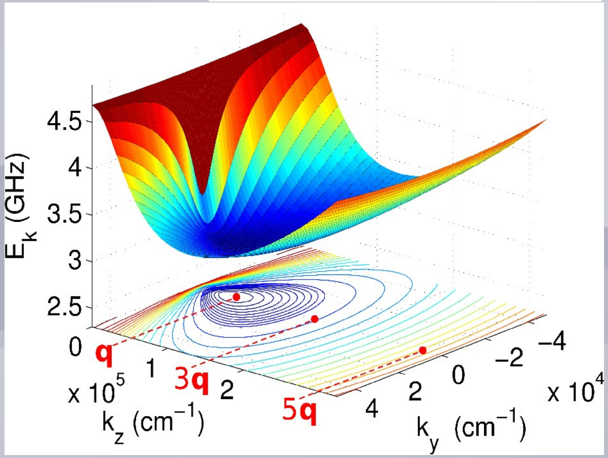


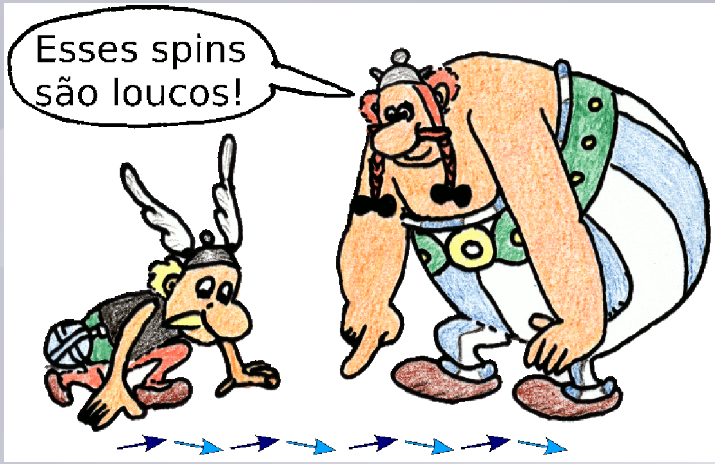


3 Summary

- description of magnetic insulators: Spin-wave theory
- development of **interacting spin-wave theory** with dipole dipole interactions
- interesting properties of the energy dispersion
- interactions: possible **condensation** of bosons at finite wave-vectors and integer multiples







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

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Phys. Rev. B **88**, 094522 (2013)

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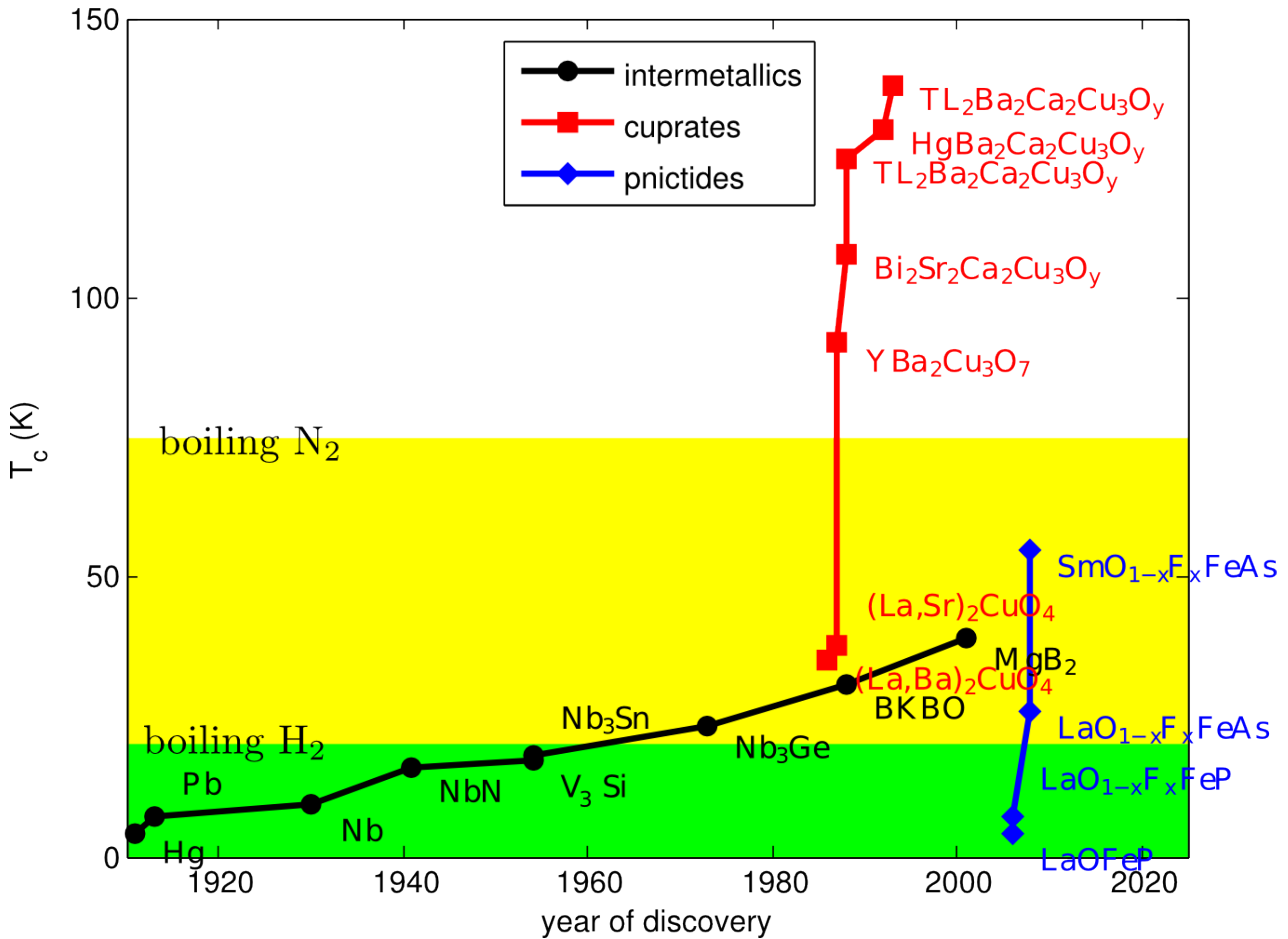
A) Fe based superconductors

