Gap symmetry in different iron based superconductors

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Ronny Thomale (Princeton), C. Platt, W. Hanke (Aachen/Würzburg), J. Hu (Purdue, IOP Beijing)

Seo, BAB, JP Hu, PRL 101, 206404 (2008)

Ronny Thomale, C. Platt, J. Hu, C. Honerkamp and B. A. B., PRB 80, 180505(R) (2009).

Ronny Thomale, C. Platt, W. Hanke, and B. A. B., arXiv:1002.3599.

KITP, January 2011

Fe-based Superconductors

- 1111 Series:

  Electron doped:

  $CeO_{1-x}F_xFeAs$: 41K $SmO_{1-x}F_xFeAs$: 55K

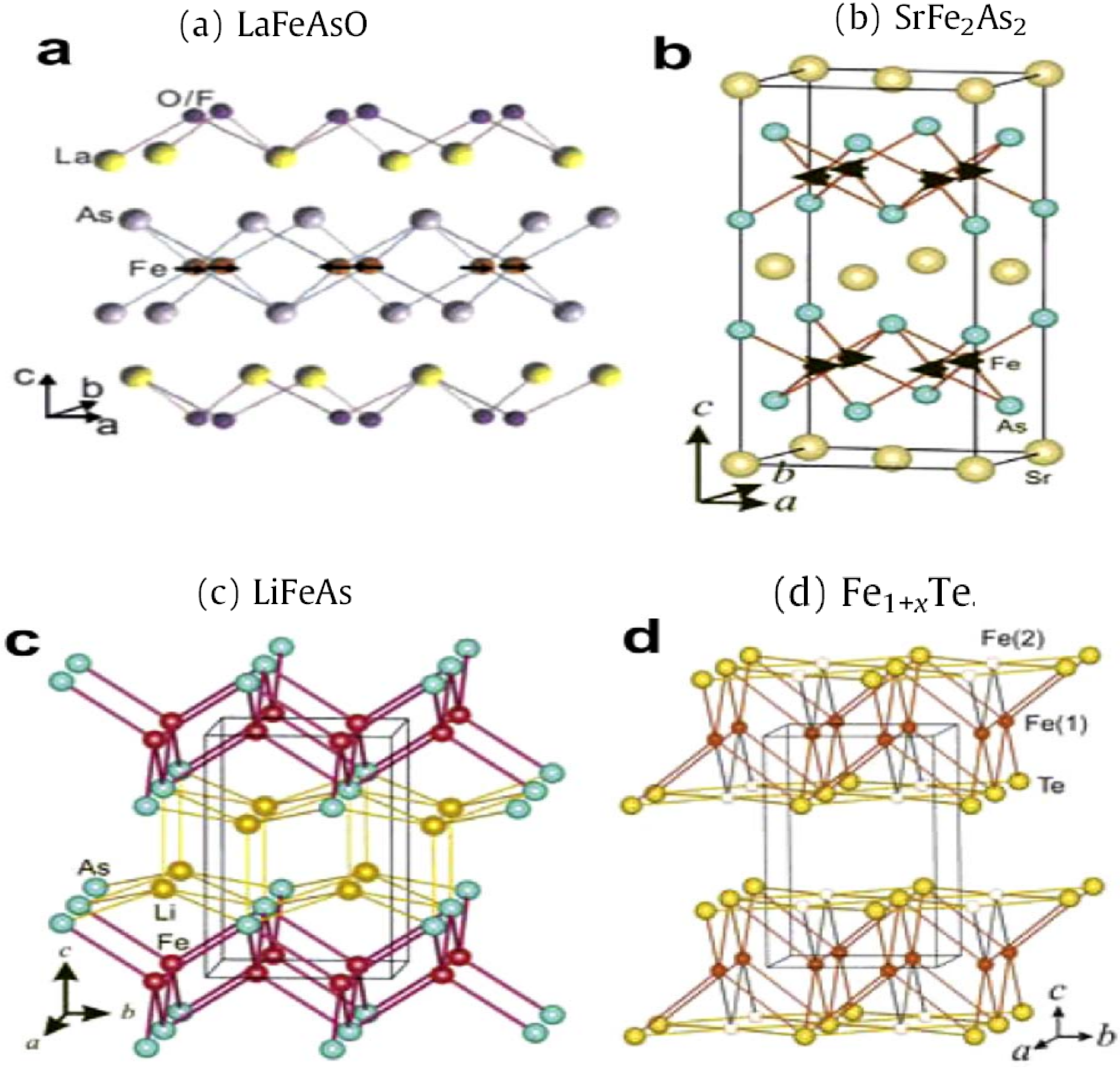
  $PrO_{0.89}F_{0.11}FeAs$: 52K $SmFeAsO_{1-x}$ 55k CaFFeAs: 36K

  Hole Doped: $La_{[1-x]}Sr_xOFeAs$
- 122 Series: (both Hole and Electron Doped)

  $BaFe_2As_2$, 38K
- 11 Series: (Taiwan)

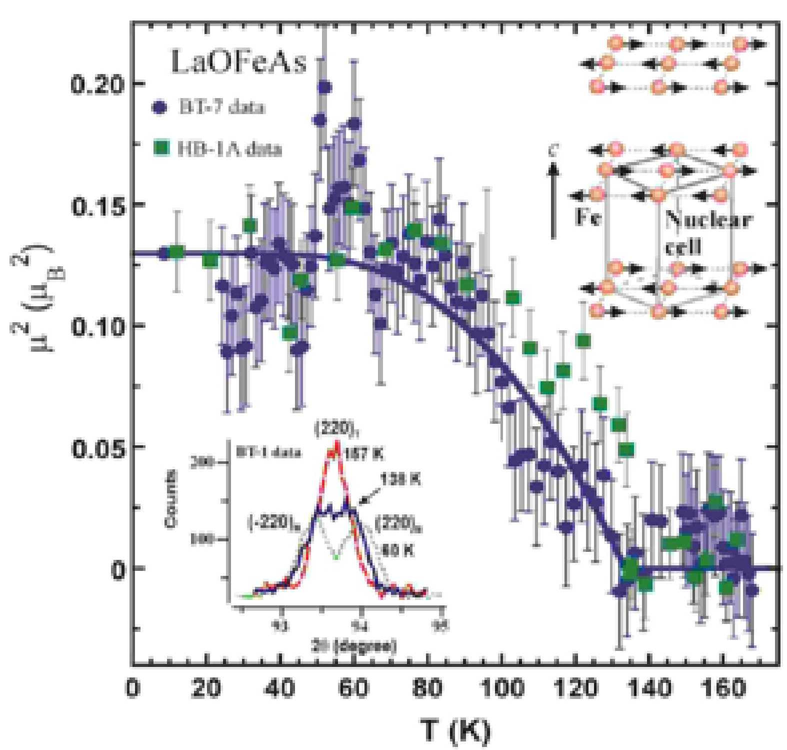
  FeSe, 8k - 37k (with pressure)
- 111 Series: LiFeAs 16k
- LaFePO: 6K

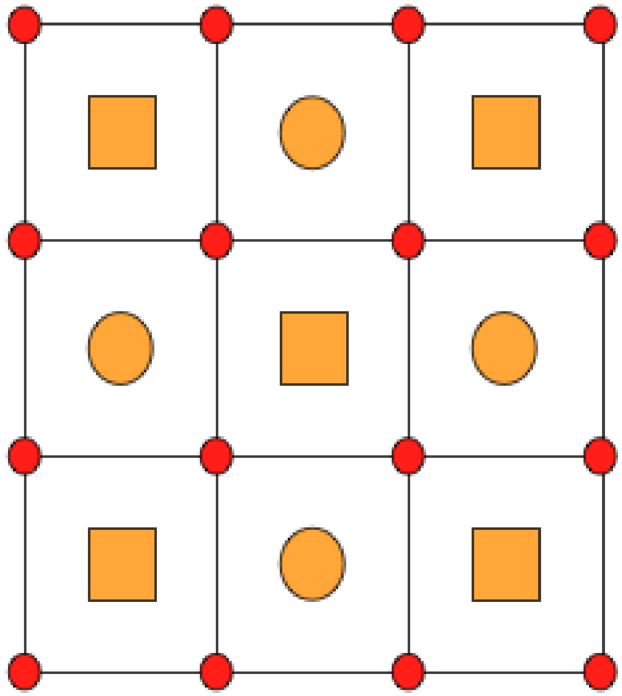
X.H. Chen et al, Nature 453, 761 (2008)



In the following, we concentrate on the 1111 and 122 compounds (a)

Exchange Can Explain Normal State Magnetism





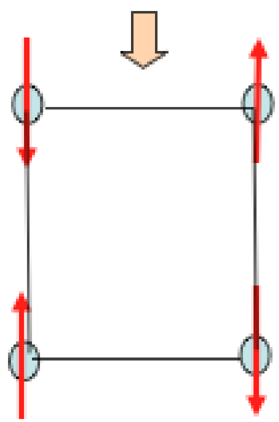
a. As bridges four nearest neighbor Fe atoms
b. Two magnetic exchange coupling parameters

$$H = J_1 \sum_{<ij>_{NN}} S_i S_j + J_2 \sum_{<ij>_{NNN}} S_i S_j$$

Magnetic Order in J_1-J_2 Model

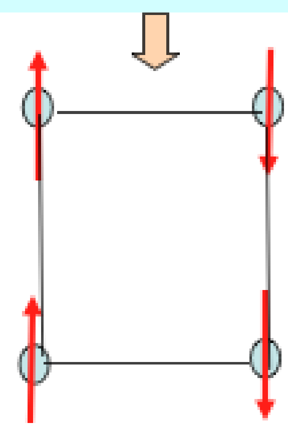
$$H = J_1 \sum_{<ij>_{NN}} S_i S_j + J_2 \sum_{<ij>_{NNN}} S_i S_j$$

$J_1 > 2J_2$, $E = -2J_1 + 2J_2$



AFM

$J_1 < 2J_2$, $E = -2J2$

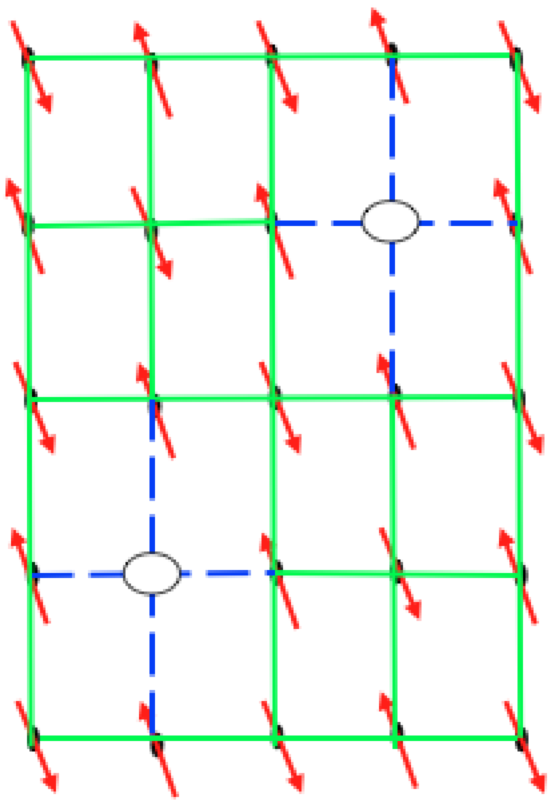


Collinear-AFM

C.Fang, Hu, Kivelson, 2008
Xu, Sachdev, 2008

If magnetism is origin of supercond., what predictions?

Doping effect and t-J model



$$H = -\tilde{t} \sum_{<ij>\sigma} C_{i\sigma}^{+} C_{j\sigma} + J \sum_{<ij>} S_i S_j$$

Kinetic energy

Magnetic exchange energy

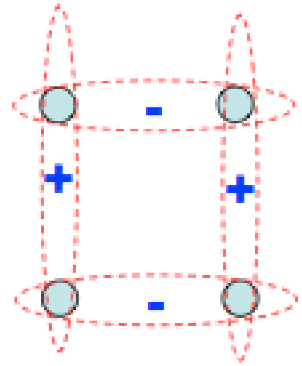
A: Doping destroys the long range AFM order
B: Short spin correlations survive.
C: Magnetic exchanges provide the force gluing electron pairs.

$$\Delta(k) = < C_{k\uparrow} C_{-k\downarrow} >$$

Cuprate D-wave Pairing Symmetry

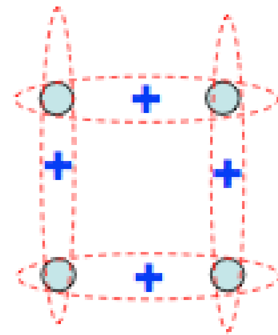
$$J\sum_{<ij>} S_i S_j$$

$$-J\,|\Delta_d|^2$$



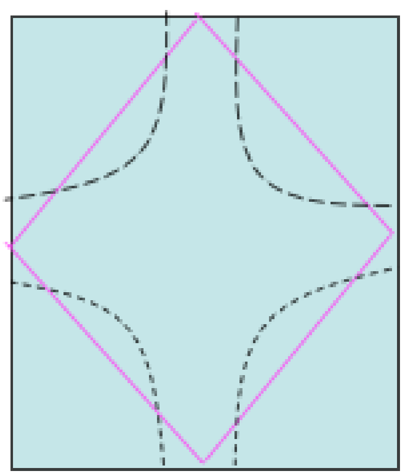
$$\Delta_d \propto (\cos k_x - \cos k_y)$$

$$-J\,|\Delta_s|^2$$



$$\Delta_s \propto (\cos k_x + \cos k_y)$$

Band structure



a. D-wave pairing is favored over S-wave pairing.
b. D-wave was really a prediction from the meanfield solution of t-J model.

