Superconductivity from repulsion in LiFeAs: novel s-wave symmetry and time-reversal symmetry breaking

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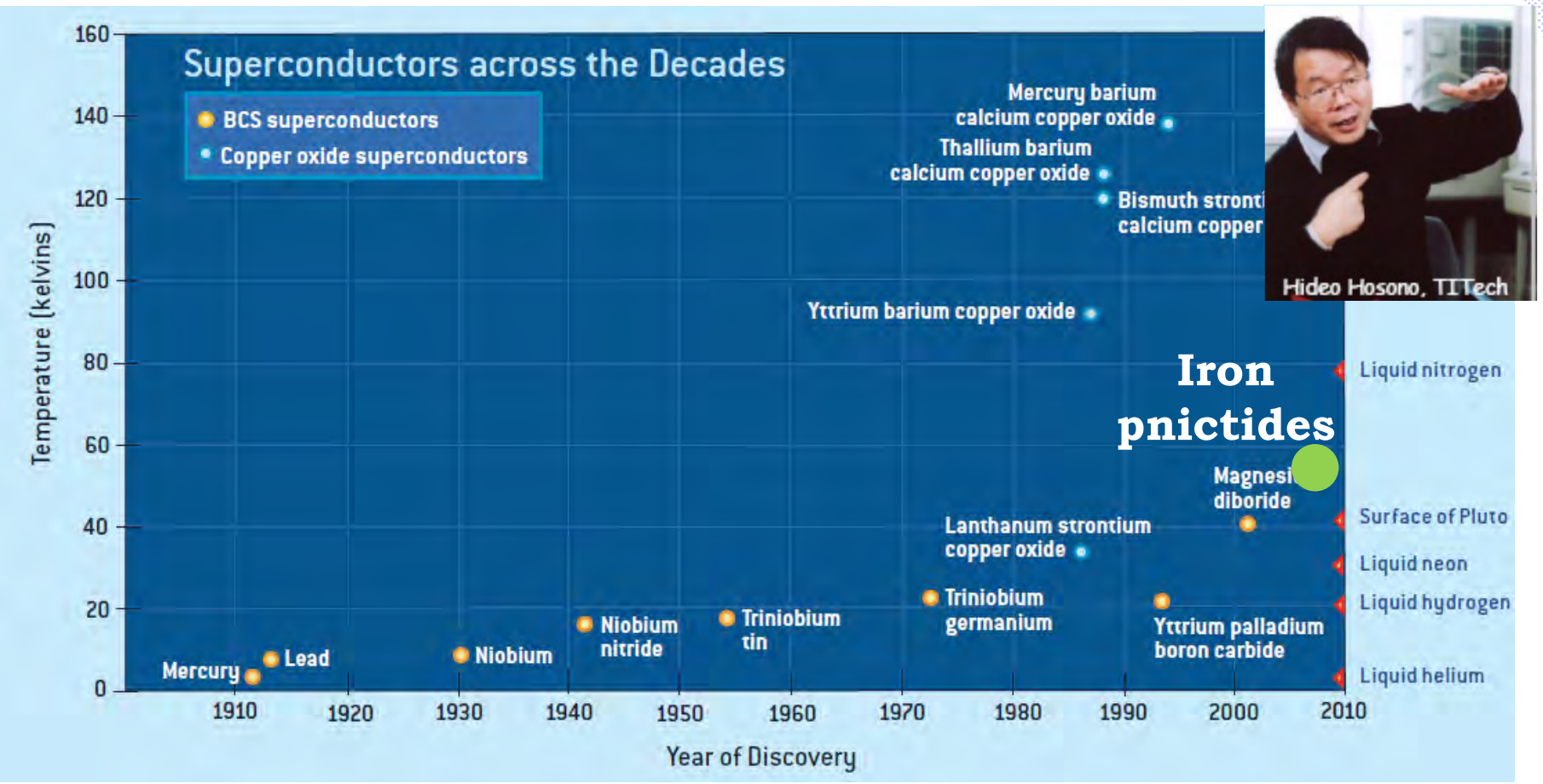
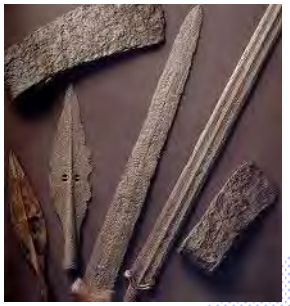
- A.V. Chubukov @ *University of Wisconsin, Madison*
- J. Knolle @ *MPI Physik komplexer Systeme, Dresden*
- S. Borisenko, V. Zabolotnyy, B. Büchner @ *IFW Dresden*

[МГУ-Январь-2014]

Superconductivity reaches the iron age



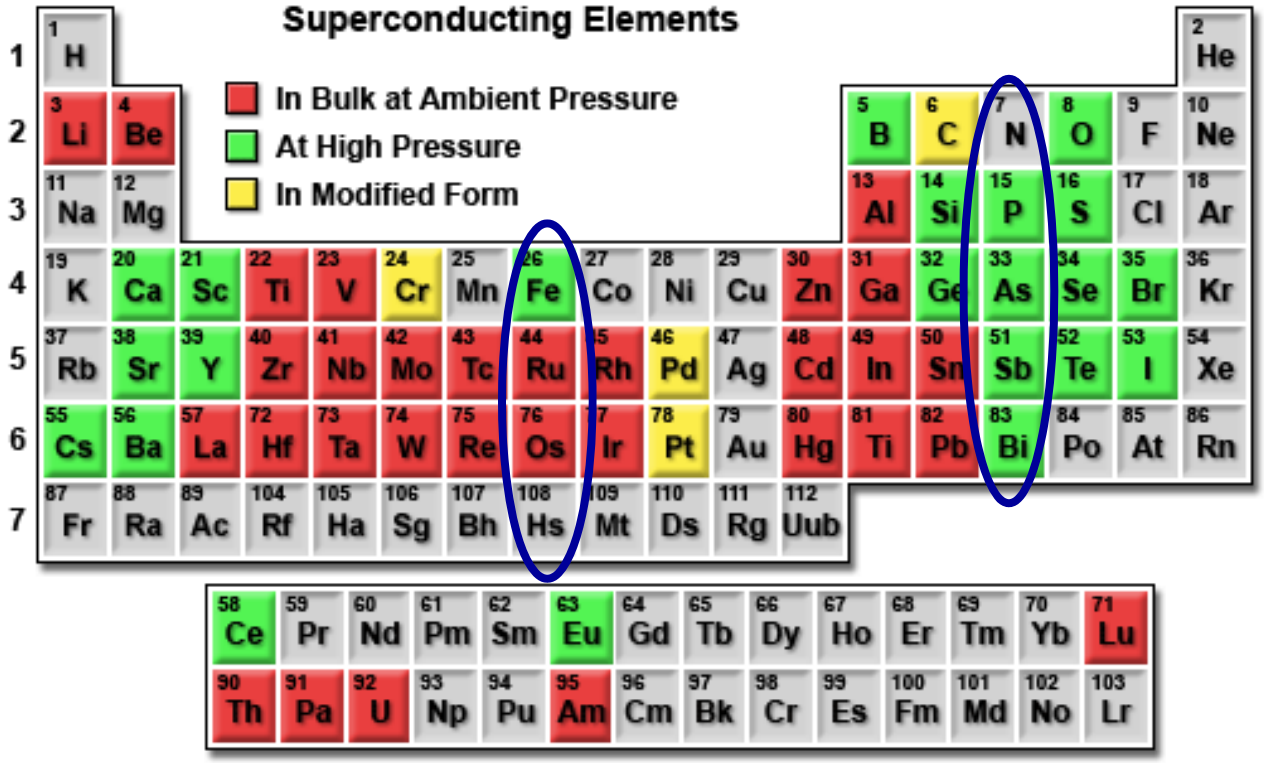
stone age ➡ copper age ➡ iron age

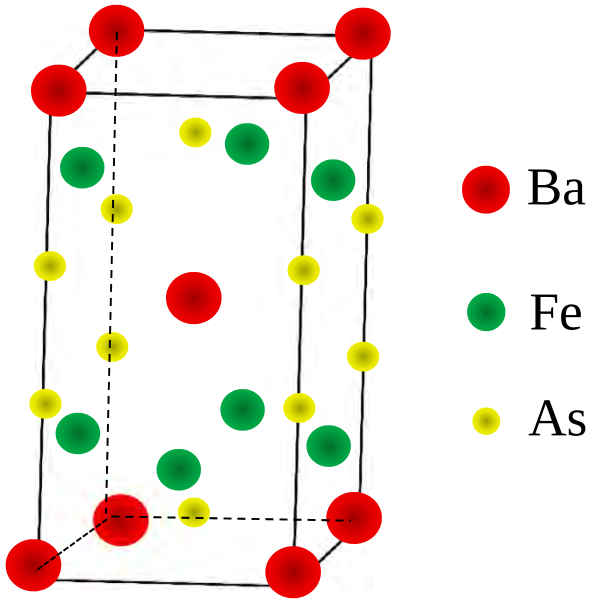


first high-temperature superconductors since the cuprates!

Iron-based superconductors

- Layered materials: transition metal (**Fe**) plus pnictogen (nitrogen group, such as **As**)





$BaFe_2As_2$

[МГУ-Январь-2014]

Iron-based superconductors

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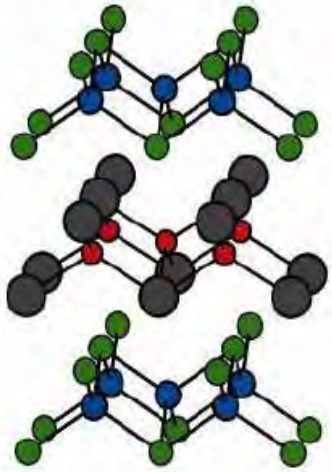
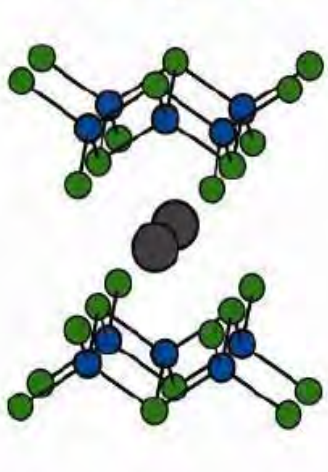


T_c=28K

(55K for Sm)

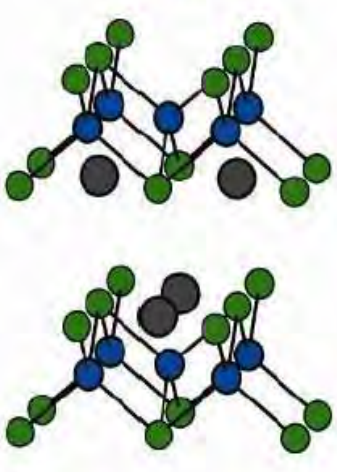
- **Kamihara et al JACS (2008)**
- **Ren et al Chin. Phys. Lett. (2008)**



T_c=38K

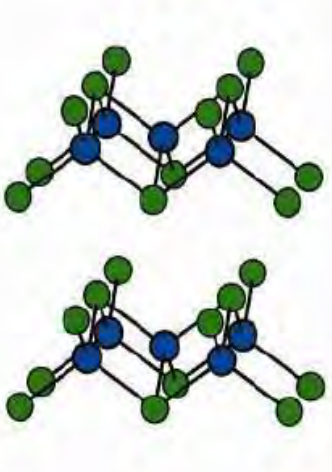
- **Rotter et al. PRL (2008)**
- **Ni et al Phys. Rev. B 2008**

(single xtals)



T_c=18K

Wang et al Sol. St. Comm. 2008



T_c=8K

Hsu et al PNAS 2008

No arsenic ☺!

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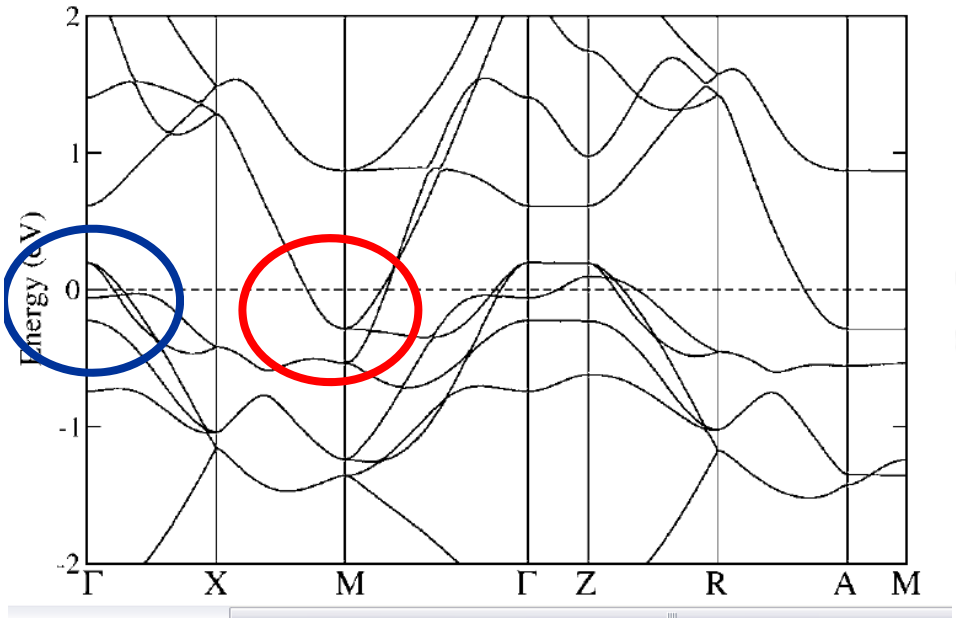
Iron-based superconductors: what are the common electronic features?