- discovery: $LaO_{1-x}F_xFeAs$ T_c=26K

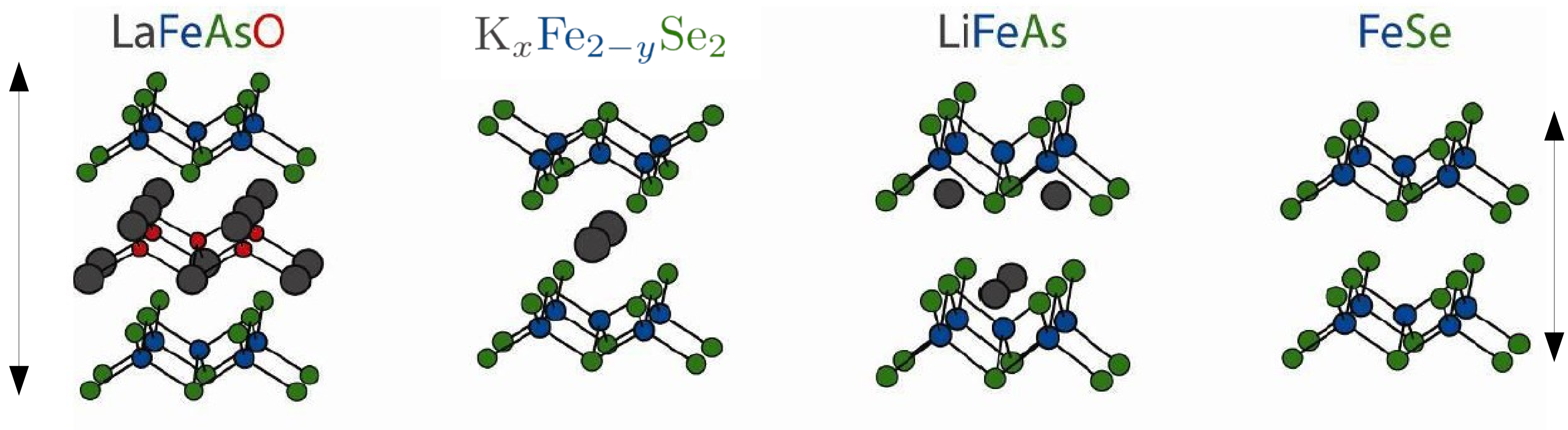
Kamihara *et al.* JACS 2006



A.1 Fe based superconductors: Materials

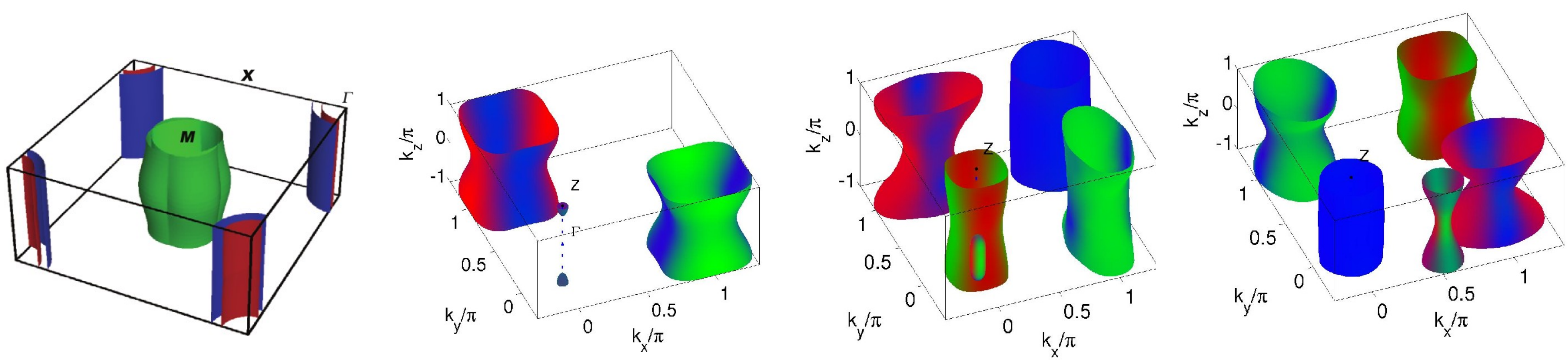
- Materials

Crystal structure



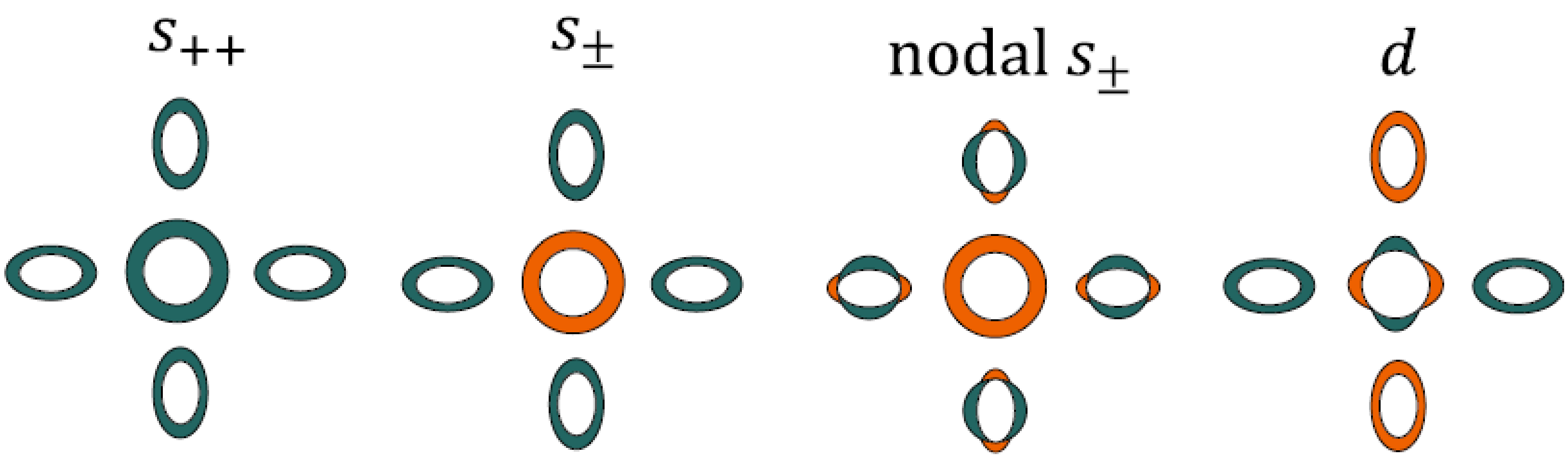
Tc	28 K (55 K for Sm)	38 K	18 K	8 K

Fermi surface (DFT)



A.2 Open questions (many)