Kotliar and Liu (1988), Gros, C.(1988)

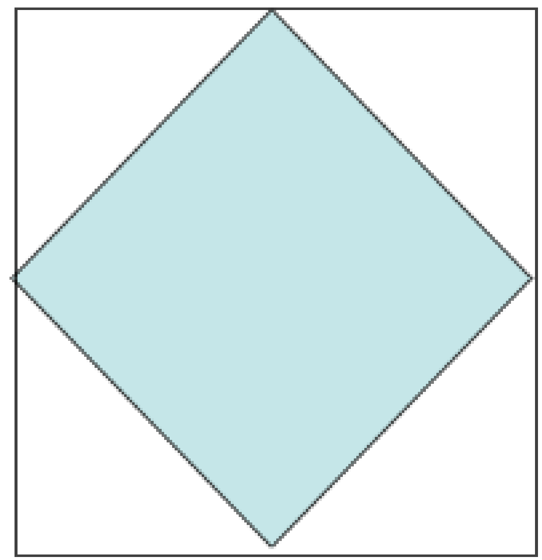
Anderson et al, J Phys.Cond. Mat 16 (2004) R755

Van Harlingen DJ. *Rev. Mod. Phys, 67, 515, 1995*

D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch, Phys. Rev. B 34, 8190–8192 (1986)

Pairing symmetry in one band-t-J_1-J_2 model

- Pairing symmetry for a *single* band t-J_1-J_2



$$d_{x2-y2} + id_{xy}$$

S.Sachdev, Physica A 313, 252 (2002)
Jian Li and Y. Wang, Chin. Phys. Lett 25, 2232 2008

FeAs Cos(kx)Cos(ky) Pairing Symmetry

J_1

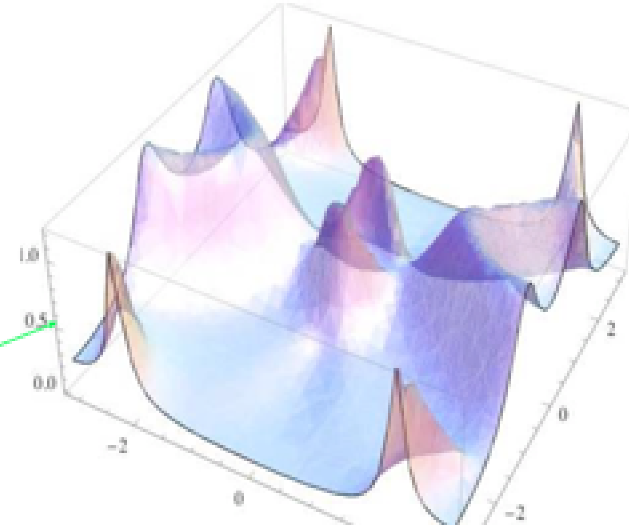
S wave pairing
$\cos k_x + \cos k_y$

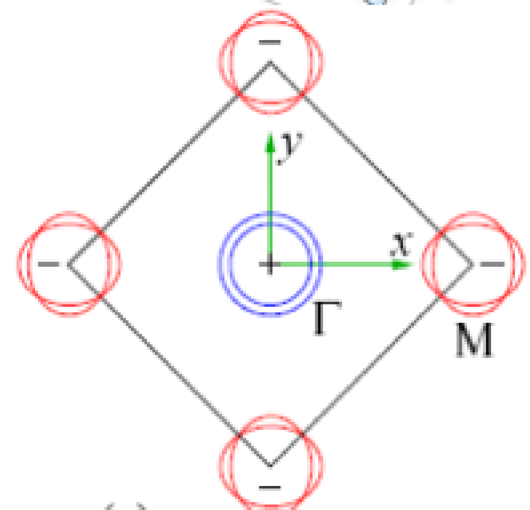
d wave pairing
$\cos k_x - \cos k_y$

J_2

S wave pairing
$\cos k_x \cos k_y$

d wave pairing
$\sin k_x \sin k_y$





(a)

$$2T_c = J_2 \sum_k (f(k))^2 g(x(k, T_c))$$

Symmetry factors

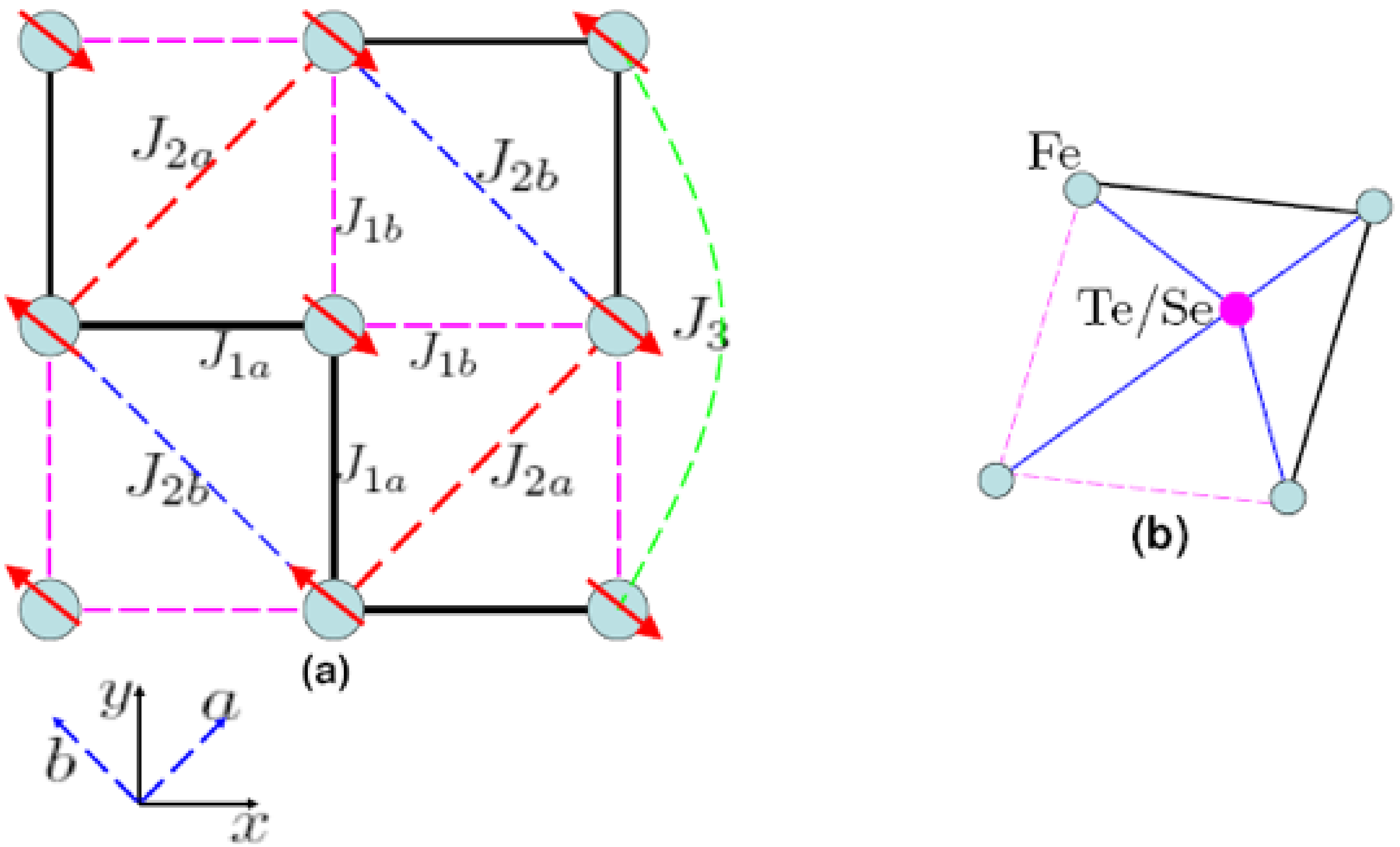
Function peaks at
Fermi surfaces

S-wave $\cos k_x \cos k_y$ wins over other symmetry pairing.

K. Seo, A. B. Bernevig, J. Hu PRL 101, 206404 (2008)

Pallab Goswami, Predrag Nikolic, Qimiao Si, EPL 91, 37006 (2010)

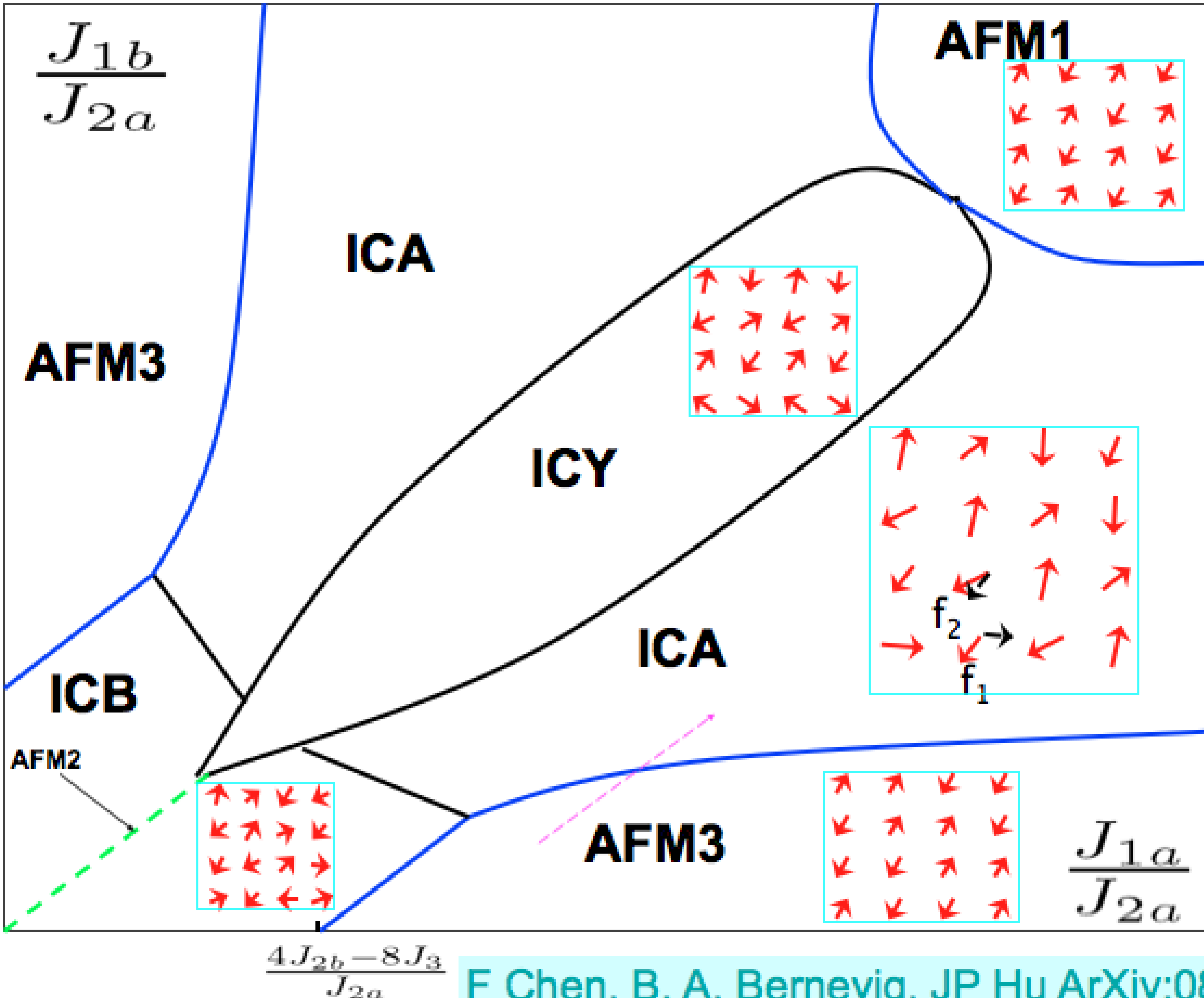
Magnetism in FeTe



Hard to understand it from Fermi surface nesting picture!

J2a>J2b, J1a>J1b; (J2a, J2b)>0, J1a>0

Phase Diagram



F Chen, B. A. Bernevig, JP Hu ArXiv:0811.1294

Weak coupling RG/RPA/Mean Field approaches

Vladimir Cvetkovic, Zlatko Tesanovic Europhysics Letters 85, 37002 (2009)

A.V. Chubukov, D. Efremov, I. Eremin, Phys. Rev. B 78, 134512 (2008)

S. Graser, T. A. Maier, P. J. Hirschfeld, D. J. Scalapino, New J. Phys. 11, 025016 (2009)

Kazuhiko Kuroki, Seiichiro Onari, Ryotaro Arita, Hidetomo Usui, Yukio Tanaka, Hiroshi Kontani, Hideo Aoki, Phys. Rev. Lett. 101, 087004 (2008)... many others

However, the situation is much more complex than Initially thought.

