

Магнетизм в железосодержащих сверхпроводниках: взаимодействие магнитных, орбитальных и решеточных степеней свободы

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Theoretische Physik III, Ruhr-Uni Bochum

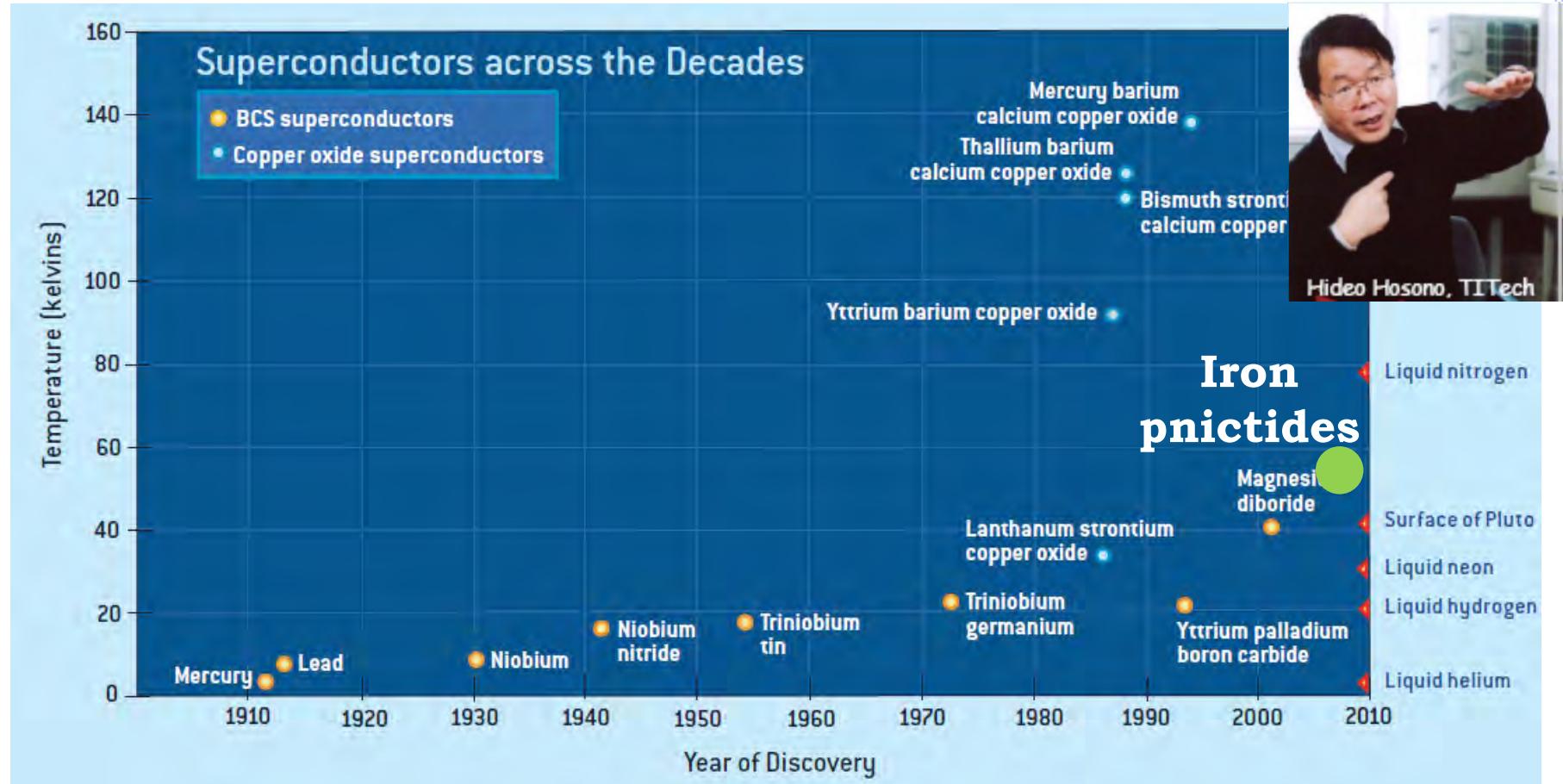


Work done in collaboration with:

- A.V. Chubukov @ *University of Wisconsin, Madison*
- R. Fernandes @ *University of Minnesota*
- J. Schmalian @ *KIT Karlsruhe*.
- J. Knolle, R. Moessner @ *MPI Physik komplexer Systeme, Dresden*

[ОФН РАН-Январь-2014]

Superconductivity reaches the iron age



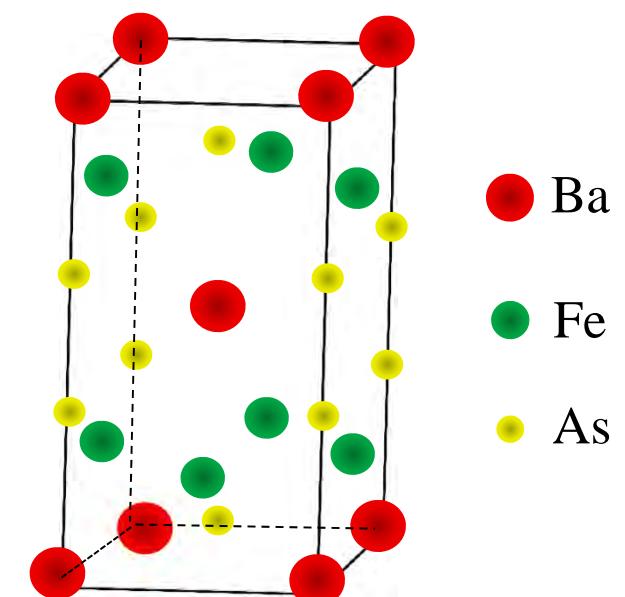
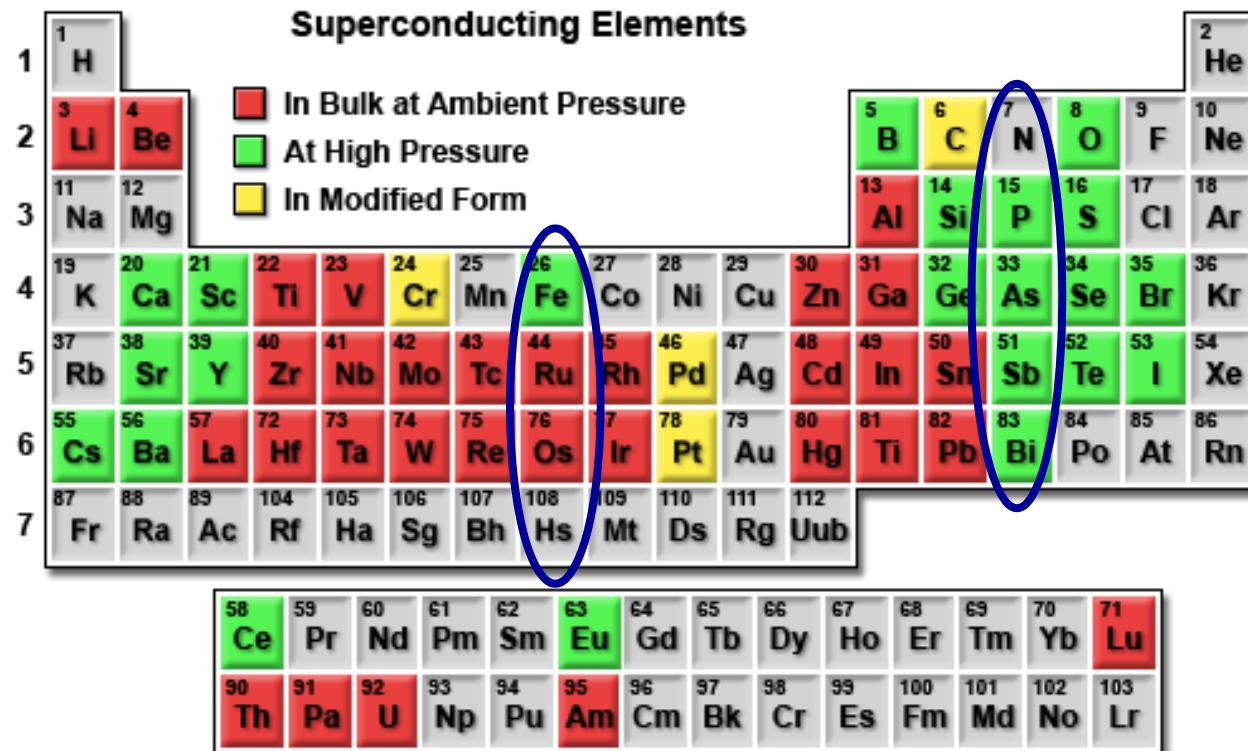
first high-temperature superconductors since the cuprates!

stone age → copper age → iron age



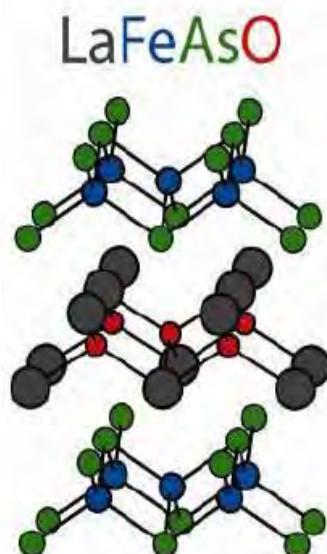
Iron-based superconductors

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



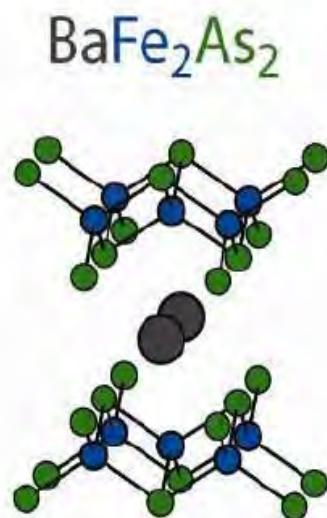
Iron-based superconductors

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



$T_c=28\text{K}$
(55K for Sm)

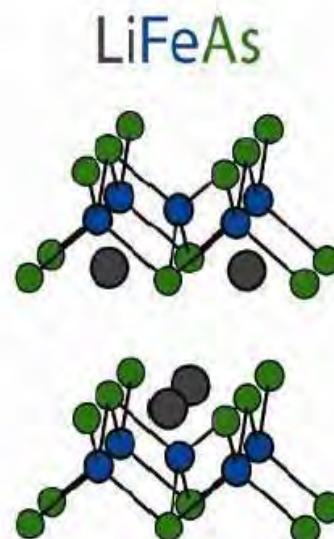
- Kamihara et al
JACS (2008)
- Ren et al
Chin. Phys. Lett.
(2008)



$T_c=38\text{K}$

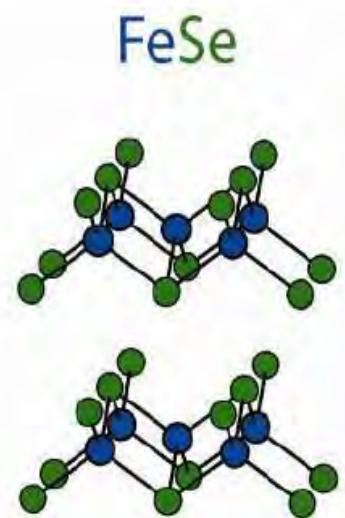
- Rotter et al.
PRL (2008)

- Ni et al Phys. Rev. B 2008
(single xtals)



$T_c=18\text{K}$

- Wang et al
Sol. St. Comm. 2008



$T_c=8\text{K}$

- Hsu et al
PNAS 2008

No arsenic ☺!

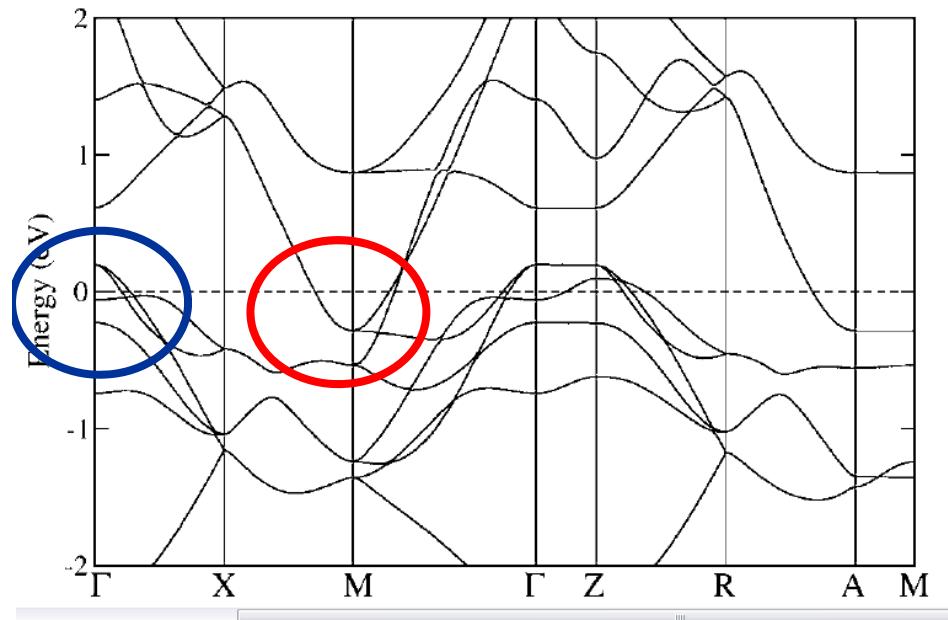
[ОФН РАН-Январь-2014]