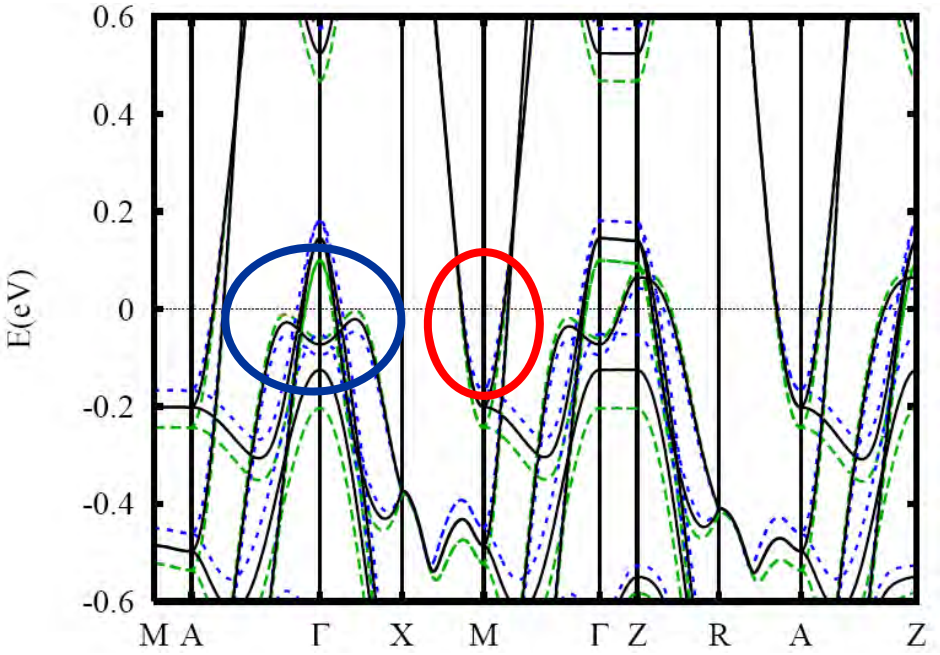
[МГУ-Январь-2014]

Electronic-structure calculations

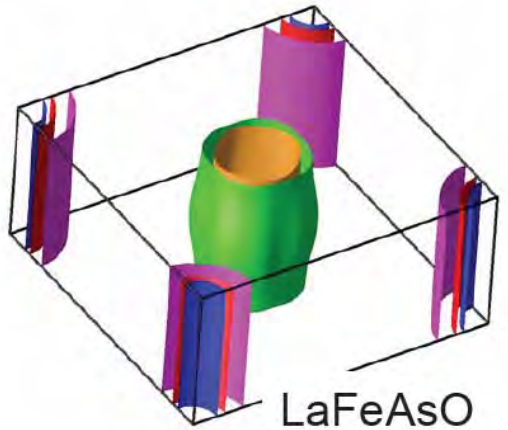
LaFePO Lebegue 2007 (T_c=6K)



LaFeAsO Singh & Du 2008 (T_c=26K)



Band structures for 2 materials nearly identical!
Hole pocket near Γ, electron pocket near M



2D!

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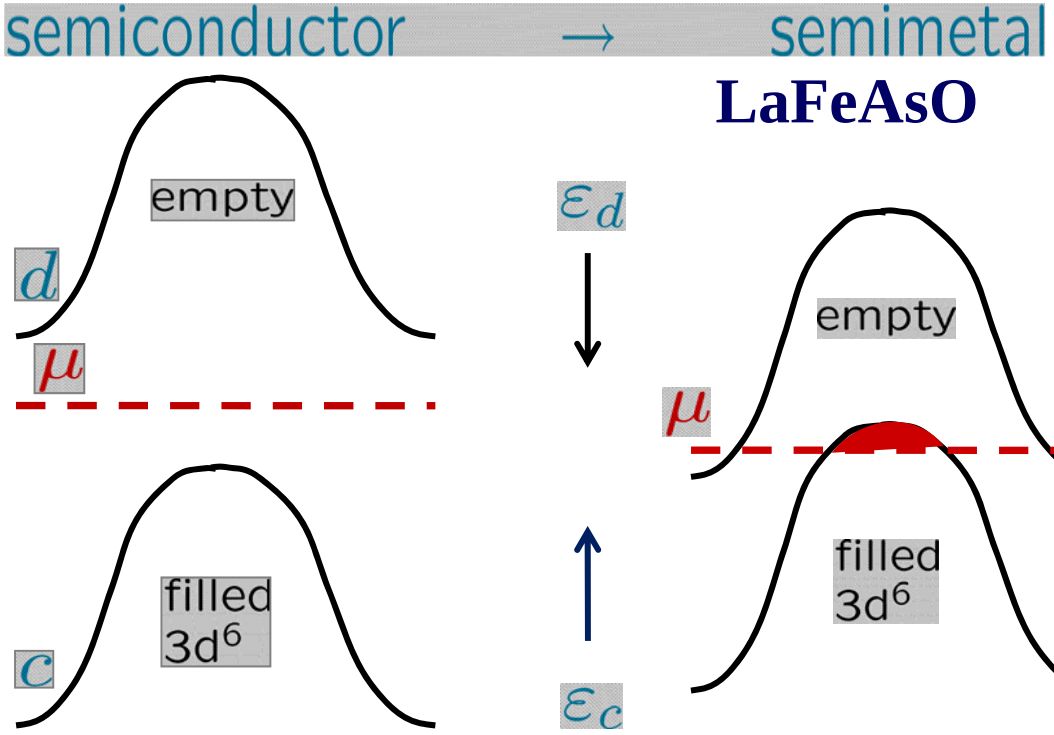
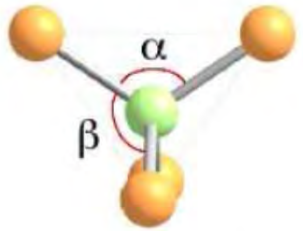
Electronic-structure: multiorband structure

$Fe^{2+} \Rightarrow 3d^6$

4 holes per site – multiband structure.
chemical potential lies in the gap





$FeAs_4$-tetrahedron

Crystalline electric field of the tetrahedra is weak

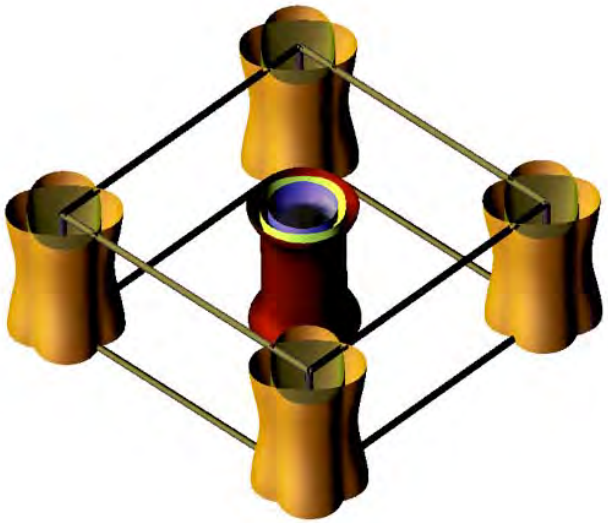
All 5 Fe d-orbitals are near the Fermi level

[МГУ-Январь-2014]

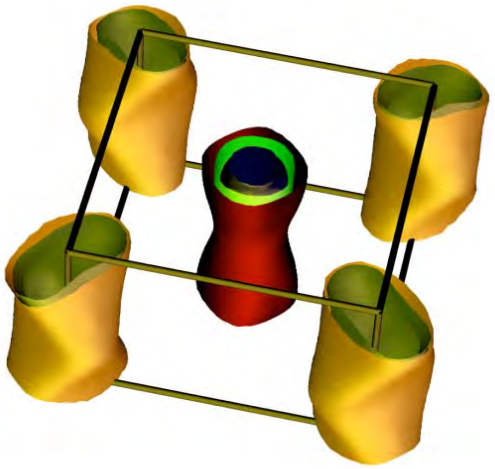
Comparison with other materials

Hole pockets near (0,0)
Electron pockets near (π,π)

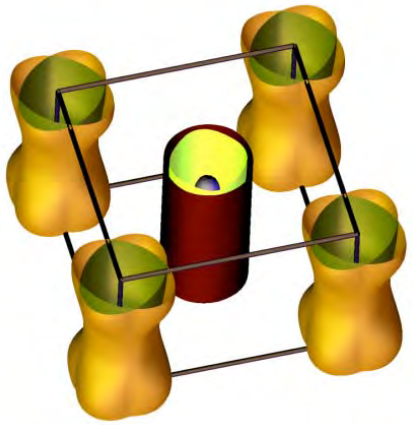
La-1111



Ba-122



FeTe



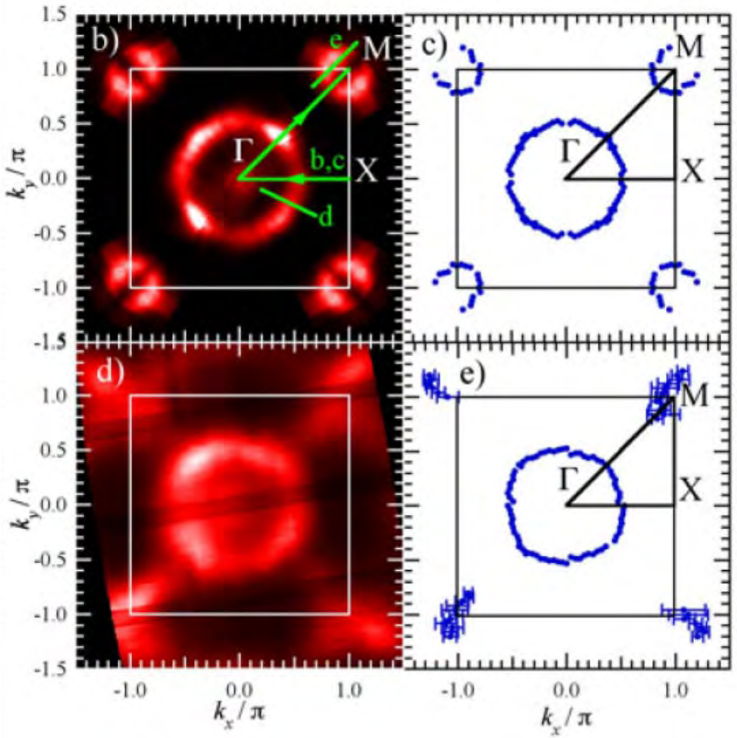
courtesy of I. Mazin

ARPES

dHVa

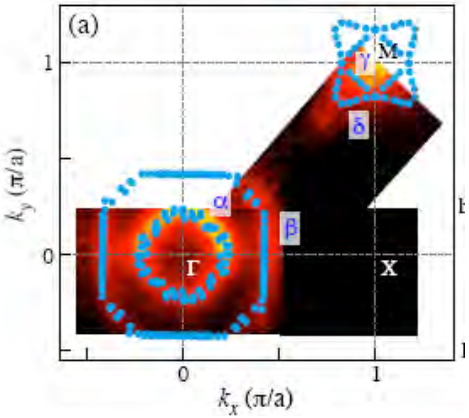
$NdFeAs(O_{1-x}F_x)$ (x=0.1)

