UNIVERSITY OF MINNESOTA

Competing orders in quantum materials

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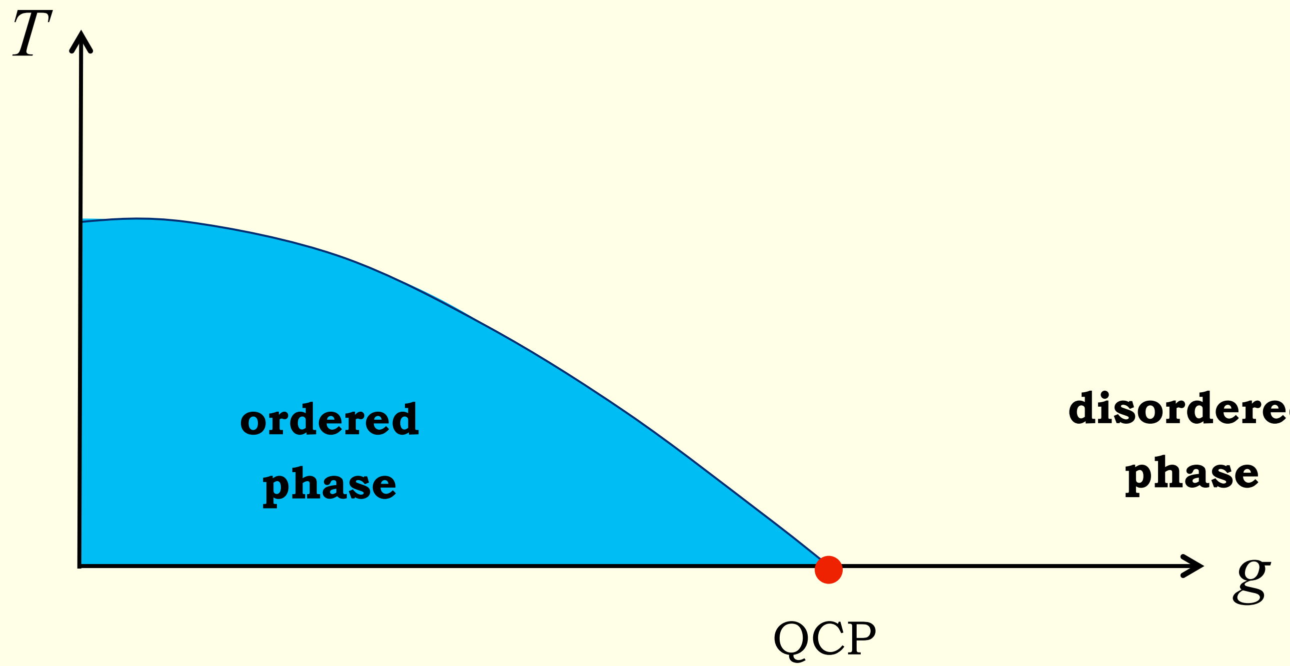
CIFAR Summer School

May, 2013

Quantum phase transitions and critical fluctuations

- Tuning of a continuous phase transition down to T=0



Quantum phase transitions and critical fluctuations

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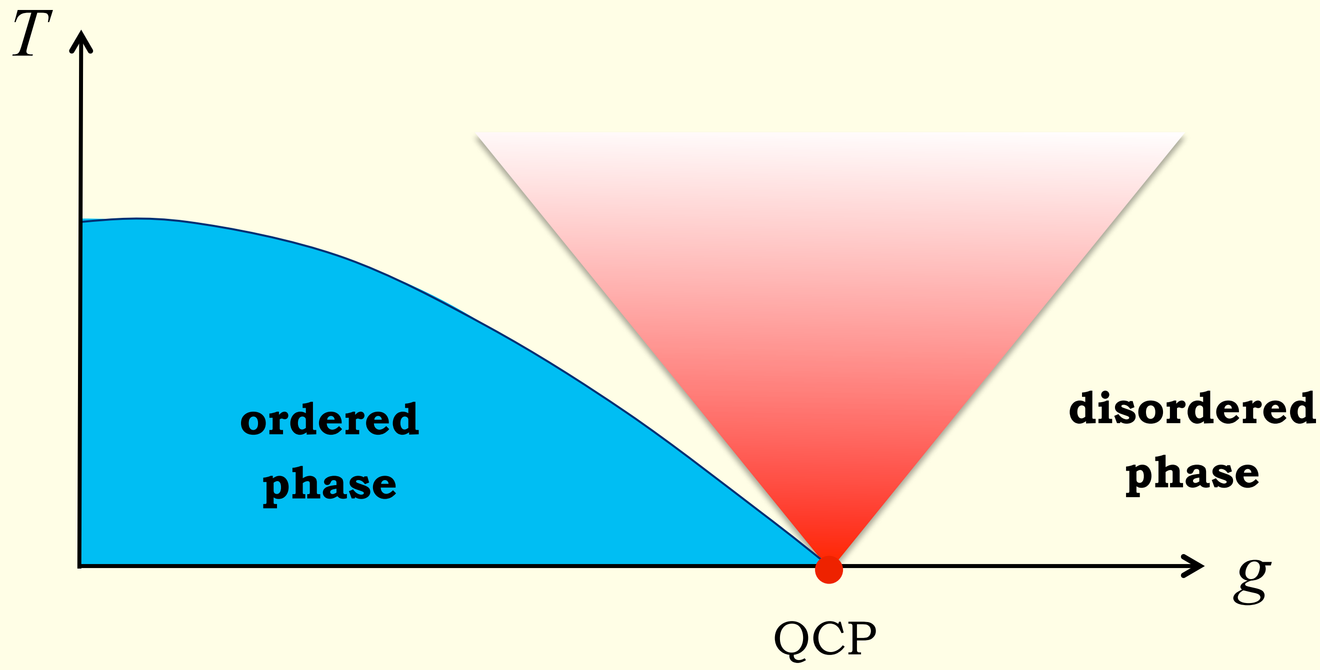