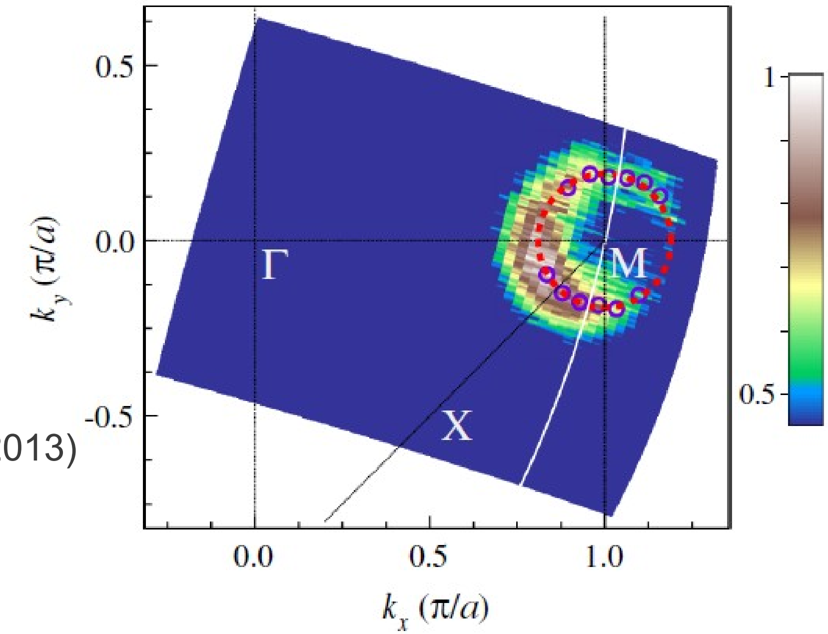
- here we concentrate on
  - symmetry of the order parameter

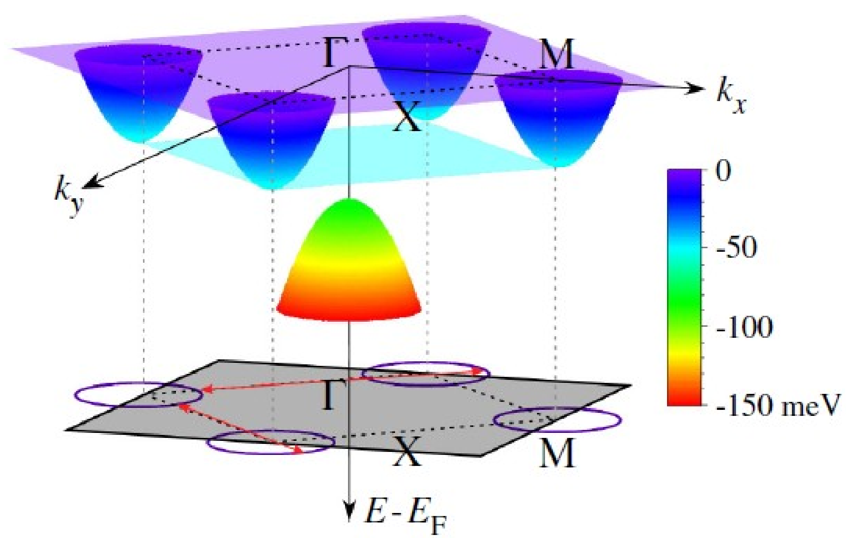


  - realistic models that capture main parameters of materials under investigation

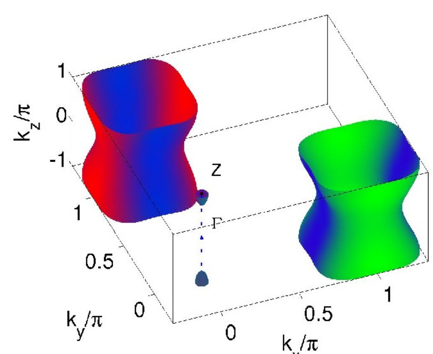
B.1 $K_xFe_{2-y}Se_2$

- 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)