A. Kaminski et al.



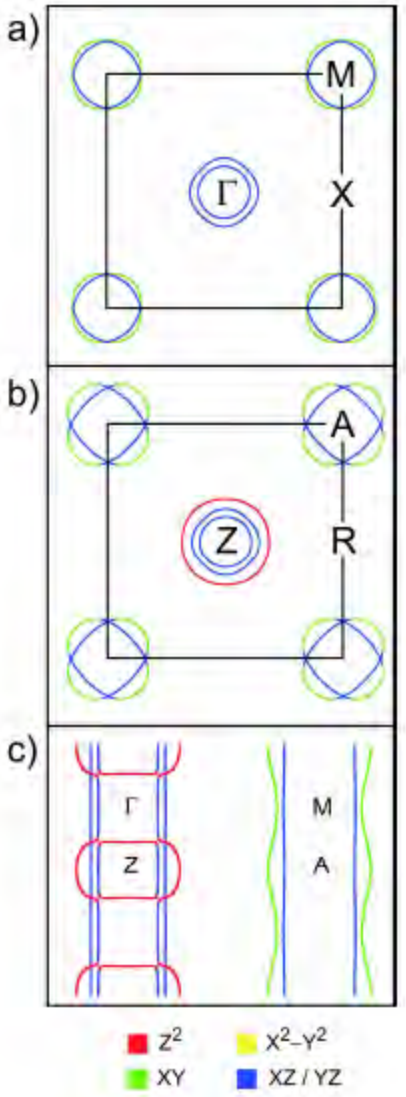
$Ba_{06}K_{04}Fe_2As_2$

H. Ding et al.



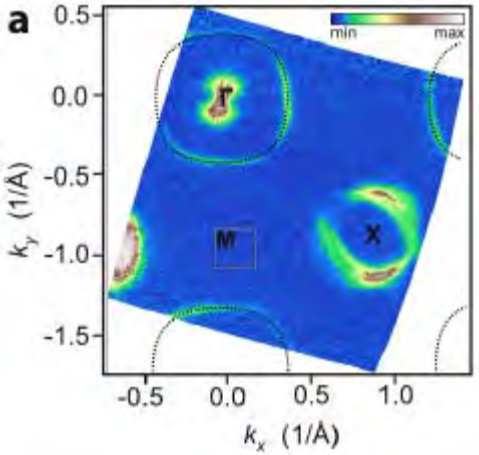
LaFePO

A. Coldea et al,



LiFeAs

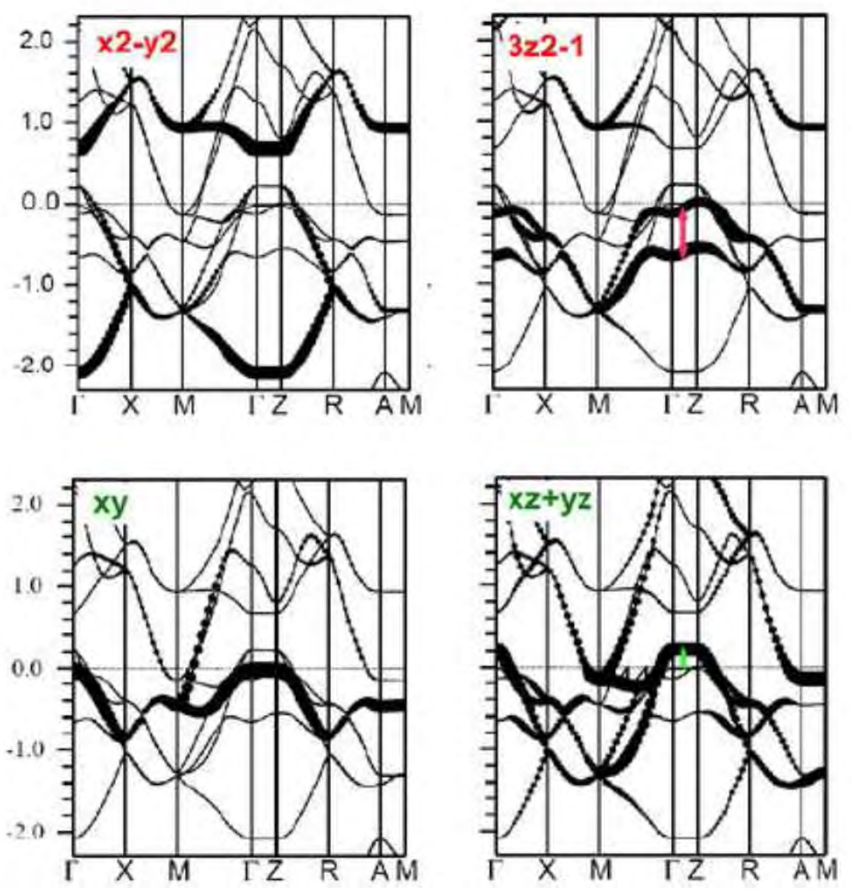
A. Kordyuk et al



Hole pockets near (0,0)
Electron pockets near (π,π)

Multiorbital structure

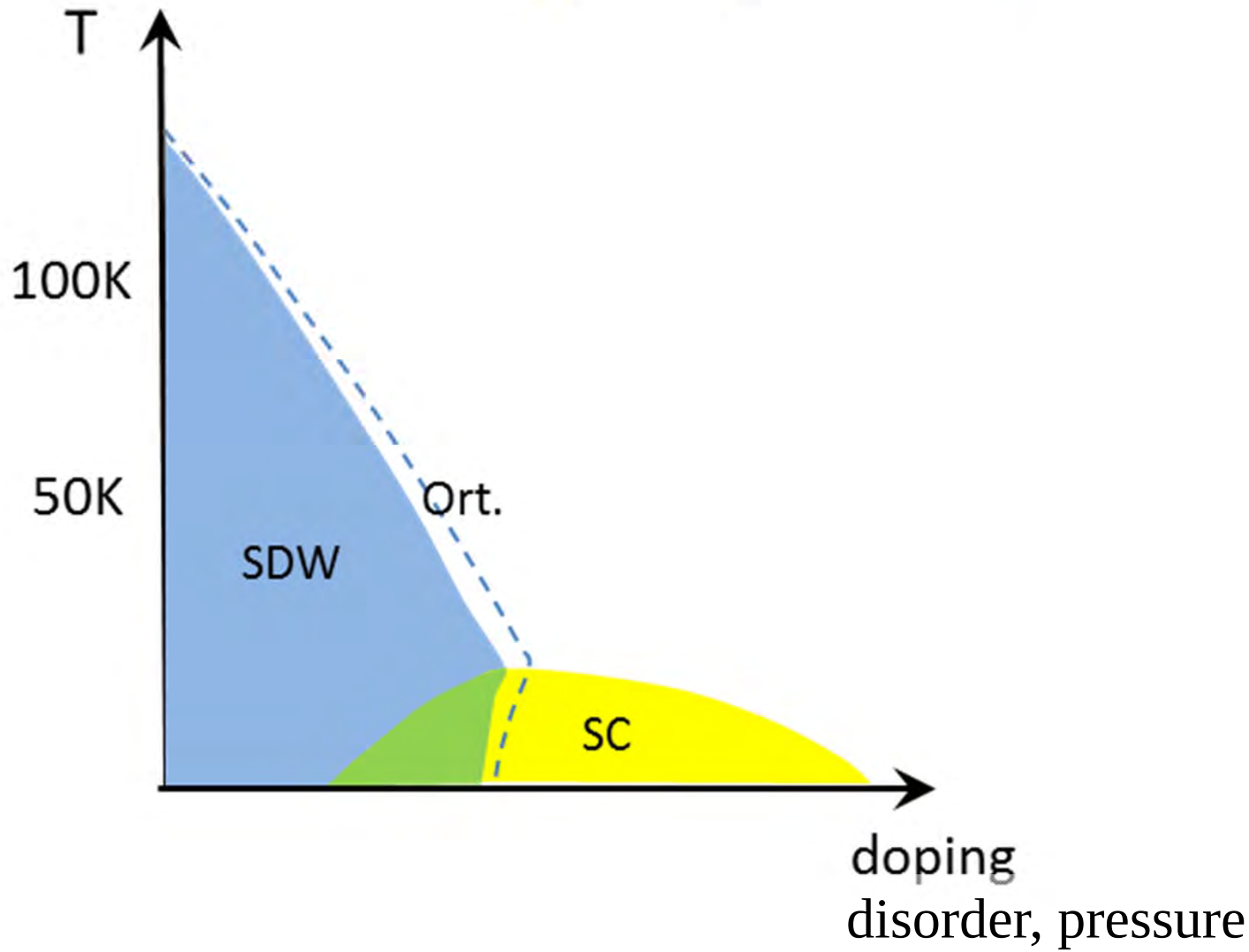
Mutiorbital and multiband physics: several d-orbitals close to E_F



L. Boeri, O.V. Dolgov, and A.A. Golubov,
PRL 101, 026403 (2008)

[МГУ-Январь-2014]

Iron-Pnictides: typical phase diagram



magnetic, structural, and superconducting order

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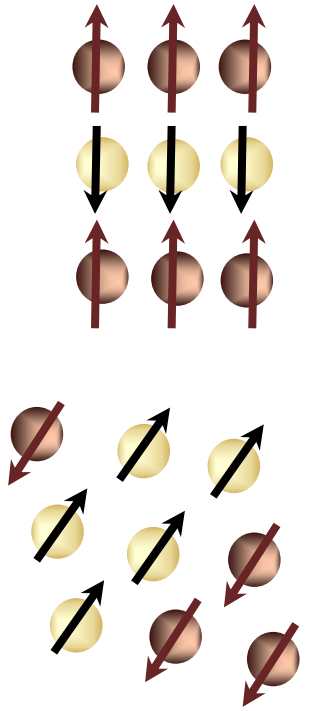
Iron pnictides: structural and magnetic transitions

I) Structural Transition

II) Magnetic Transition



DFT correctly reproduces (or even predicts) correct magnetic and structural ground states, but requires magnetism as a prior condition for distortion

transitions are simultaneous for FeTe and almost for parent 122's, but structural transition is first in 1111's and doped 122's

[МГУ-Январь-2014]

Is the physics behind superconductivity universal or model dependent?

[МГУ-Январь-2014]

Universality due to electron-phonon interaction? NO

Electron-phonon interaction is probably too weak

L. Boeri, O.V. Dolgov, and A.A. Golubov,
PRL 101, 026403 (2008)

$$\lambda = 0.21$$

λ=0.44 for Al

$\lambda \lesssim 0.35$, still not enough

including magnetism

L. Boeri et al., PRB 82, 020506 (2010)

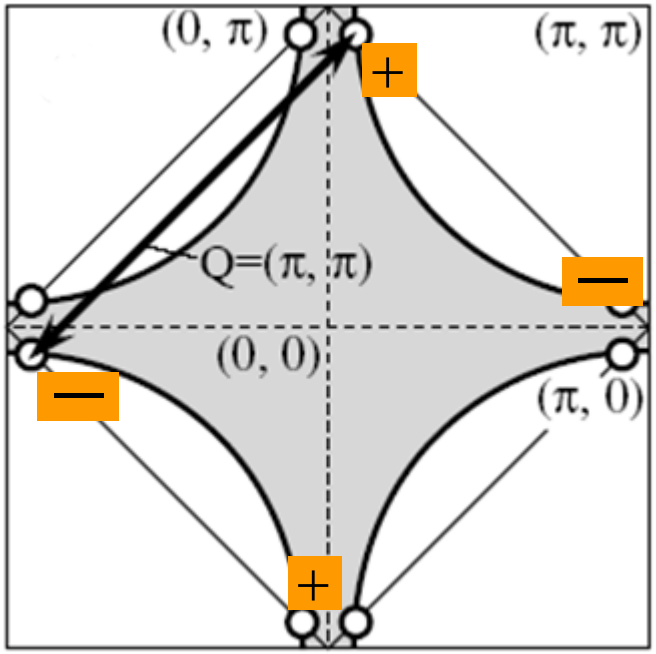
Too small to account
for Tc ~ 50K

Is there any universality in these systems?

[МГУ-Январь-2014]

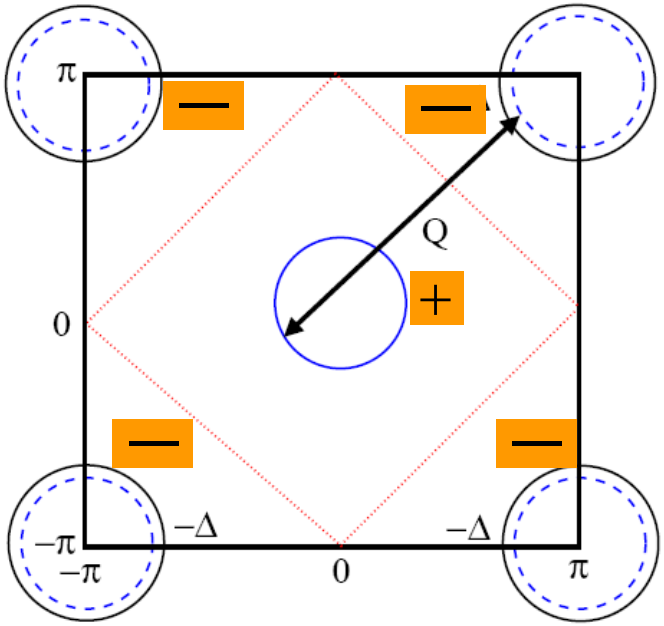
Universality due to proximity to antiferromagnetism?
Pairing due to spin fluctuations?

Cuprates



$$\Delta(\theta) = \Delta_0 (\cos k_x - \cos k_y)$$

Pnictides



$$\Delta(\theta) = \Delta_0 (\cos k_x + \cos k_y)$$

Mazin et al.

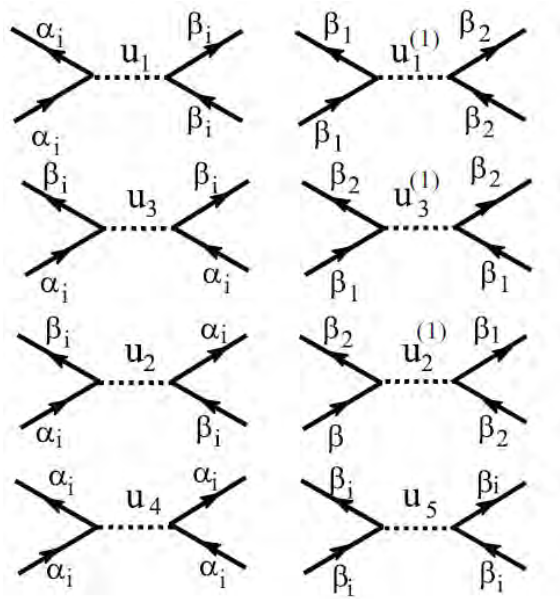
$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} \frac{V_{eff}(\mathbf{k}-\mathbf{k}')}{2E(\mathbf{k}')} \Delta(\mathbf{k}')$$