Experimental evidence for LaOFeAs and LaOFeP:

LaOFeAs	LaOFeP
High Tc (50K)	Low Tc (7K)
Nodeless, but anisotropic gap	Nodal gap
(π,0) parent magnetic order	No parent magnetic order

fRG method

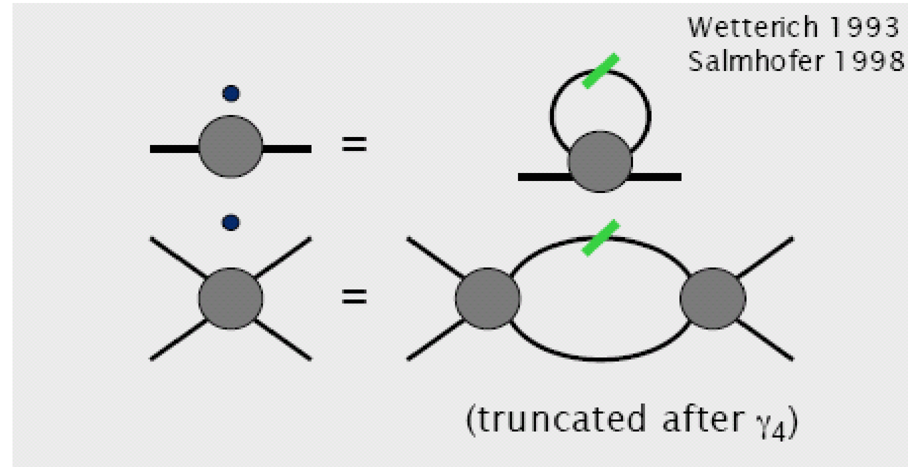
- Polchinski's flow equations: hierarchy of m-point functions

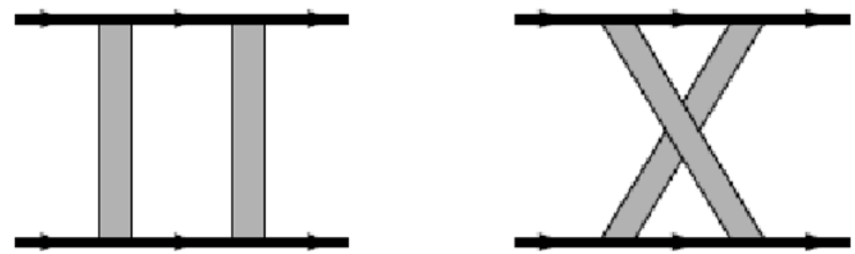
- Infinitesimal steps of mode integration: fRG solution of fermionic action

$$Z = \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi \; e^{S\{\Psi\}}$$

- Consider diagrams contributing to 4 point function: 2nd order plaquet terms

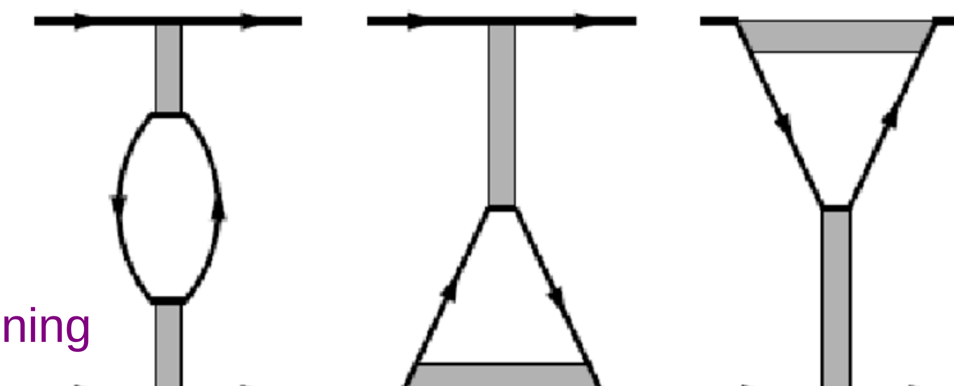
- Suitable method to detect FS instabilities starting from bare weak coupling





Cooper

Peierls



Screening

Vertex corrections

fRG method

- Flow to FS IR fixed point manifold w.r.t. cutoff Λ:
4-point function V(k1, k2, k3) diverges

- Symmetry and general properties of diverging channels of V(k1, k2, k3) specify the type of observed instability

- $T_c \sim \Lambda_c$ where V diverges

- Unbiased description of all FS instabilities, subset of diagrams maps back to other methods (Cooper channel: fRG ~ BCS ladder summation $V=U+U^2 \chi(k-q)$ (Kohn-Luttinger))

- SC instabilities emerge from magnetic fluctuations

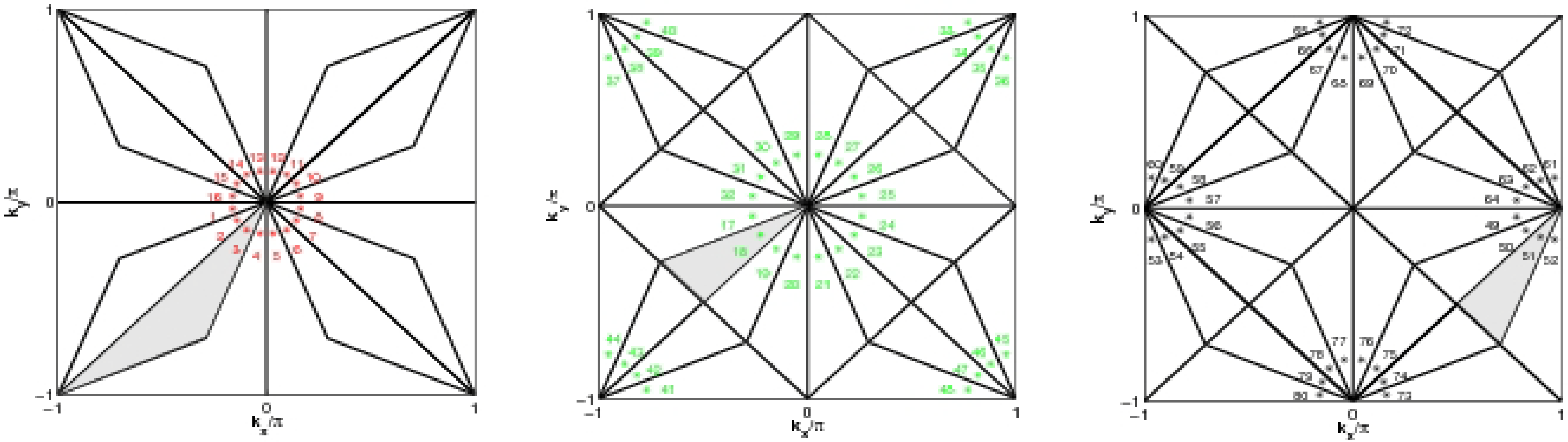
- Pioneered for cuprates by Honerkamp, Salmhofer, Metzner, for pnictides by Fa Wang, Dung-Hai Lee

Approximations in fRG

- Projection of 4-point momenta on Fermi surface

$$V(k_1, k_2, k_3) \rightarrow V(k_{1,\mathrm{F}}, k_{2,\mathrm{F}}, k_{3,\mathrm{F}})$$

- (numerically demanded) patch discretization of BZ



- Neglection of higher m-point functions
(≡ weak coupling approach)

Interactions as starting condition for 4PF bare level

- orbital symmetry is crucial for the phenomenology of the pnictides (nodal SDW instability)

- for SC orbital interaction trigger the potentially strong gap anisotropy

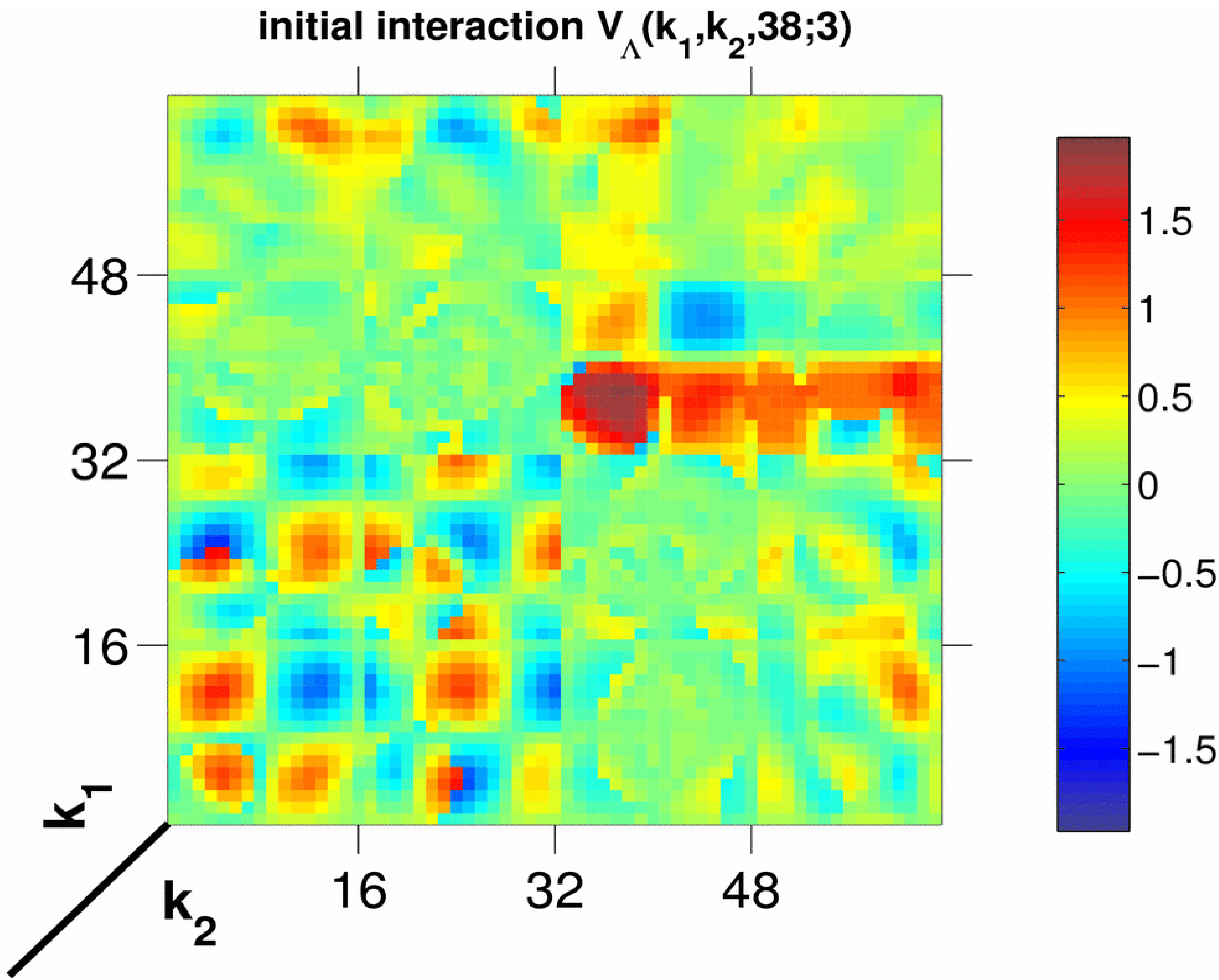
- Constant band interaction: Detect FS topology effects (Thomale et al., PRB 2009)

- Inter-and intra-orbital interaction (a,b orbital indices)

$$U_{\text{intra}} = \sum_i \sum_a n_{ia\uparrow} n_{ia\downarrow}; \quad U_{\text{inter}} = \sum_i \sum_{a<b} \sum_{s,s'} n_{i,a,s} n_{i,b,s'}$$

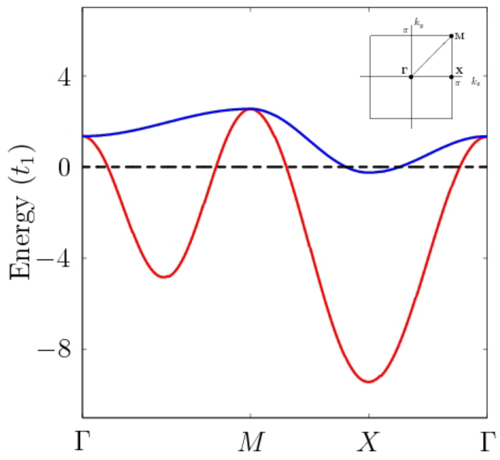
- Hund's coupling and orbital pair hopping

$$J_H = \sum_i \sum_{a<b} \sum_{s,s'} c^\dagger_{i,a,s} c^\dagger_{i,b,s'} c_{i,a,s'} c_{i,b,s}; \quad J_{\text{pair}} = \sum_i \sum_{a<b} \sum_{s,s'} (c^\dagger_{i,a,s} c^\dagger_{i,a,s'} c_{i,b,s'} c_{i,b,s} + \text{h.c.})$$

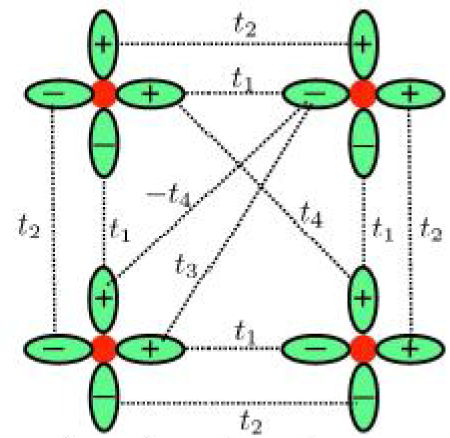

initial interaction $V_\Lambda(k_1,k_2,38;3)$
k_1
k_2
16
32
48
16
32
48
1.5
1
0.5
0
−0.5
−1
−1.5