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

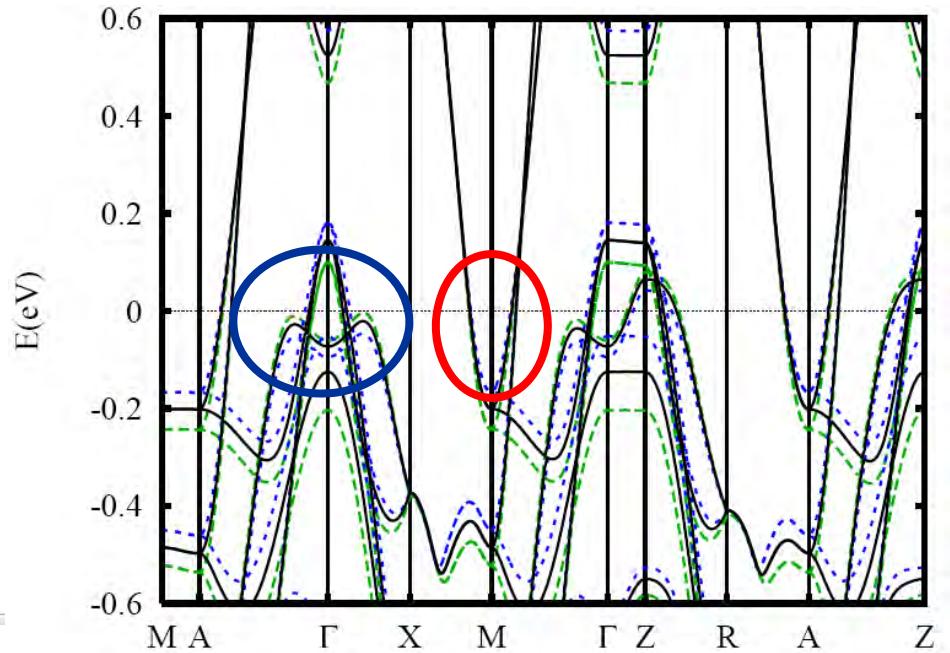
[ОФН РАН-Январь-2014]

Electronic-structure calculations

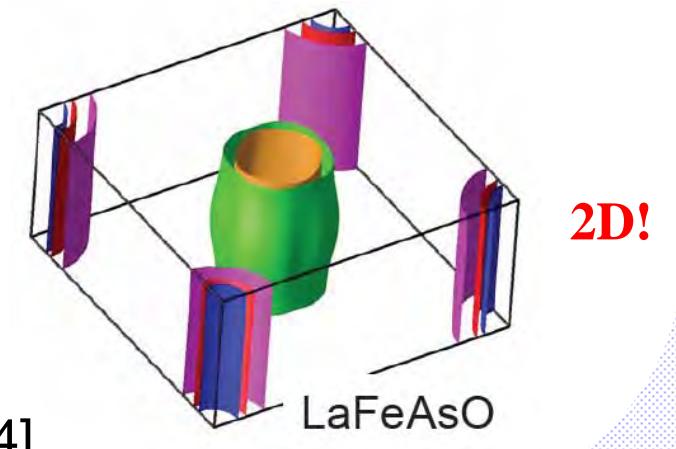
LaFePO Lebegue 2007 ($T_c=6\text{K}$)



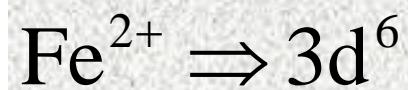
LaFeAsO Singh & Du 2008 ($T_c=26\text{K}$)



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



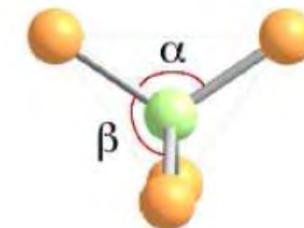
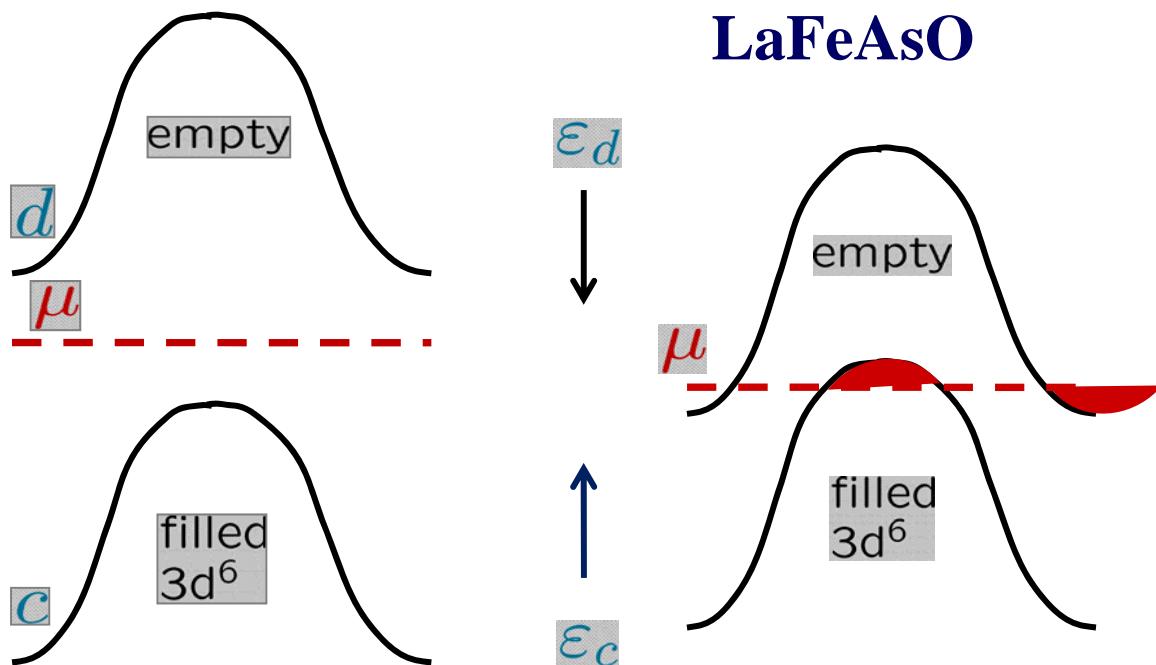
Electronic-structure: multiorband structure



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

semiconductor → semimetal

LaFeAsO



FeAs_4 -tetrahedron

Crystalline electric
field of the tetrahedra
is weak

All 5 Fe d-orbitals are near the Fermi level

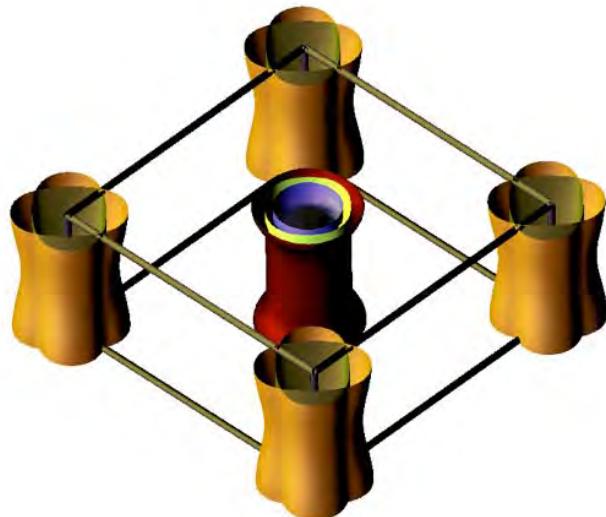
[ОФН РАН-Январь-2014]

Comparison with other materials

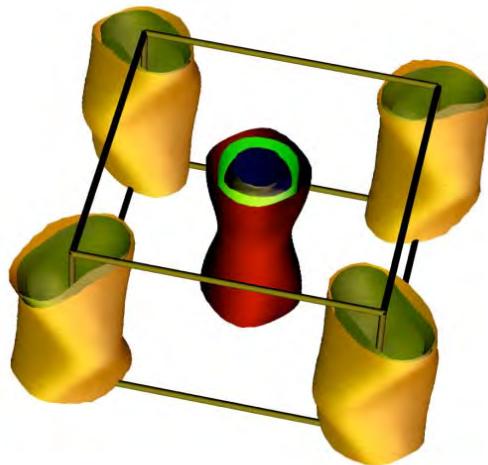
Hole pockets near $(0,0)$

Electron pockets near (π,π)

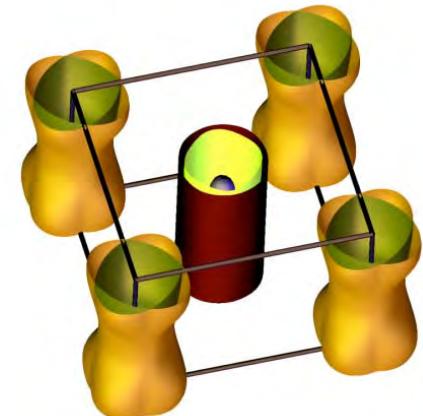
La-1111



Ba-122



FeTe

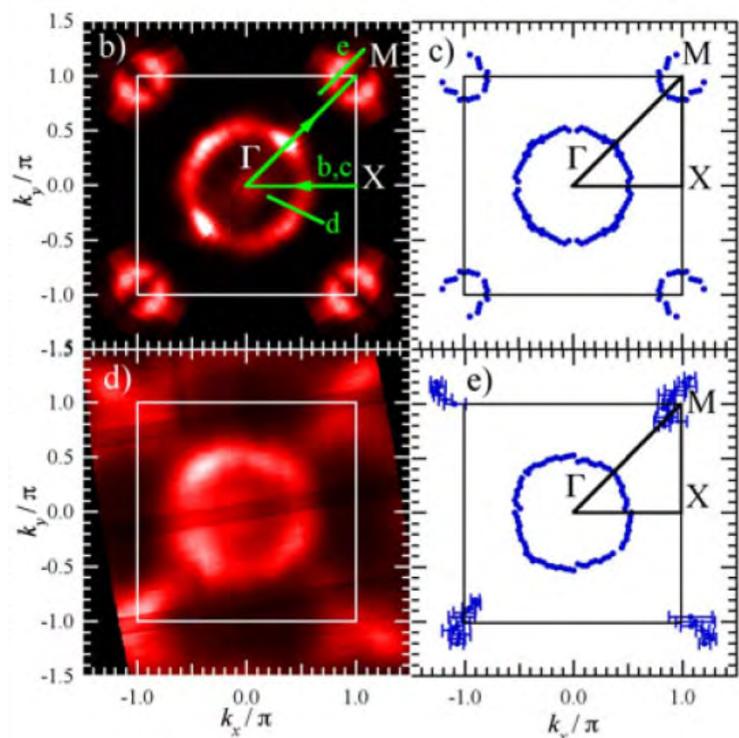


courtesy of I. Mazin

ARPES

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

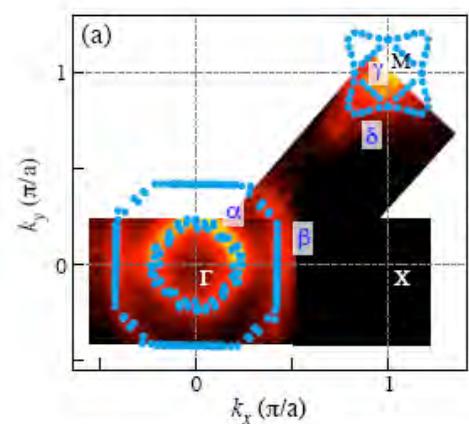
A. Kaminski et al.



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

Ba_{0.6}K_{0.4}Fe₂As₂

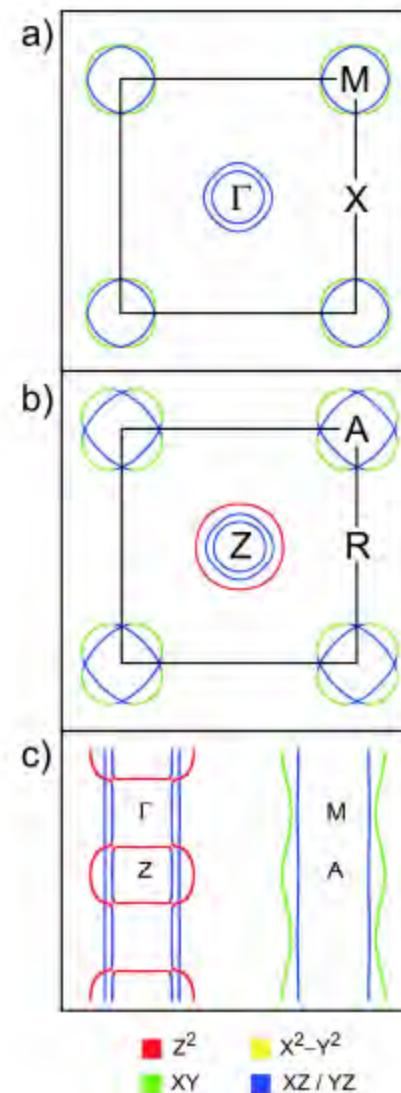
H. Ding et al.



dHVa

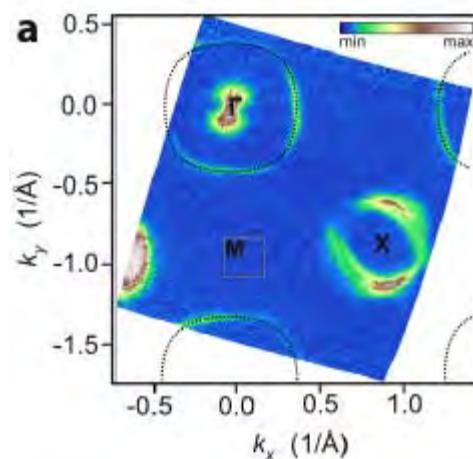
LaFePO

A. Coldea et al,



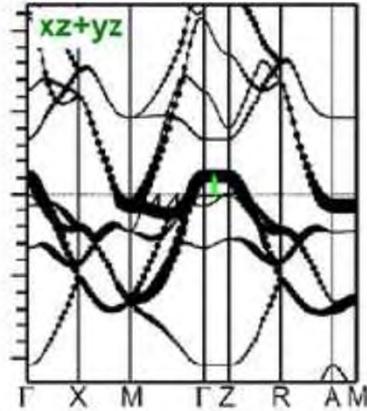
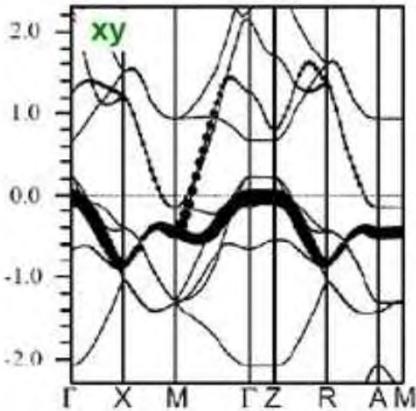
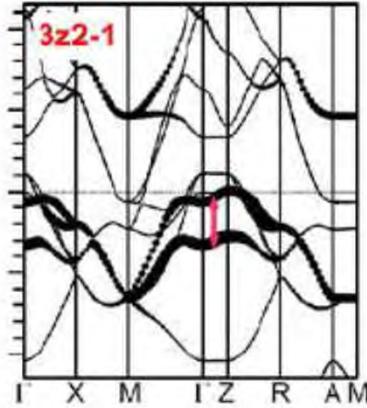
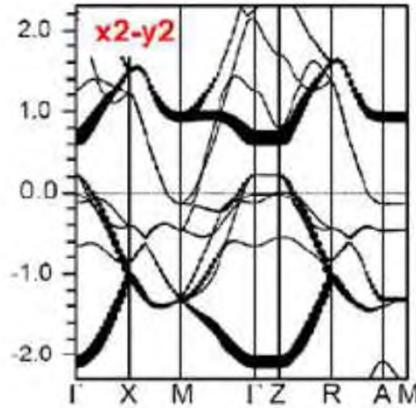
LiFeAs