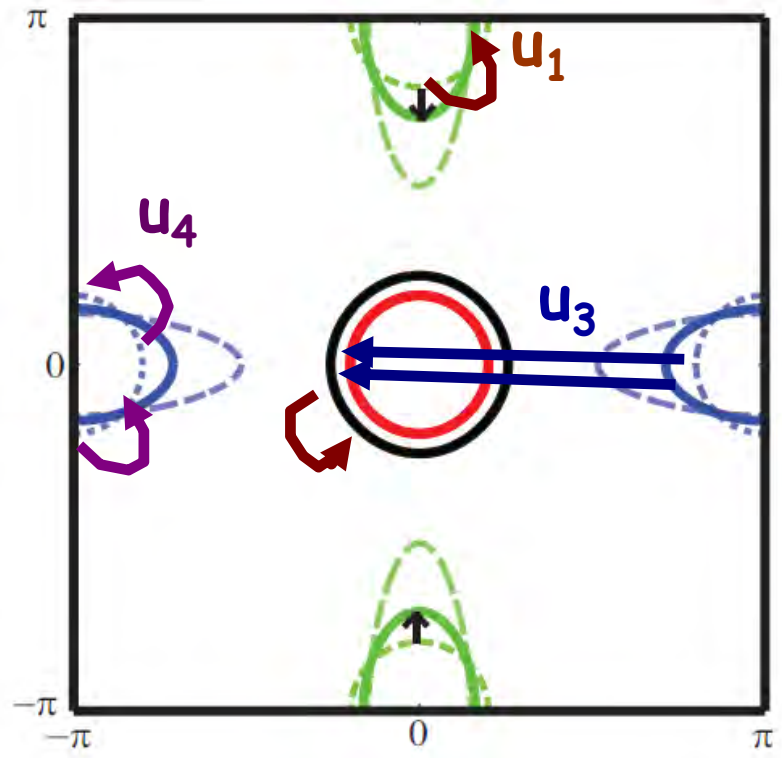
Although in some materials this may give a reasonable explanation – this is not the true origin of universality

Universality due to initial electronic structure ⇒ impact on the interactions

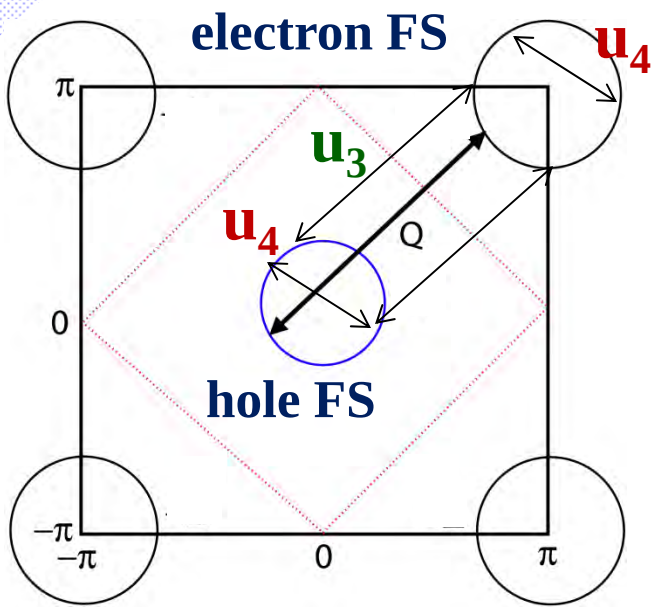
2-body Hamiltonian with intrasite interactions only!

$$H_{int}^{orb} = U \sum_i \sum_\nu n_{i\nu\uparrow} n_{i\nu\downarrow} + V \sum_{\nu \neq \mu, \sigma, \sigma'} n_{i\nu\sigma} n_{i\mu\sigma'}$$
$$- J \sum_{\nu \neq \mu} \mathbf{S}_{i\nu} \cdot \mathbf{S}_{i\mu} + J' \sum_{\nu \neq \mu} d^\dagger_{i\nu\uparrow} d^\dagger_{i\nu\downarrow} d_{i\mu\downarrow} d_{i\mu\uparrow}$$



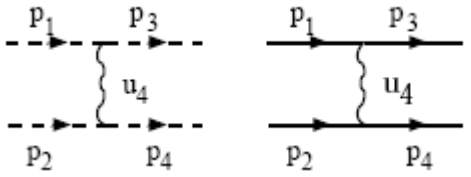


L. Benfatto, P. Hirschfeld, S. Graser, A. Chubukov, K. Kuroki, H. Aoki, R. Thomale, C. Honerkamp, Ch. Platt, W. Hanke, …

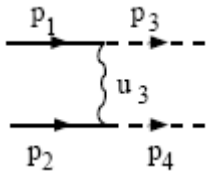


toy model: one hole and one electron FSs

Pairing interactions:



Intra-band repulsion u_4



Pair hopping

(π,π) interaction

s^{+-} superconductivity, BCS theory

$$(\Gamma_{SC}^{s+-}) = u_3 - u_4,$$

need $(\Gamma_{SC}^{s+-}) > 0$

If the intra-pocket repulsion (u_4) is stronger than the pair hopping (u_3), the pairing interaction is repulsive

In general, intra-pocket interaction should be the largest
(u_4 is Coulomb repulsion at a small momentum transfer)

Intra-orbital interactions are bigger than the interorbital ones

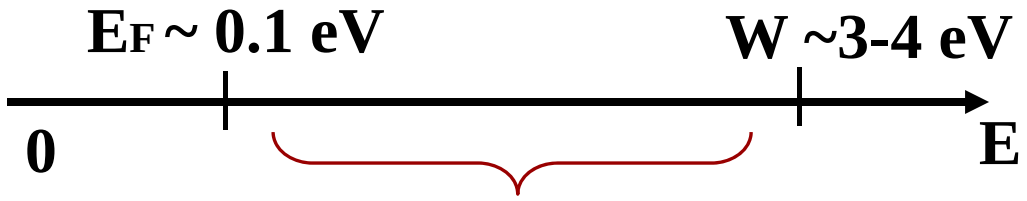
A.V. Chubukov, D. Efremov, and I. Eremin, PRB (2008)

fRG and/or one-loop RG is extremely important

A.V. Chubukov, I. Eremin, F. Wang, D.-H. Lee, C. Platt, R. Thomale, C. Honerkamp, W. Hanke, …

u_{ee} and u_{he} are bare interactions at energies of a bandwidth

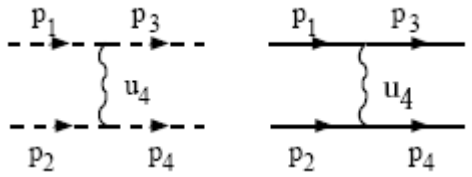
For SC we need interactions at energies smaller than the Fermi energy



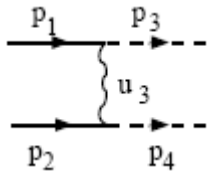
Couplings flow due to renormalizations in particle-particle and particle-hole channels

[МГУ-Январь-2014]

One-loop parquet RG

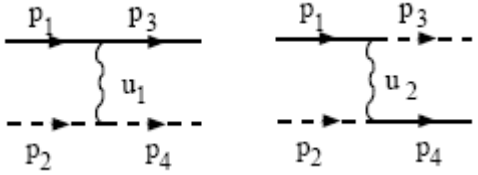


Intra-band repulsion u_4



Pair hopping

(π,π) interaction

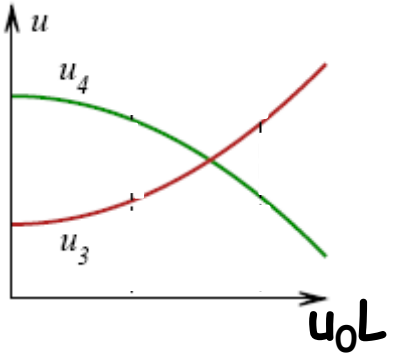


Inter-band density-density and exchange interaction

$$\dot{u}_1 = u_1^2 + u_3^2$$
$$\dot{u}_2 = 2u_2(u_1 - u_2)$$
$$\dot{u}_3 = 2u_3(2u_1 - u_2 - u_4)$$
$$\dot{u}_4 = -u_3^2 - u_4^2$$

(H. Shultz, Dzyaloshinskii & Yakovenko, Rice, Honerkamp…)

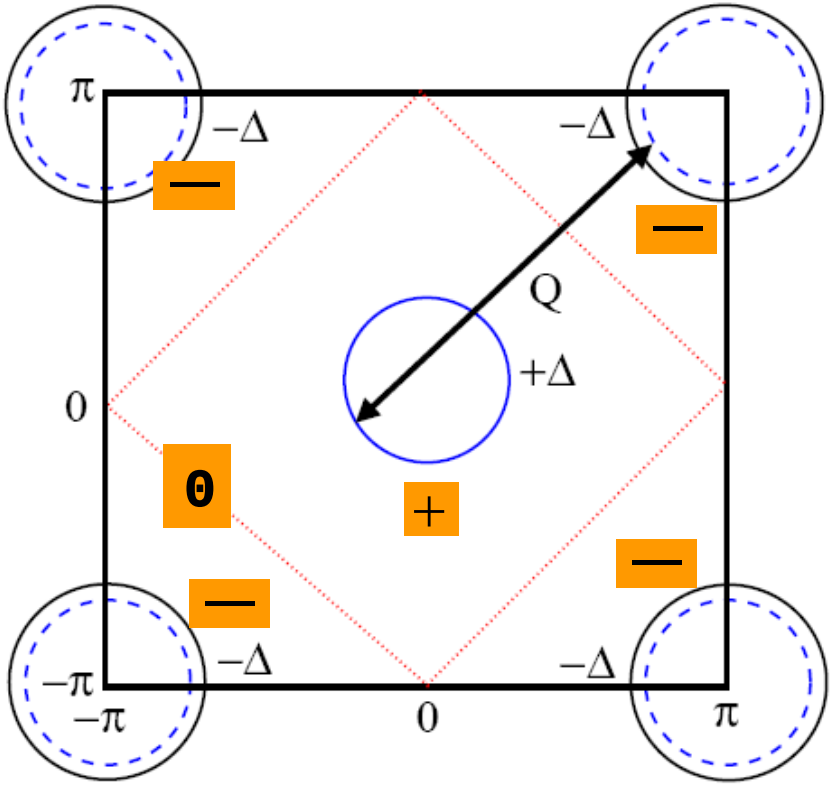
SDW



u_3 is pushed up by u_1, which gives rise to SDW

If the tendency towards SDW is strong, u_3 becomes larger than u_4, leading to an attraction in s^{+-} superconducting channel

Tests for pairing symmetry (s^{+-})

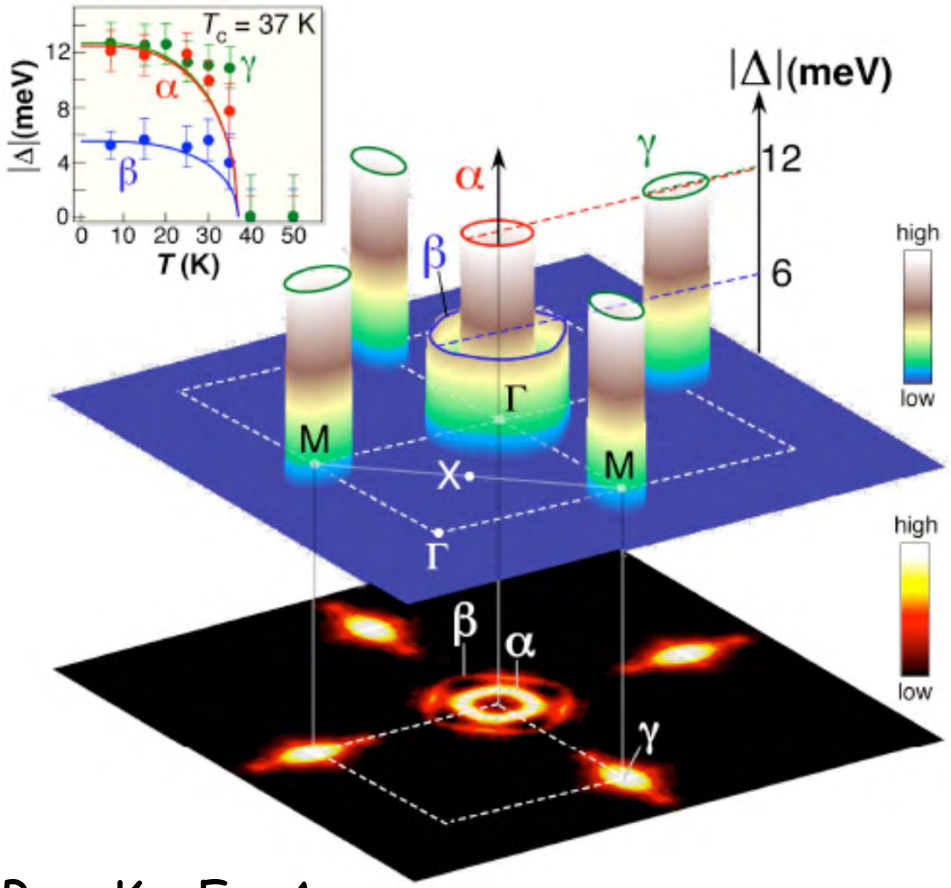


$$\Delta_h = -\Delta_e$$

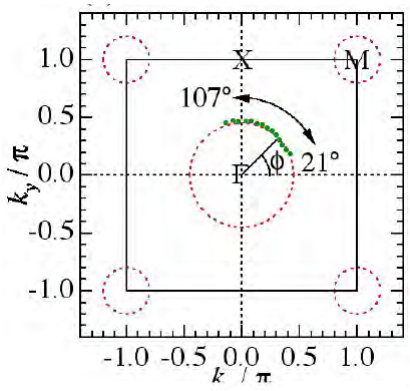
[МГУ-Январь-2014]