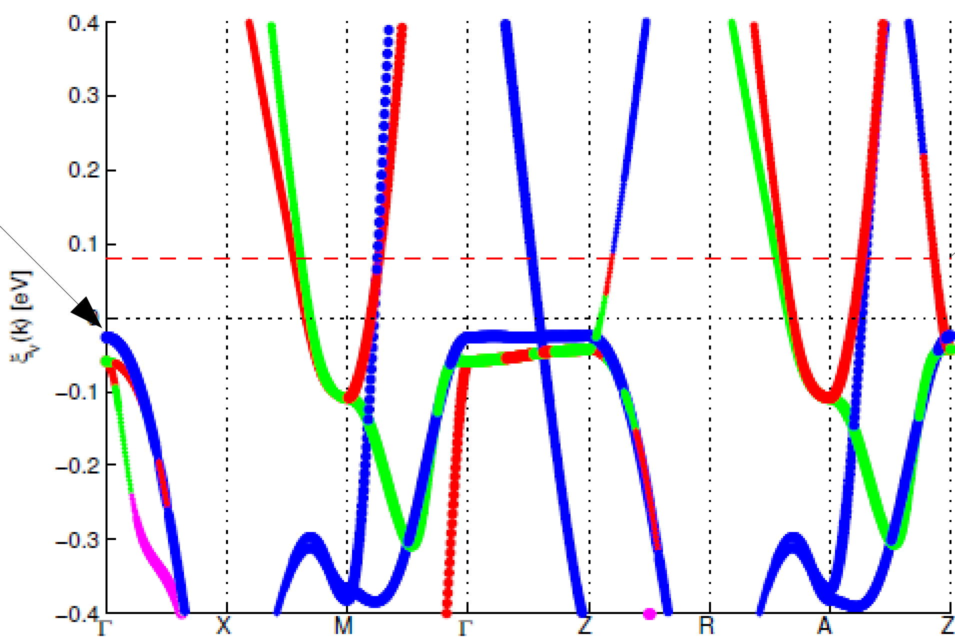


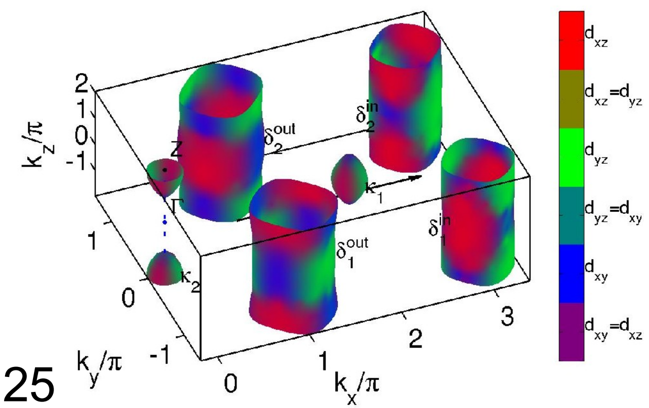
B.2 Band structure: Tight binding model

- 10 orbital, *I4/mmm* for K-122
- Wannier projection of DFT results

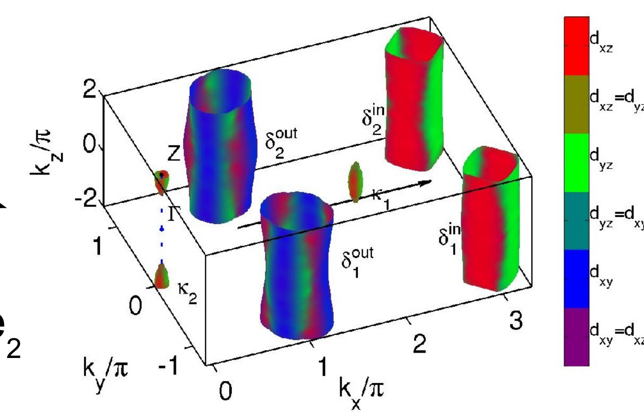
$$H_0 = \frac{1}{N}\sum_{ij}\sum_{\ell_1,\ell_2=1}^{10} t_{ij}^{\ell_1\ell_2} c_{i\ell_1}^{\dagger} c_{i\ell_2}$$

no hole pocket





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



n=6.12
$K_{0.85}Fe_{1.8}Se_2$

B.2 Interactions

- Hubbard-Hund Hamiltonian

extended Hubbard model

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

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

Kuroki *et al.* PRL (2008)

exchange interaction

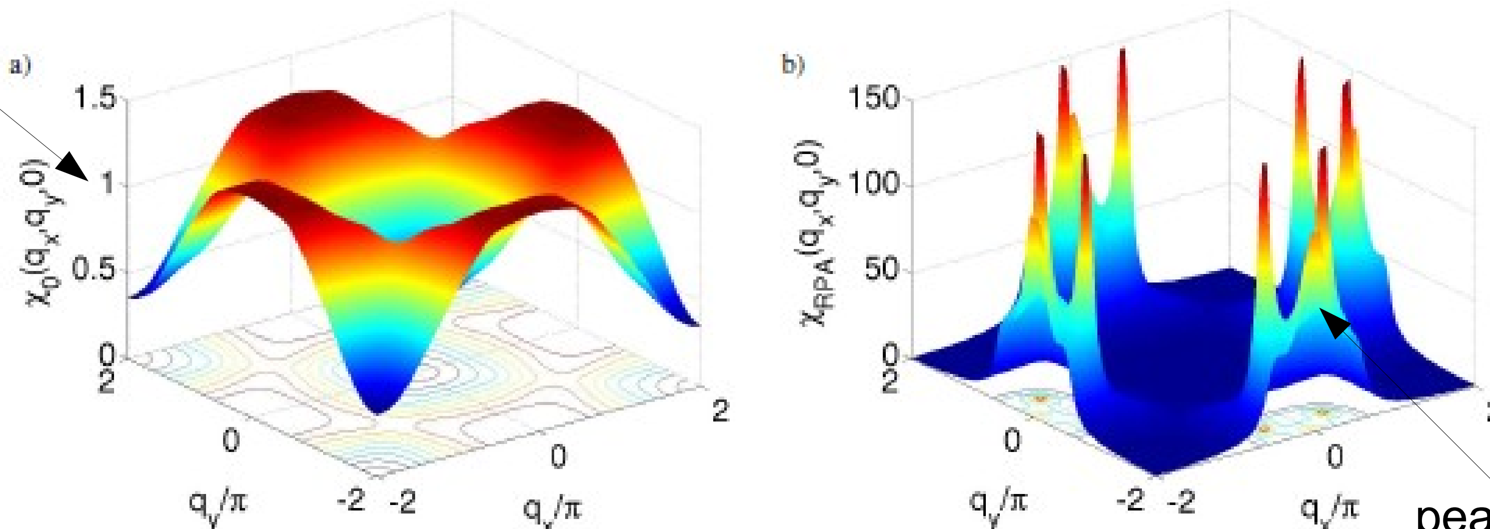
pair hopping

B.3 Spin fluctuation mediated pair scattering

- Susceptibility in normal state (orbital resolved)

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

periodic with 1 Fe zone



peaked at Q=(1.65,0.35) pi

- Interactions: RPA approximation

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

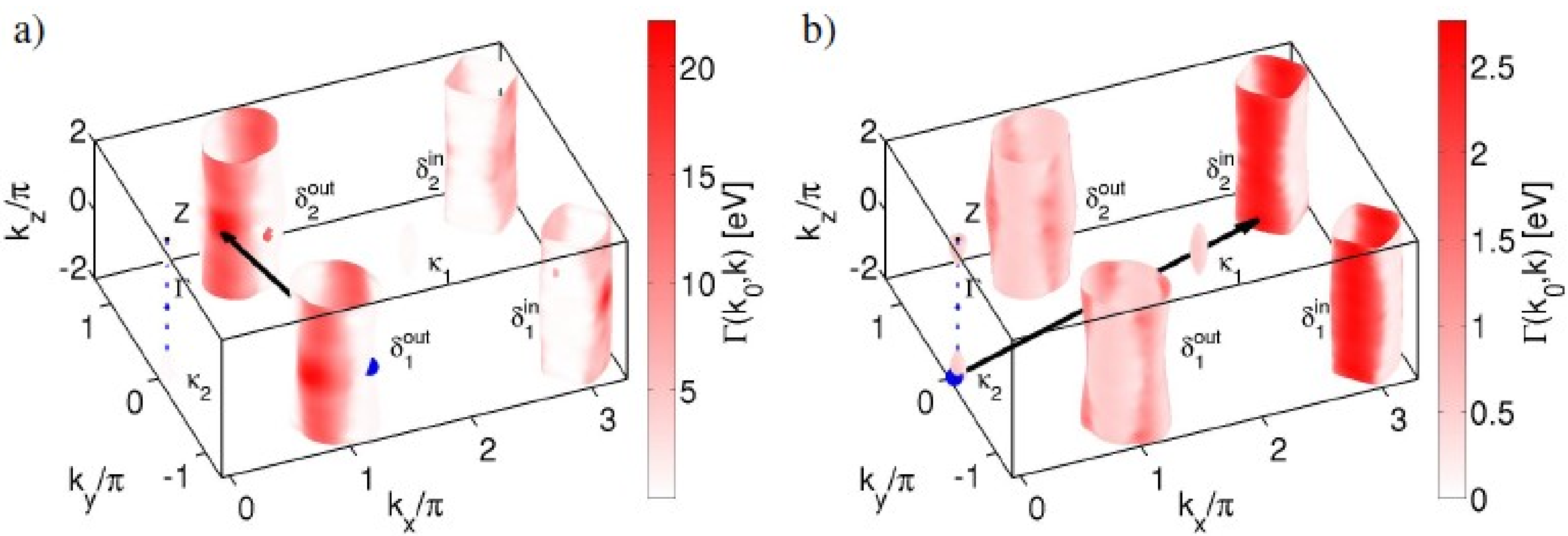
B.4 Spin fluctuation mediated pair scattering