critical fluctuations around the quantum critical point

Quantum phase transitions and critical fluctuations

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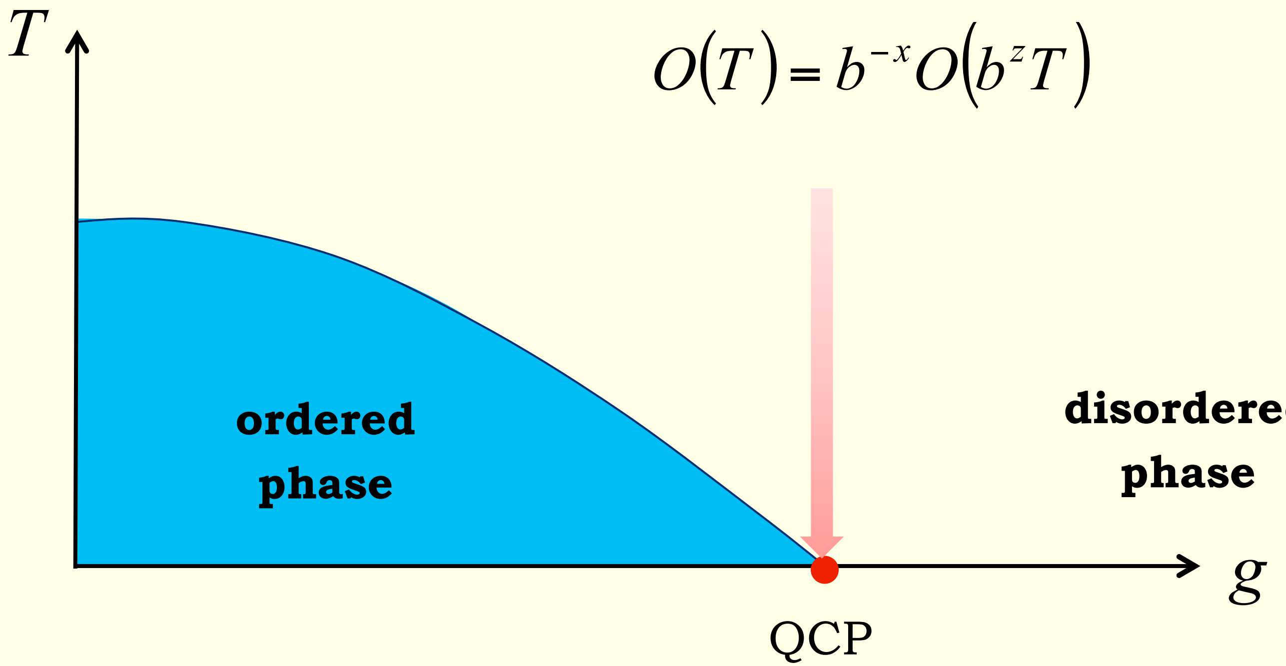
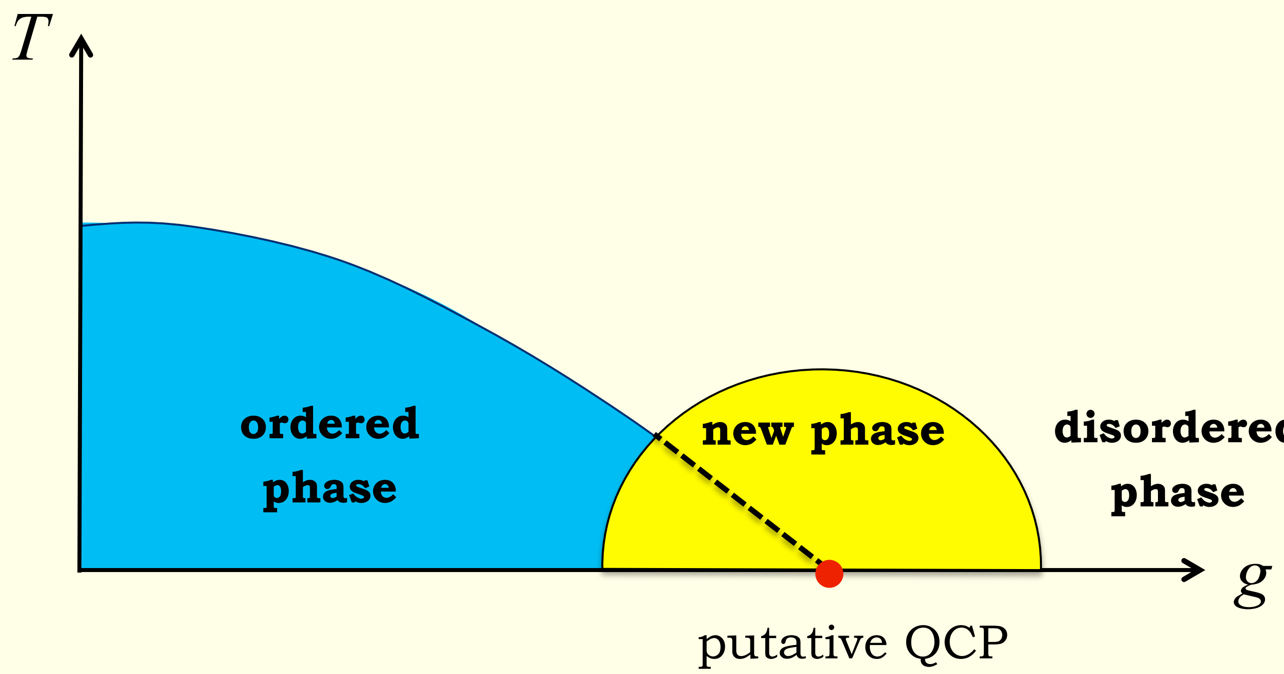


scale invariance: critical exponents

Quantum phase transitions in metals

- Unusual behavior near the onset of putative QCPs: non-Fermi liquid behavior, **unconventional SC**,…



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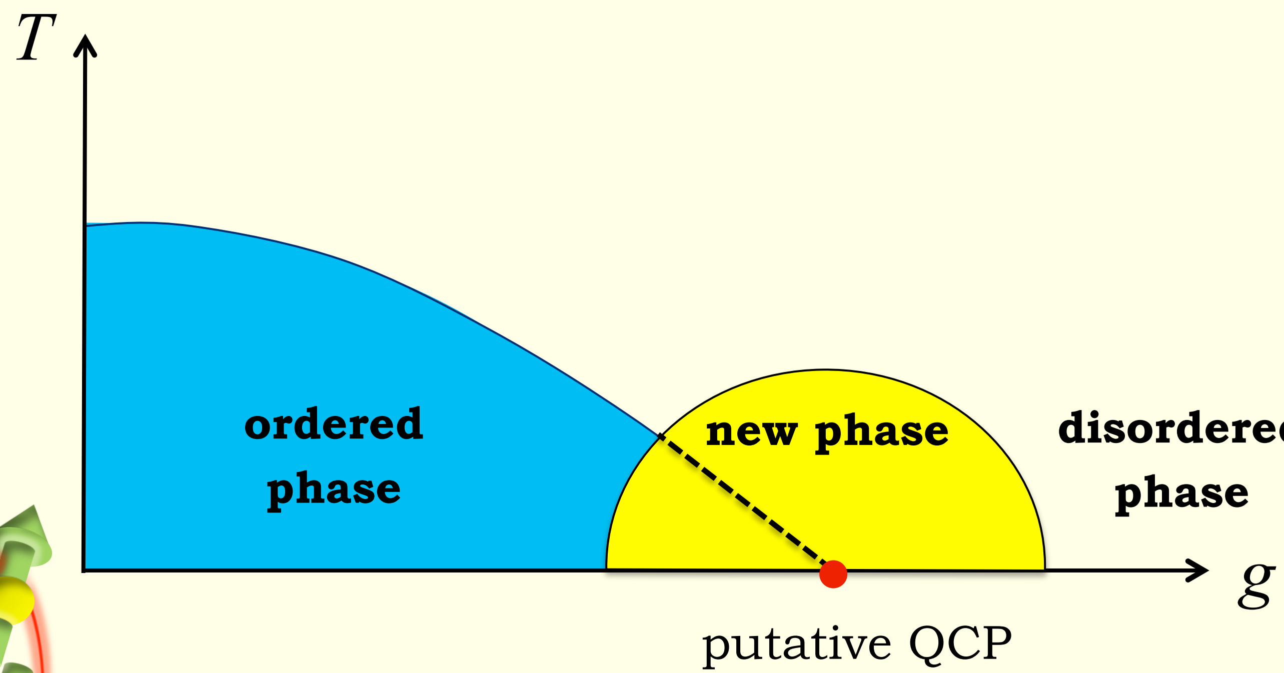
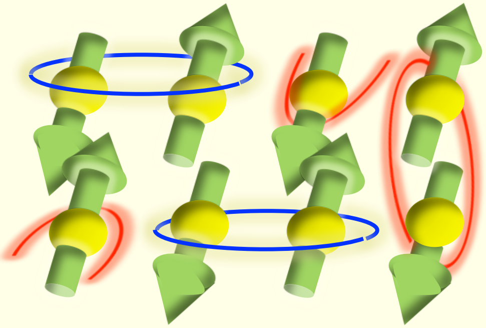