A. Kordyuk et al



Multiorbital structure

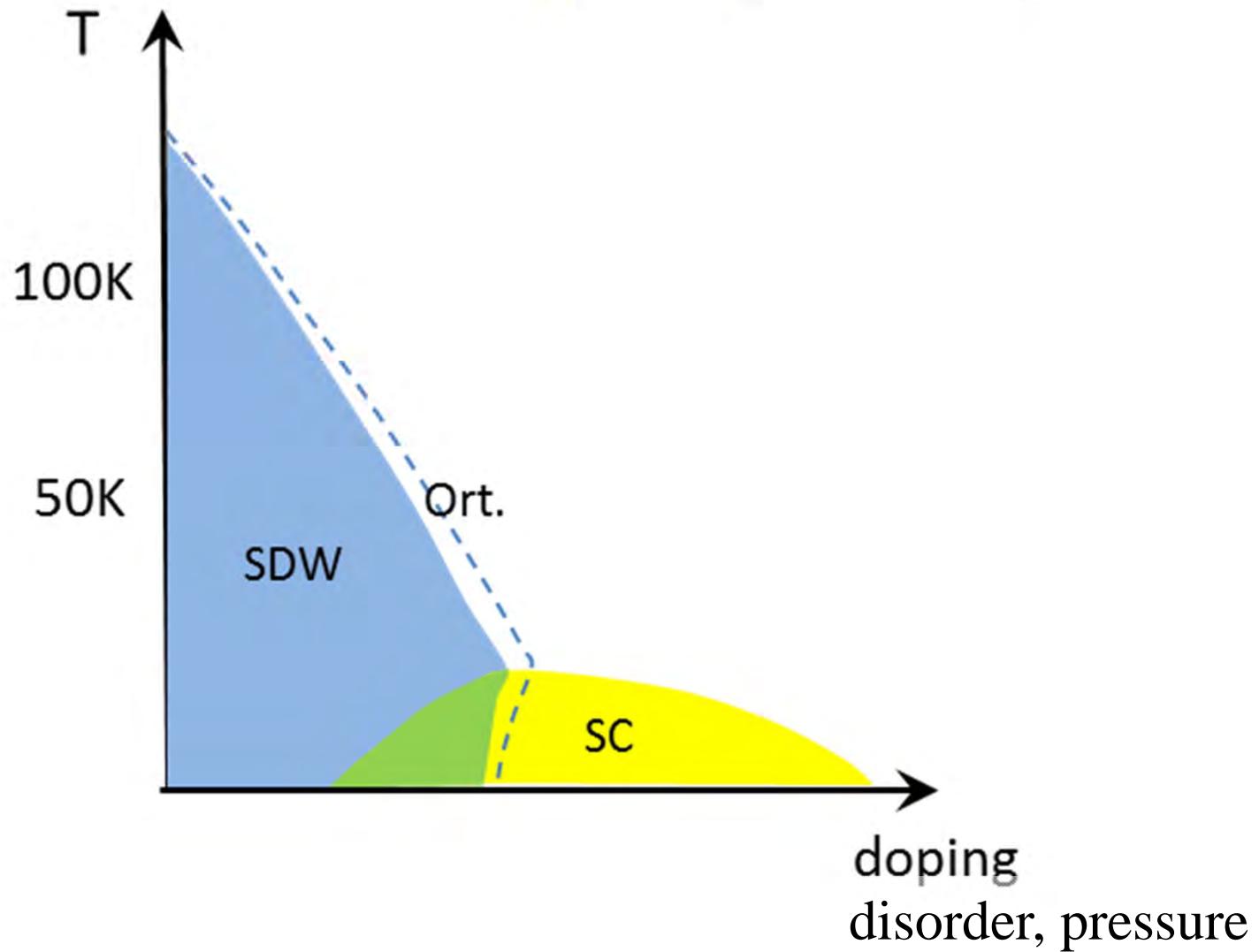
Multiorbital and multiband physics: several d-orbitals close to E_F



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

[ОФН РАН-Январь-2014]

Iron-Pnictides: typical phase diagram

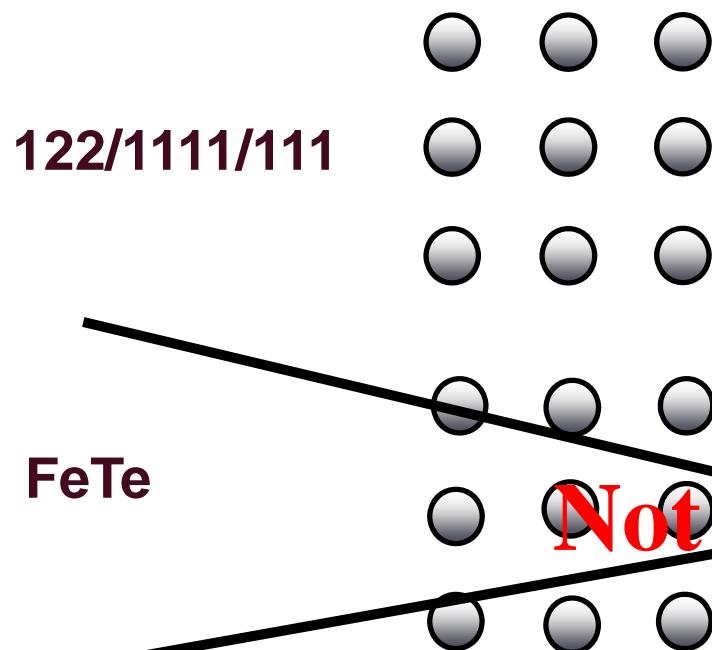


magnetic, structural, and superconducting order

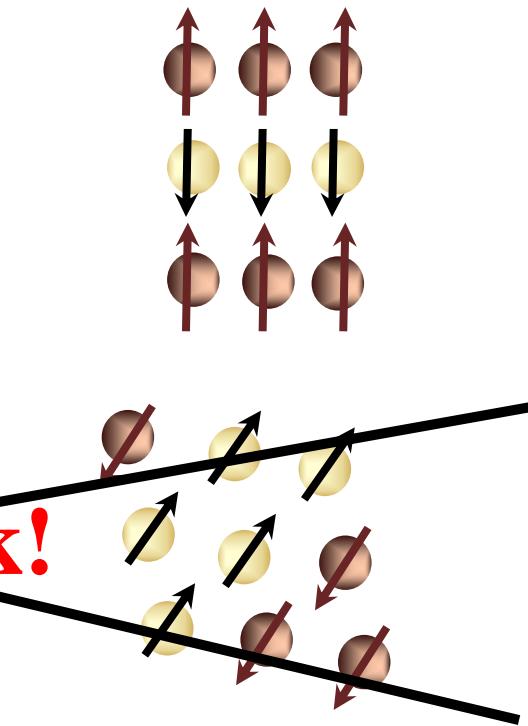
[ОФН РАН-Январь-2014]

Iron pnictides: structural and magnetic transitions

I) Structural Transition



II) Magnetic Transition



FeTe

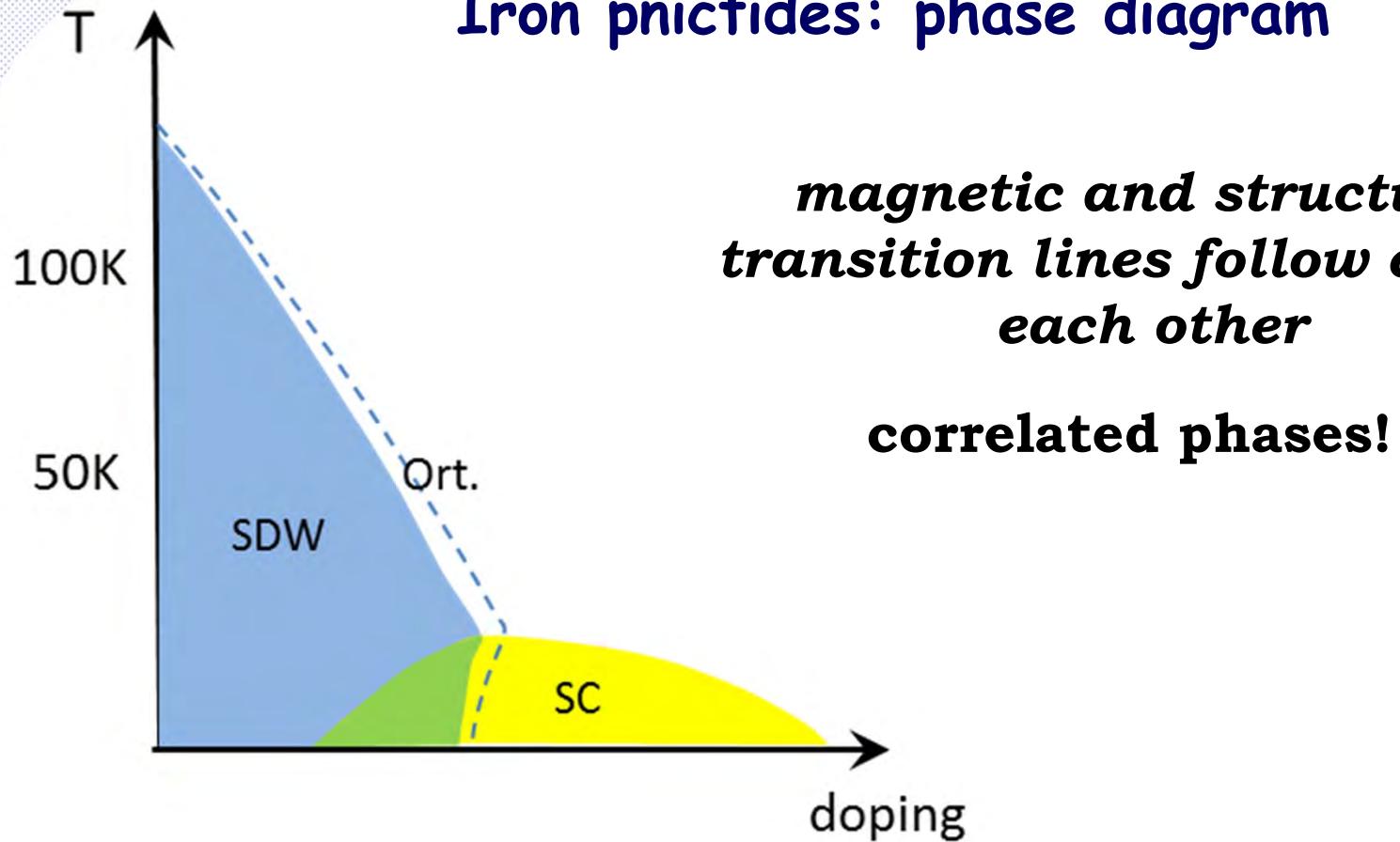
Not in this talk!

DFT calculations reproduce (or even predict) magnetism and structural ground states but requires magnetism as prior condition for distortion
and doped 223

Outline

- **Selection of the magnetic ‘stripe’ order within itinerant picture**
- **Ising nematic degree of freedom**
- **Manifestation of the nematic state: structural and orbital instabilities**

Iron pnictides: phase diagram



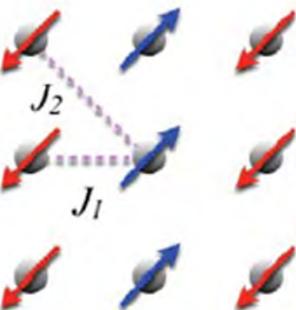
- The systems are metals in the normal state
study magnetism in the system with no local moments 'a-priori'
- rich phase diagram with hidden degeneracy
selection of the magnetic order and resulting interaction with the structural degrees of freedom

[ОФН РАН-Январь-2014]

Magnetism in ferropnictides: strong coupling description

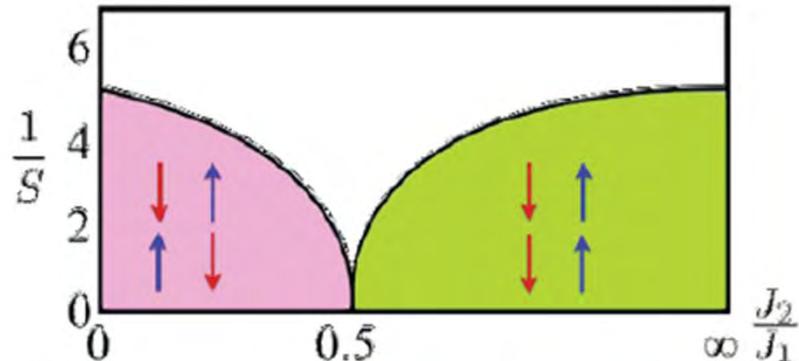
Frustrated J_1 - J_2 model

$$H = \frac{J_1}{2} \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{J_2}{2} \sum_{\ll i,j \gg} \mathbf{S}_i \cdot \mathbf{S}_j$$



Ising nematic $\sigma = \langle \vec{M}_1 \cdot \vec{M}_2 \rangle \neq 0$

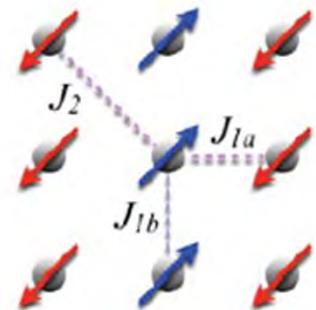
Ch. Henley, PRL 62, 2056 (1989)



Collinear AF order for $J_2 > 0.5 J_1$.