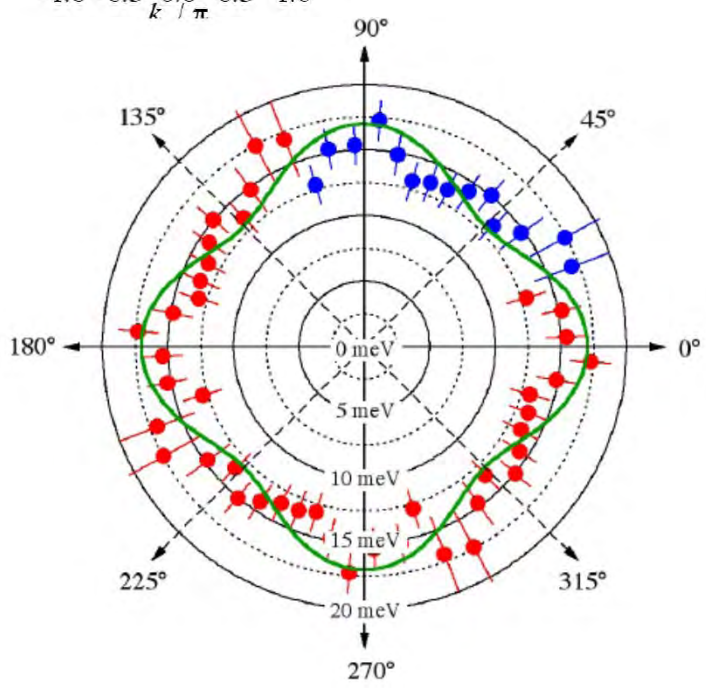
ARPES: Symmetry of the superconducting gap

- nearly isotropic gap in ARPES



$Ba_{0.6}K_{0.4}Fe_2As_2$
H. Ding et al., EPL (2008)



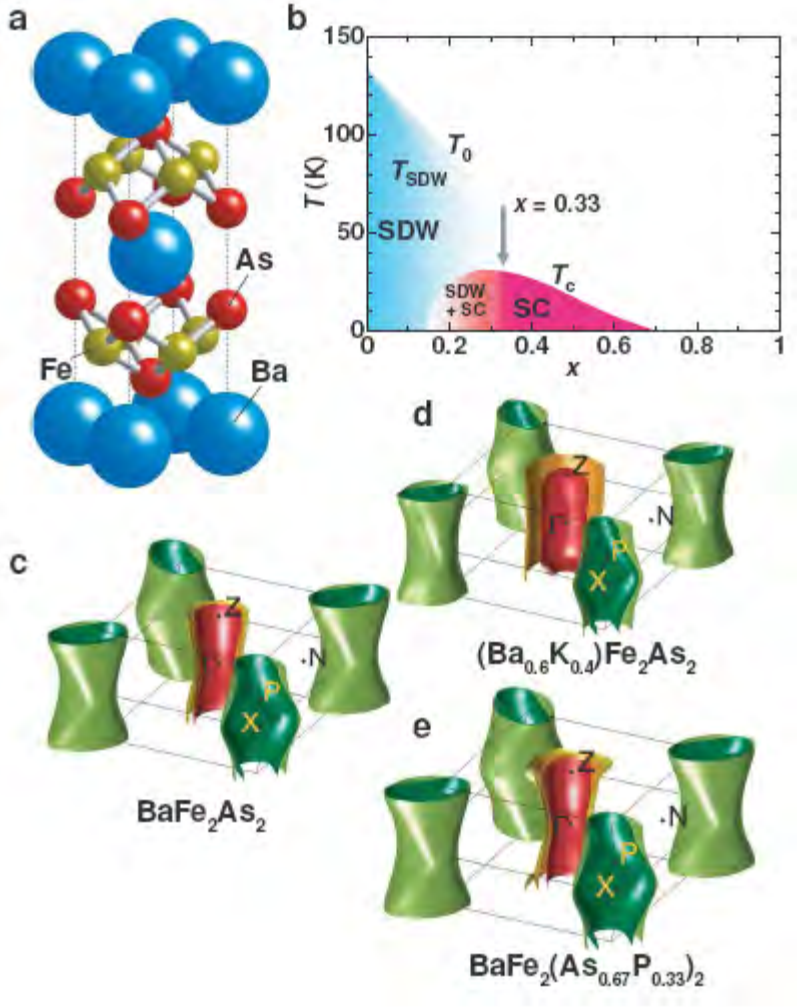


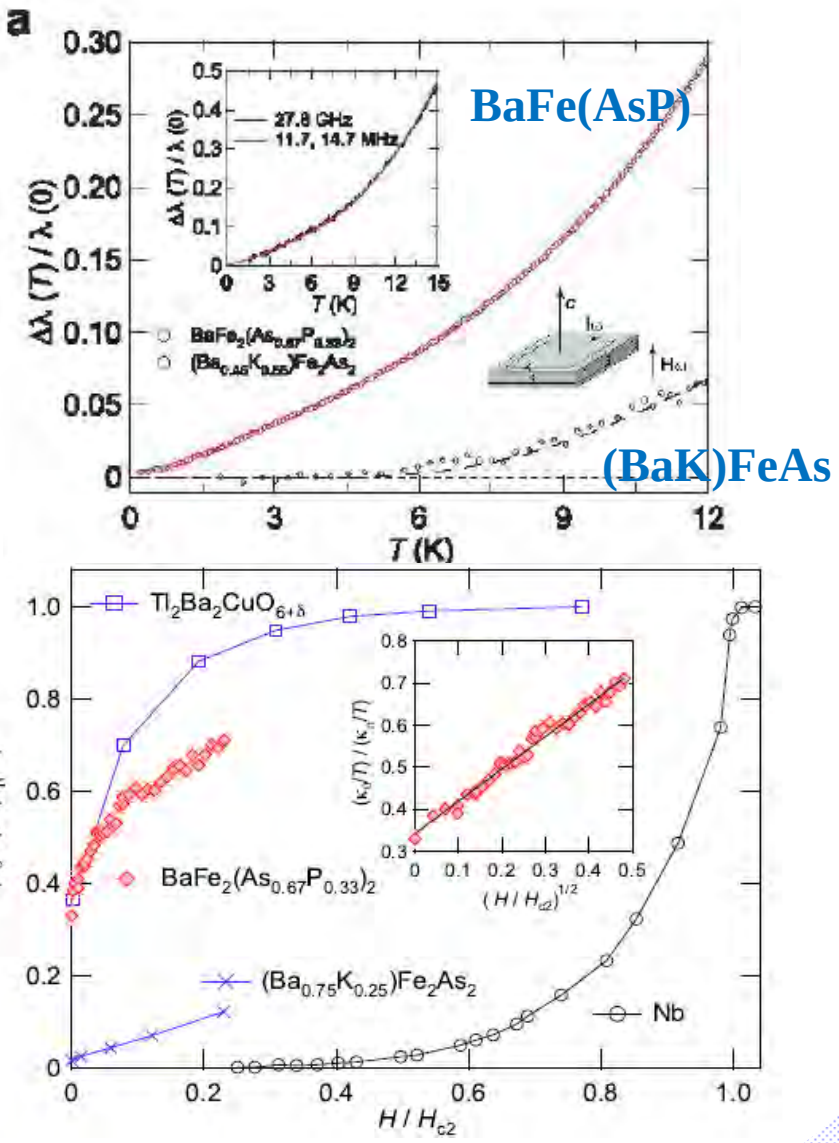
$NdFeAsO_{1-x}F_x$
T. Kondo et al., PRL 101 (2008)

[МГУ-Январь-2014]

Nodal gap: the behavior of $BaFe_2(As_{1-x}P_x)_2$, Tc =30K

Y. Matsuda et al





Consistent with line nodes

Extension for the realistic model

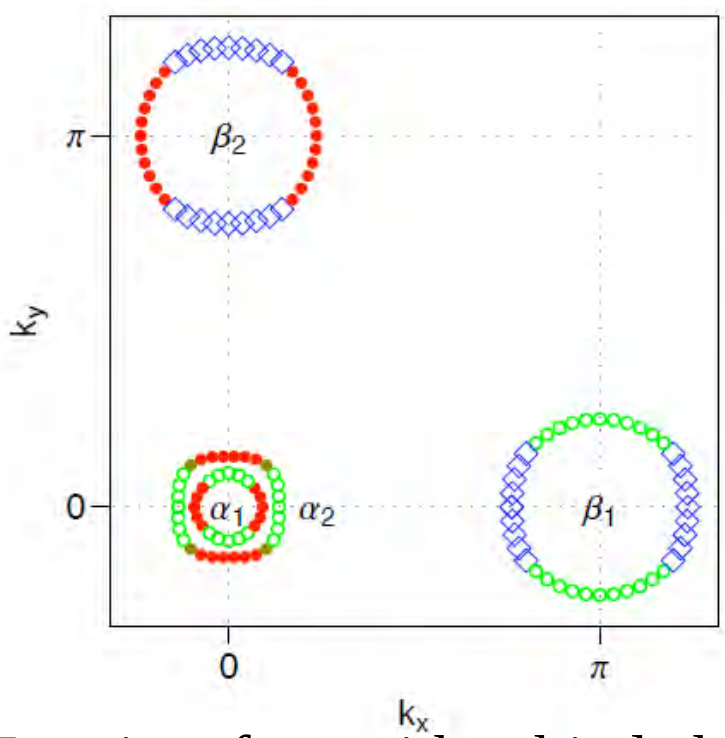
- **convert the model into band basis,**
- **fit the interactions by the lowest angular harmonics, and extracted parameters u_{eh},u_{ee}, etc.**
- **solve and analyze the gap equations for moderate and large hole and electron dopings**
- **for a bare interaction and for interaction dressed by the higher order bubble and ladder diagrams (spin fluctuations)**

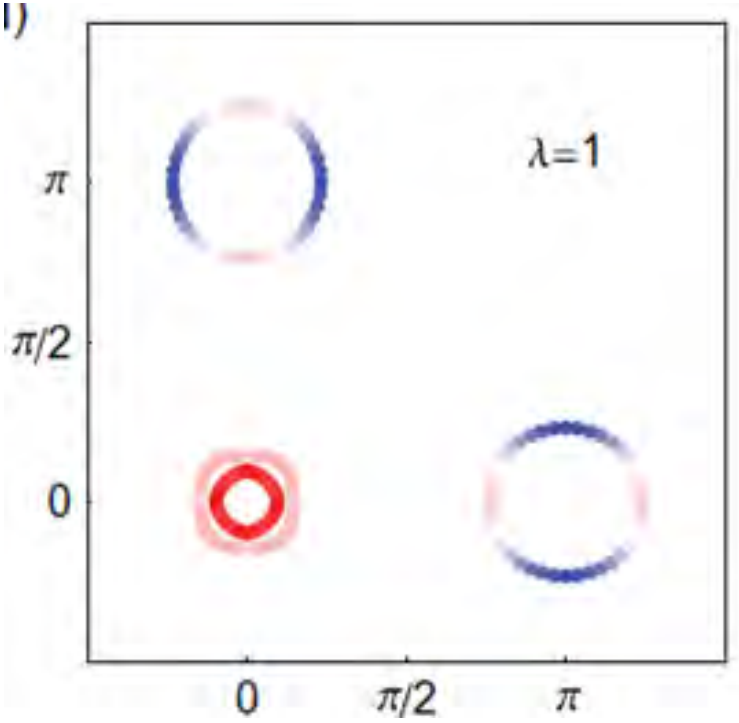
[МГУ-Январь-2014]

Multiorbital physics is missing ⇒ Origin of the gap anisotropy

1. **importance of orbital character on Fermi sheets**
2. **scattering between β_1 and β_2 sheets**
3. **intraband Coulomb repulsion**

See also: Chubukov et al 2009, Thomale et al 2009, 2011 (band picture), Kemper et al 2010, P. Hirschfeld et al.(orbital picture)



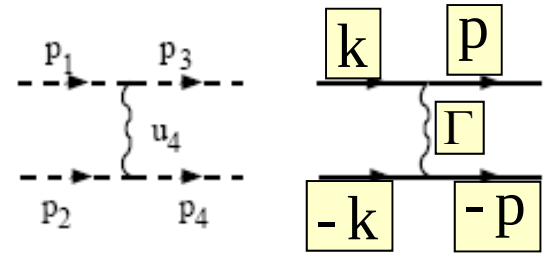


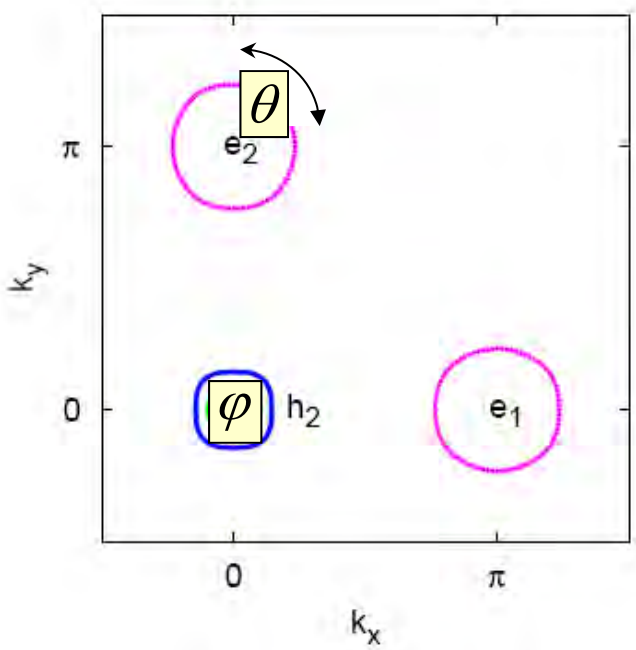
Fermi surface with orbital character

Gap

Pairing vertex in multiband (multiorbital) systems

S-wave pairing





$$\Gamma(k,p)=\sum_{n,m}\Gamma_{n,m}\,\psi_n(k)\,\psi_m(p)$$

$$\psi_{n,m}(\pm k_x,\pm k_y)=\psi_{n,m}(\pm k_y,\pm k_x)$$

Near k=0,

$$\psi_n(k)=A_n+B_n\cos 4\varphi+C_n\cos 8\varphi+\ldots$$

φ along hole FS

Near p=(π,0) ,

$$\psi_n(p)=(\tilde{A}_n+\tilde{B}_n\cos 4\theta+\tilde{C}_n\cos 8\theta+\ldots)$$
$$\pm(D_n\cos 2\theta+E_n\cos 6\theta+\ldots)$$