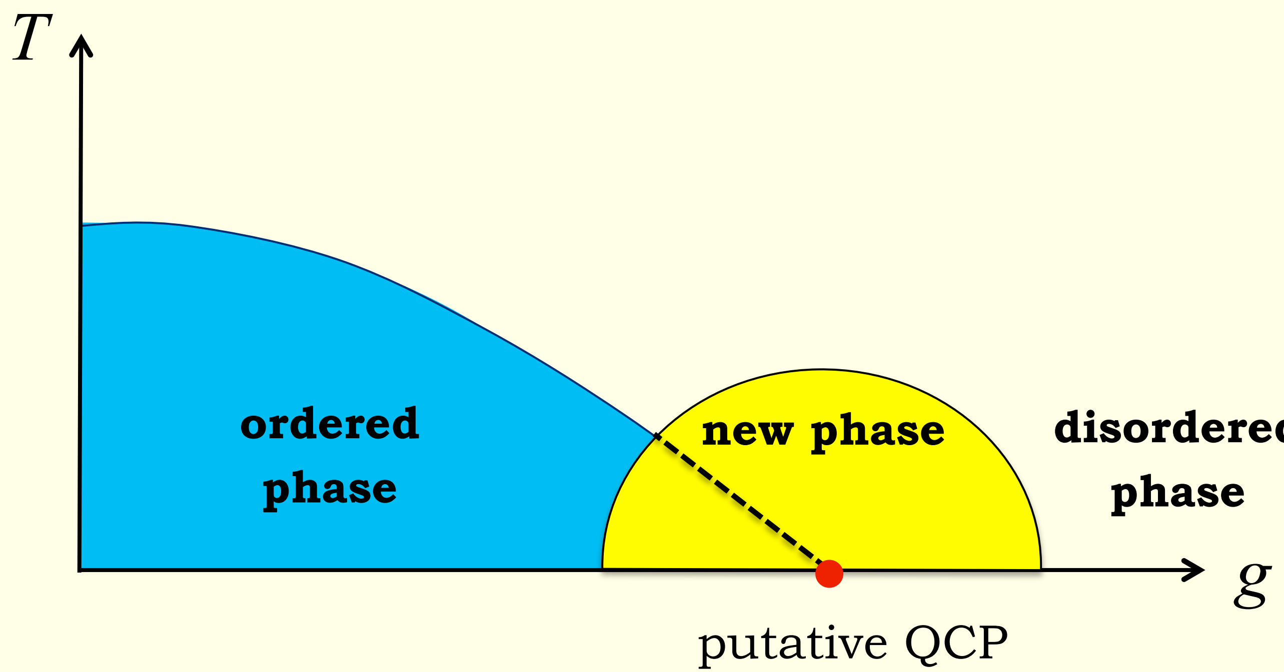


pairing mediated by quantum critical fluctuations?

Sachdev, Chubukov, Schmalian, Lonzarich, Taillefer, and many others...

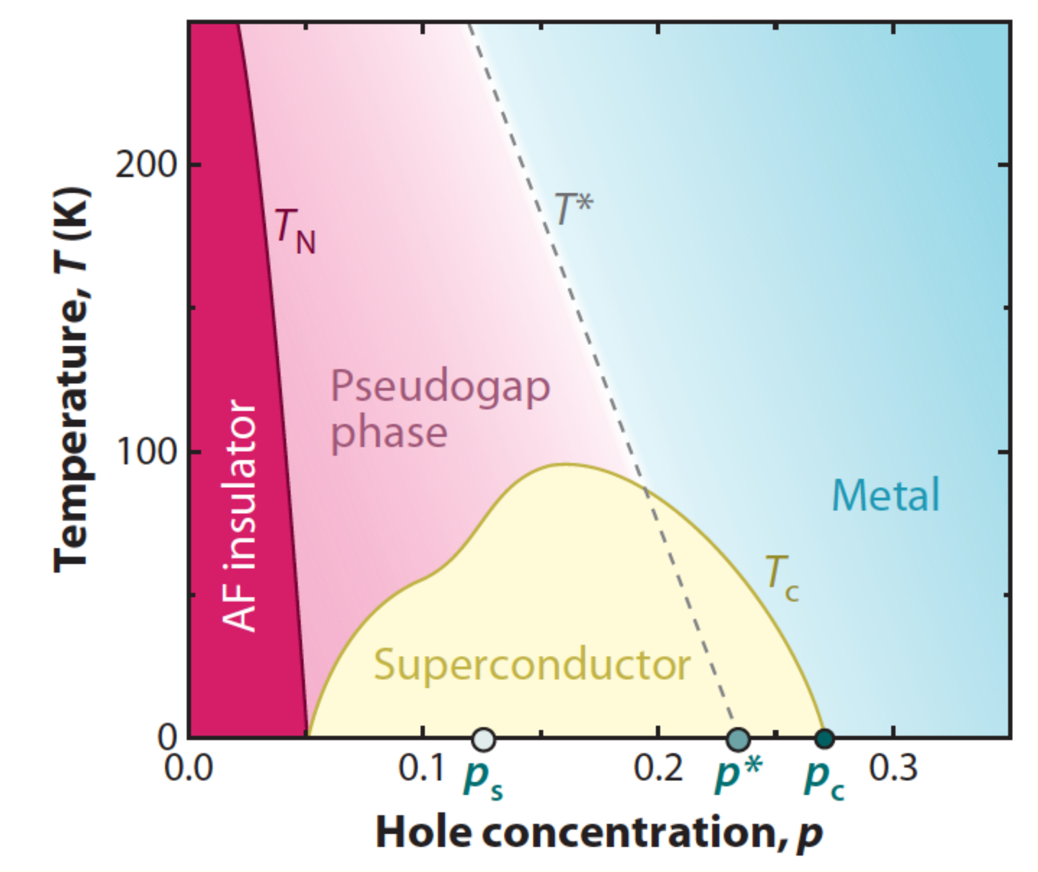
Quantum phase transitions in metals

- However, the phases are usually associated with different broken symmetries and **compete** with each other



Quantum phase transitions in metals

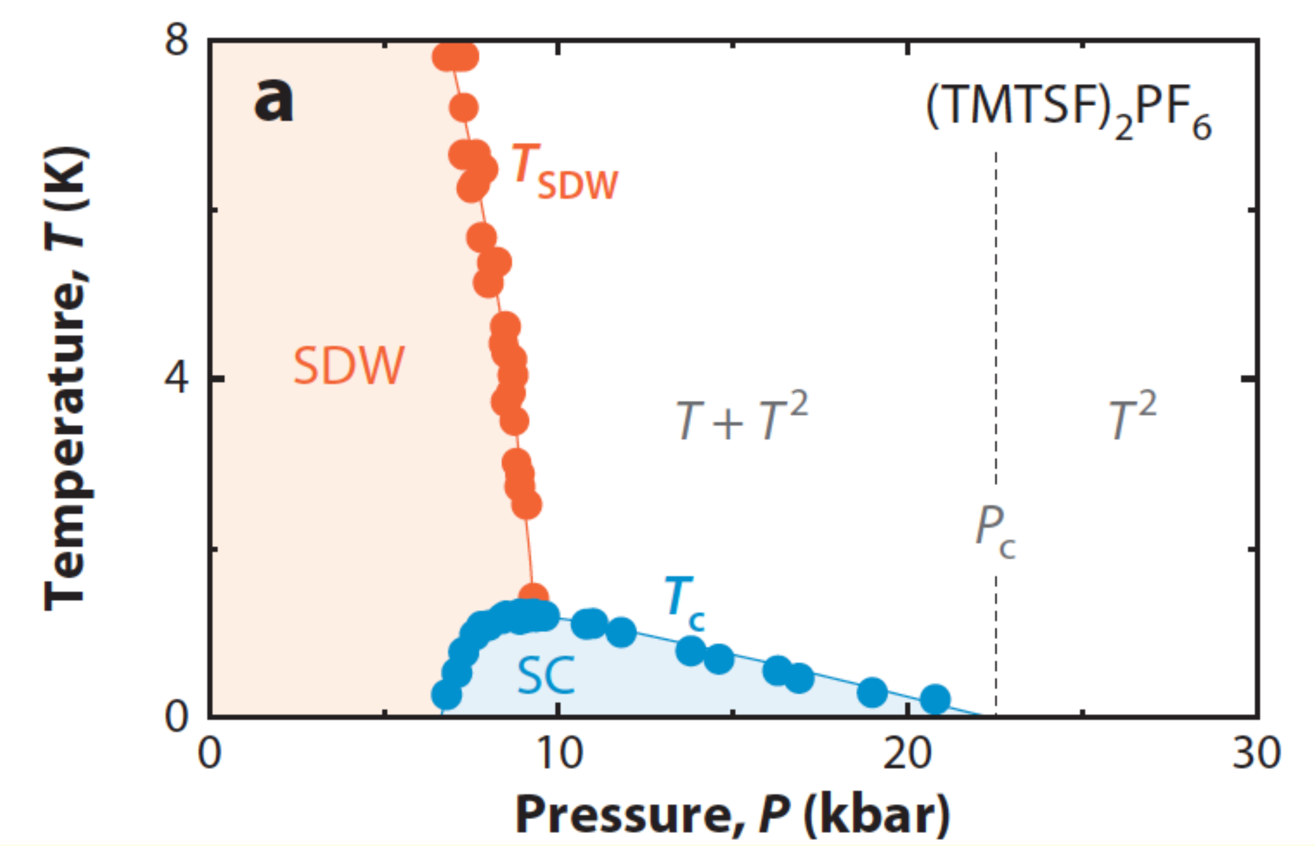
- Competing phases: examples in real materials
  - cuprates