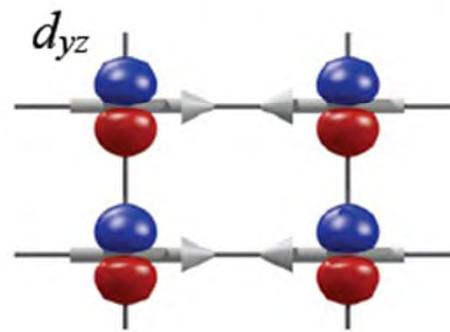
Anisotropic J_{1a} - J_{1b} - J_2 model

$$H = \sum_i J_{1a} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}} + \sum_i J_{1b} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}} + \sum_{\ll i,j \gg} \frac{J_2}{2} \mathbf{S}_i \cdot \mathbf{S}_j$$



$$J_{1a} > 0, J_{1b} < 0.$$

Orbital Order (Polarization)

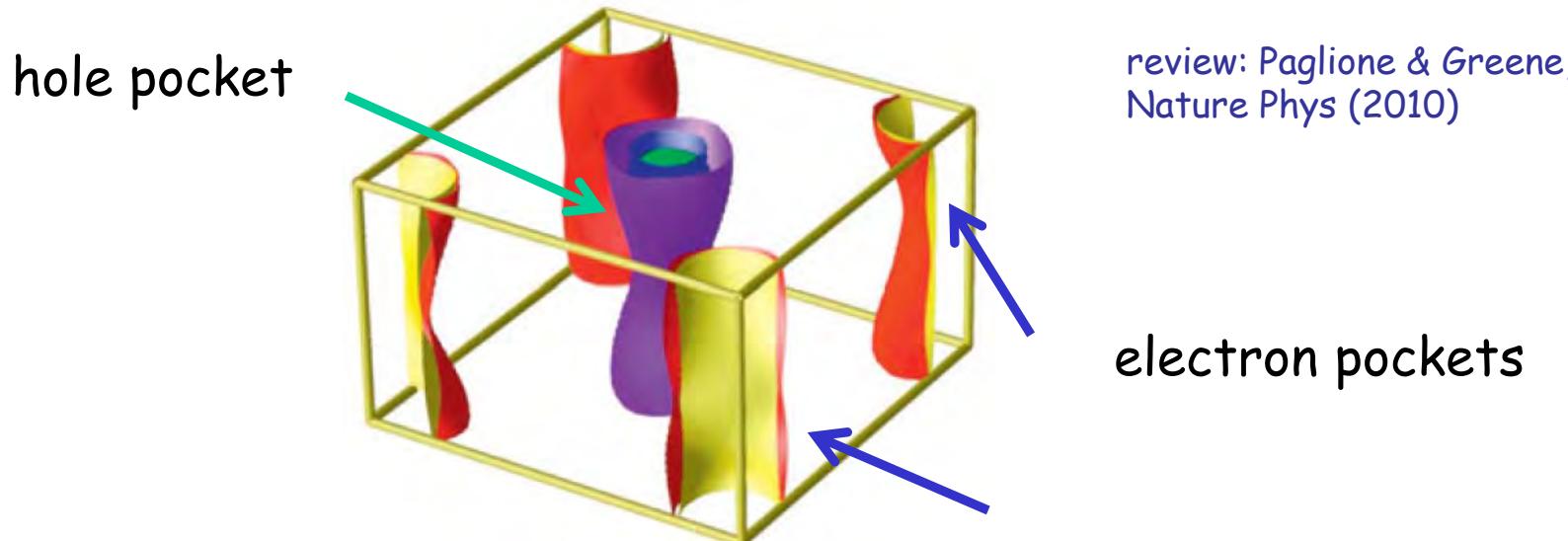


F. Krüger et al., PRB 79 (2009);
W. G. Yin, C. C. Lee, and W. Ku, PRL 105 (2010)

Orbital order breaks C_4 symmetry.

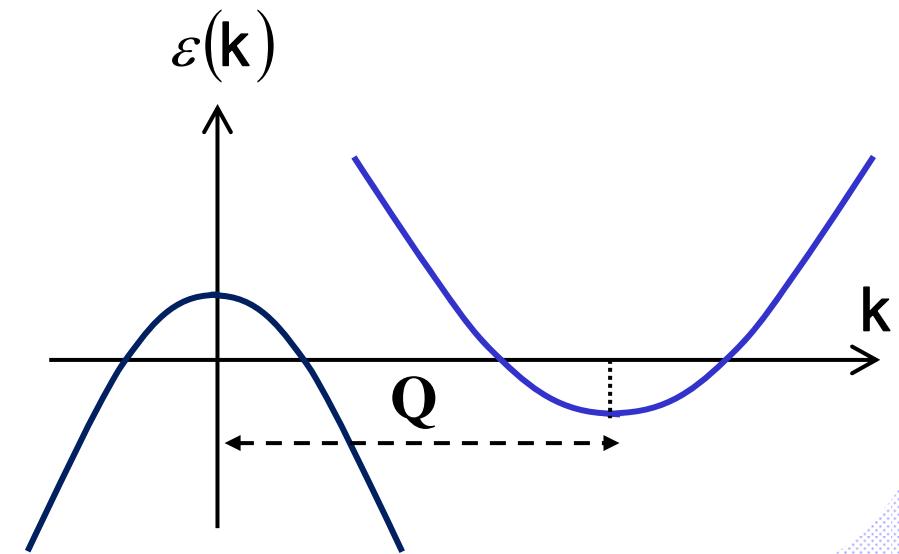
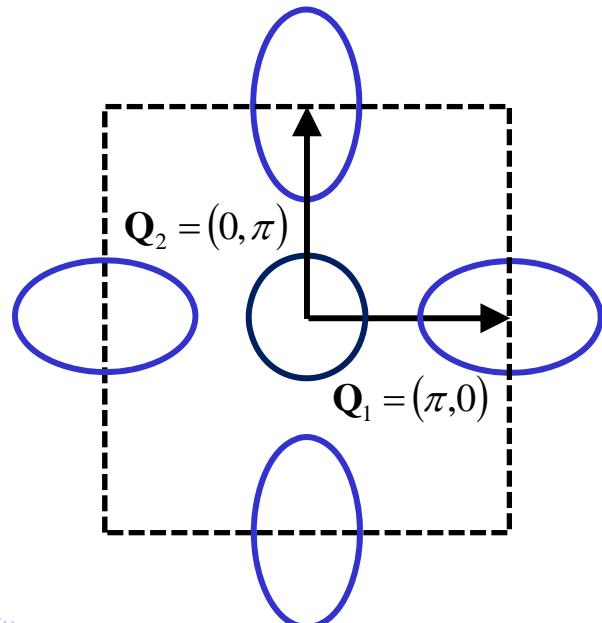
Iron pnictides: band structure

disconnected Fermi surfaces 2Fe ions per unit cell



review: Paglione & Greene,
Nature Phys (2010)

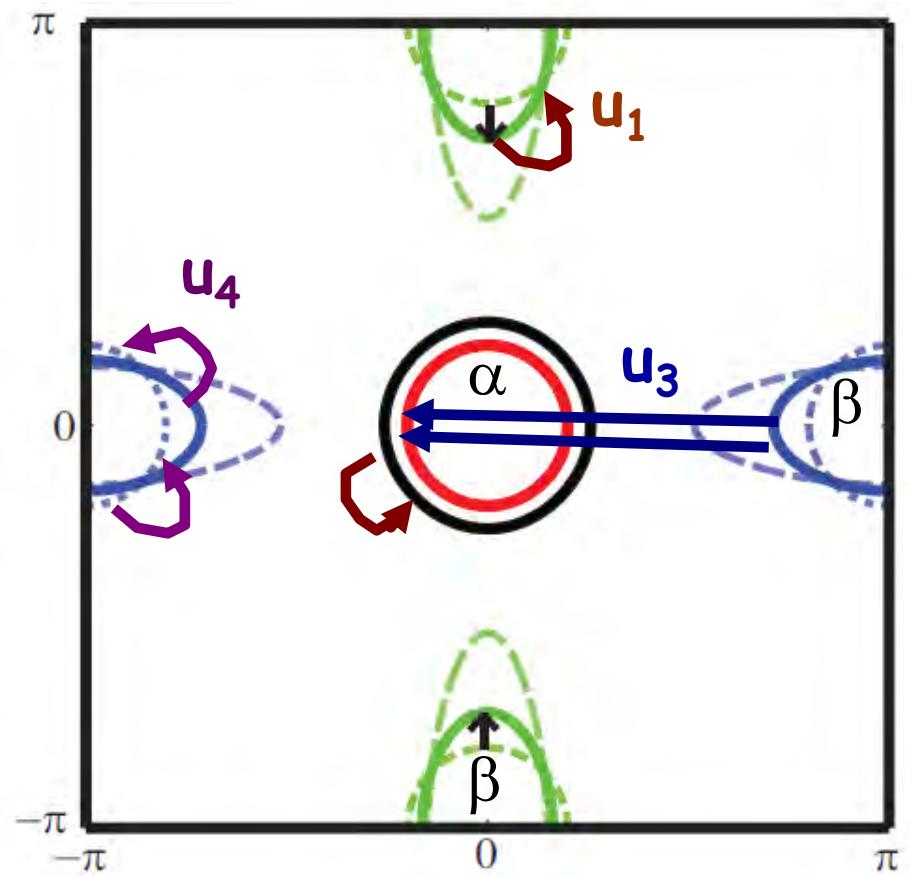
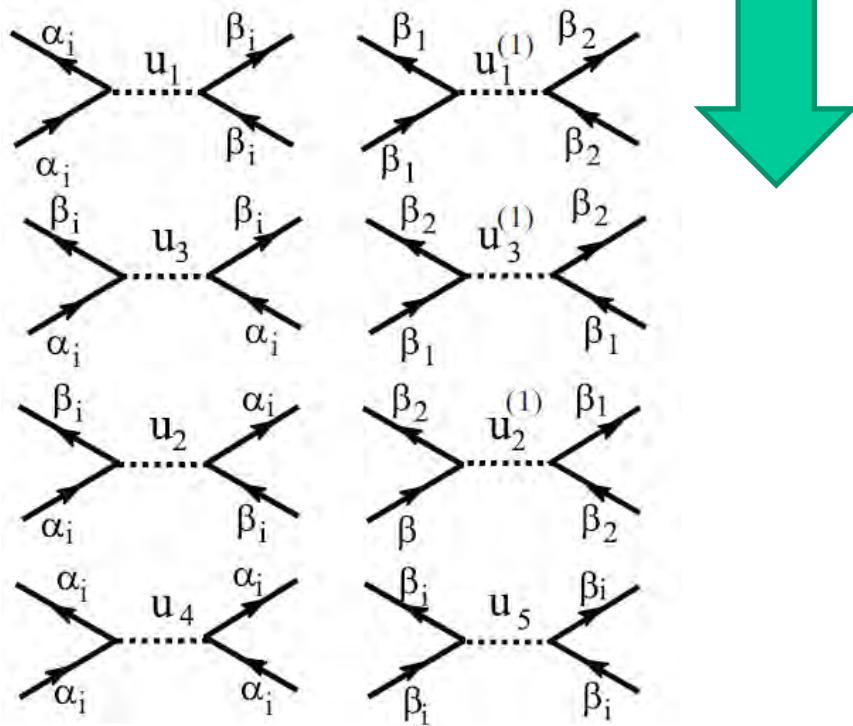
unfolded BZ (1 Fe atom)



The model: from orbital to the band description

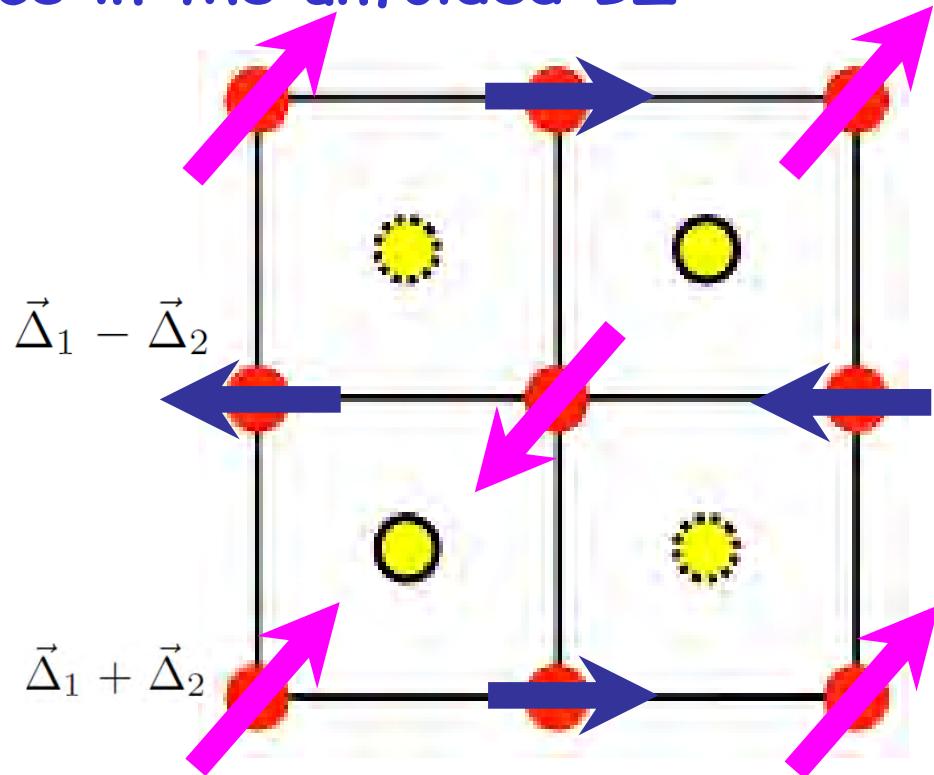
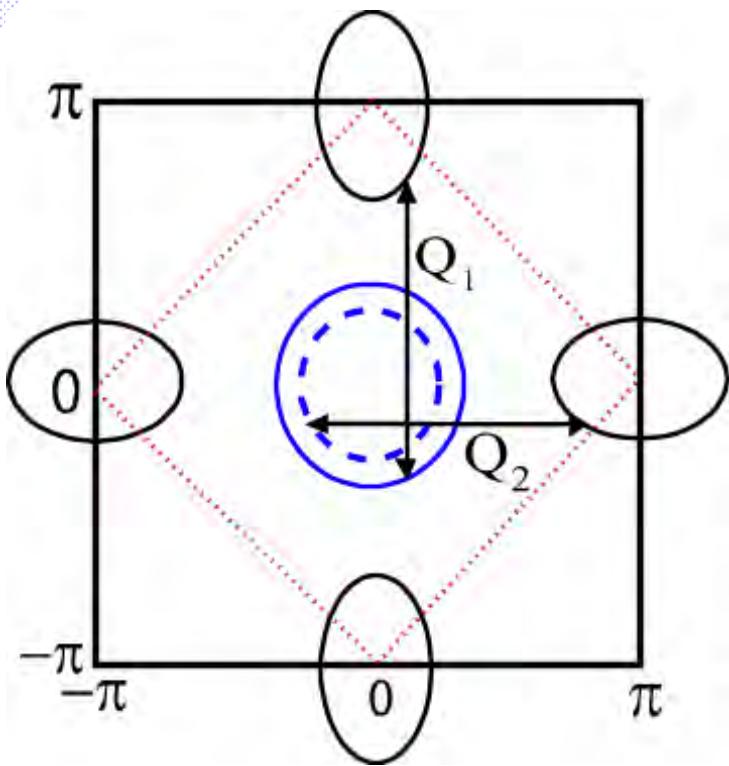
$$H_{int}^{orb} = U \sum_i \sum_{\nu} n_{i\nu\uparrow} n_{i\nu\downarrow} + V \sum_{\nu \neq \mu, \sigma, \sigma'} n_{i\nu\sigma} n_{i\mu\sigma'} - J \sum_{\nu \neq \mu} \mathbf{S}_{i\nu} \cdot \mathbf{S}_{i\mu} + J' \sum_{\nu \neq \mu} d_{i\nu\uparrow}^\dagger d_{i\nu\downarrow}^\dagger d_{i\mu\downarrow}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