Two band model

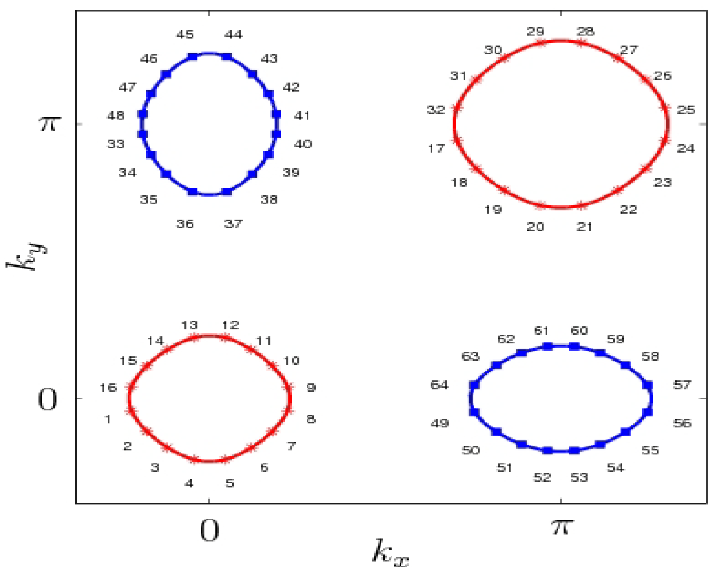
Raghu et. al., PRL 08

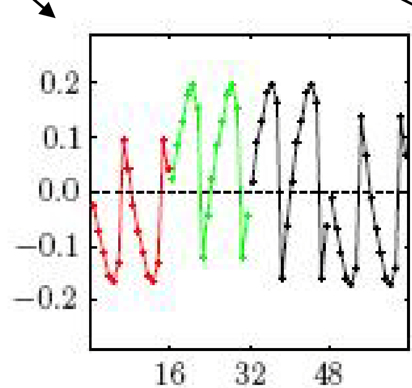


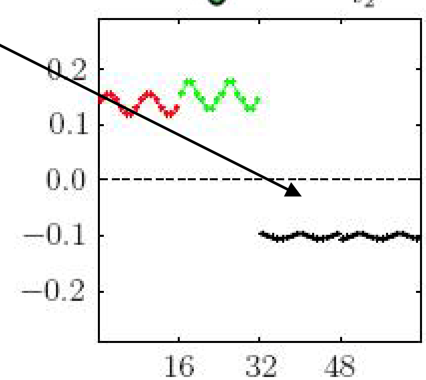
- Minimal model featuring electron pockets at X and hole pockets at Γ and M
- Sensitive to tight binding parameters t_i (in/decreasing nesting -> favor SDW/SC)
- Nodal SDW



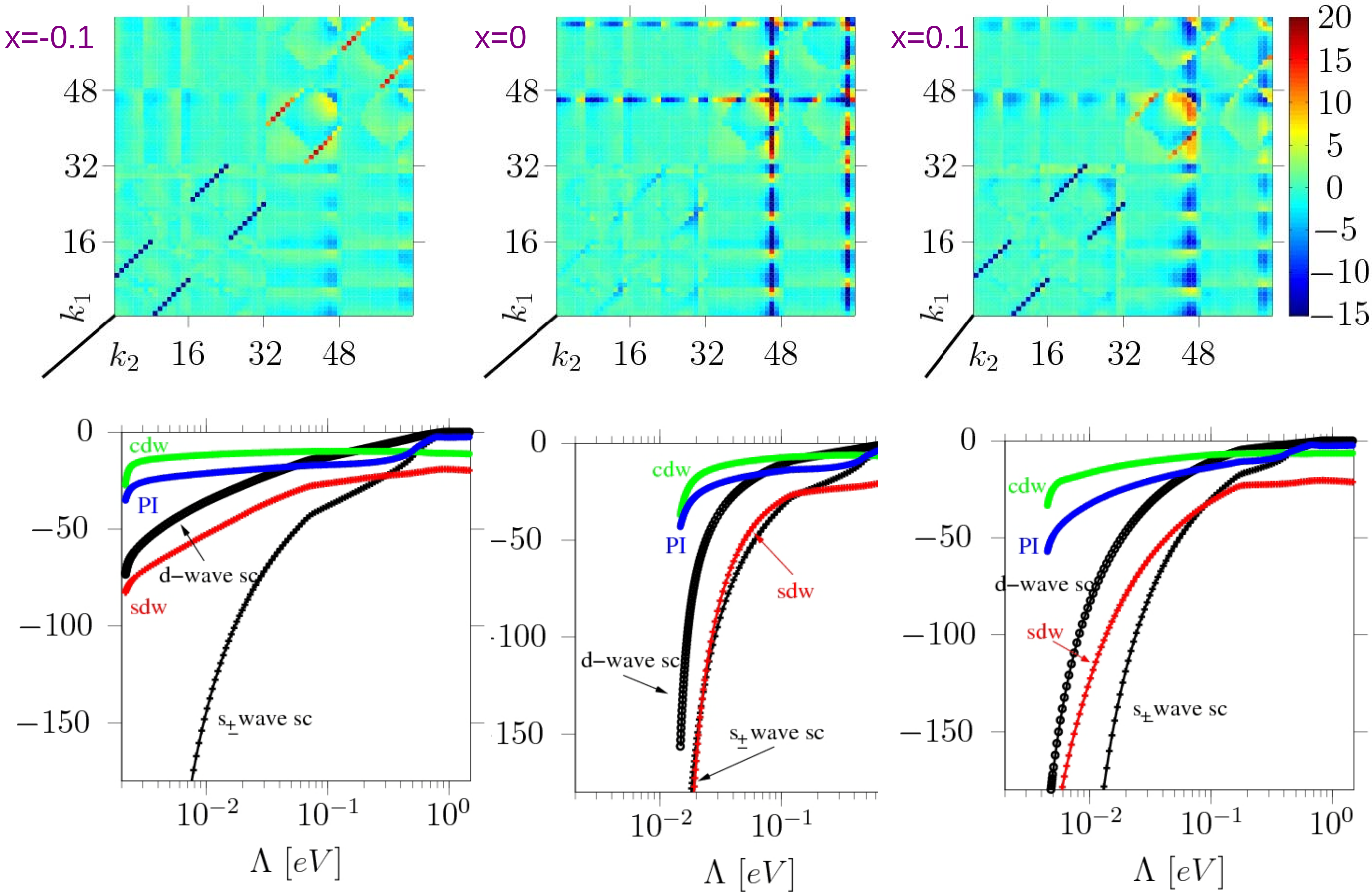
- Nodeless SC; anisotropy changing t_i varies from touching node to plain gapped







Doping-induced SC/SDW transition in 2-band model



5 orbital models

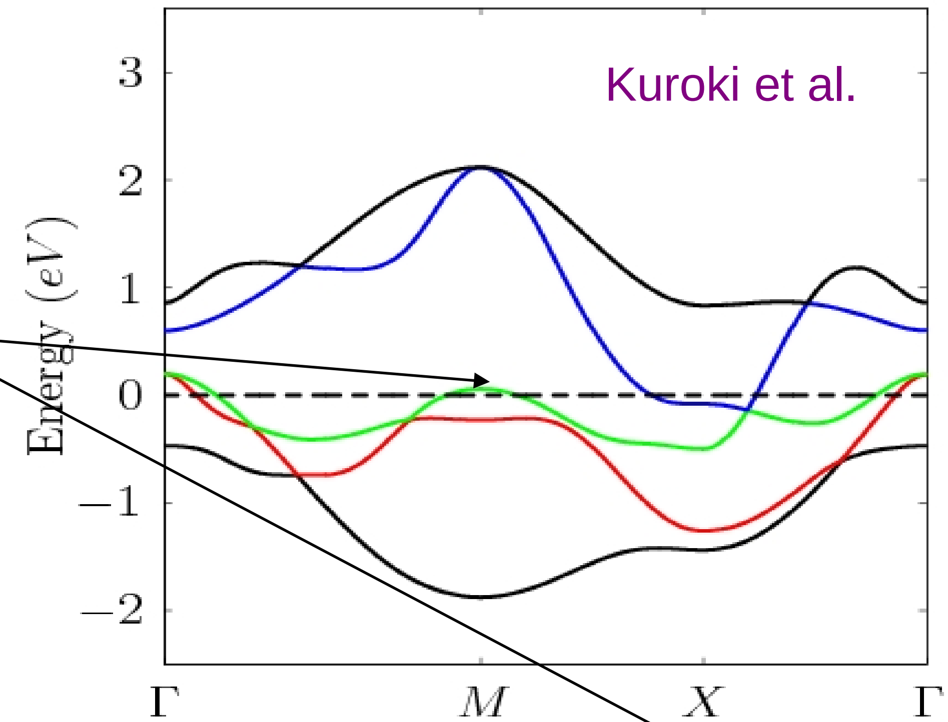
- Kuroki et al., Graser et al.
Kuroki: more SDW tendency

- As-based: vicinity of broad Fermi level band at (π,π)

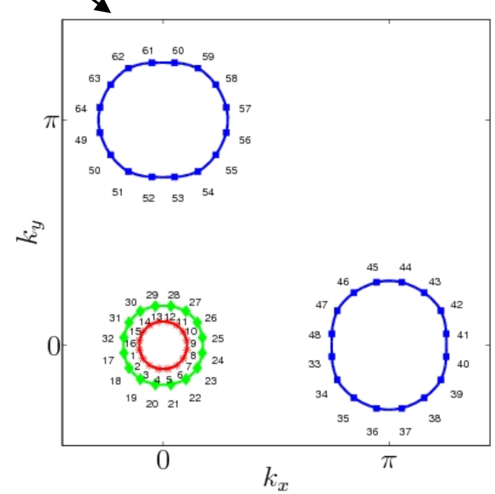
- P-based: band shifted away from Fermi level

- Orbital content: Hole pockets at (0,0): d_xz, d_yz, at (π,π): d_x^2-y^2, electron pockets admixture of all three

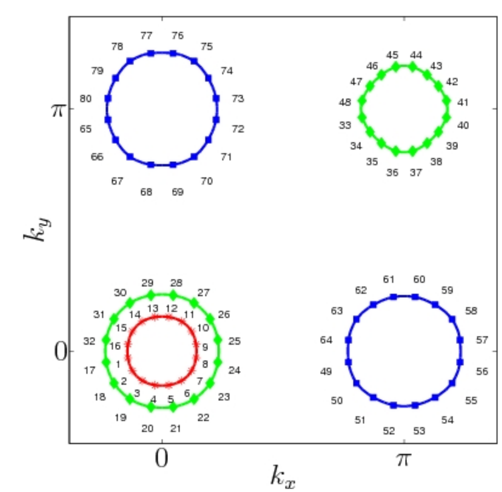
- fRG: study the orbital signature of instabilities