θ along electron FS

[МГУ-Январь-2014]

Leading harmonics in the superconducting s-wave gap

$$\psi_n(k) = A_n + B_n \cos 4\psi + C_n \cos 8\psi + \ldots \Rightarrow A_n$$

Near hole FSs

$$\psi_n(p) = \tilde{A}_n + \tilde{B}_n \cos 4\theta + \tilde{C}_n \cos 8\theta + \ldots$$
$$\pm(\tilde{D}_n \cos 2\theta + \tilde{E}_n \cos 6\theta + \ldots) \Rightarrow \tilde{A}_n \pm \tilde{D}_n \cos 2\theta$$

Near electron FSs

effective interactions dependent on the angles along electron FSs

$$\Gamma_{h,h}(k,p) = u_{h,h}, \quad \Gamma_{e,h}(k,p) = u_{e,h}\,(1 \pm 2\alpha \cos 2\theta),$$

$$\Delta_h(q) = \Delta_h, \qquad \Delta_{e,1,2}(q) = \Delta_e \pm \bar{\Delta} \cos 2\theta$$

Depending on the ratio the gap is just anisitropic or nodal

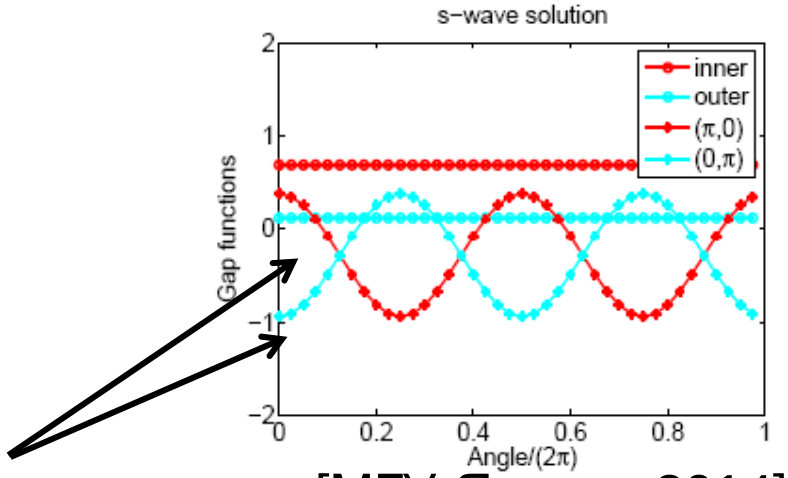
[МГУ-Январь-2014]

Leading harmonics in the superconducting s-wave gap

combination of magnetic fluctuations and angle-dependence of the interaction between hole and electron pockets
⇒ attraction in s-wave channel for all electron and hole dopings.

S^{+-} gap with or without nodes

interaction is necessary angle-dependent,
the gaps on electron FSs have cos 2θ components
and may have accidental nodes



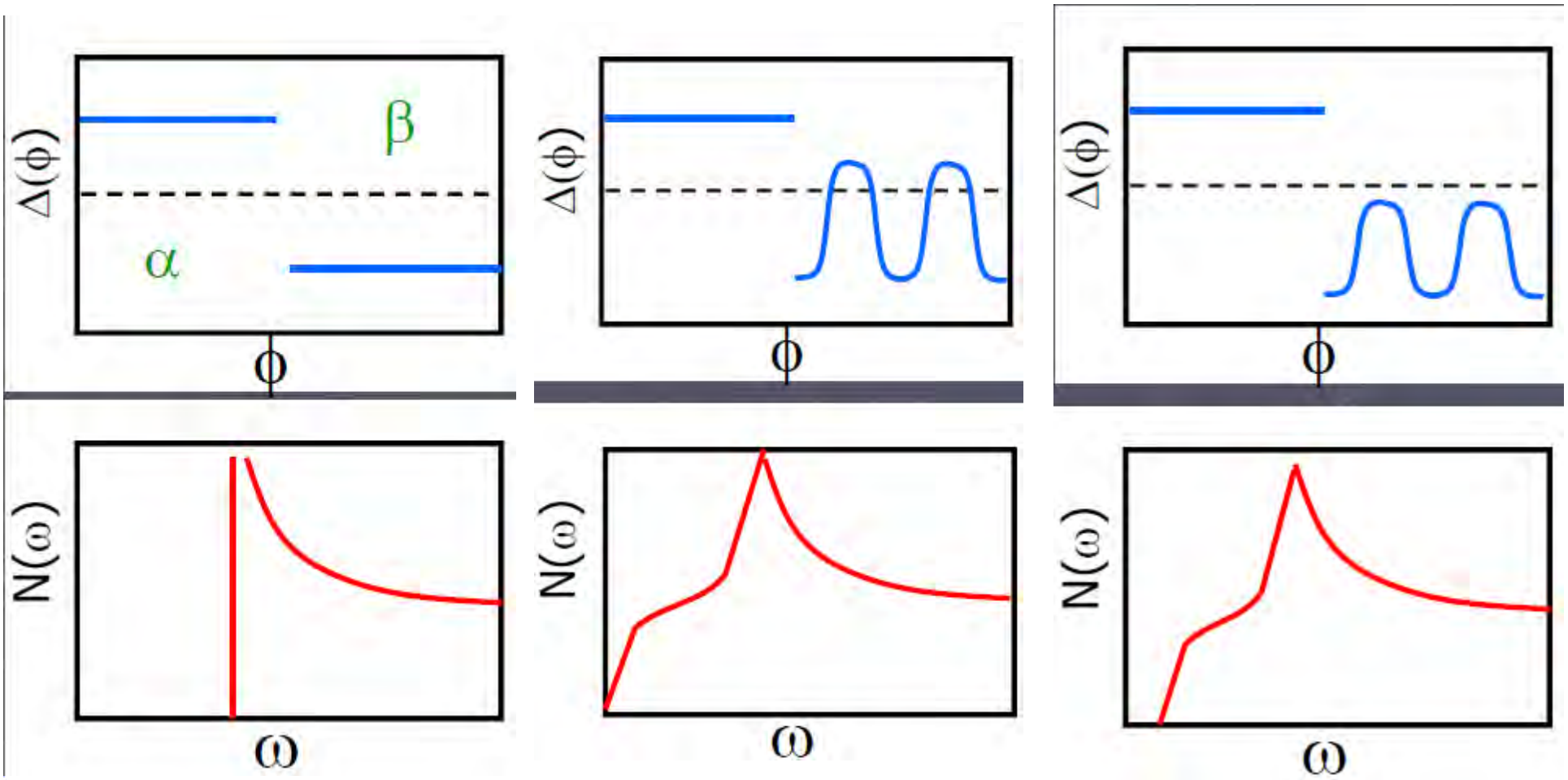
electron FSs

[МГУ-Январь-2014]

Sensitivity to the relatively small changes

Nevertheless the physics is still universal

a) isotropic $s_{+/-}$ **b) nodes** **c) deep minima**



s_{+-} solution exists for ANY $u^2_{he}/u_{hh}\, u_{ee}$

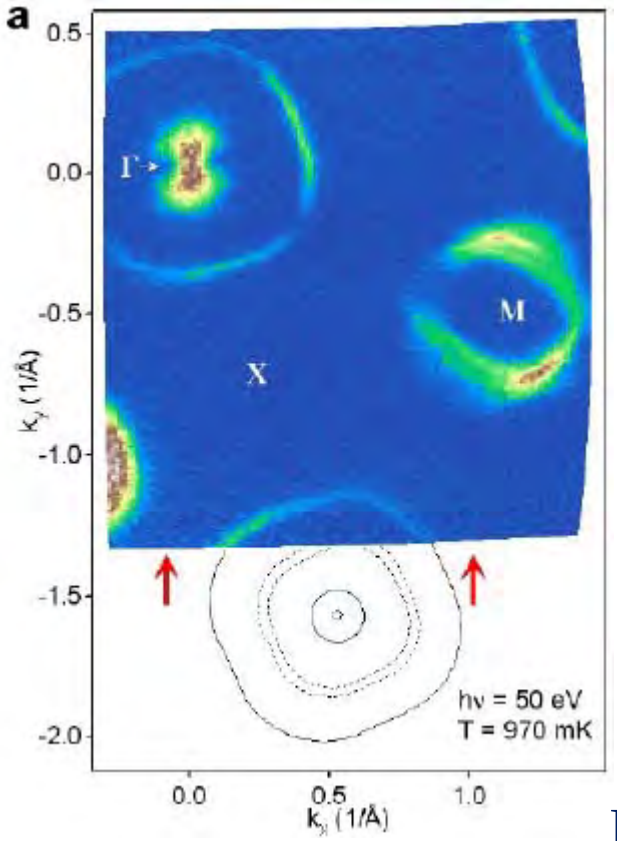
[МГУ-Январь-2014]

Another example:

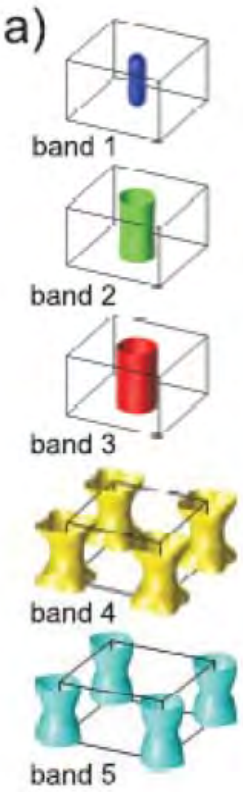
LiFeAs

[МГУ-Январь-2014]

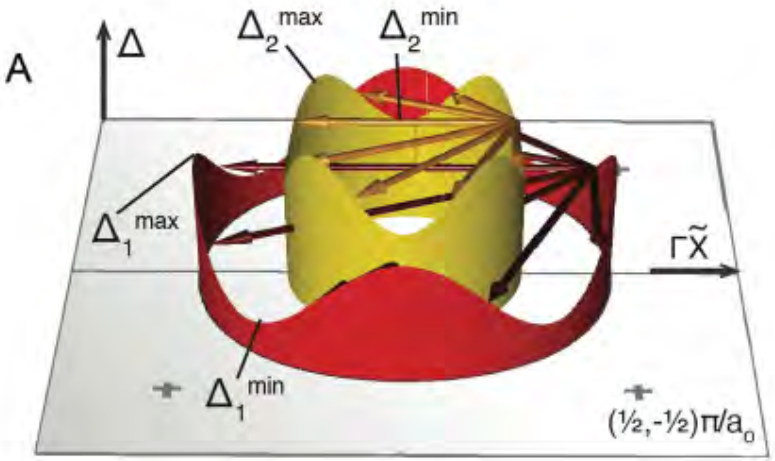
LiFeAs: weak-characterized electronic structure



Borisenko et al.



Putzke et al



Exp STM: Allan et al

Near hole FSs

$$\psi_n(k) = A_n + B_n \cos 4\psi + C_n \cos 8\psi + \ldots \Rightarrow A_n$$

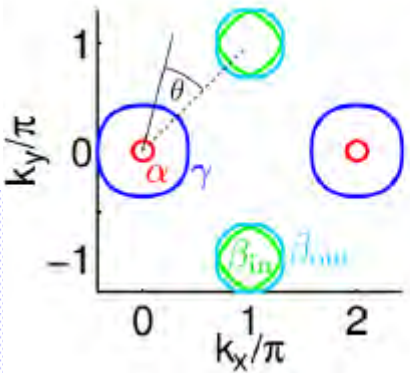
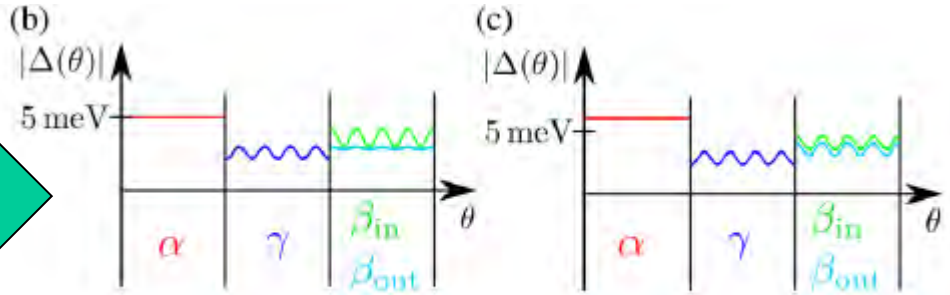