S. Graser et al New J. Phys. 11, 025016 (2009)



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

Fermi surface in the unfolded BZ

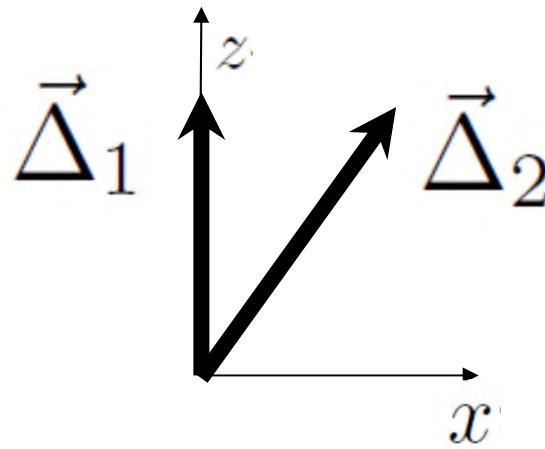
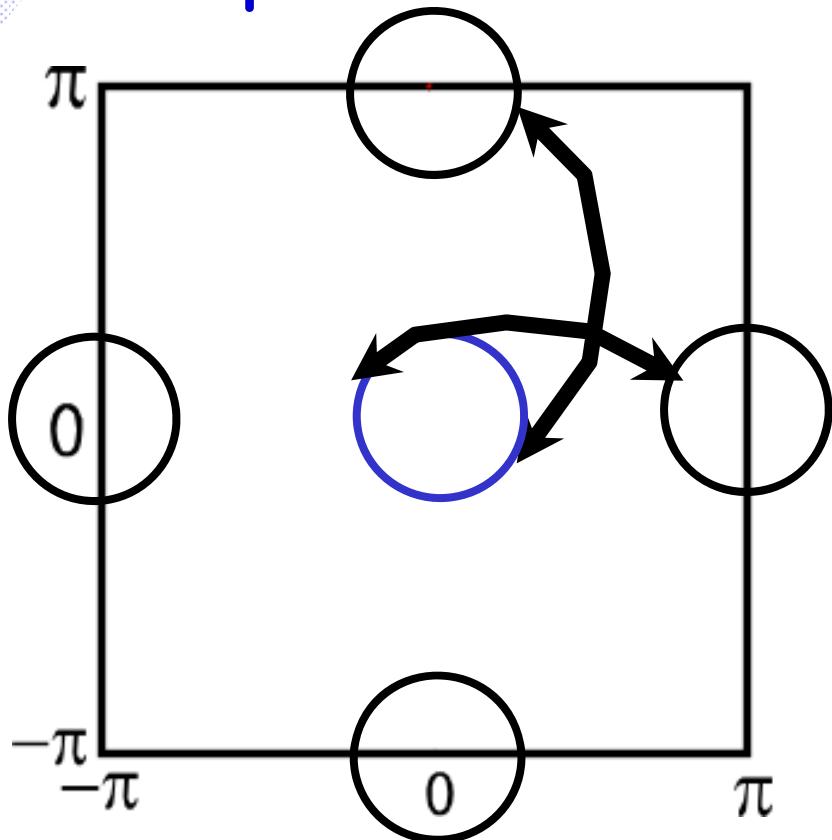


- two nesting wave vectors $\mathbf{Q}_1=(0,\pi)$ and $\mathbf{Q}_2=(\pi,0)$
- two vector SDW order parameters

$$\vec{S}(\mathbf{R}) = \vec{\Delta}_1 e^{i\mathbf{Q}_1 \cdot \mathbf{R}} + \vec{\Delta}_2 e^{i\mathbf{Q}_2 \cdot \mathbf{R}}$$

- two sublattice order parameters $\vec{\Delta}_1 + \vec{\Delta}_2$ $\vec{\Delta}_1 - \vec{\Delta}_2$

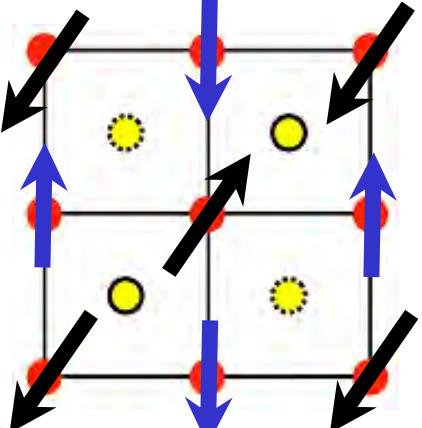
Simplest model to solve: hole and electron pockets



$$1 = \frac{(U_1 + U_3)}{2N} \sum_{\mathbf{p}} \frac{1}{\sqrt{(\varepsilon_{\mathbf{p}}^-)^2 + \Delta^2}}$$

$$\Delta^2 = \vec{\Delta}_1^2 + \vec{\Delta}_2^2$$

- sets the value of the total order parameter but does not specify $\vec{\Delta}_1$ or $\vec{\Delta}_2$

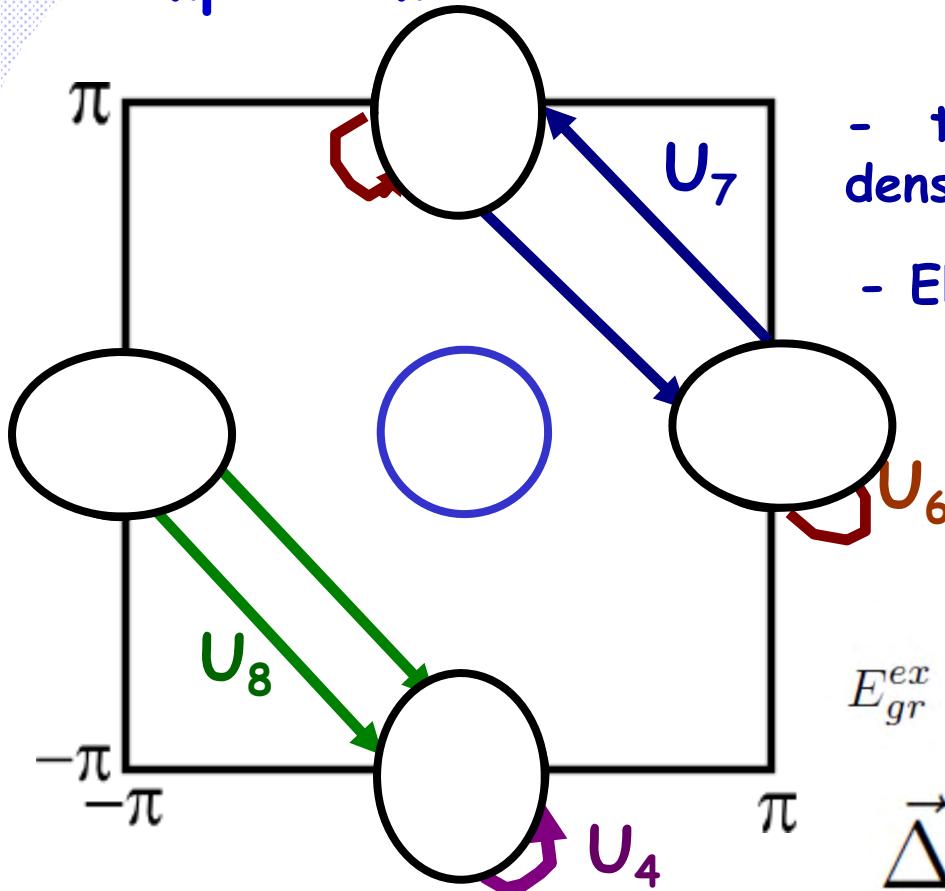


- the ground state degeneracy is even larger than in the J₁-J₂ model of localized spins

O(6) degeneracy [5 Goldstone modes]

(0, π) or (π, 0) are two of many possibilities

Simplest model to solve: 1 hole and 2 electron pockets



- to add the interaction (density-density) between electron pockets
- Electron pockets are elliptic, ε

$$\text{Positive} \propto (m_x - m_y)^2$$

$$E_{gr}^{ellipt} = C |\vec{\Delta}_1|^2 |\vec{\Delta}_2|^2$$

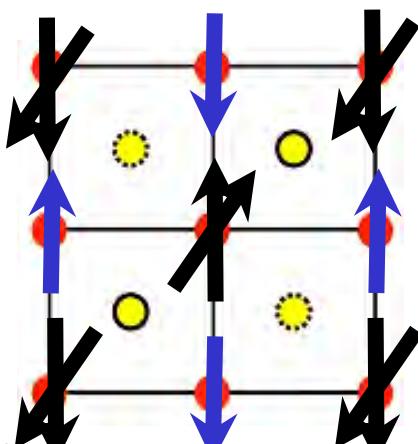
$$E_{gr}^{ex} = 2A^2 [(U_6 + U_8 - U_7 - U_4)] \frac{|\vec{\Delta}_1|^2 |\vec{\Delta}_2|^2}{\Delta^4} < 0$$

$$\vec{\Delta}_1 = 0 \quad \text{or} \quad \vec{\Delta}_2 = 0$$

I. Eremin and A.V. Chubukov, PRB 81, 024511 (2010)

(0, π) or (π , 0) is selected !

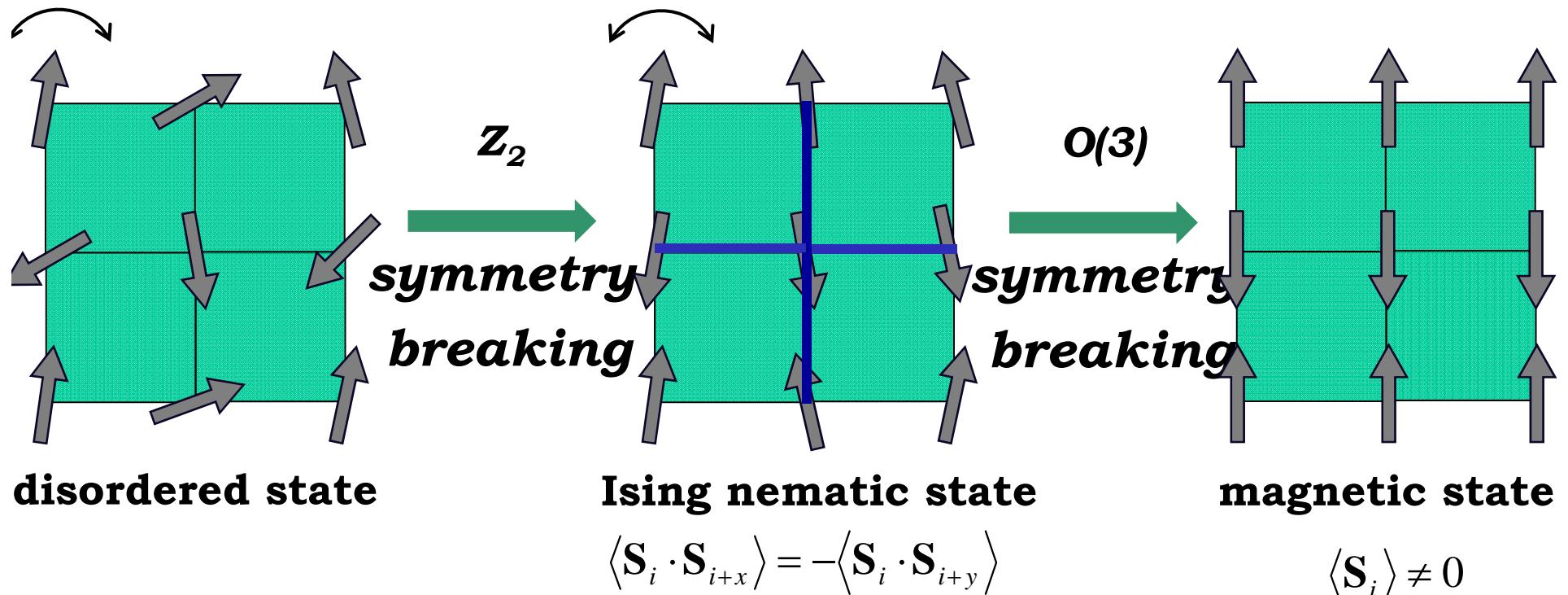
- no need for quantum fluctuations in itinerant picture
- charge fluctuations are crucial



Ising nematic order and magnetism

- A state that breaks Z_2 symmetry but remains paramagnetic

spontaneous tetragonal symmetry breaking



Electronic nematic phase

- ⇒ the point-group symmetry from C_4 (tetragonal) to C_2 (orthorhombic),
- ⇒ is equivalent to the orthorhombic phase
- ⇒ "nematic" is used to emphasize that the phase transition is of purely electronic origin

How to treat the Ising nematic order in the itinerant picture

$$\Delta_{\text{SDW}} \sum_k c_{\mathbf{k},\alpha}^\dagger \sigma_{\alpha\beta}^z f_{\mathbf{k}+\mathbf{Q},\beta}$$