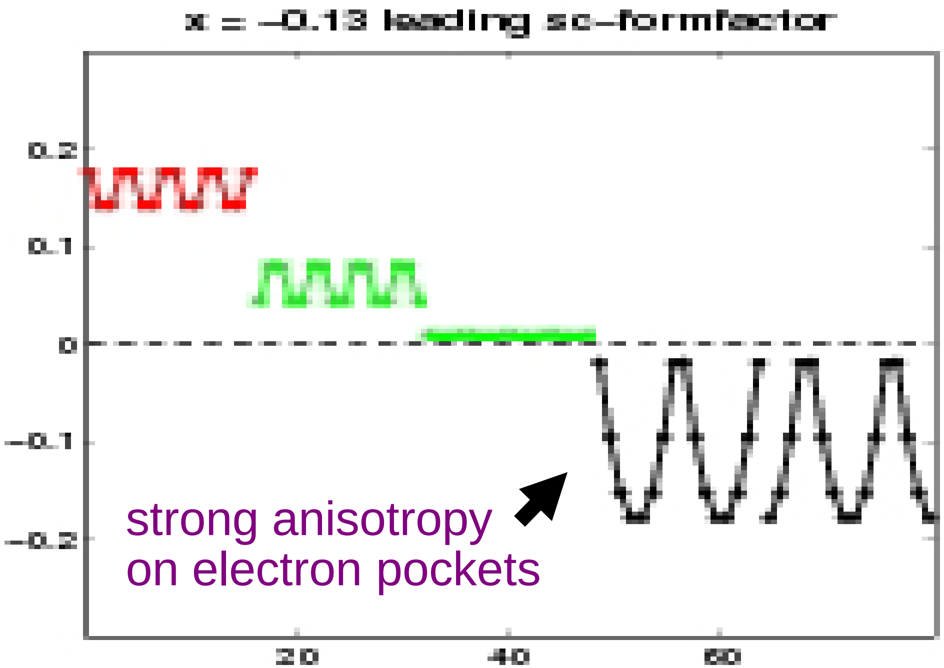
4 pocket scenario

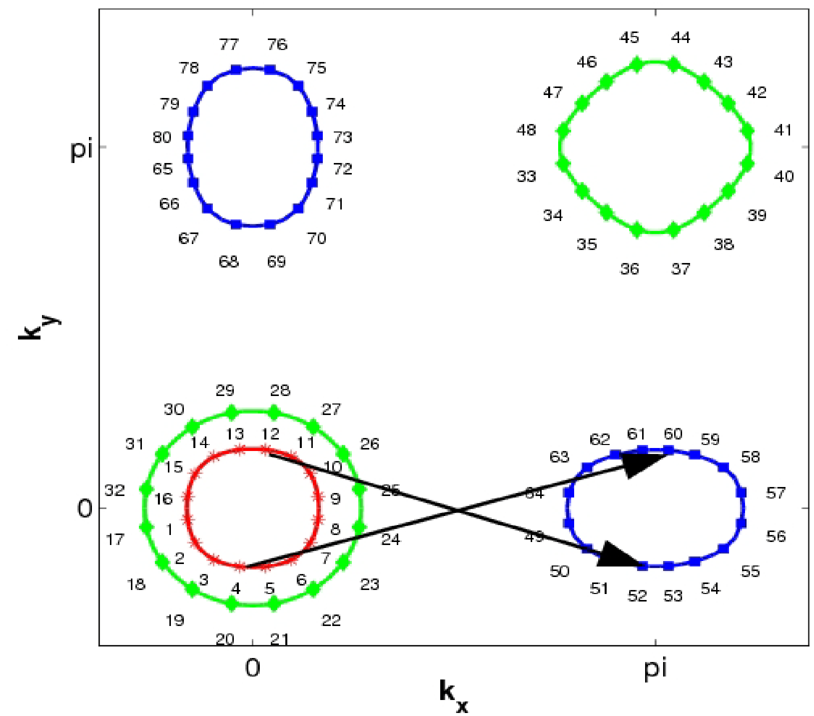


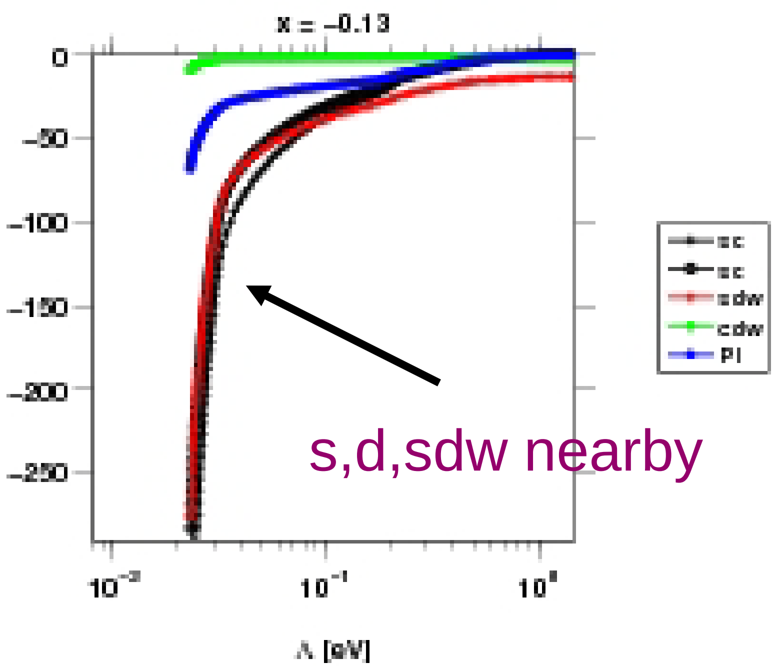
5 pocket scenario



5 pocket scenario: band notation



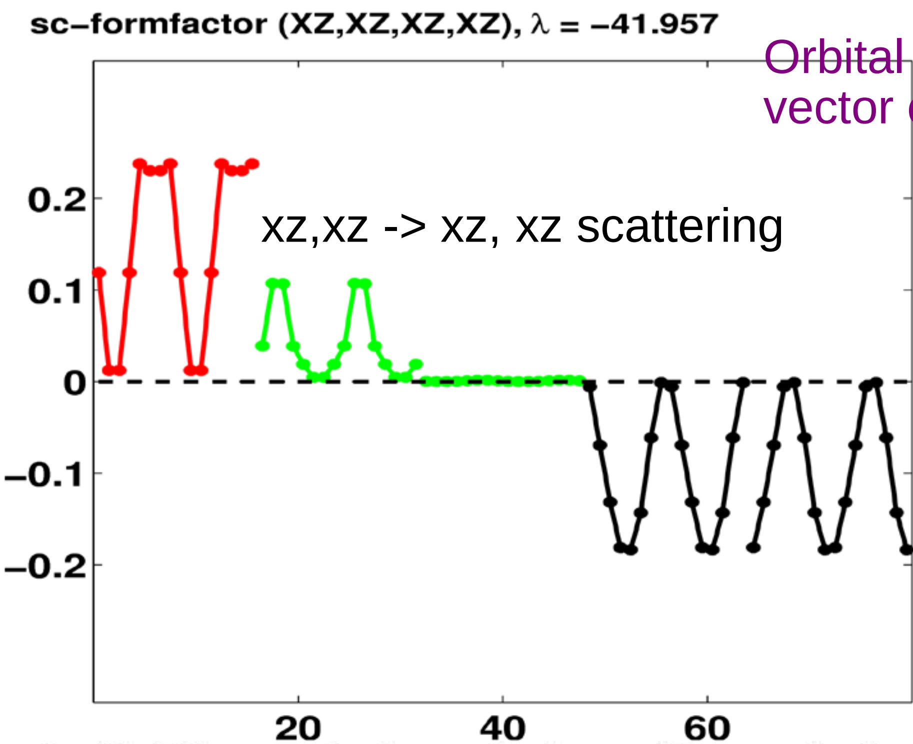




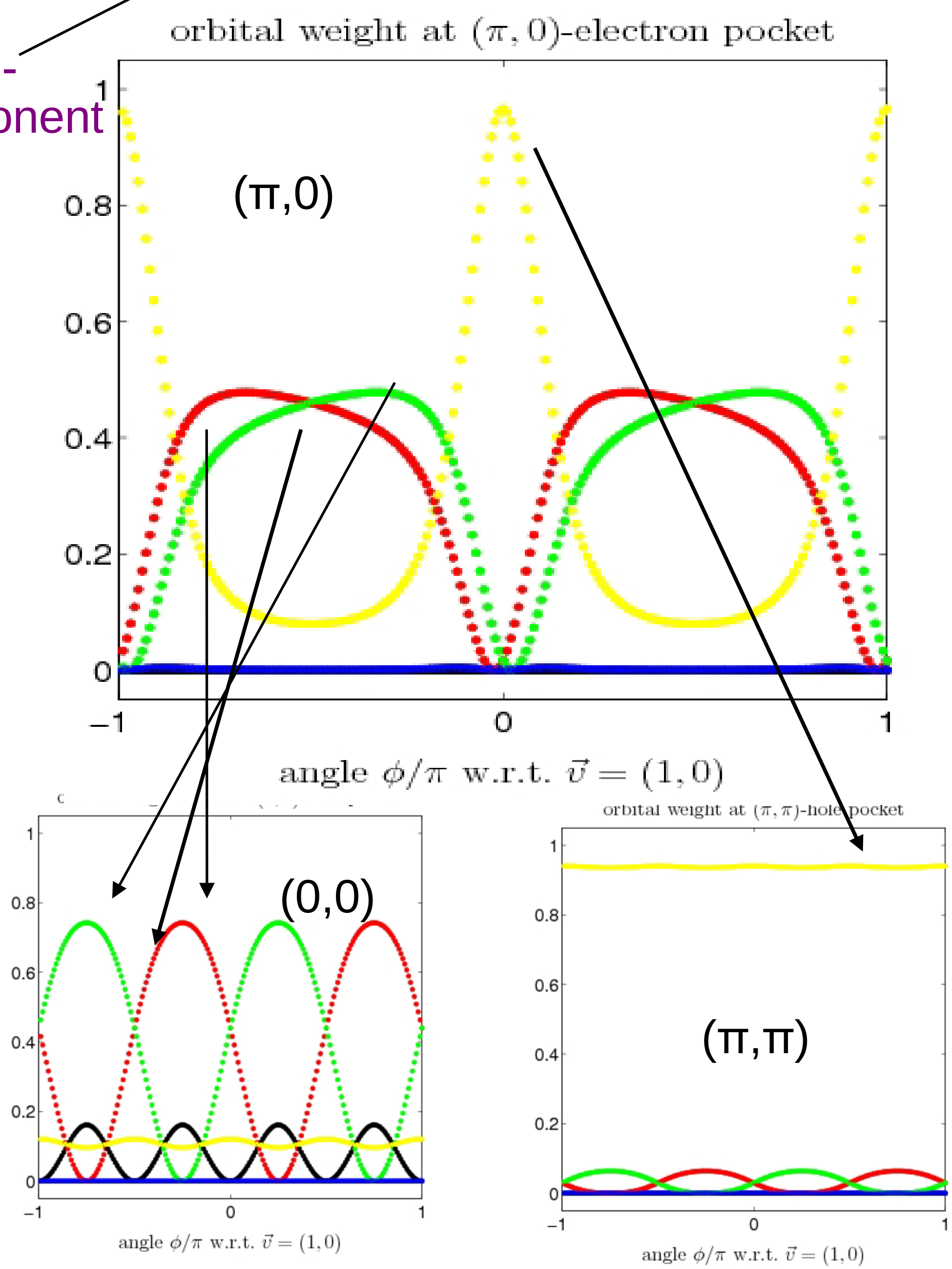
Extended s-wave and d-wave diverge in close proximity to each other

5 pocket scenario: orbital notation

$$V^{\rm orb}(\boldsymbol{k},a;-\boldsymbol{k},a;\boldsymbol{q},b;-\boldsymbol{q},b) \approx V(k_{1,\rm F},k_{2,\rm F},k_{3,\rm F})u^*_{\alpha,a}(\boldsymbol{k})u^*_{\beta,a}(-\boldsymbol{k})u_{\gamma,b}(\boldsymbol{q})u_{\delta,b}(-\boldsymbol{q})$$