Figure taken from Wang et al. 2013

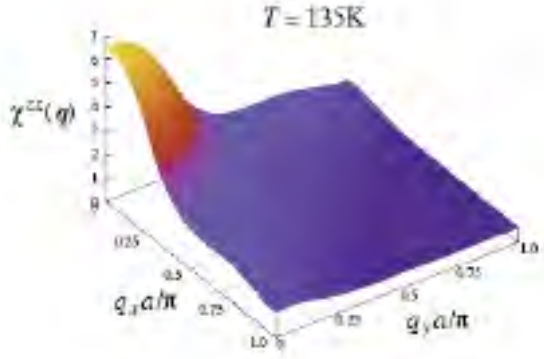


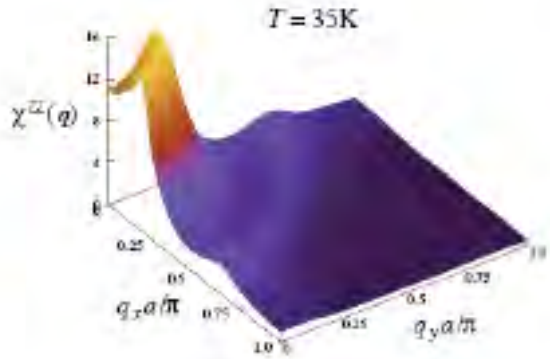
Umewaza et al

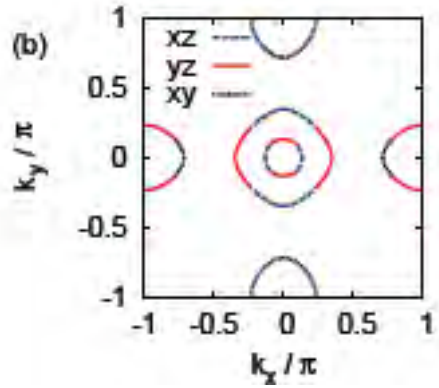
Borisenko et al

LiFeAs: low-q fluctuations competing with incommensurate AF fluctuations

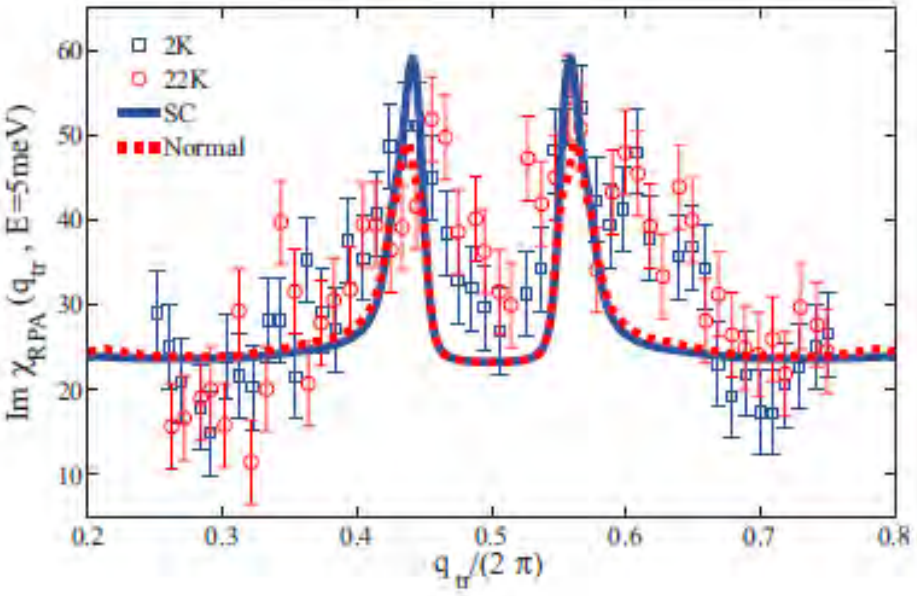
Low-q fluctuations (almost FM): Brydon et al PRB 83 (2011)

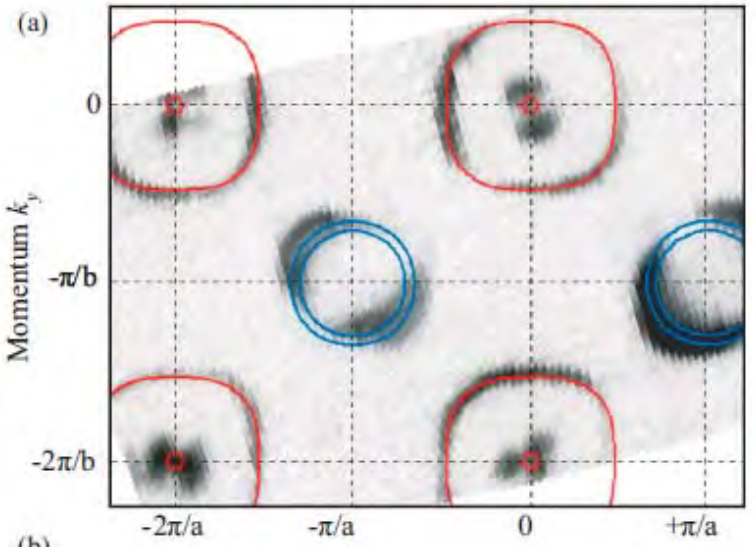






Incommensurate AF fluctuations: J. Knolle, I. Eremin, et al PRB 86 (2012)





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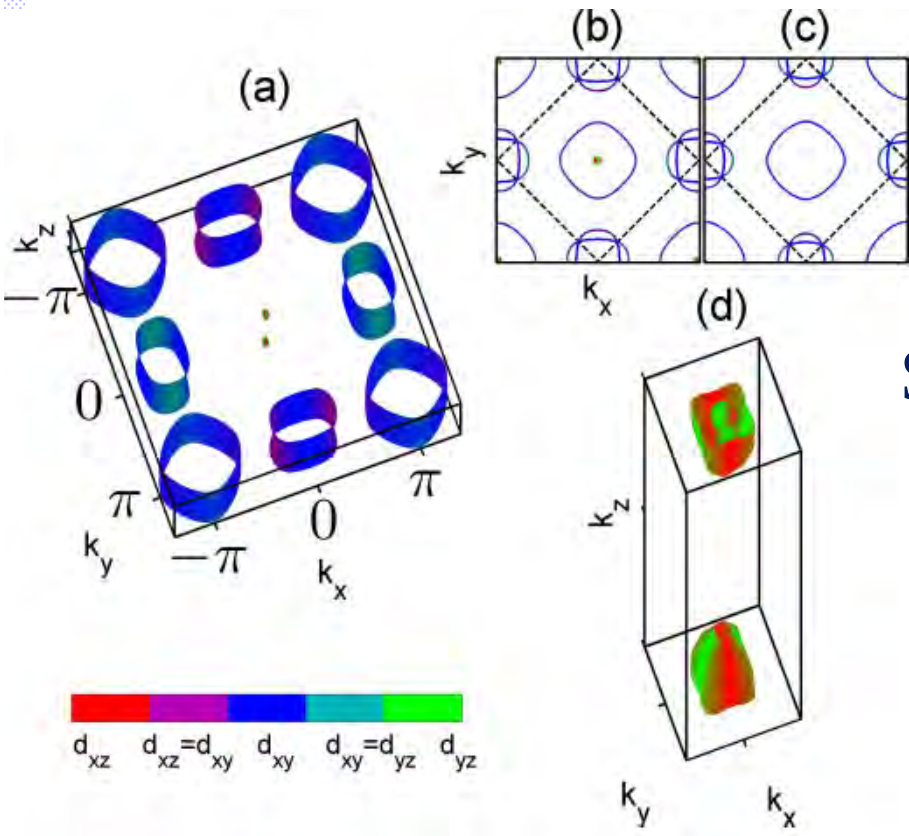
How the superconducting instability arises in this case



Subset 1: two hole pockets mainly of xz and yz character

$$\Delta_{h1}, \Delta_{h2}$$

Subset 2: large hole pocket and two electron pockets with strong admixture of xy orbital

$$\Delta_{h3}, \Delta_{e1,e2} = \Delta_e \pm \overline{\Delta}_e \cos 2\theta$$

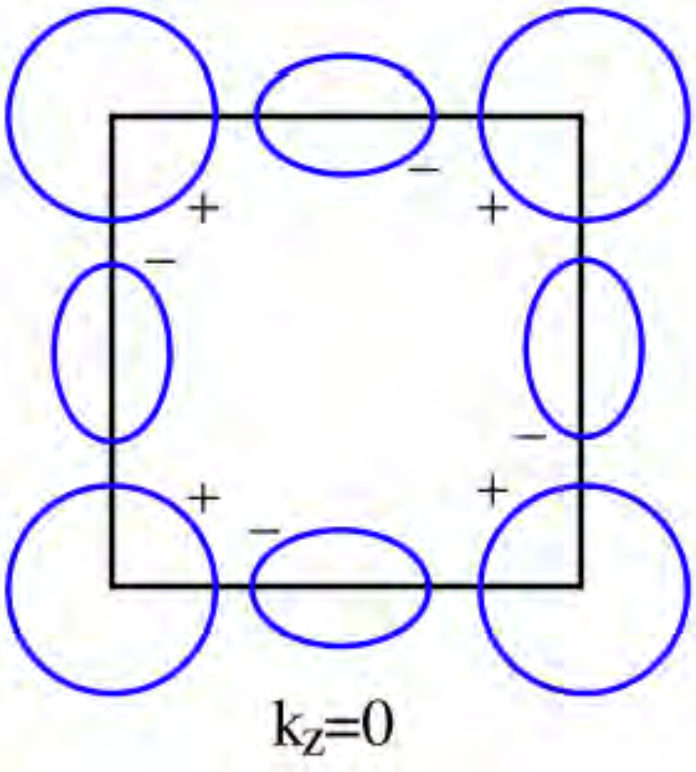
The coupling between two subsets is relatively weak without taking into account spin fluctuations

Possibility for the time-reversal symmetry breaking

s+is

[МГУ-Январь-2014]

Subset 2, k_z=0



Subset 2: large hole pocket and two electron pockets

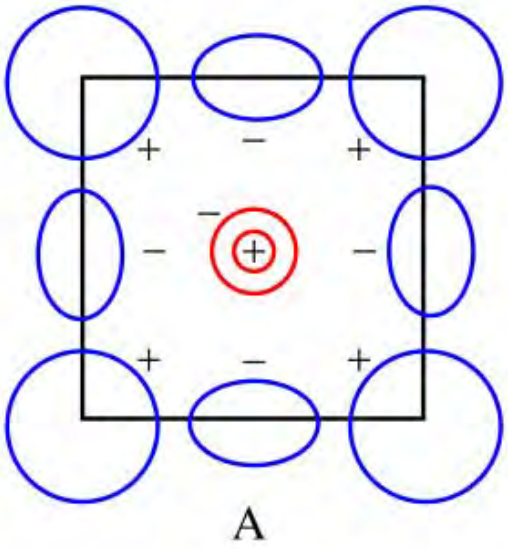
For γ – pocket and β - pockets

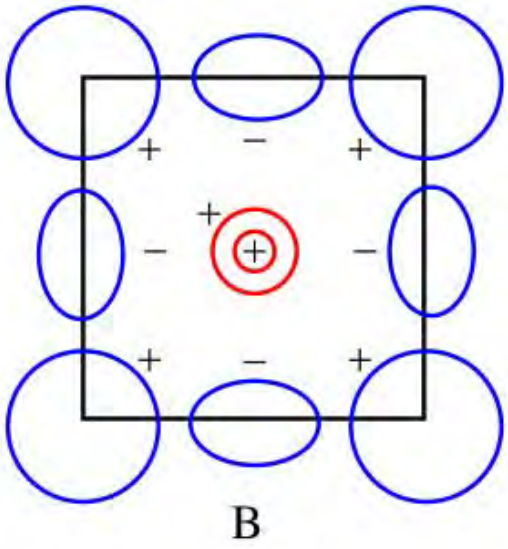
$$\lambda \begin{pmatrix} \Delta_h \\ \Delta_e \\ \bar{\Delta}_e \end{pmatrix} = -L \begin{pmatrix} U_{hh} & 2U_{he} & 2U_{he}\alpha_{he} \\ U_{he} & 2U_{ee} & 2U_{ee}\alpha_{ee} \\ 2U_{he}\alpha_{he} & 4U_{ee}\alpha_{ee} & 4U_{ee}\beta_{ee} \end{pmatrix} \begin{pmatrix} \Delta_h \\ \Delta_e \\ \bar{\Delta}_e \end{pmatrix}$$

If only the γ – pocket and two β – pockets are present, the gap changes sign between them

[МГУ-Январь-2014]

Weakly coupled subsets, degeneracy of various s-wave states





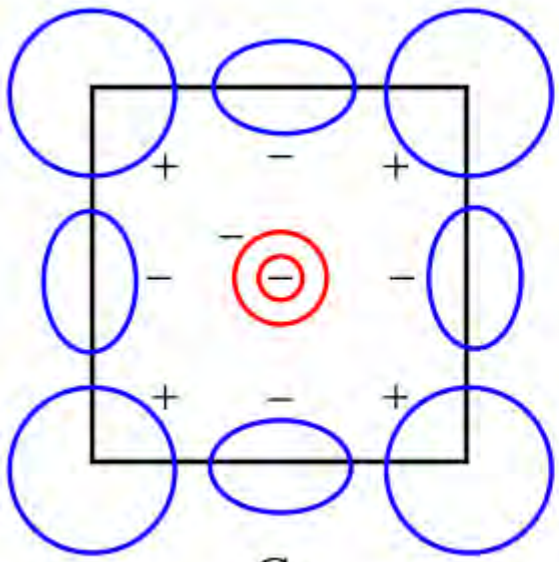
Subset I: red
Subset II: blue

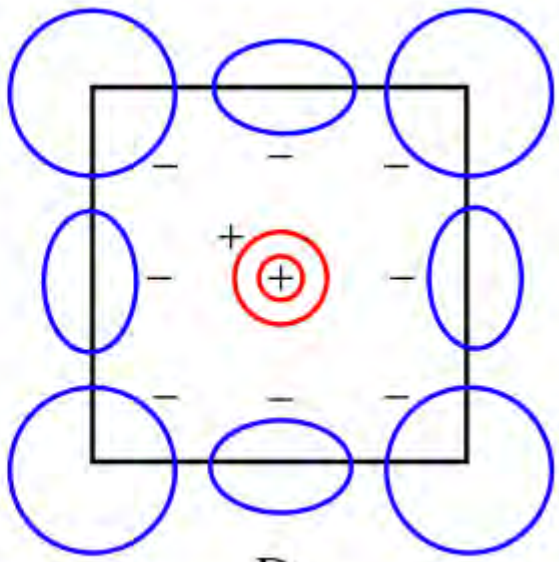
s-wave A state:
If the coupling via α - β and α – γ interactions is small, both subset are effectively uncoupled and the pairing state is s^{+-} in each subset

s-wave B state: (conventional s^{+-} – state)
If α - β and γ – β interactions are enhanced, both subsets are coupled and the gap changes sign between electron and hole pockets