- Ising variable: $\sigma = \langle \vec{M}_1 \cdot \vec{M}_2 \rangle \neq 0$

[R. Fernandes et al., PRL 105 (2010)]

Ising nematic transition

$$\sigma = \langle \vec{M}_1 \cdot \vec{M}_2 \rangle = \langle \vec{\Delta}_1^2 - \vec{\Delta}_2^2 \rangle = \langle \vec{\Delta}_X^2 - \vec{\Delta}_Y^2 \rangle$$

General procedure: introduce two bosonic fields

$$\Delta_{(X,Y)} \propto \sum_{\mathbf{k}} c_{\Gamma,\mathbf{k}\alpha}^\dagger \sigma_{\alpha\beta} c_{(X,Y),\mathbf{k}\beta}$$

Partition function as an integral over Grassmann variables

$$Z \propto \int dc_{i,\mathbf{k}} dc_{i,\mathbf{k}}^\dagger e^{-\beta \mathcal{H}}$$

[ОФН РАН-Январь-2014]

How to treat the Ising nematic order in the itinerant picture

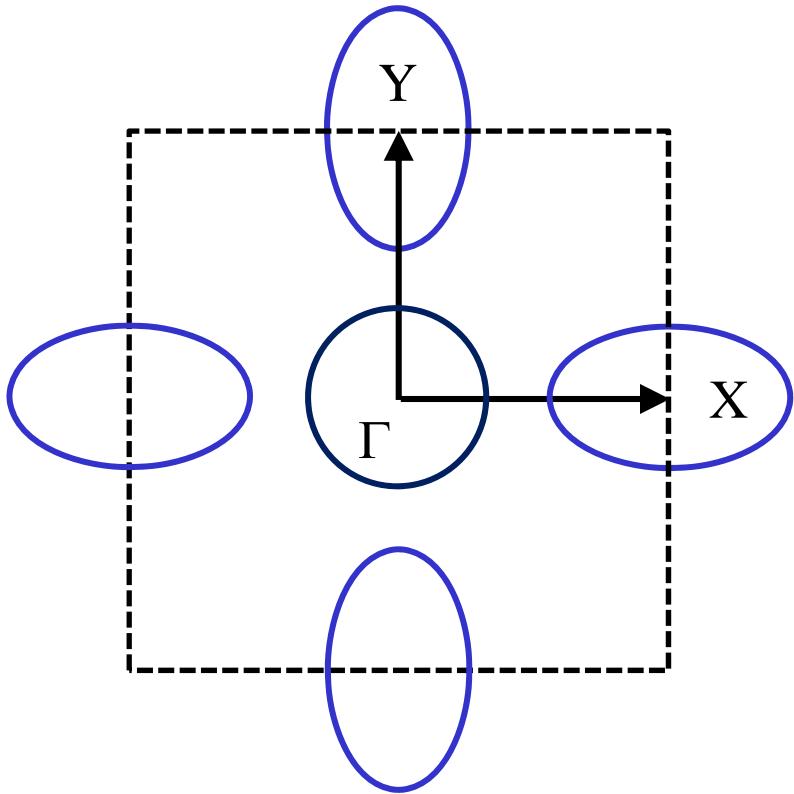
decouple the quartic term in fermionic operators using the Hubbard-Stratonovich transformation

$$Z \propto \int d\Delta_X d\Delta_Y e^{-S_{\text{eff}}[\Delta_X, \Delta_Y]}$$

Expand S_{eff} in powers of Δ_X and Δ_Y and obtain the Ginzburg-Landau type of action

$$\begin{aligned} S_{\text{eff}} [\Delta_X, \Delta_Y] = & r_0 (\Delta_X^2 + \Delta_Y^2) + \frac{u}{2} (\Delta_X^2 + \Delta_Y^2)^2 \\ & - \frac{g}{2} (\Delta_X^2 - \Delta_Y^2)^2 + v (\Delta_X \cdot \Delta_Y)^2 \end{aligned}$$

Itinerant approach to the nematic state



$$G_{i,k}^{-1} = i\omega_n - \varepsilon_{\mathbf{k}}$$

$$\left. \begin{aligned} r_0 &= \frac{2}{u_{\text{spin}}} + 2 \int_k G_{\Gamma,k} G_{X,k} \\ u &= \frac{1}{2} \int_k G_{\Gamma,k}^2 (G_{X,k} + G_{Y,k})^2 \\ g &= -\frac{1}{2} \int_k G_{\Gamma,k}^2 (G_{X,k} - G_{Y,k})^2 > 0 \end{aligned} \right\}$$

Finite ellipticity

**Away from
perfect nesting:**

$$F_{\text{mag}} = \frac{r_0}{2} (\Delta_1^2 + \Delta_2^2) + \frac{u}{4} (\Delta_1^2 + \Delta_2^2)^2 - \frac{g}{4} (\Delta_1^2 - \Delta_2^2)^2$$

Itinerant approach to the nematic state

To consider the possibility of a nematic state,
we need to include fluctuations

$$F_{\text{mag}} = \chi_{\text{mag}}^{-1}(\mathbf{q}) (\Delta_1^2 + \Delta_2^2) + \frac{u}{4} (\Delta_1^2 + \Delta_2^2)^2 - \frac{g}{4} (\Delta_1^2 - \Delta_2^2)^2$$
$$\underbrace{\psi \propto \Delta_1^2 + \Delta_2^2}_{\text{nematic order parameter}}$$
$$\underbrace{\varphi \propto \Delta_1^2 - \Delta_2^2}_{\text{nematic order parameter}}$$

Itinerant approach to the nematic state

$$\frac{\partial F}{\partial \varphi} = 0$$

Equation of state for the nematic order parameter:

$$\varphi^3 = \varphi \left[g \int \chi_{\text{mag}}^2(\mathbf{q}) - 1 \right]$$

$\varphi \neq 0$ solution already in the paramagnetic phase,
when the magnetic susceptibility is large enough

$$\langle \Delta_1^2 \rangle \neq \langle \Delta_2^2 \rangle$$

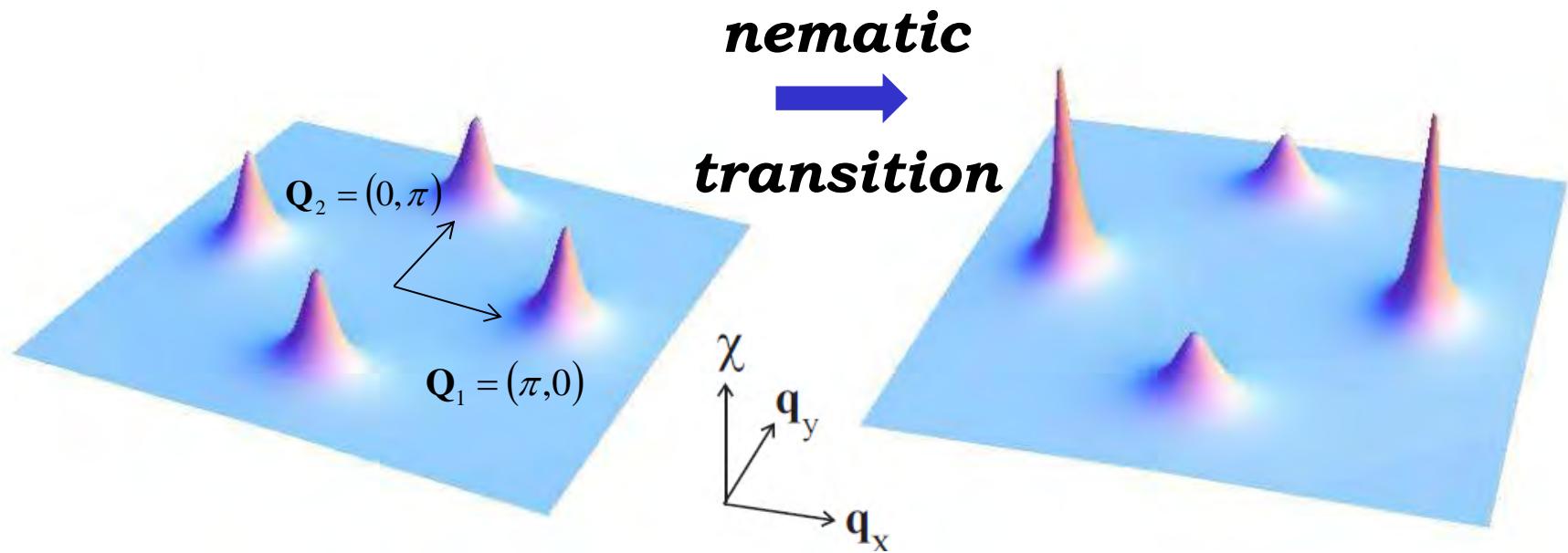
magnetic
fluctuations



nematic order

Itinerant approach to the nematic state

- Magnetic fluctuations become stronger around one of the ordering vectors in the paramagnetic phase



$$\chi_X(q=0) = \frac{1}{r-\phi}, \quad \chi_Y(q=0) = \frac{1}{r+\phi}$$

**x and y directions become inequivalent:
tetragonal symmetry breaking**

Fernandes, Chubukov, Eremin, Knolle, Schmalian, PRB (2012)

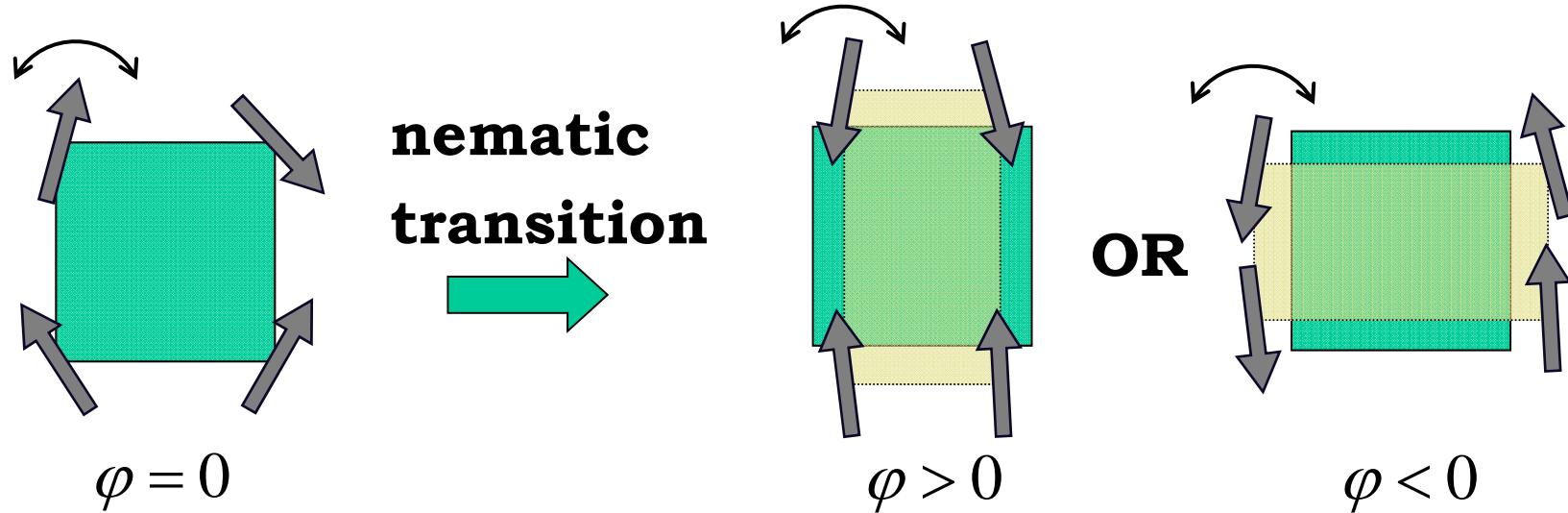
[ОФН РАН-Январь-2014]

Ising nematic transition triggers structural transition

magneto-elastic coupling: $H_{\text{mag-el}} = \lambda \sum_{\mathbf{k}} \delta(c_{X,\mathbf{k}\alpha}^+ c_{X,\mathbf{k}\alpha} - c_{Y,\mathbf{k}\alpha}^+ c_{Y,\mathbf{k}\alpha})$

$$\delta = \frac{a-b}{a+b}$$

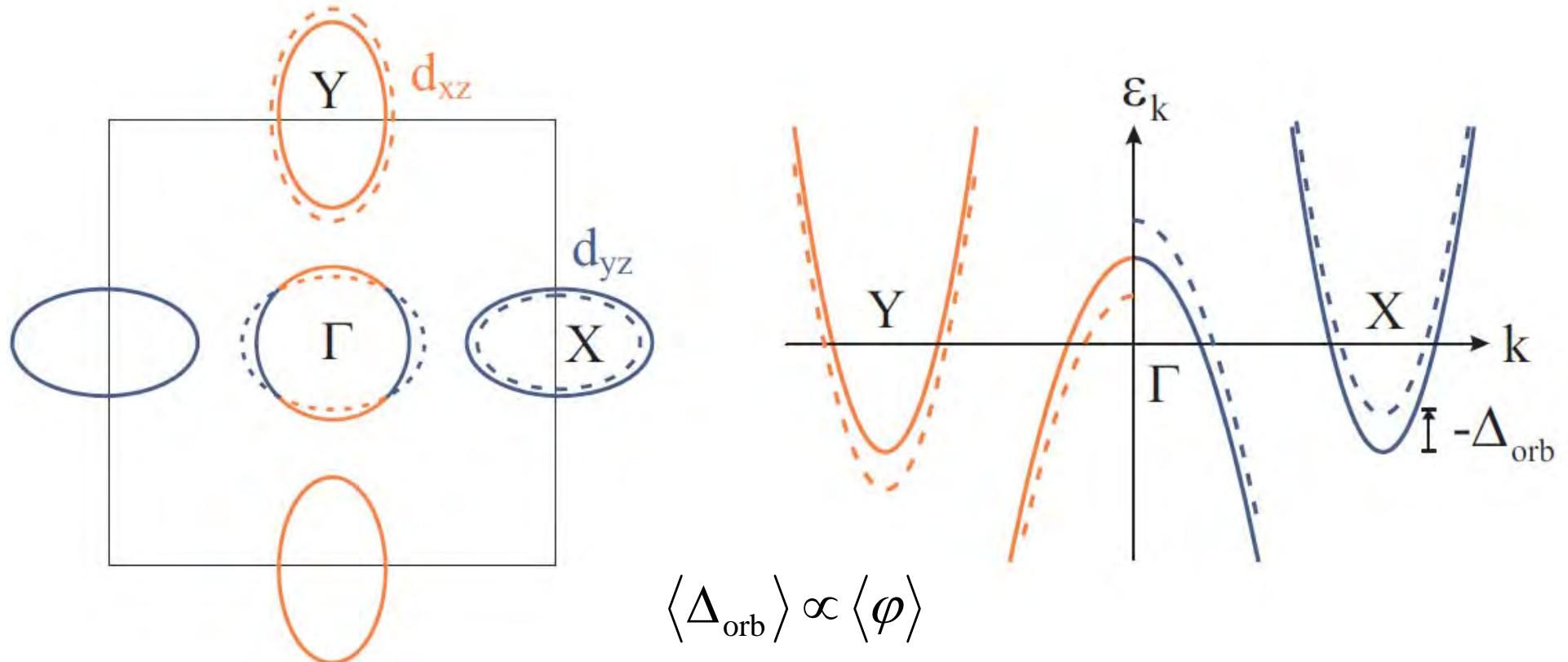
$$\Rightarrow \langle \delta \rangle \propto \langle \varphi \rangle$$