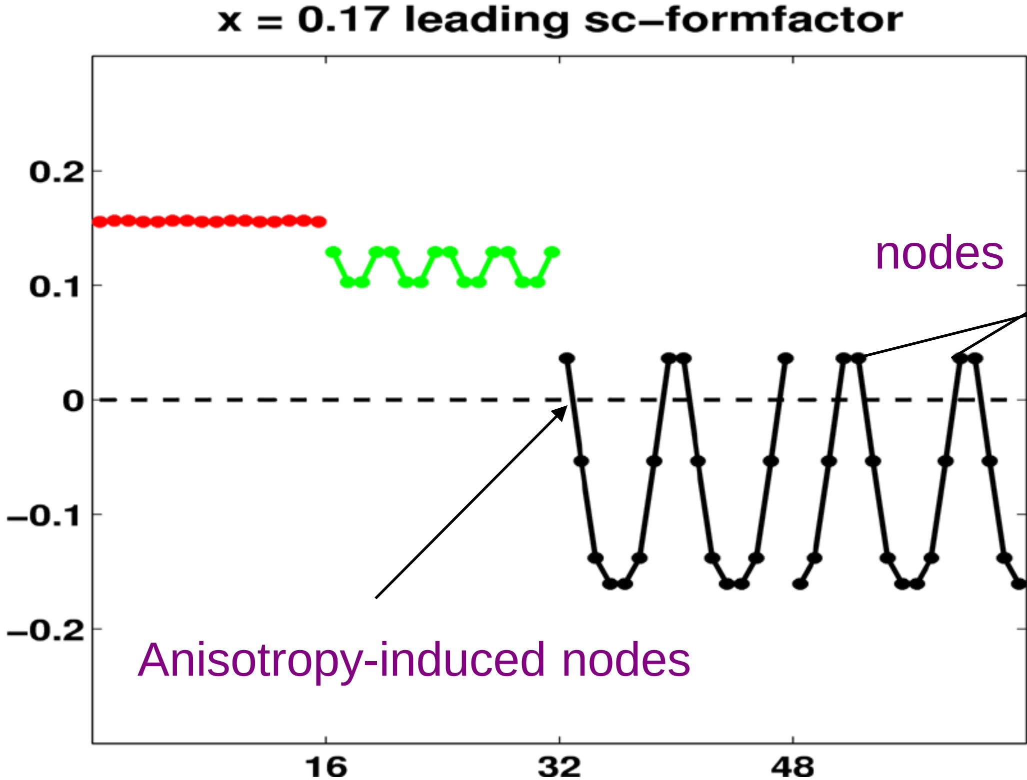
Orbital Eigen-
vector component

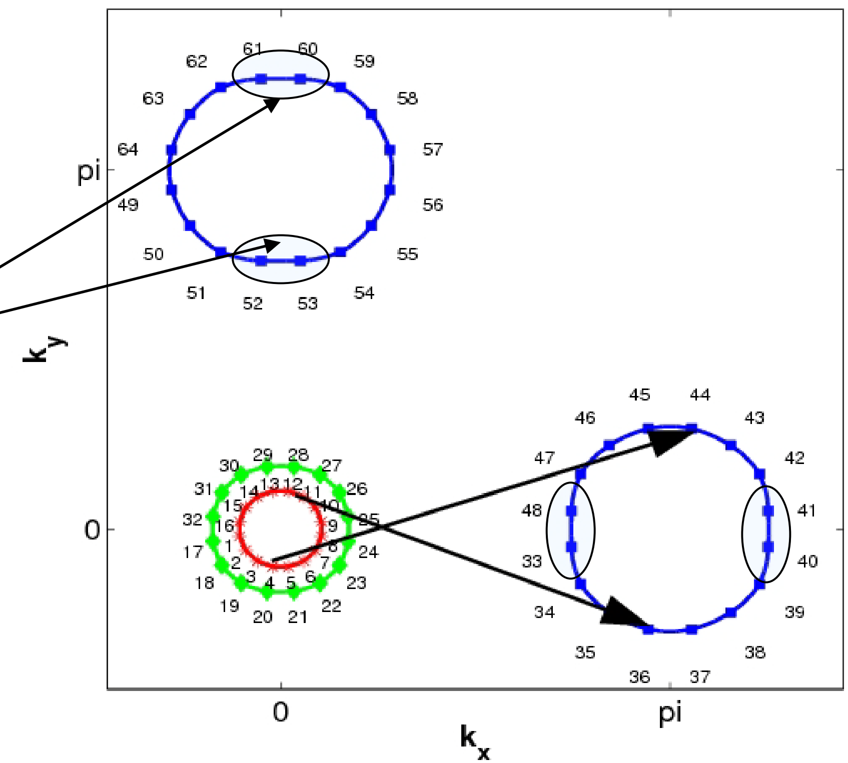


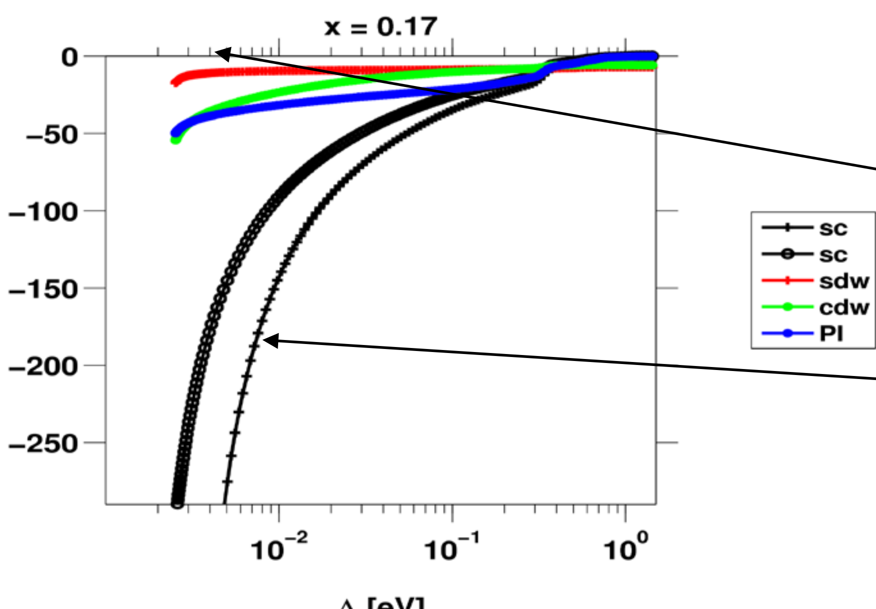
(a,b)	$d_{3z^2-r^2}$	d_{XZ}	d_{YZ}	$d_{X^2-Y^2}$	d_{XY}
$d_{3z^2-r^2}$	-0.4401	-2.1500	-2.1500	-1.0491	-0.2945
d_{XZ}	-2.1500	-41.9571	-35.9939	-4.6217	-2.6863
d_{YZ}	-2.1500	-35.9939	-41.9572	-4.6217	-2.6863
$d_{X^2-Y^2}$	-1.0491	-4.6217	-4.6217	-20.7482	-1.4694
d_{XY}	-0.2945	-2.6863	-2.6863	-1.4694	-0.6105

Leading eigenvalues

4 pocket scenario: band notation



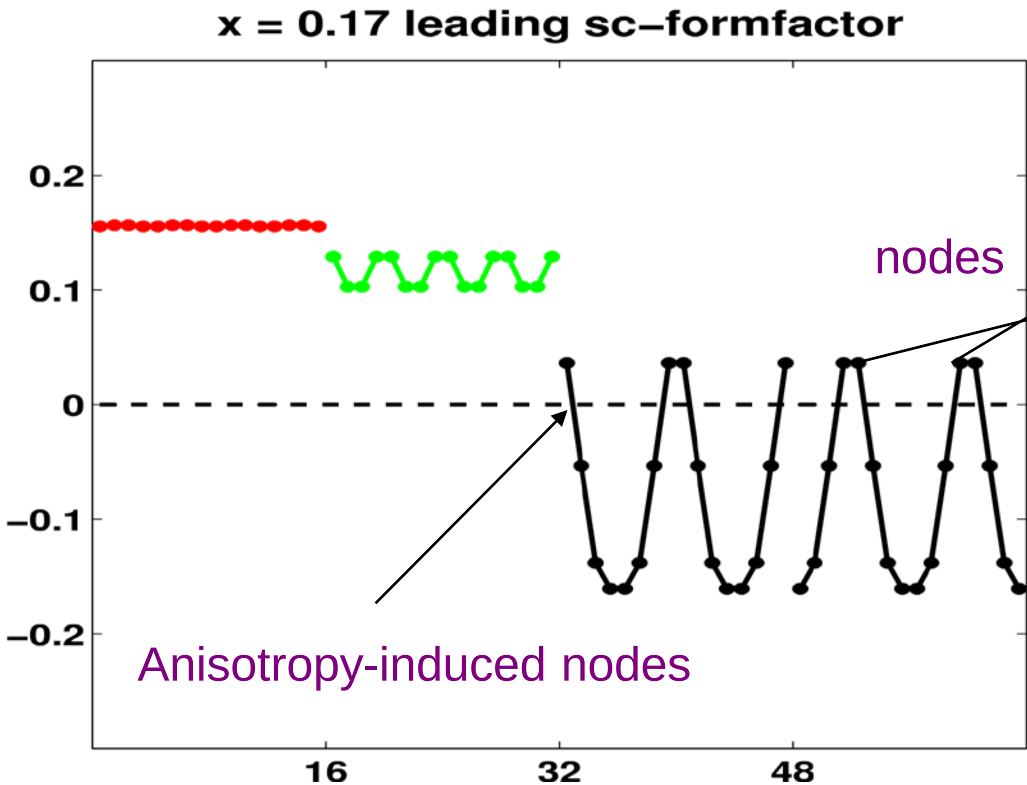


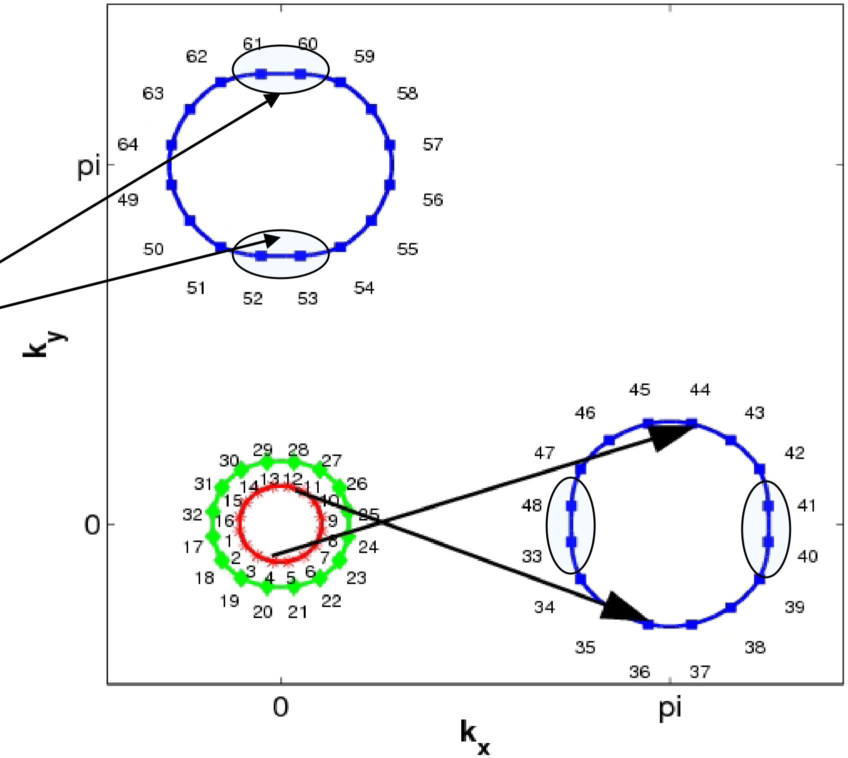


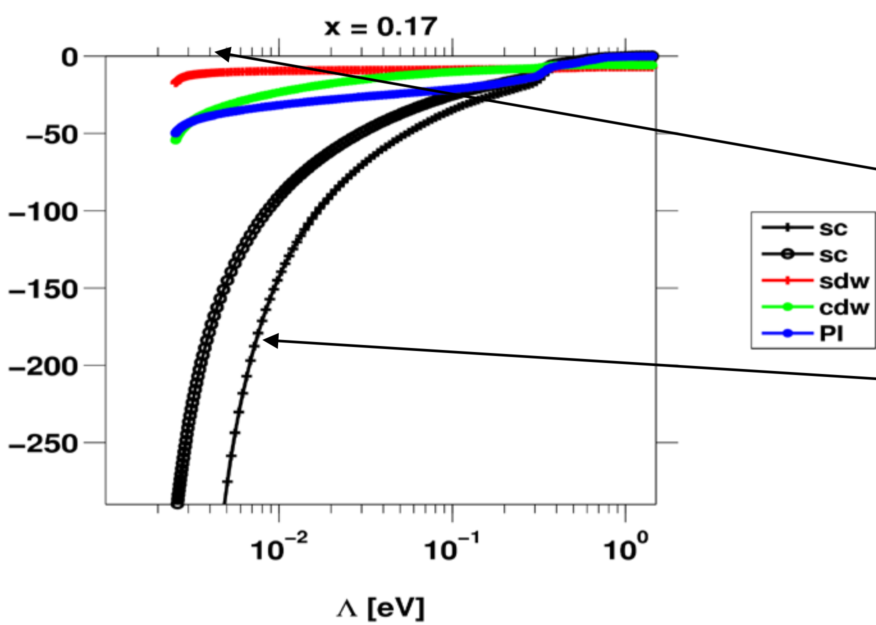
Change of orbital character in electron pockets reduces SDW fluctuations