[МГУ-Январь-2014]

Weakly coupled subsets, degeneracy of various s-wave states



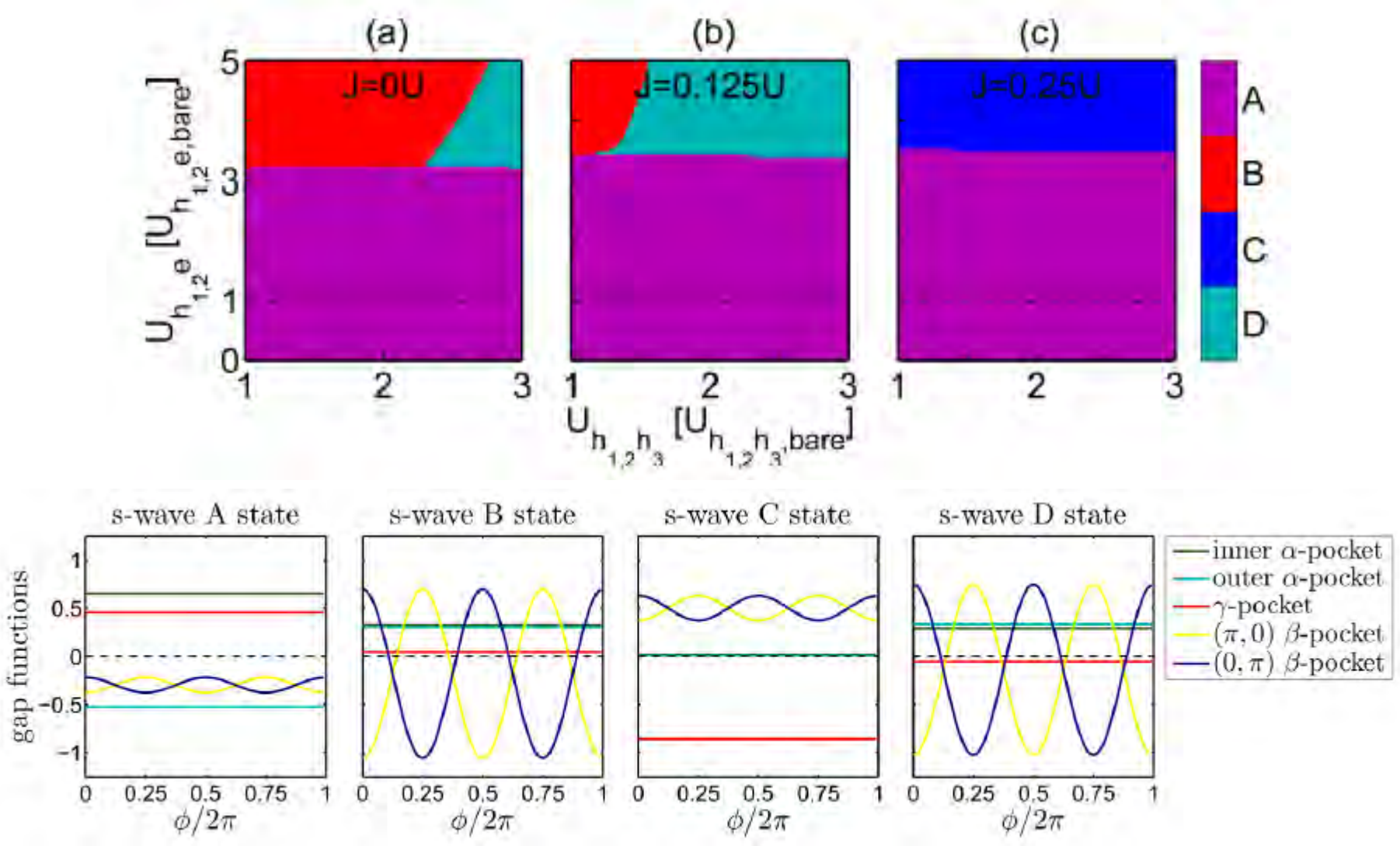


s-wave C state:
If the coupling via α - γ interaction is larger than by α – β interaction, the gaps changes sign between α and γ instead of α and β pockets

s-wave D state:
If the the intra-subet β - γ interaction is small, the gap changes sign between both subset I and II

[МГУ-Январь-2014]

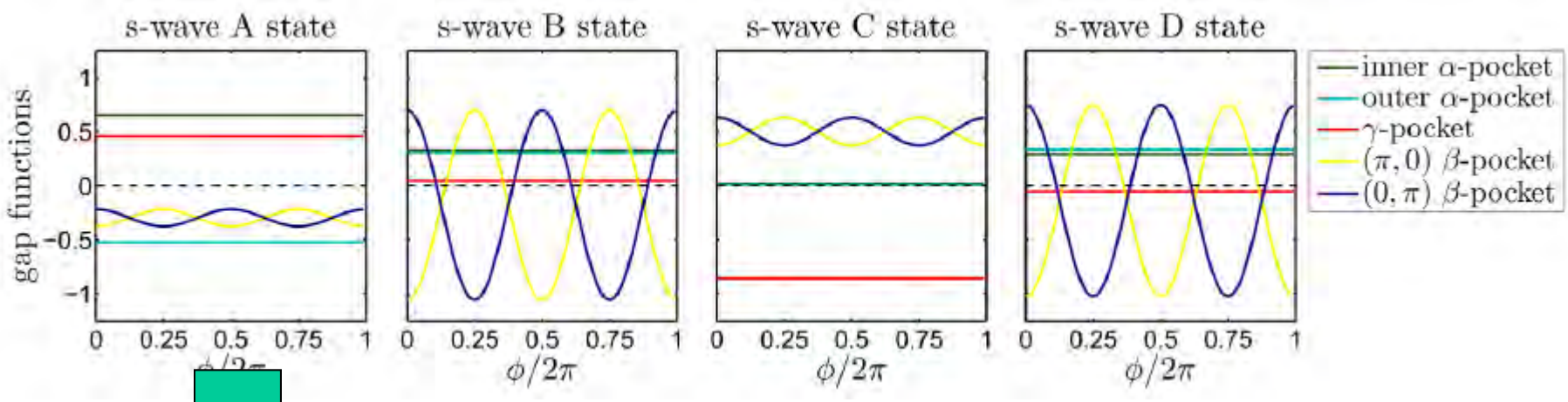
Weakly coupled subsets, degeneracy of various s-wave states



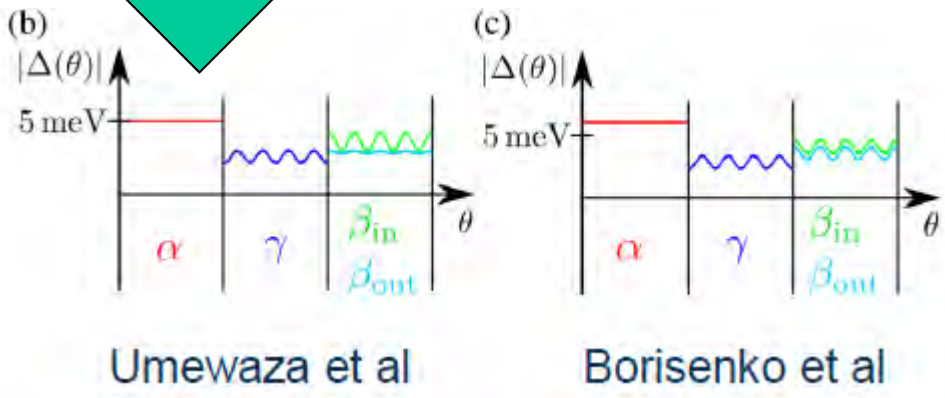
[МГУ-Январь-2014]

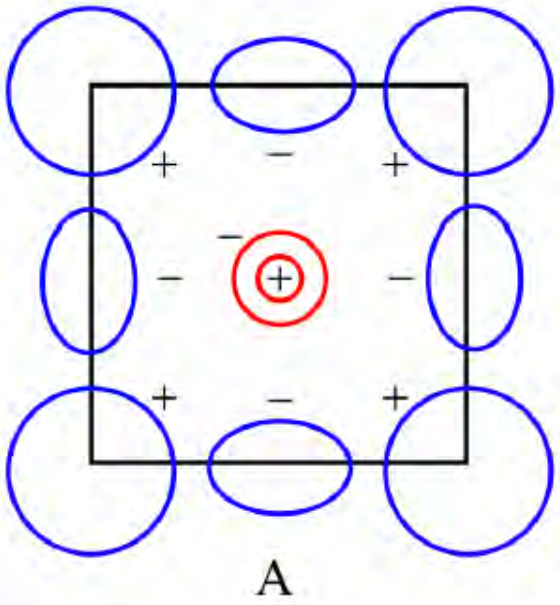
Weakly coupled subsets, degeneracy of various s-wave states

Theory



Experiment





A-state matches the experimental results

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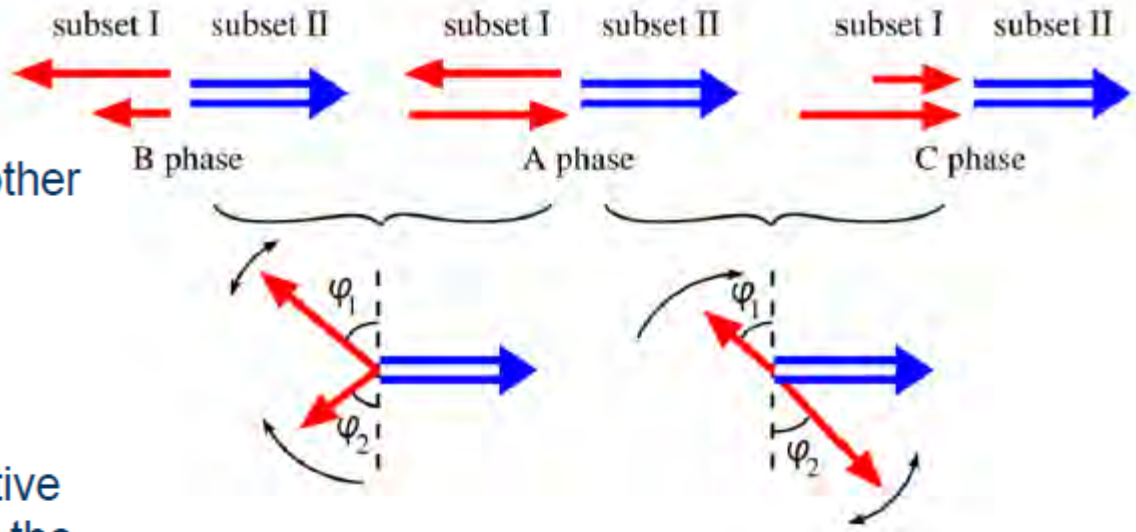
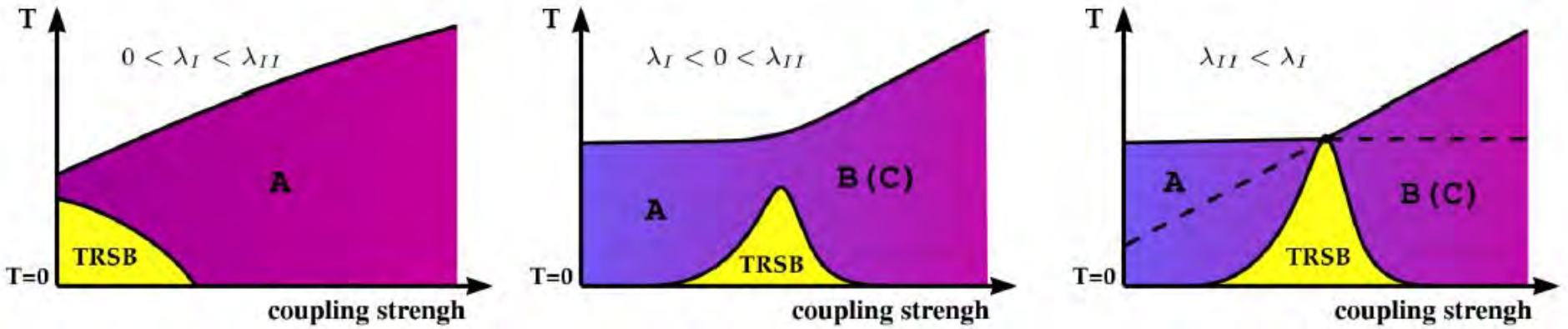
Possible time-reversal symmetry breaking

The transition from one state to another might also occur discontinuously.



Possible scenario: at some $T < T_c$, existence of an s+is state with relative phases $\varphi_{1,2} \neq (\pi \; or \; 0)$ (Figure on the right).



[МГУ-Январь-2014]

Superconductivity in iron-based systems

- Inter-band interaction (enhanced by spin fluctuations) ⇒
glue for the pairing for all dopings,
gap structure and symmetry may change

-if both h and e pockets are present ⇒ driving force is electron-hole interaction. [SC gap has s+- form, d-wave is a competitor, s-wave gap with accidental nodes on electron FS]

LiFeAs ⇒ orbital character may change the character of the s-wave state

- Novel effects due to multiorbital structure