Structural transition driven by magnetic fluctuations

Ising nematic transition triggers orbital order

- Distinct orbital content of different Fermi pockets leads to **orbital order** (Fe configuration: $3d^6$)



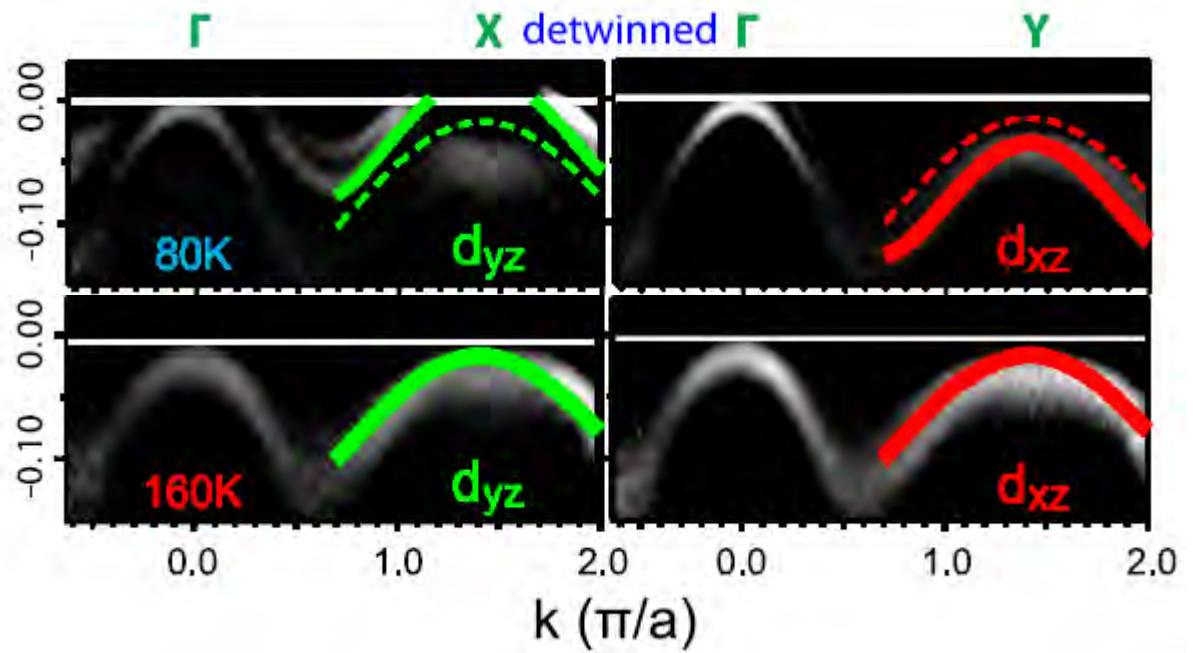
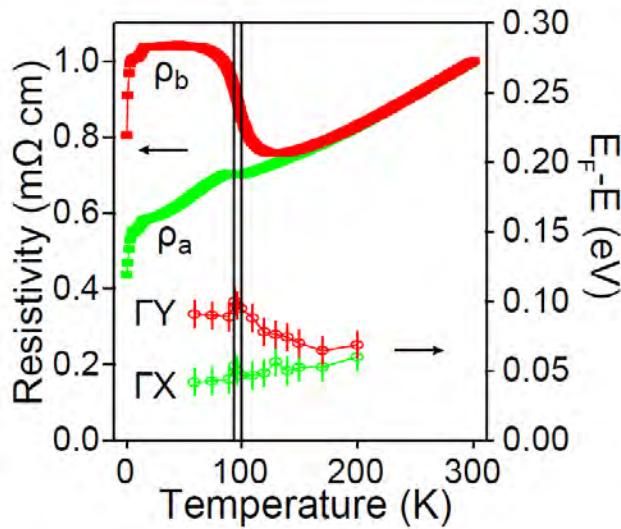
Fernandes, Chubukov, Eremin, Knolle, Schmalian, PRB (2012)

See also: M. Daghofer, A. Nicholson, and A. Moreo, Phys. Rev. B 85, 184515 (2012)

[ОФН РАН-Январь-2014]

Ising nematic transition triggers orbital order

- explains the experimentally observed sign of the orbital splitting in BaFe_2As_2

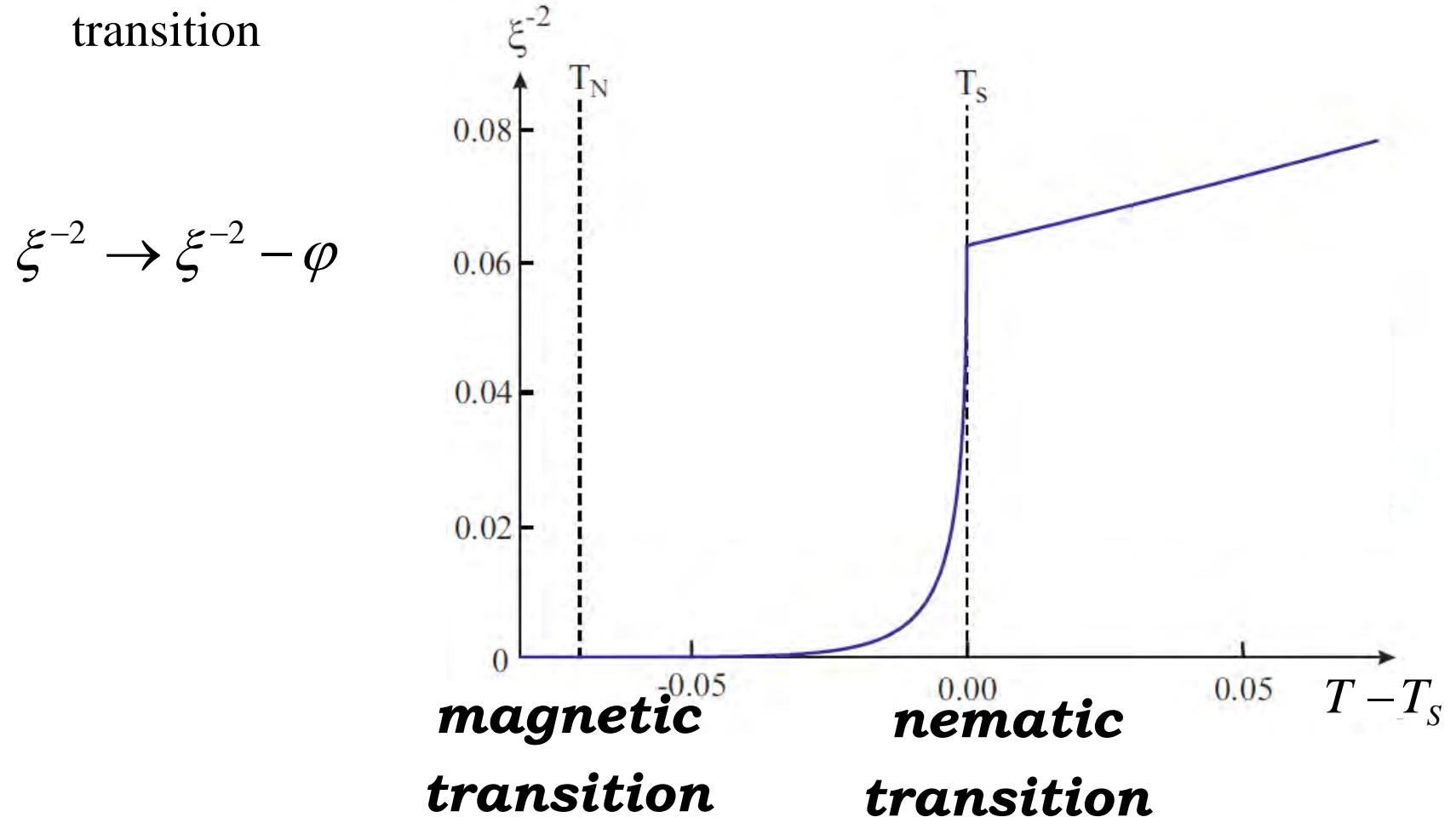


Yi et al, PNAS (2011)

[ОФН РАН-Январь-2014]

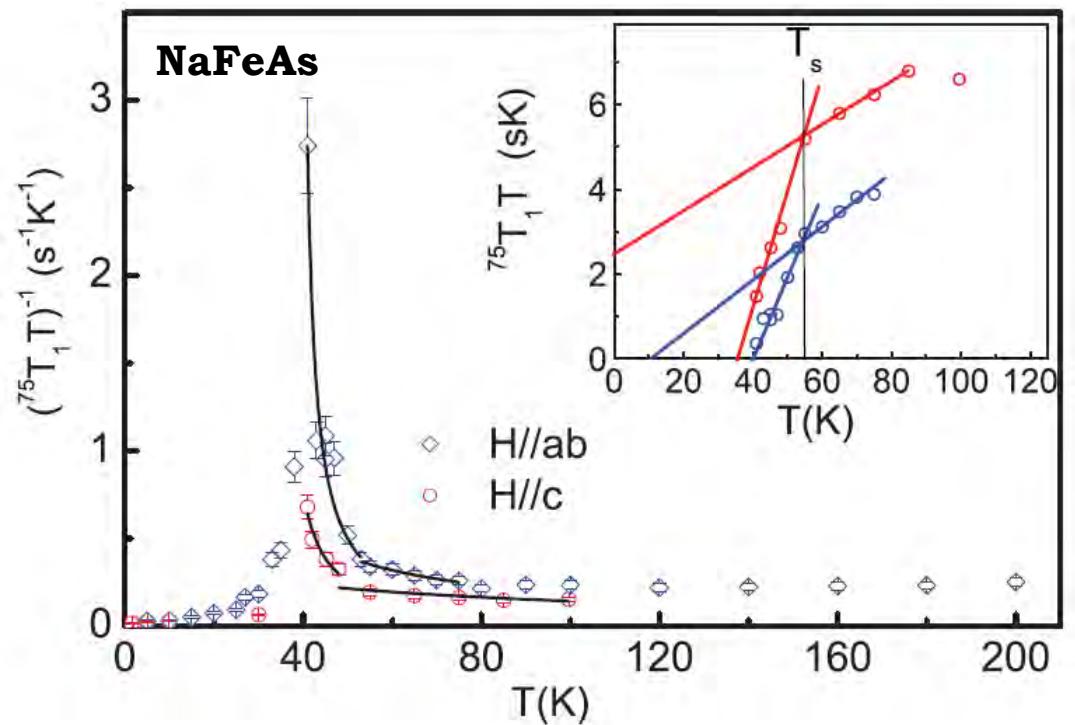
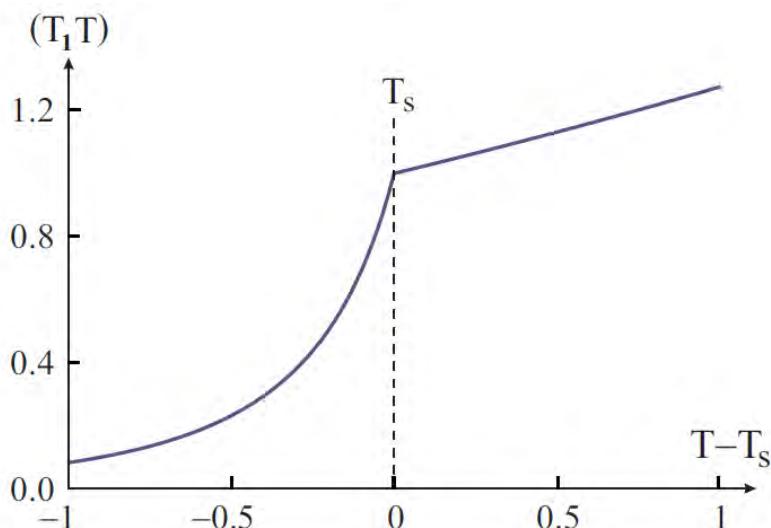
Nematic order enhances magnetic fluctuations

- Strong increase of the magnetic correlation length at the nematic transition



Nematic order enhances magnetic fluctuations

- NMR reveals the enhancement of magnetic fluctuations at the nematic transition



Fernandes, Chubukov, Eremin, Knolle, Schmalian, PRB (2012)