nodal s^+- is the dominant instability

4 pocket scenario: band notation



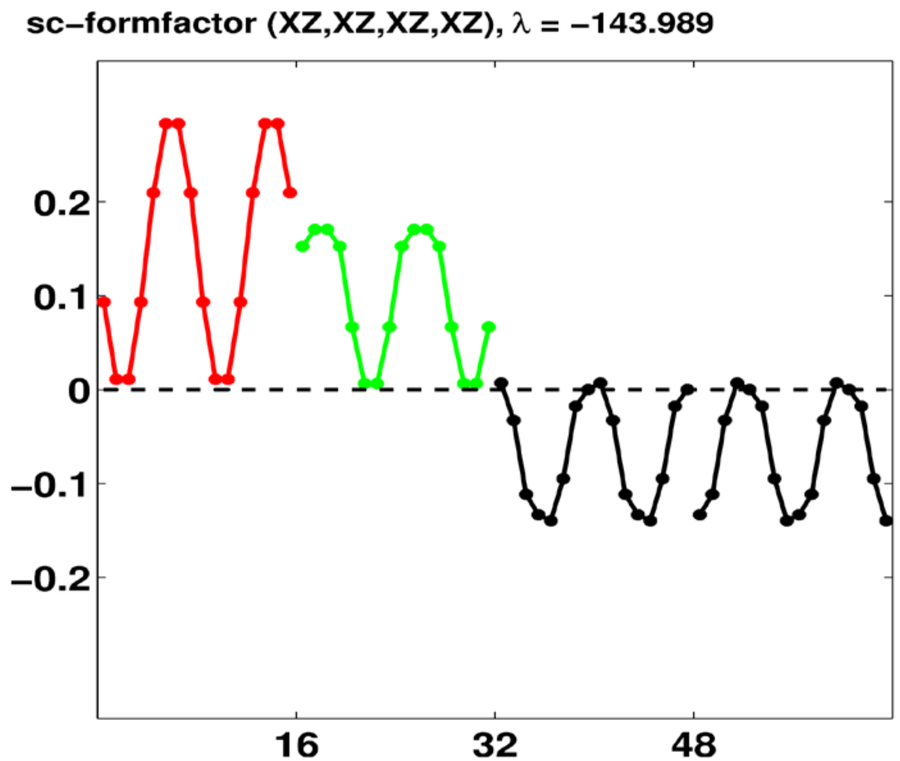


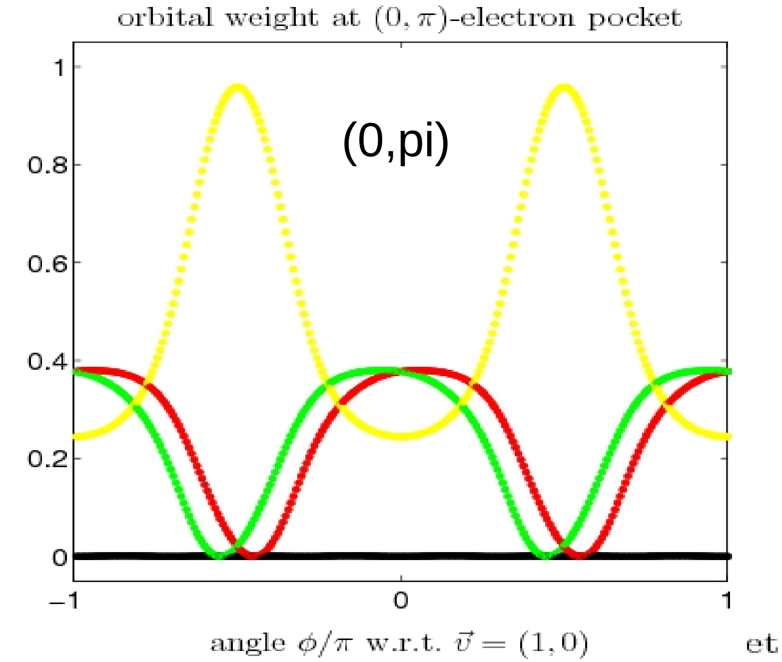


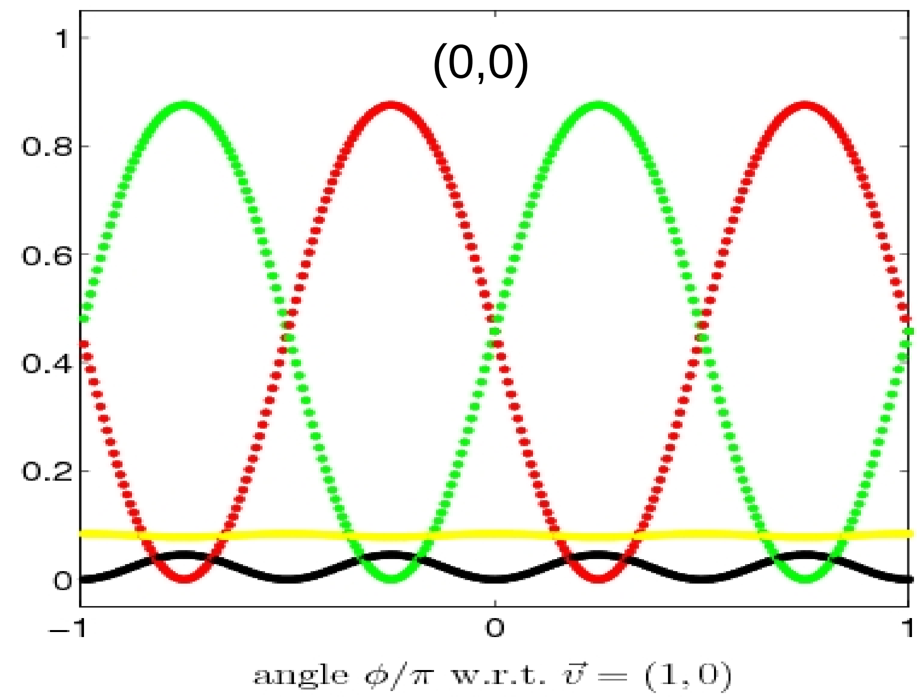
Change of orbital character in electron pockets reduces SDW fluctuations

nodal s^+- is the dominant instability

4 pocket scenario: orbital notation







d_xz/yz becomes dominant to d_x^2-y^2

(a,b)	$d_{3z^2-r^2}$	d_{XZ}	d_{YZ}	$d_{X^2-Y^2}$	d_{XY}
$d_{3z^2-r^2}$	-0.3463	-1.4706	-1.4706	-2.0388	-0.9476
d_{XZ}	-1.4706	-143.9886	-108.8343	-17.7601	-7.0638
d_{YZ}	-1.4706	-108.8343	-143.9886	-17.7601	-7.0638
$d_{X^2-Y^2}$	-2.0388	-17.7601	-17.7601	-28.8951	-6.5970
d_{XY}	-0.9476	-7.0638	-7.0638	-6.5970	-4.3055

Nodal-driving scattering contributions

Attractive channels in the Cooper sector: scattering of d_x^2-y^2 electron pocket content from (pi,0) to (0,pi)

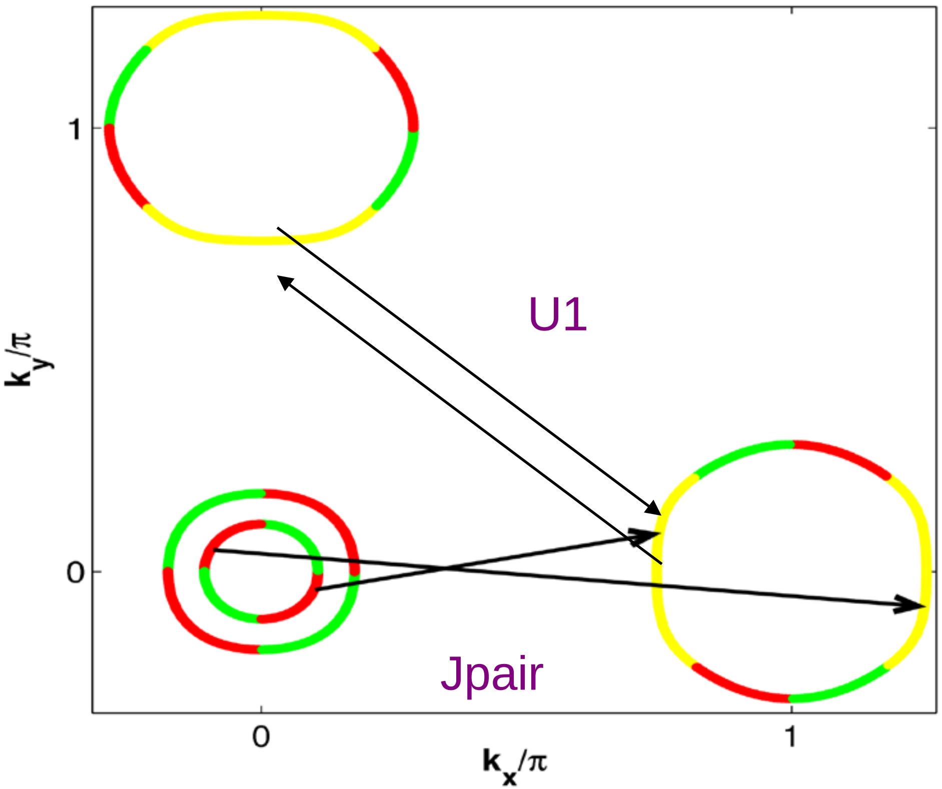
- Decisively driven by U1

- Jpair and U2 (previously subleading) become important

- Stable against variation of interaction parameters (see Thomale/Hanke talk)

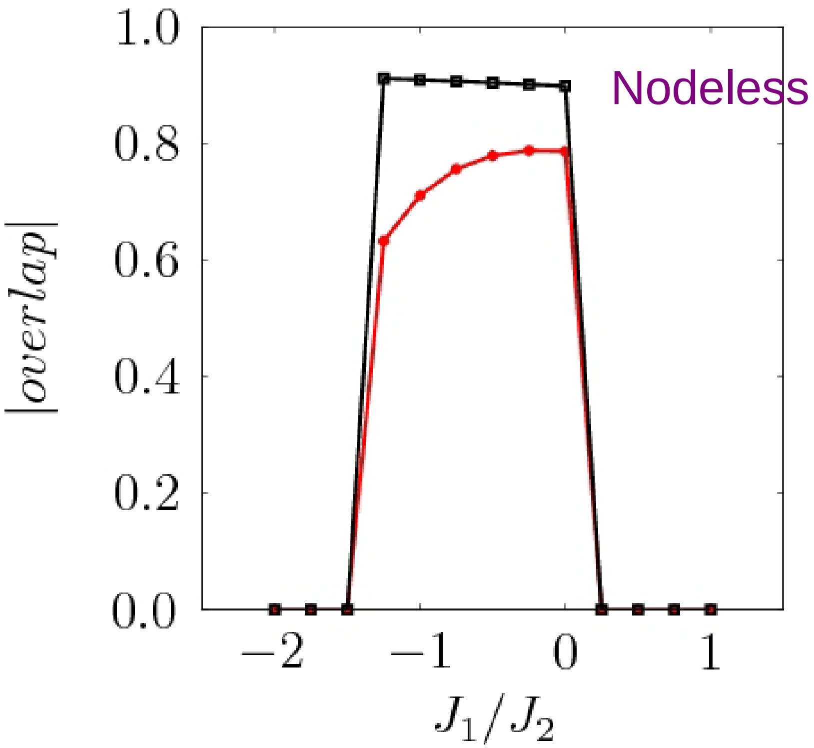
- Comparison to 5 pocket scenario: intra orbital scattering from (π,π) is absent

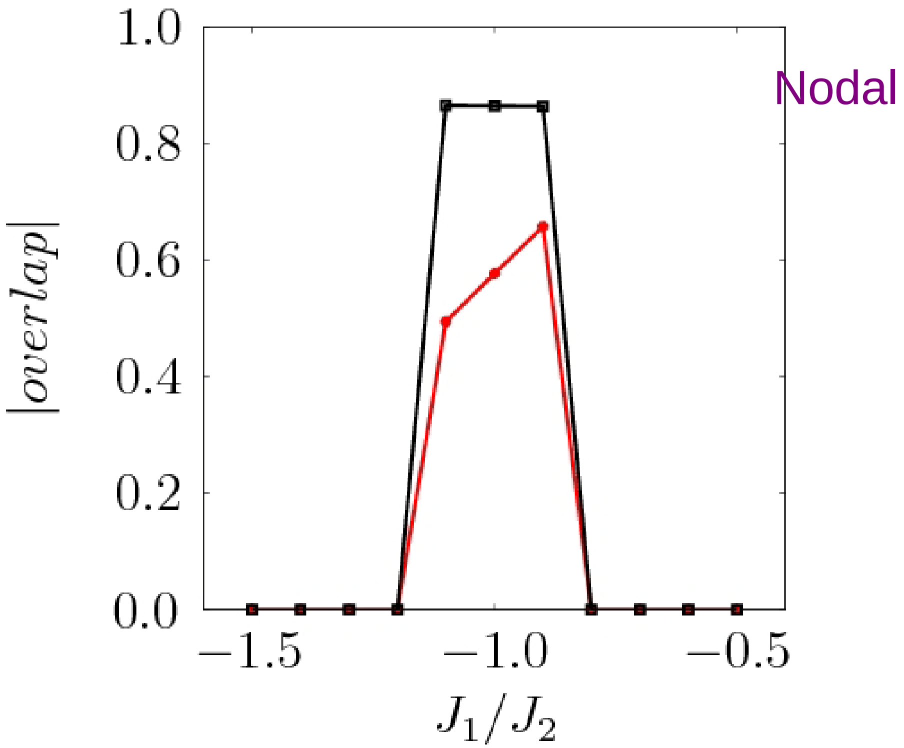
- Explains nodal propensity of Phosphor-based compounds



Correspondence to J1 J2 model

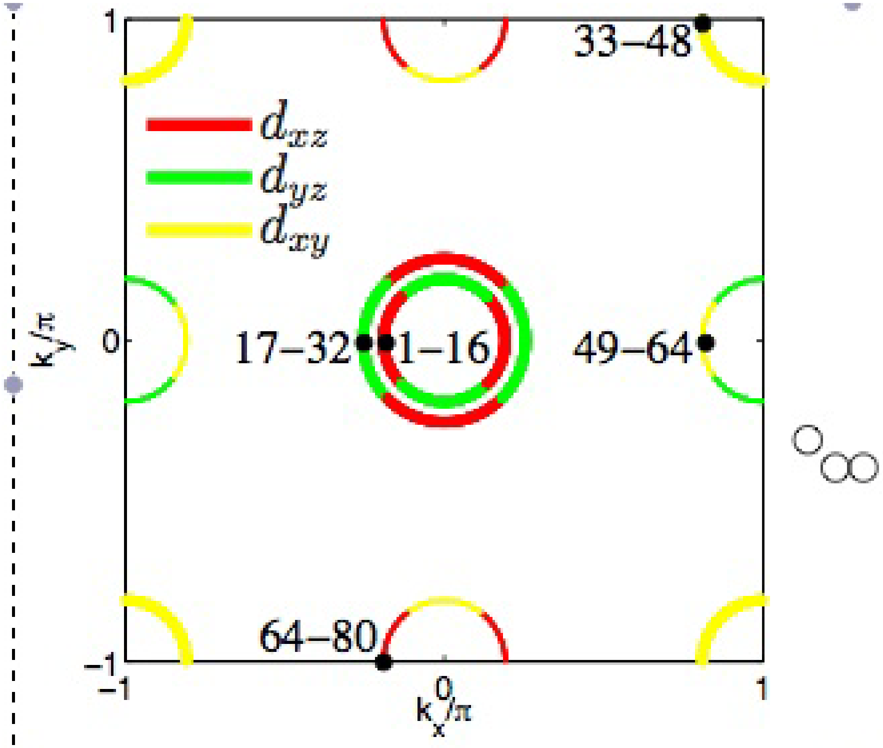
- Low energy correspondence of J1 J2 model and fRG results: Good agreement for the nodeless 5 pocket scenario, insufficient for 4 pocket scenario