Taillefer, ARCMP (2010)

Quantum phase transitions in metals

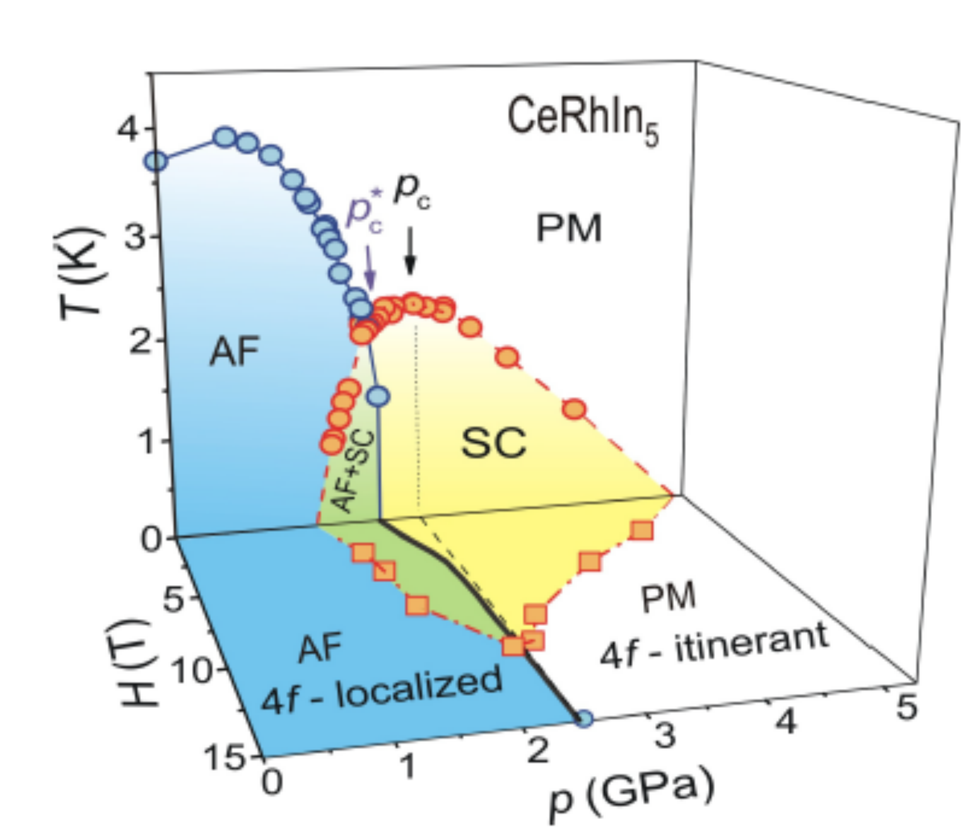
- Competing phases: examples in real materials
  - organics



Taillefer, ARCMP (2010)

Quantum phase transitions in metals

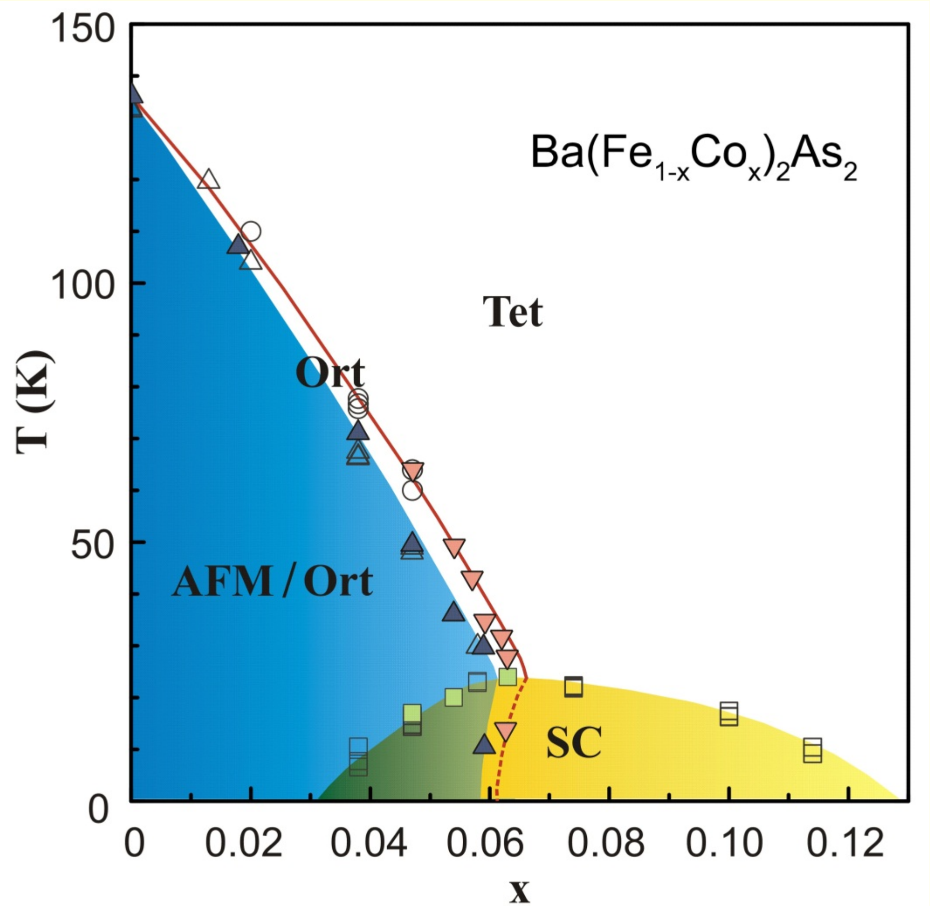
- Competing phases: examples in real materials
  - heavy fermions



Flouquet, 2009

Quantum phase transitions in metals

- Competing phases: examples in real materials
  - iron pnictides



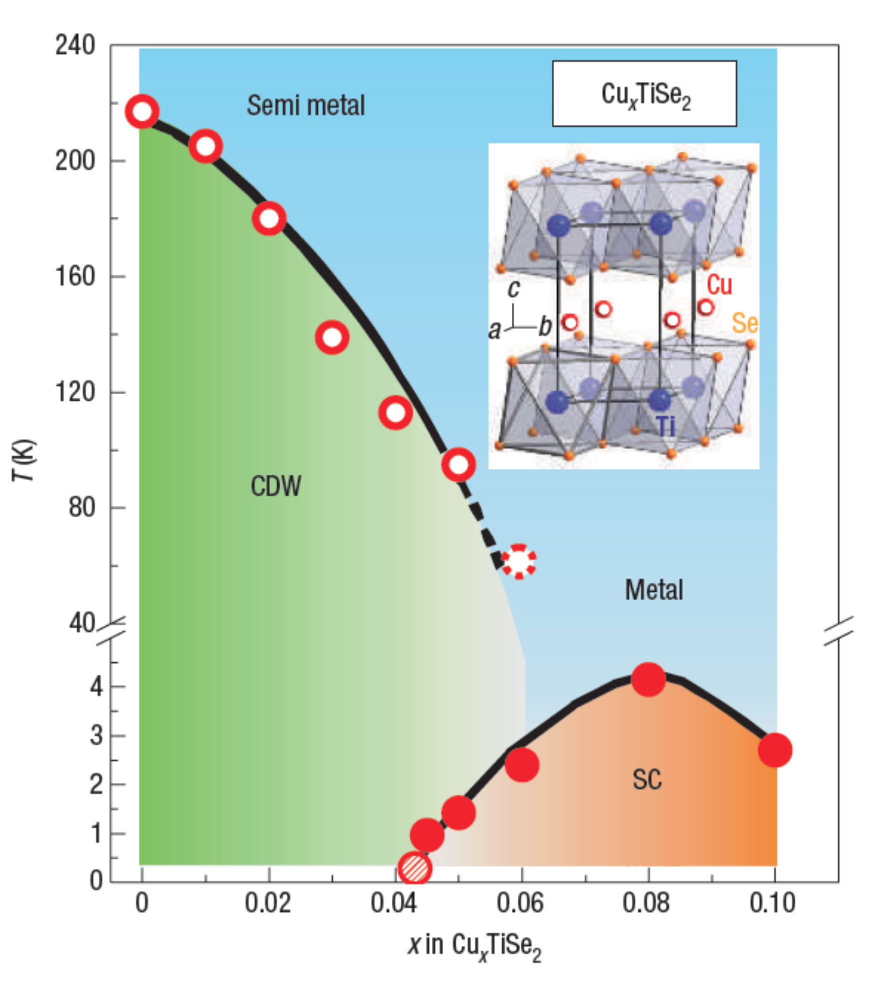
Ni et al, PRB (2008)