- Scattering vertex in singlet channel

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

band space

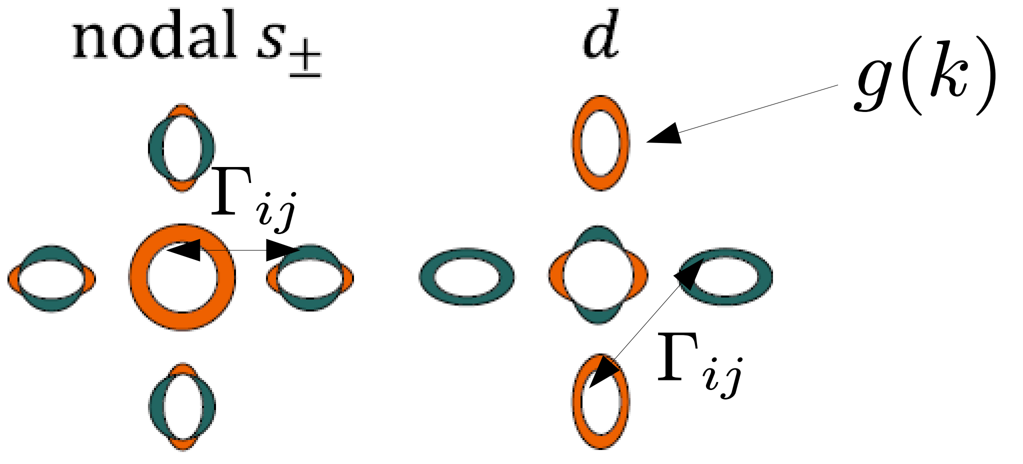
Graser *et al.* NJP (2009)