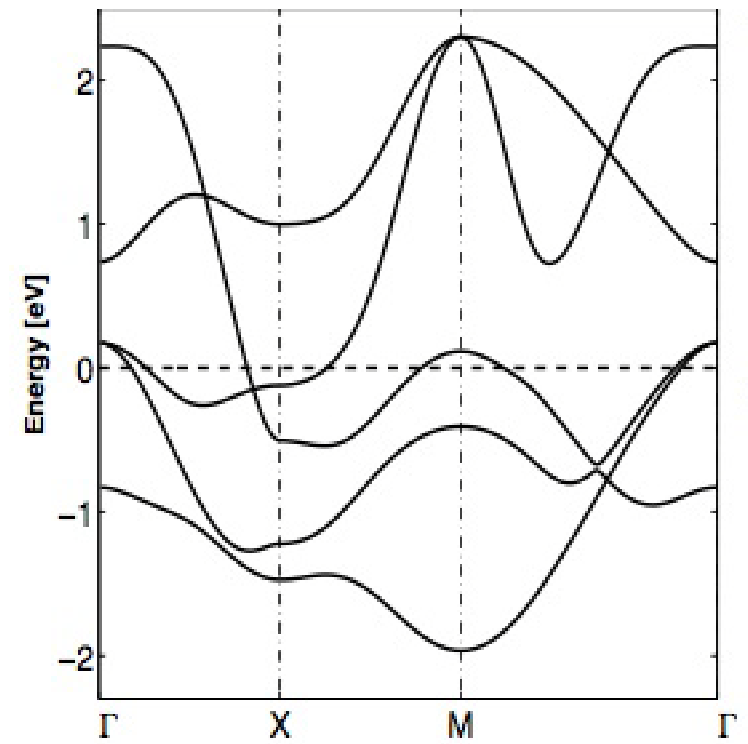




Better understanding of magnetic phases needed in pnictides → Pseudofermion RG?
(Reuther & Wölfle, PRB 2010; Reuther & Thomale, arXiv 2010)

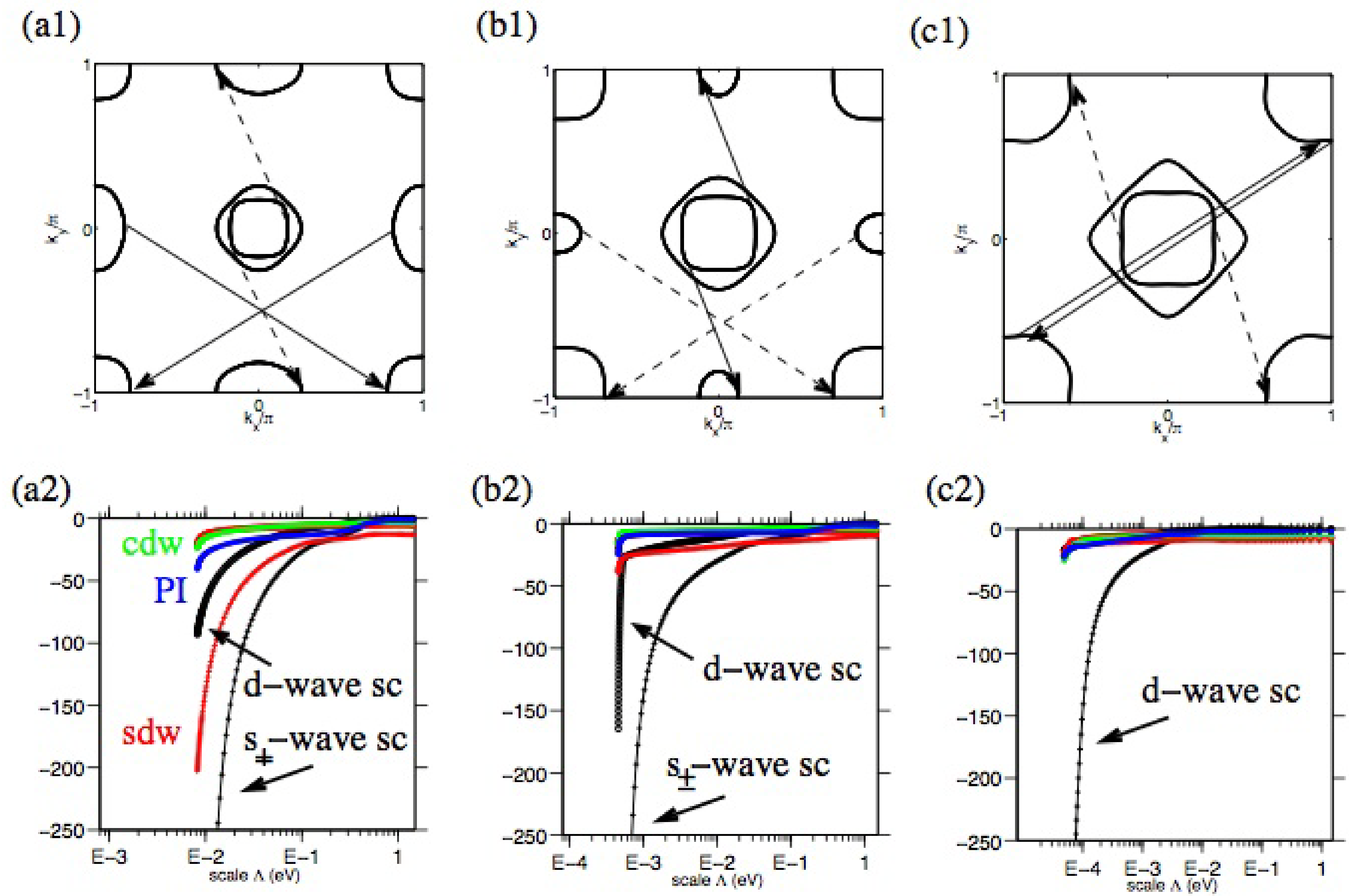
Fully k-doped KFe2As2





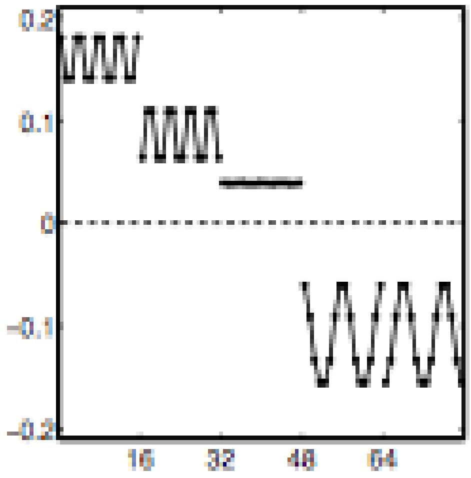
U1>U2>JH~Jpair
U1=3eV, U2=2eV, Jh=Jpair=0.6eV

Extreme hole doping induces d-wave SC



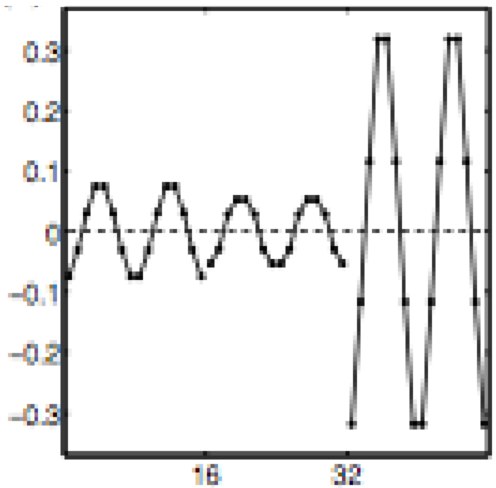
Form factors as hole-doping increases

(a)



(b)

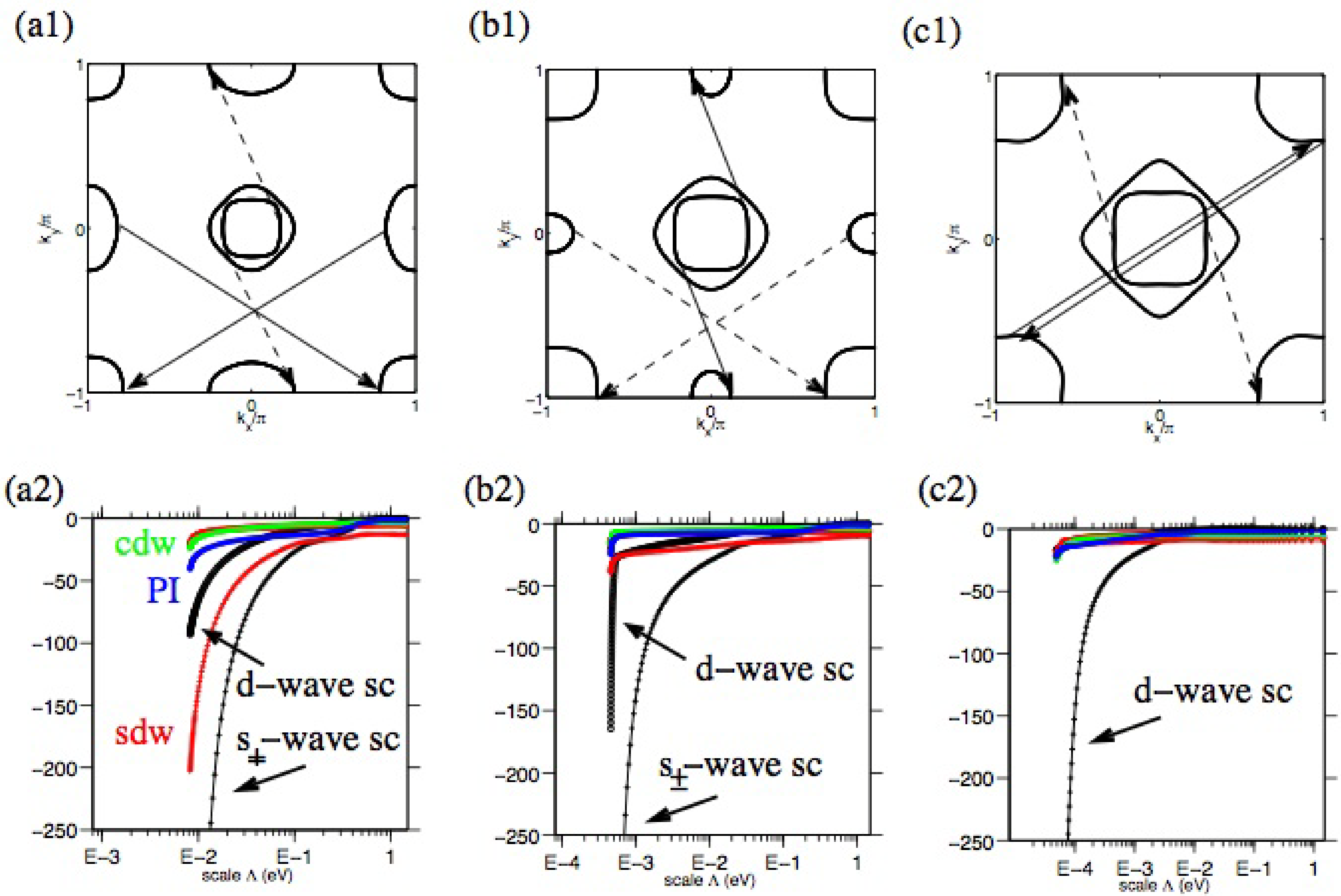
(a,b)	d_{xz}	d_{yz}	$d_{x^2-y^2}$	d_{xy}	$d_{3z^2-r^2}$
d_{xz}	-845.326	-436.185	-67.482	-142.778	-13.076
d_{yz}	-436.185	-845.326	-67.482	-142.778	-13.076
$d_{x^2-y^2}$	-67.482	-67.482	-33.036	-27.675	-5.542
d_{xy}	-142.778	-142.778	-27.675	-87.978	-6.087
$d_{3z^2-r^2}$	-13.076	-13.076	-5.542	-6.087	-1.558



(a,b)	d_{xz}	d_{yz}	$d_{x^2-y^2}$	d_{xy}	$d_{3z^2-r^2}$
d_{xz}	-24.143	-11.829	-4.513	-41.785	-2.518
d_{yz}	-11.829	-24.143	-4.513	-41.785	-2.518
$d_{x^2-y^2}$	-4.513	-4.513	-3.798	-23.405	-1.412
d_{xy}	-41.785	-41.785	-23.405	-567.184	-23.598
$d_{3z^2-r^2}$	-2.518	-2.518	-1.412	-23.598	-1.721

At large hole doping, the xy hole pocket is
(essentially alone) responsible for the superconductivity

Extreme hole doping induces d-wave SC



Conclusion

- fRG studies on multi-orbital tight binding models yield nodal SDW and extended s-wave SC instabilities

- The anisotropy of the SC formfactor is very sensitive on the tight binding parameters, doping, and interaction parameters; it can vary from nodeless, touching nodal to nodal

- A nodeless scenario is found in the presence of relevant intraorbital scattering from a (pi,pi) hole pocket to the electron pockets

- A nodal scenario is found for the (pi,pi) hole pockets being absent and driven by electron-electron scattering from the d_xy (d_x^2-y^2) weight of the electron pockets; relates to P-based compounds

- An improved understanding of the magnetic phases is needed