RMF et al, PRB (2010)

Nandi et al, PRL (2010)

Quantum phase transitions in metals

- Competing phases: examples in real materials
  - dichalcogenides



Morosan et al, Nature Phys (2006)

Outline

- **Brief introduction to the iron pnictides**
  - experimental evidence for competing phases

- **Competition between magnetism and superconductivity**
  - symmetry of the Cooper pair wave function

- **Competition between nematicity and superconductivity**
  - indirect competition mediated by magnetism

Outline

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Collaborators:

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(Bochum)

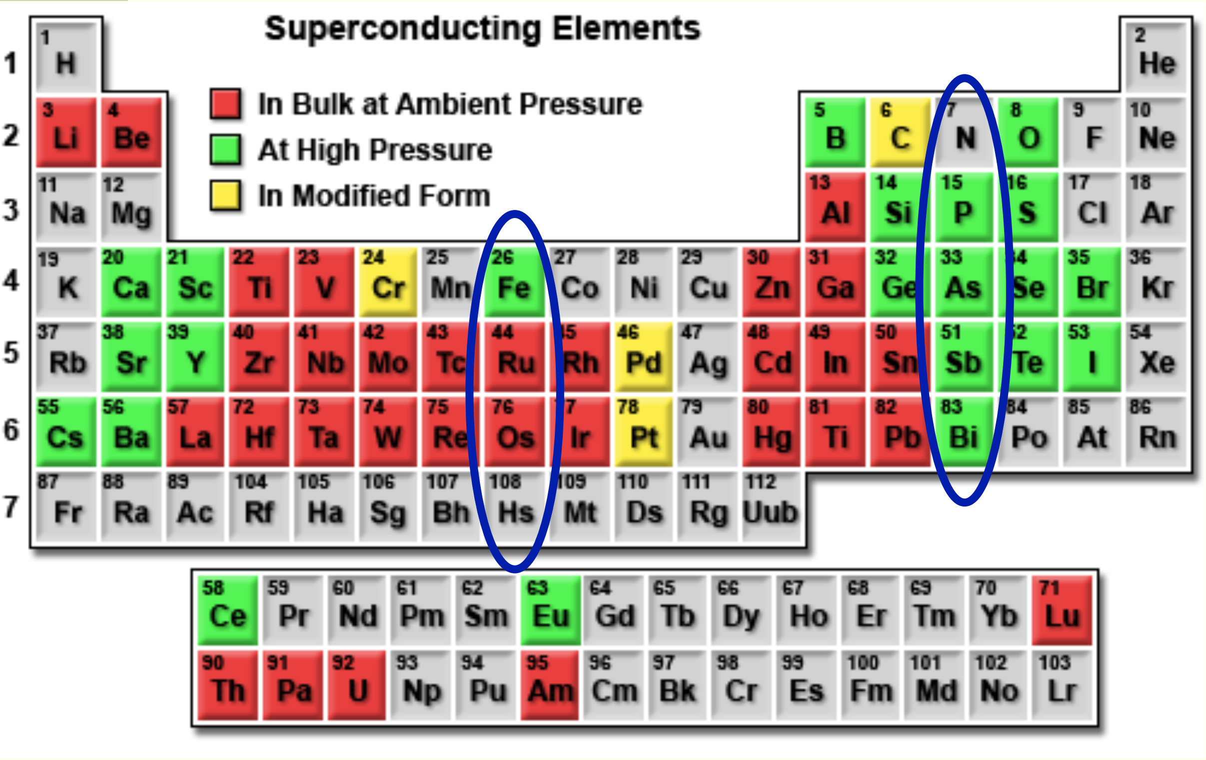
Elihu Abrahams
(UCLA)

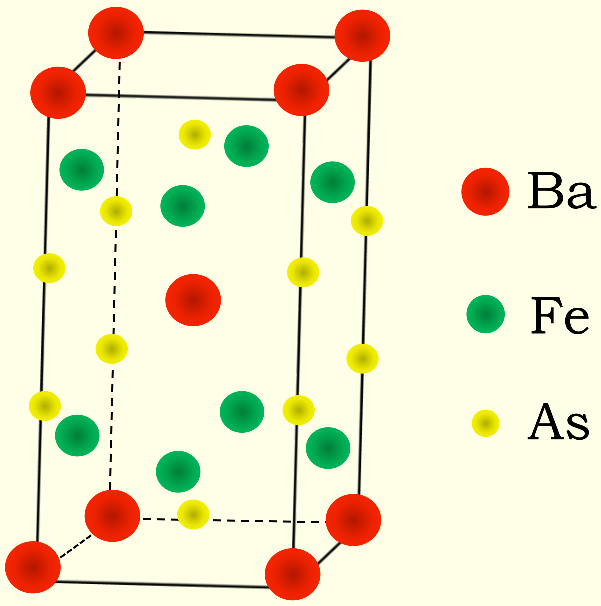
Saurabh Maiti
(Madison)

Andy Millis
(Columbia)

Iron pnictides

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



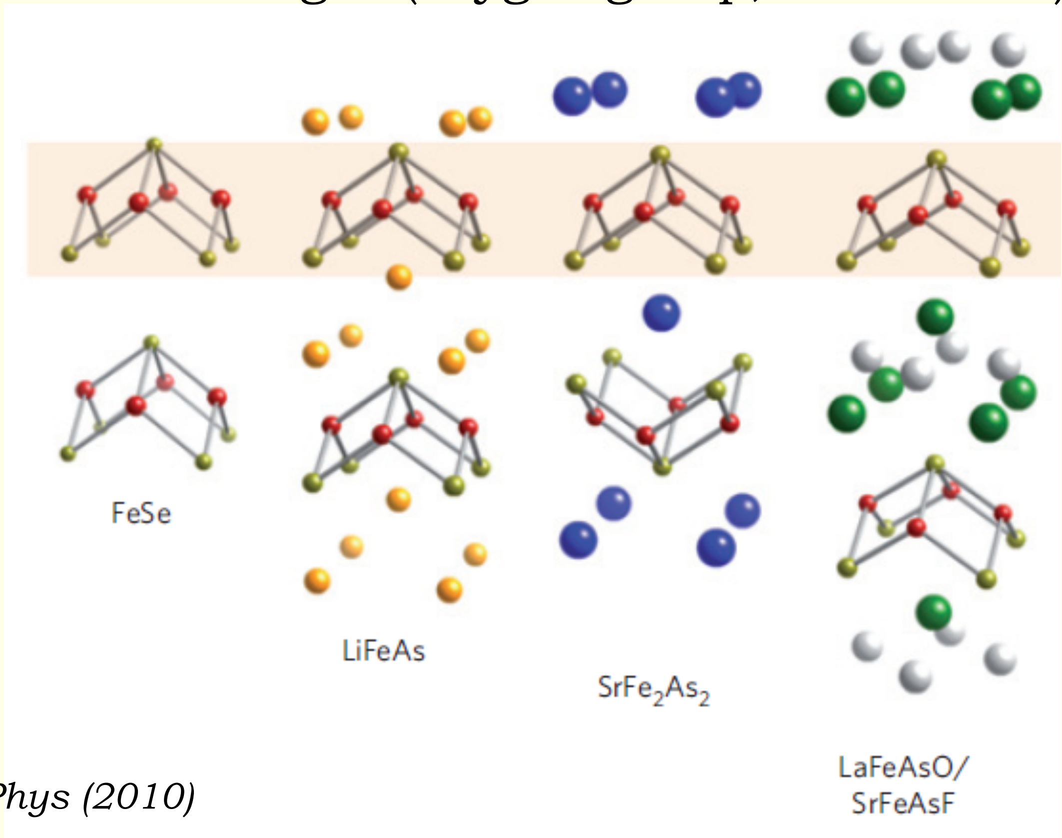


$BaFe_2As_2$

J. Schmalian, Physik Journal

Iron pnictides

- Layered materials: transition metal (**Fe**) plus pnictogen (nitrogen group, such as **As**)
  - several families
  - also with chalcogen (oxygen group, such as **Se**).