B.5 Gap equation

- Decompose gap function into magnitude and dimensionless symmetry function

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

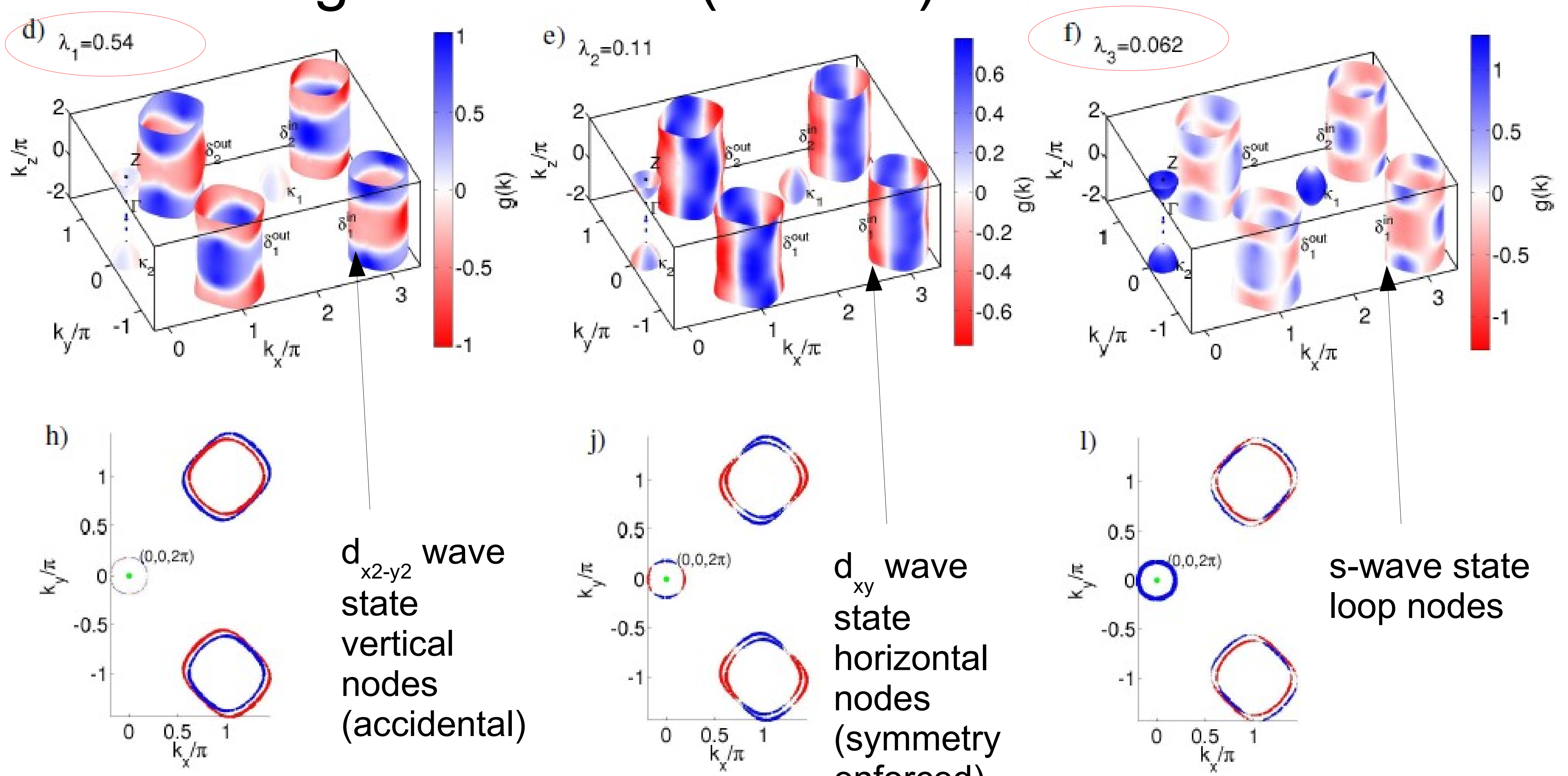


- Pairing strength functional
- variation leads to eigenvalue equation

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

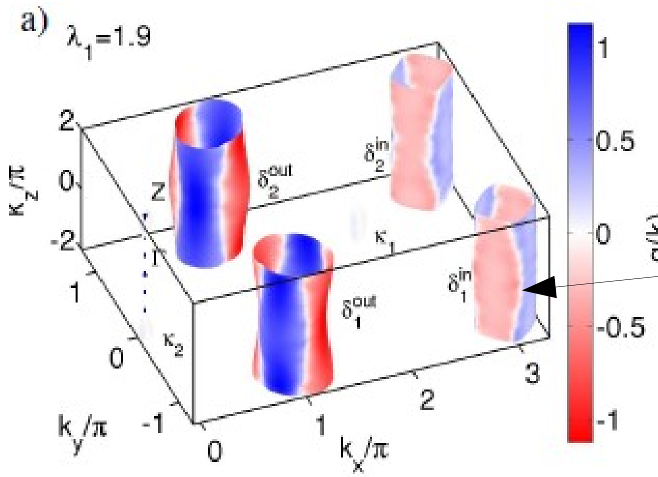
B.5 Gapfunction

- leading instabilities (n=6.25)



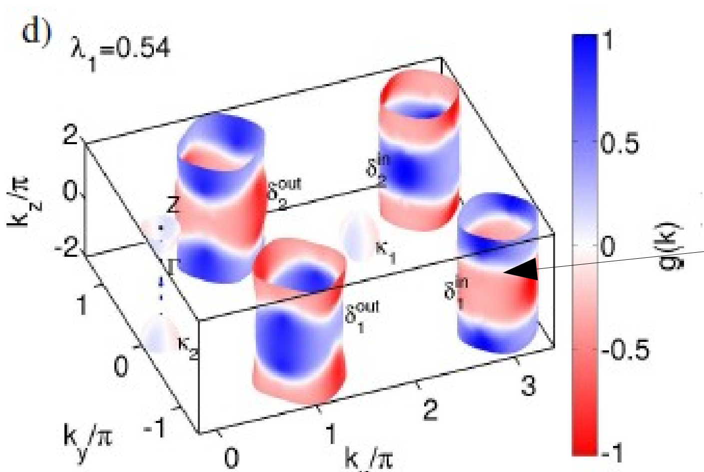
B.5 Gapfunction doping dependence

- underdoped case (n=6.12)



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

- overdoped case (n=6.25)



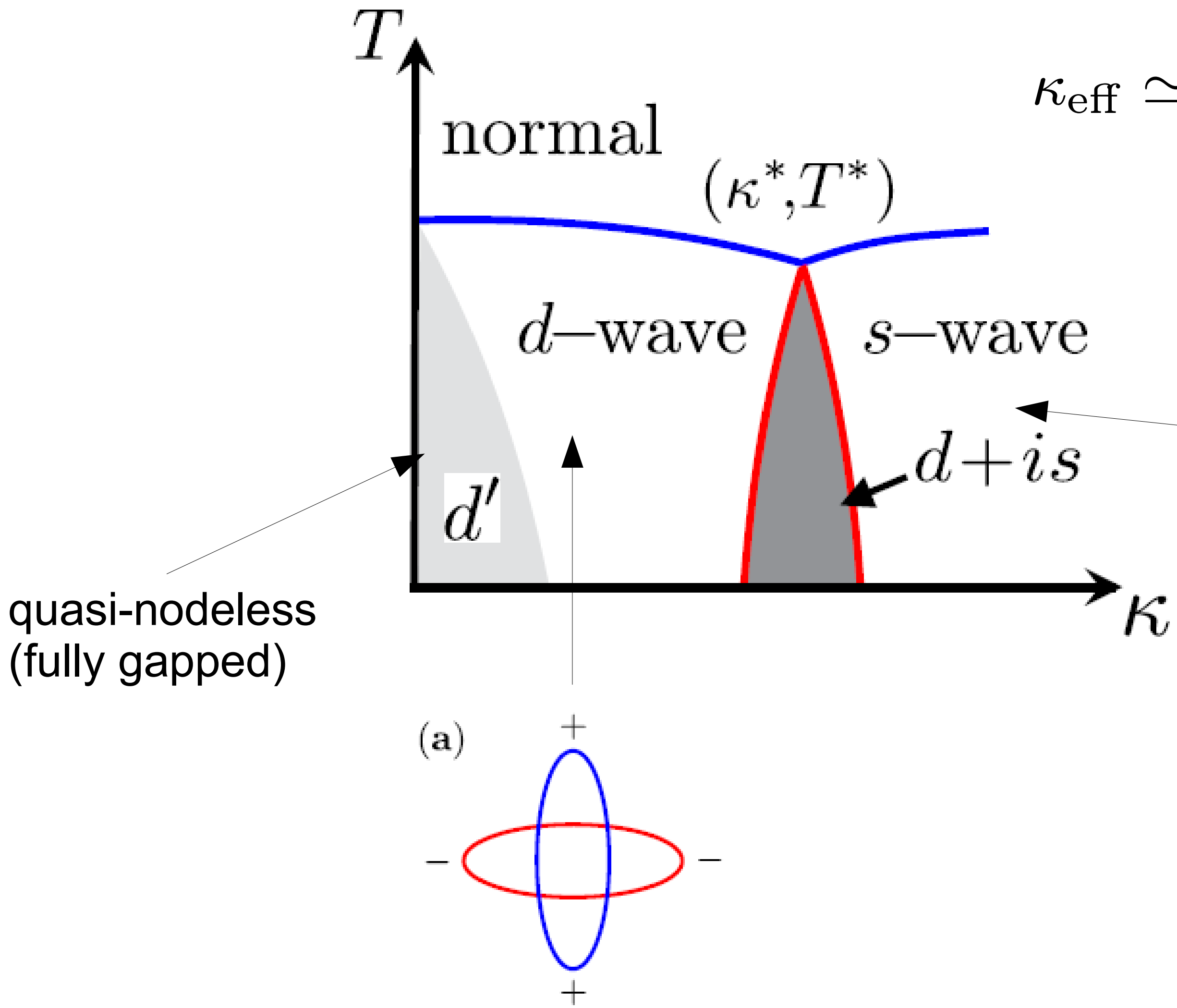
d_{x2-y2} wave state vertical nodes (accidental)