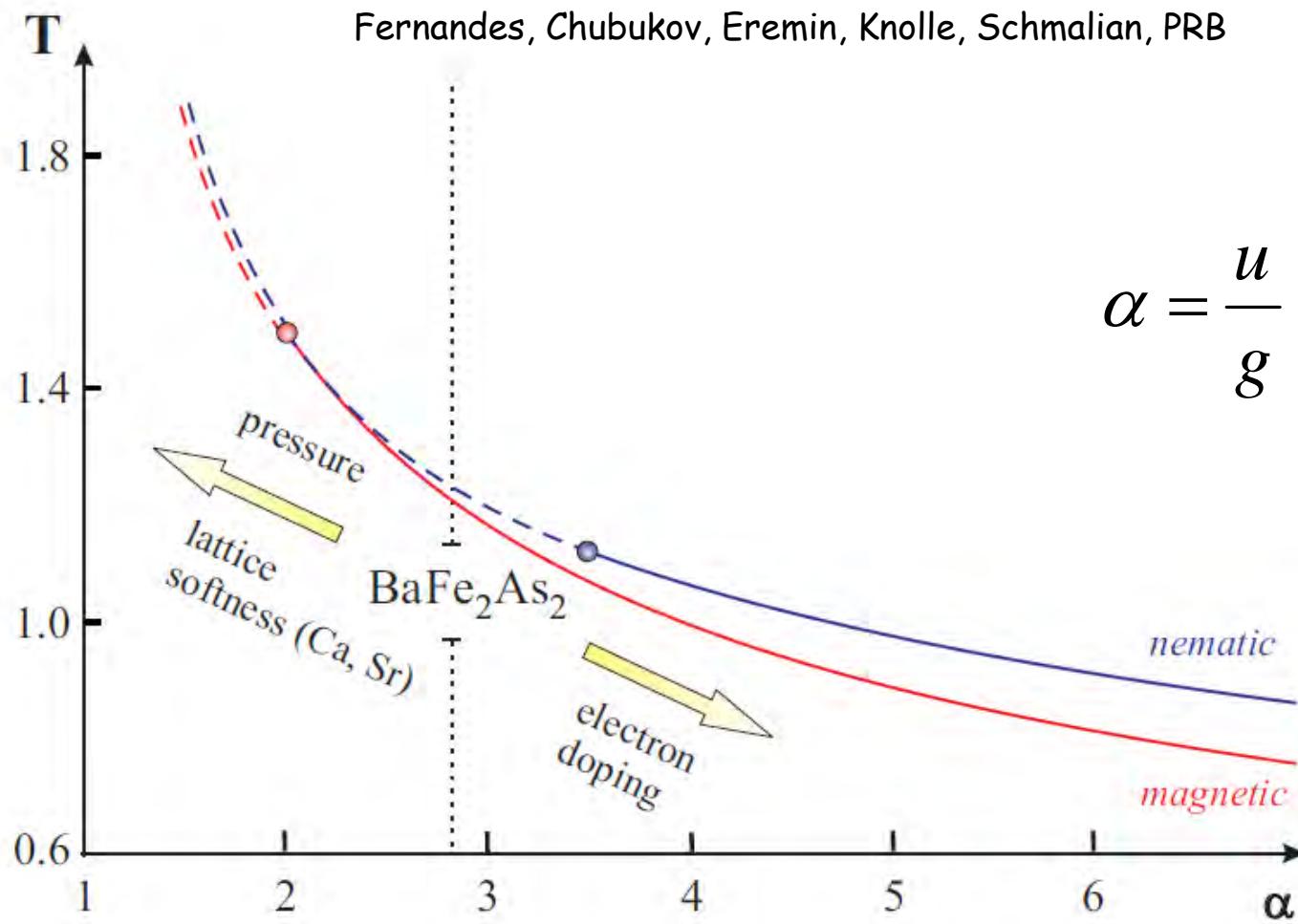
Ma et al, PRB
(2011)

Phase diagrams for the magnetic and structural transitions



transitions naturally follow each other

Magnetic and Ising 'nematic' transition temperatures



- Ising nematic order introduces orbital polarization
- magnetic correlation length jumps to a larger value at the nematic transition

[ОФН РАН-Январь-2014]

Two-component order parameter: combination $(\pi, 0)$ and $(0, \pi)$

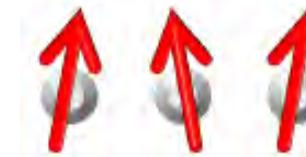
$$E_{gr} = C |\vec{\Delta}_X|^2 |\vec{\Delta}_Y|^2$$



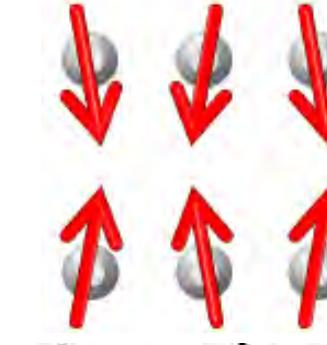
$$\vec{\Delta}_X = 0, \vec{\Delta}_Y \neq 0$$



$$|\vec{\Delta}_X| = |\vec{\Delta}_Y| \neq 0$$



or



$$|\vec{\Delta}_X| \ll |\vec{\Delta}_Y| \neq 0$$

- Ginzburg-Landau description: transition to the two-component phase if C becomes negative

G. Giovanetti, et al Nature Commun. 2, 298 (2011); I. Eremin and A.V. Chubukov, PRB 81, 024511 (2010); P.M.R. Brydon, J. Schmiedt, and C. Timm, PRB 84, 214510 (2011)

- non-linear effects inside SAF phase => phase transition at $T_{N2} < T_{N1}$

Magnetic mean-field phase diagram

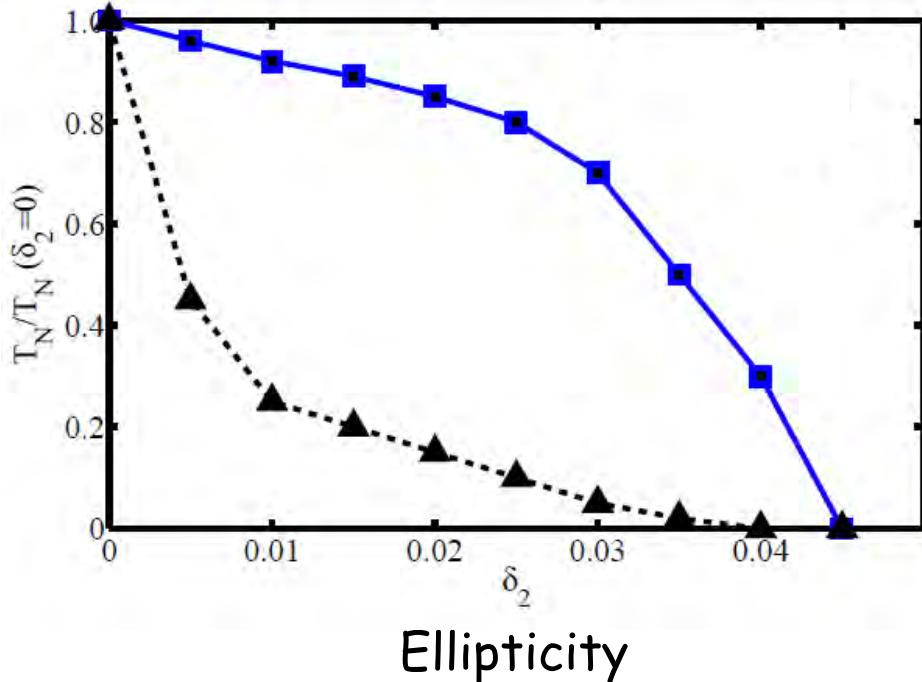
$$S_{\text{eff}} [\Delta_X, \Delta_Y] = -\text{Tr} \ln (1 - \mathcal{G}_{0,k} \mathcal{V}) + \frac{2}{u_{\text{spin}}} \int_x (\Delta_X^2 + \Delta_Y^2)$$

saddle-point equations

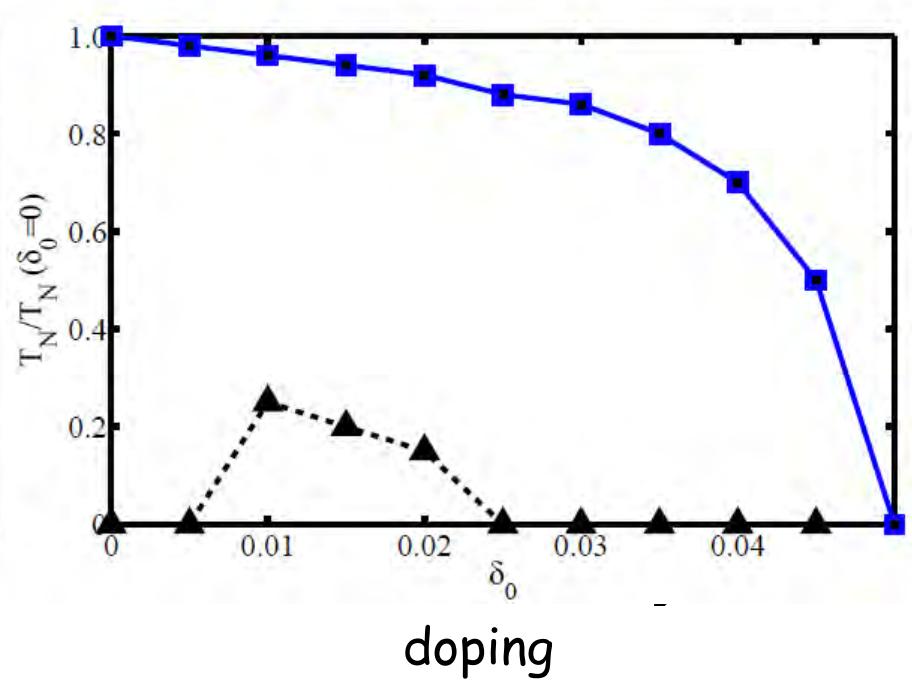
$$\frac{\delta S}{\delta \Delta_i} = 0$$

free energy analysis

Slight hole doping, 1%

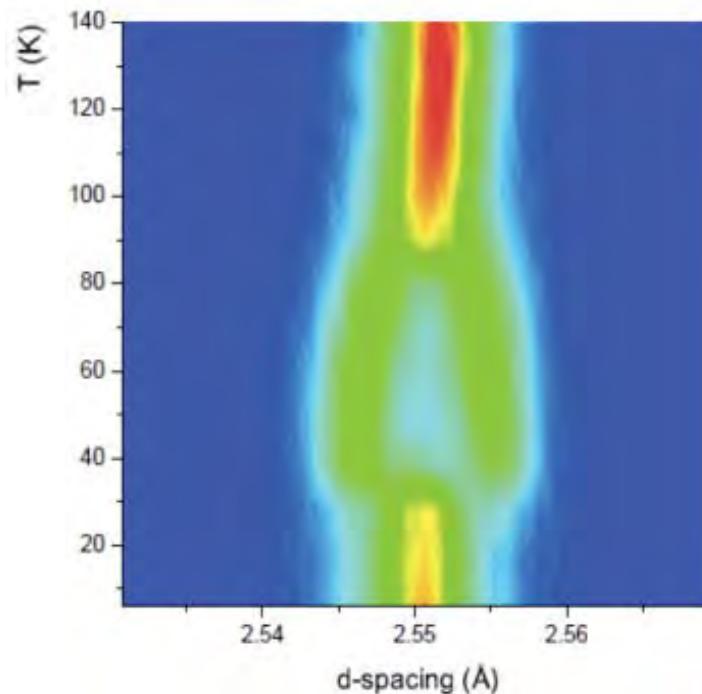
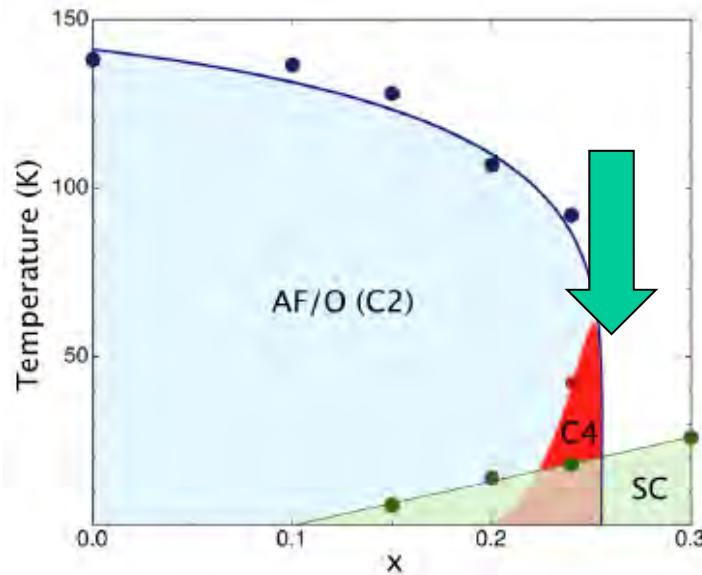


Finite ellipticity



Magnetic mean-field phase diagram: experimental situation

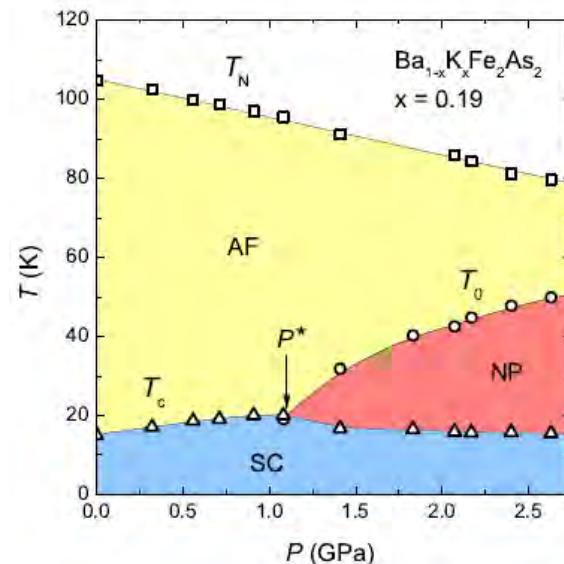
1) $\text{Ba}_{1-x}\text{Na}_x\text{Fe}_2\text{As}_2 \Rightarrow$ Neutron and X-ray diffraction



S. Avci et al., arXiv:1303.2647

2) $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ under pressure:
Resistivity measurements \Rightarrow new phase

E. Hassinger et al., PRB 86, 140502 (2012)



Iron-based superconductors: Magnetism:

- shows rich phase diagram with hidden magnetic frustration (selection of the magnetic order, preemptive Ising nematic instability)
- contains beside striped AF order also C_4 symmetric phase with two-component order parameter
- particular aspects of the itinerant physics are important and decisive for comparison with experiment

I. Eremin, and A. V. Chubukov, PRB 81, 024511 (2010)

J. Knolle, I. Eremin, A.V. Chubukov, and R. Moessner, PRB 81, 140506(R) (2010)

J. Knolle, I. Eremin, and R. Moessner, PRB 83, 224503 (2011)

R. M. Fernandes, A. V. Chubukov, J. Knolle, I. Eremin, and J. Schmalian, Phys. Rev. B 85, 024534 (2012)