Paglione & Greene, Nature Phys (2010)

- Rise of the iron pnictides

J|A|C|S COMMUNICATIONS

Published on Web 02/23/2008

Iron-Based Layered Superconductor $La[O_{1-x}F_x]FeAs$ (x = 0.05−0.12) with T_c = 26 K

Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§

- Rise of the iron pnictides

J|A|C|S

nature Vol 453|15 April 2008|**doi:10.1038/nature06972**

LETTERS

Superconductivity at 43 K in an iron-based layered compound $LaO_{1-x}F_xFeAs$

Hiroki Takahashi[1], Kazumi Igawa[1], Kazunobu Arii[1], Yoichi Kamihara[2], Masahiro Hirano[2,3] & Hideo Hosono[2,3]

- Rise of the iron pnictides

J|A|C|S
COMMUNICATIONS

nature Vol 453|15 April 2008|**doi:10.1038/nature06972**

LETTERS

2)

CHIN.PHYS.LETT. Vol. 25, No. 6 (2008) 2215

Superconductivity at 55 K in Iron-Based F-Doped Layered Quaternary Compound Sm$[O_{1-x}F_x]$FeAs *

REN Zhi-An(任治安)**, LU Wei(陆伟), YANG Jie(杨杰), YI Wei(衣玮), SHEN Xiao-Li(慎晓丽), LI Zheng-Cai(李正才), CHE Guang-Can(车广灿), DONG Xiao-Li(董晓莉), SUN Li-Ling(孙力玲), ZHOU Fang(周放), ZHAO Zhong-Xian(赵忠贤)***

- Rise of the iron pnictides

J|A|C|S

COMMUNICATIONS

nature Vol 453|15 April 2008|doi:10.1038/nature06972

LETTERS

2)

CHIN.PHYS.LETT. Vol. 25, No. 6 (2008) 2215

epl A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

September 2008

EPL, **83** (2008) 67006 www.epljournal.org

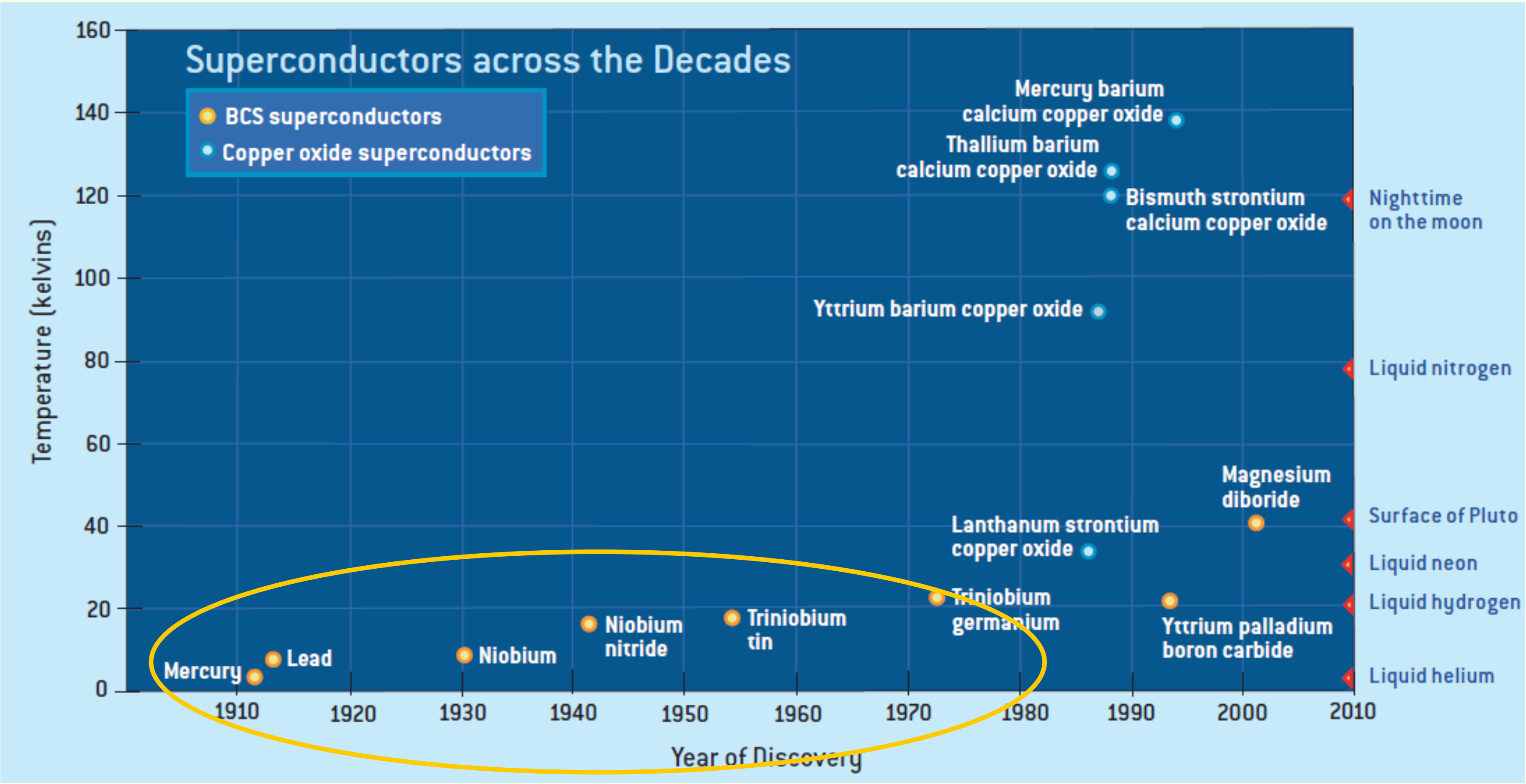
doi: 10.1209/0295-5075/83/67006

Thorium-doping–induced superconductivity up to 56 K in $Gd_{1-x}Th_xFeAsO$

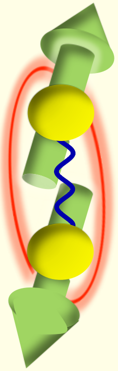
CAO WANG, LINJUN LI, SHUN CHI, ZENGWEI ZHU, ZHI REN, YUKE LI, YUETAO WANG, XIAO LIN, YONGKANG LUO, SHUAI JIANG, XIANGFAN XU, GUANGHAN CAO[a] and ZHU'AN XU[b]

Superconductivity reaches the iron age!