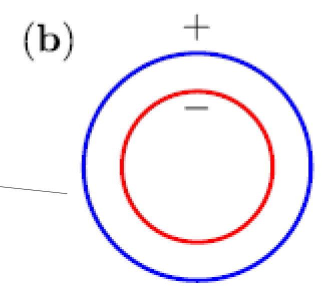
C.1 Hybridization effects

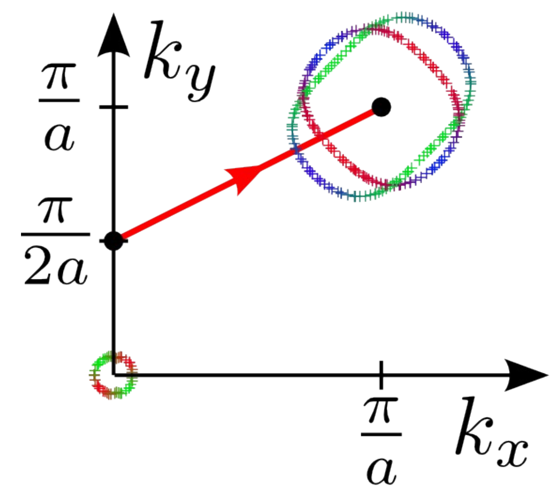
- Transition from d to s-wave

Khodas, Chubukov PRL (2012)

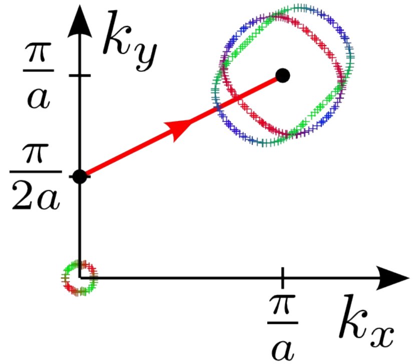
$$\kappa_{\rm eff} \simeq \frac{\delta\xi}{\left\langle \frac{\Delta\xi_{\rm k}}{v_{\rm F}({\rm k})k_{\rm F}({\rm k})}\right\rangle} = \frac{\text{hybridization}}{\text{ellipticity}}$$



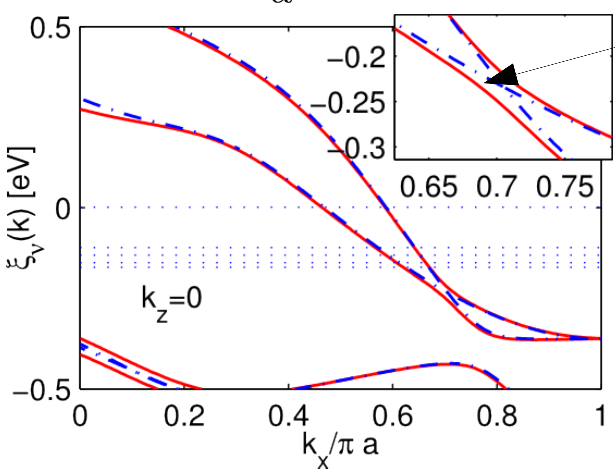


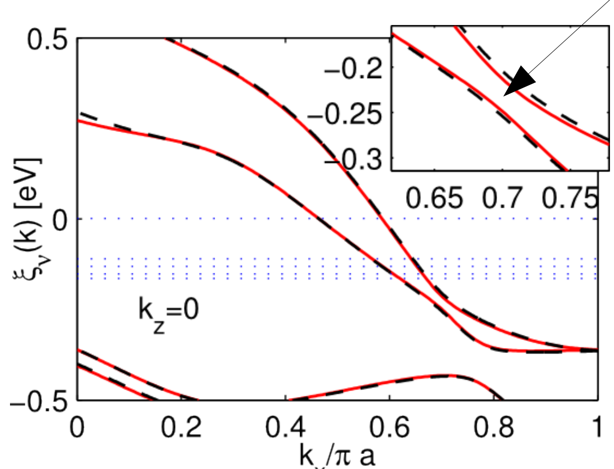


C.2 Hybridization in $K_xFe_{2-y}Se_2$



cut along non-symmetry path





- Origin of hybridization :

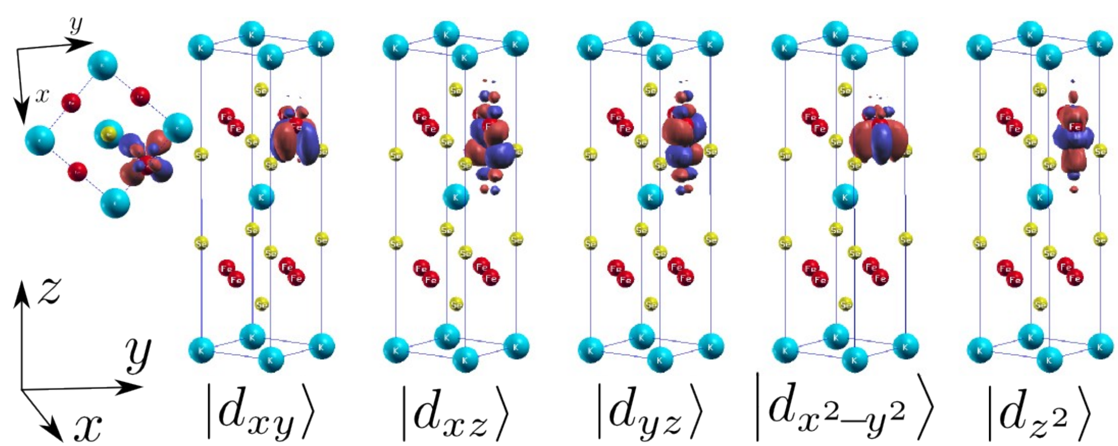
I4/mmm space group

spin-orbit coupling

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

Friedel ('64)