Canfield et al, Sci. Am. (2005)



stone age



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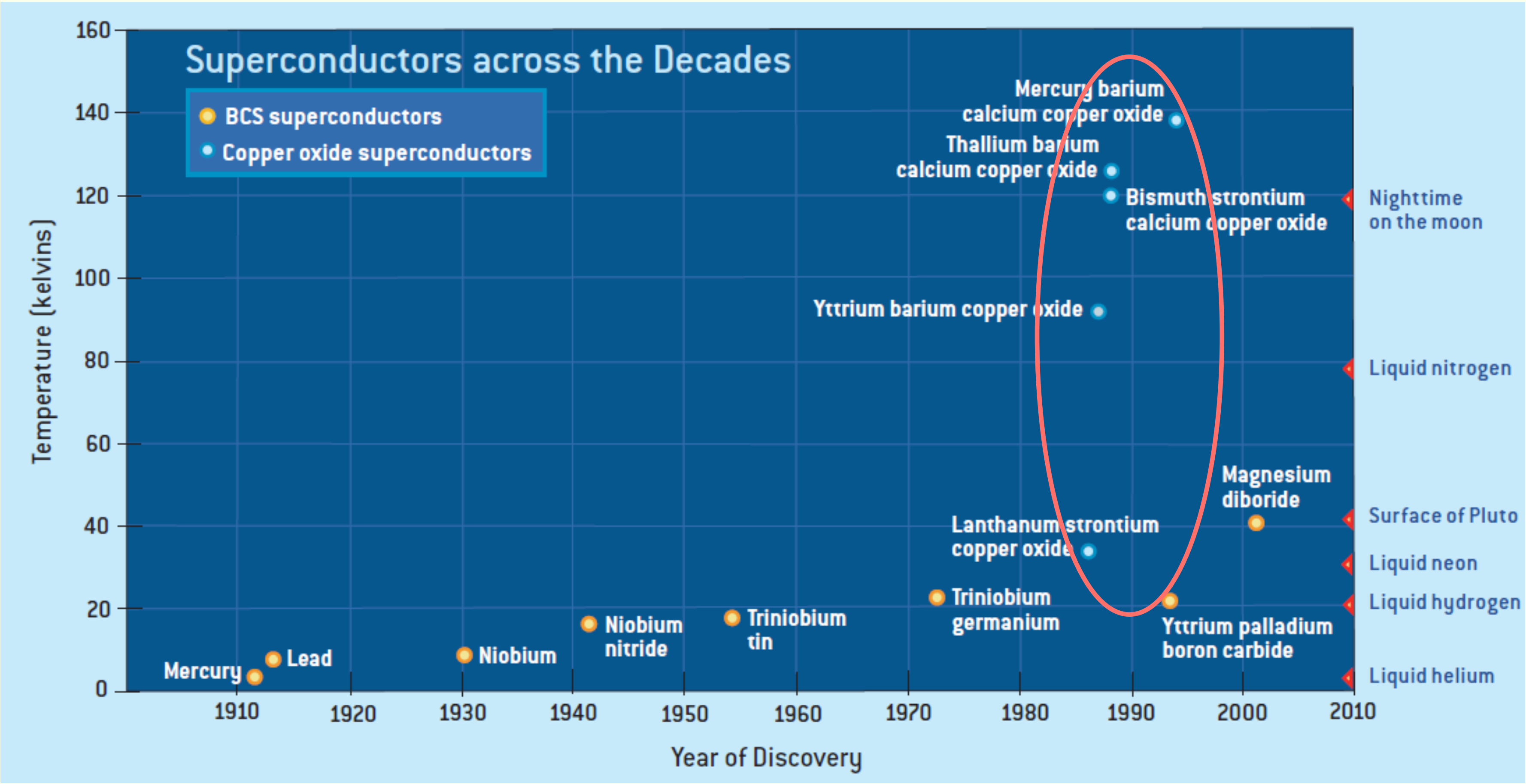
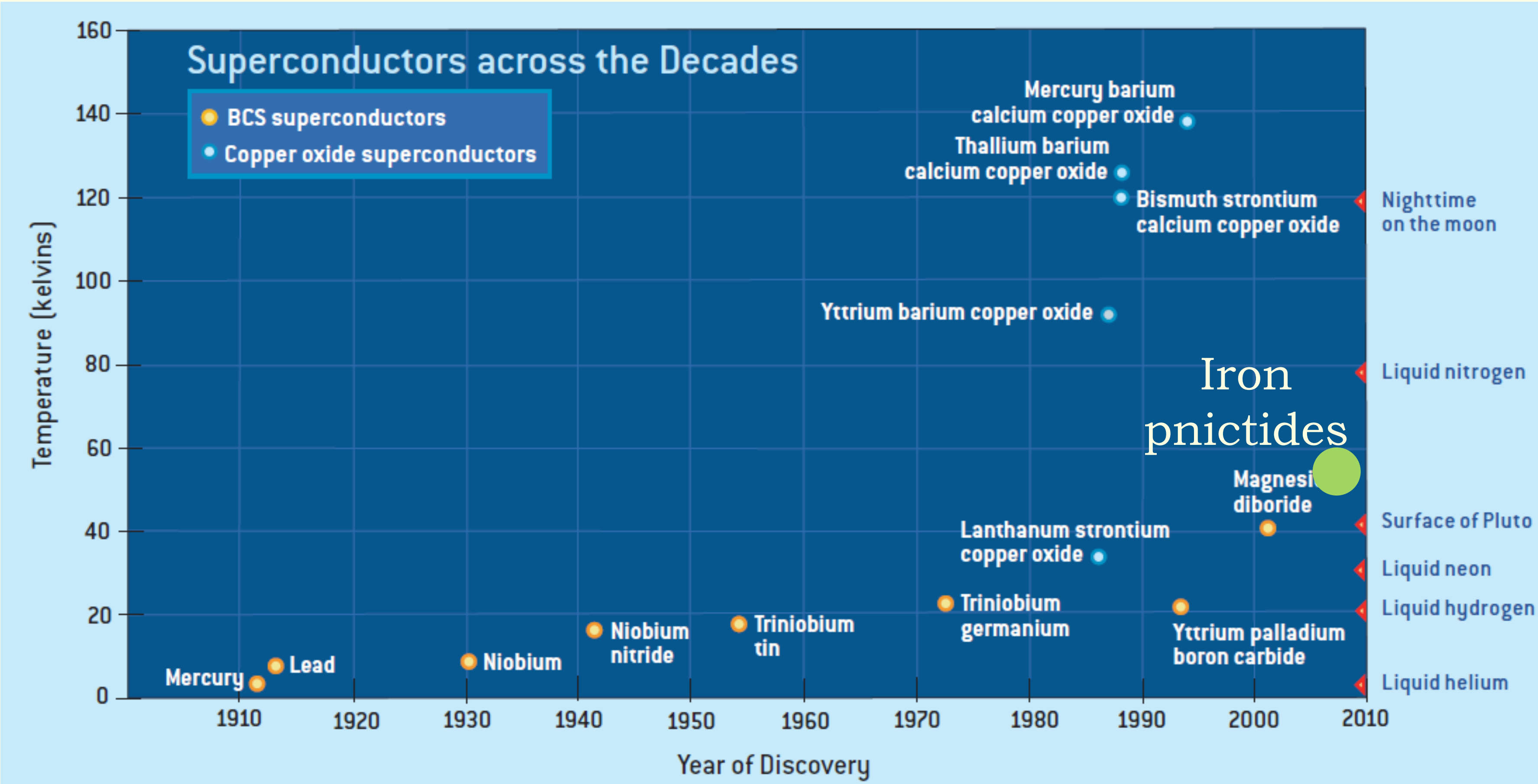


stone age → **copper age**

Superconductivity reaches the iron age!