approximate with atomic wave functions for spin-orbit coupling

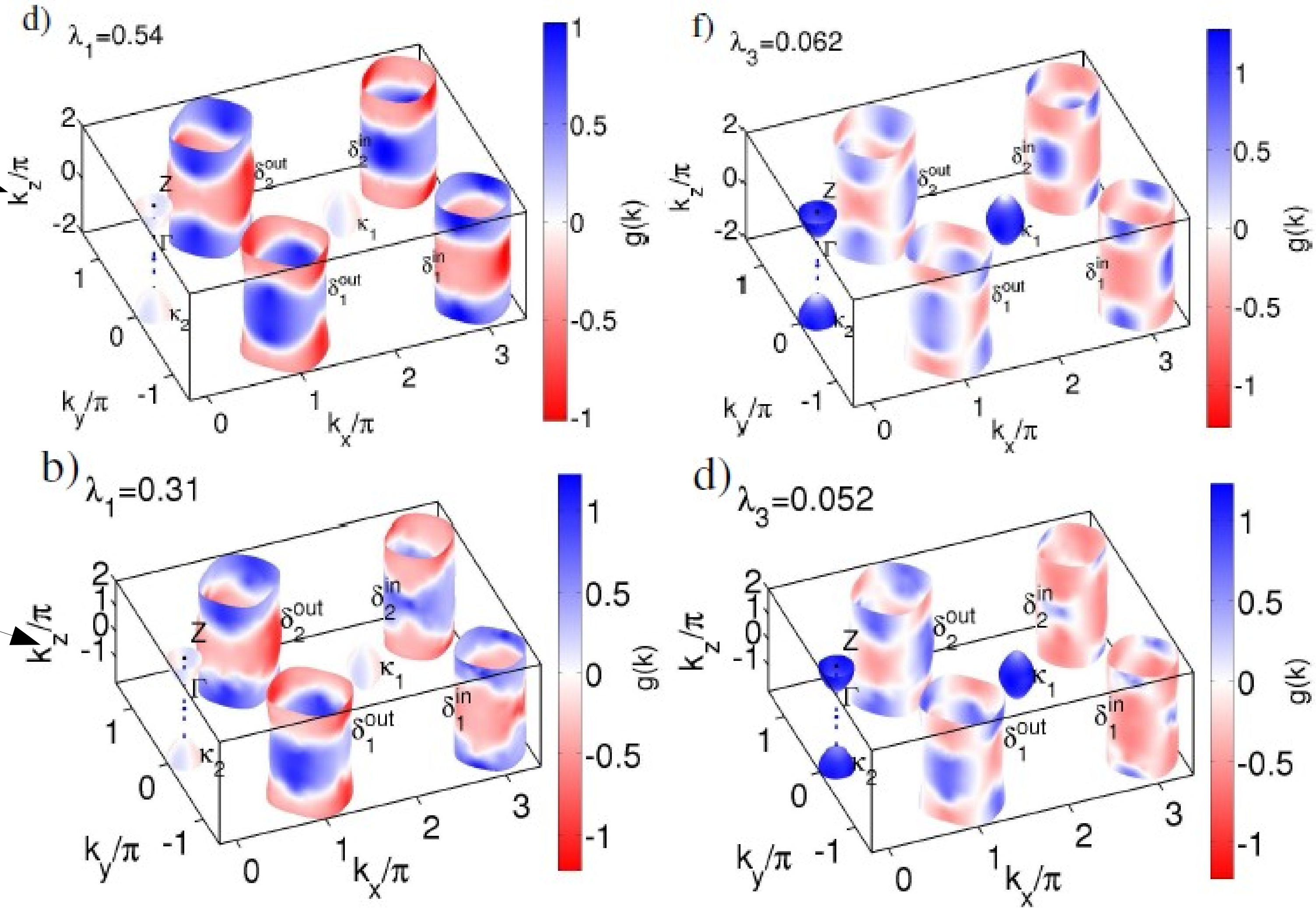


C.3 Gapfunction with spin-orbit coupling

- weakening of superconducting instability
  (all symmetries)

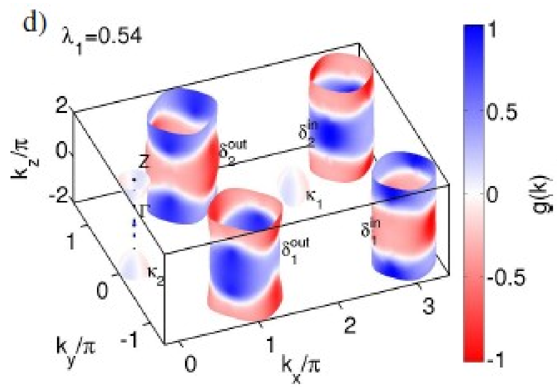
no spin-orbit coupling

spin-orbit coupling (λ=0.05 eV)



D Summary

- $K_xFe_{2-y}Se_2$ different from other Fe based SC
- missing hole-pocket makes s-wave instability less likely (spin-fluctutation 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-centrered hole pockets
  - quasinodal behavior makes detection difficult
  - missing ingredients as correlations or deviations from normal-state properties due to doping / impurities



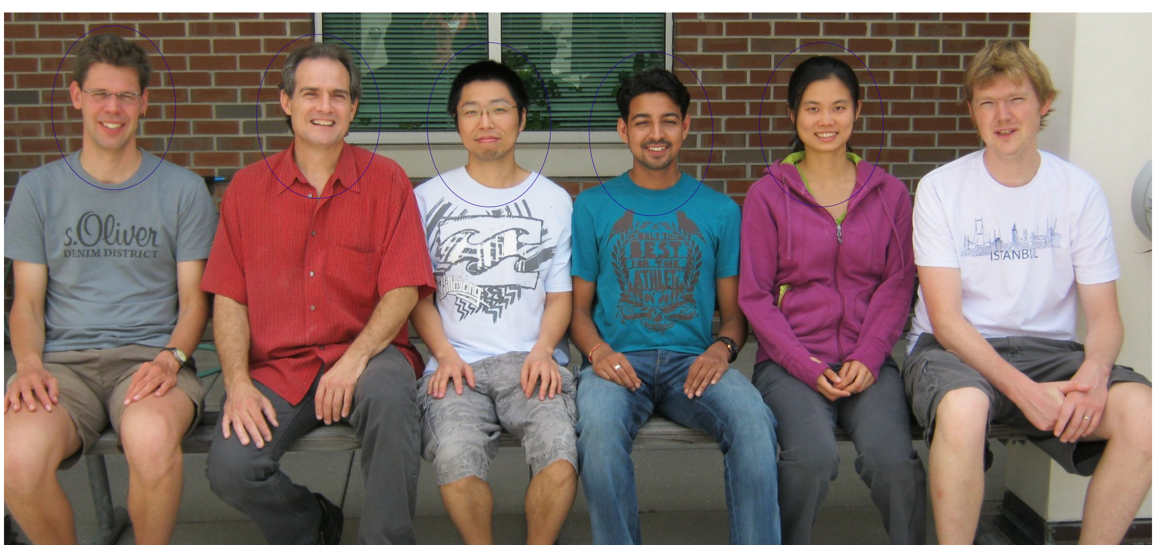
Acknowledgements

- External collaborators





- Hirschfeld group (UF)



Kopietz group (UF)