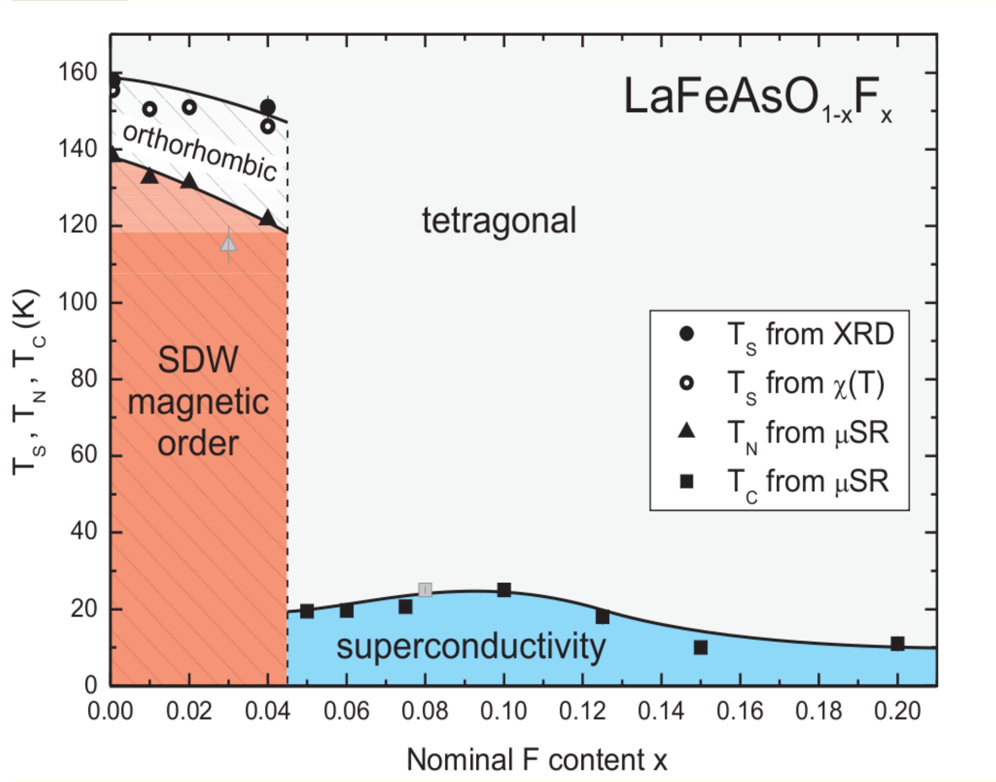


stone age → **copper age** → **iron age**

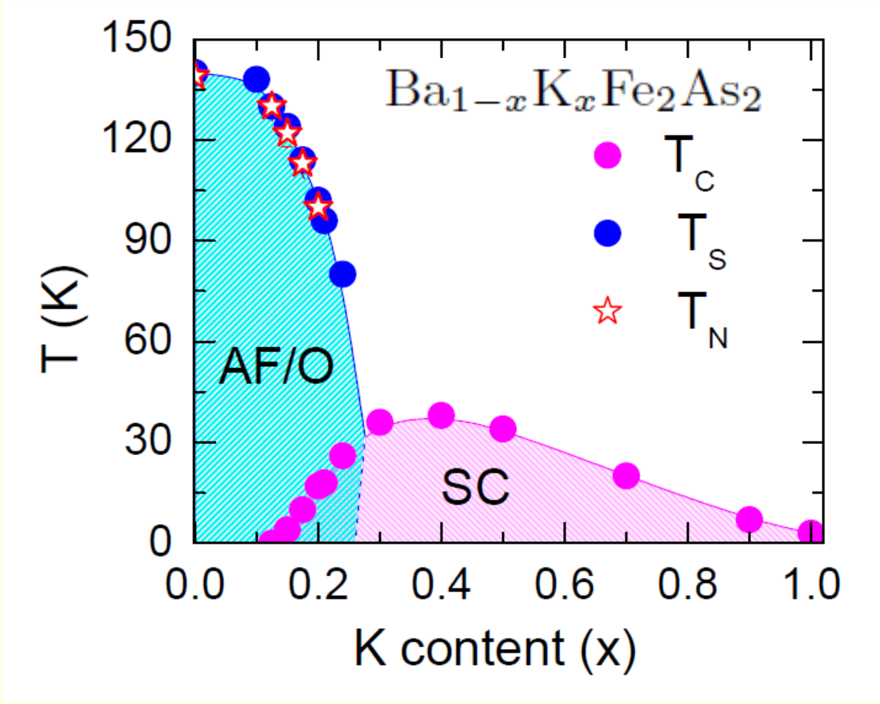
first high-temperature superconductors since the cuprates!

Iron pnictides: phase diagrams

Interplay between magnetic, superconducting and elastic degrees of freedom



Luetkens et al, Nature Mater. (2008)



Avci et al, PRB (2011)

Iron pnictides: phase diagrams

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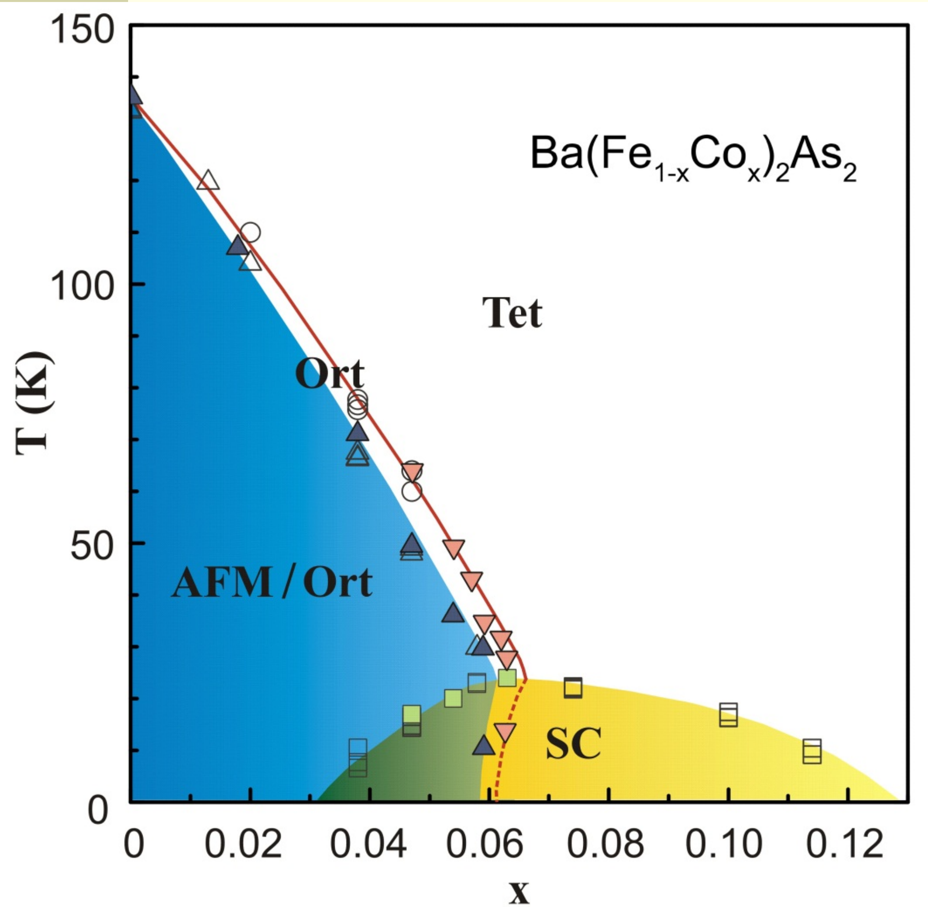
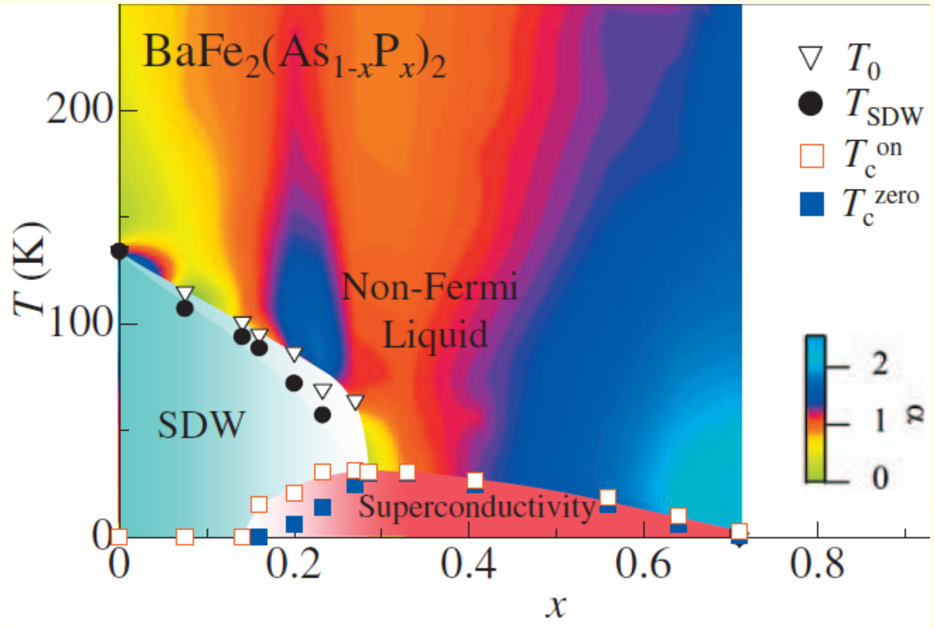


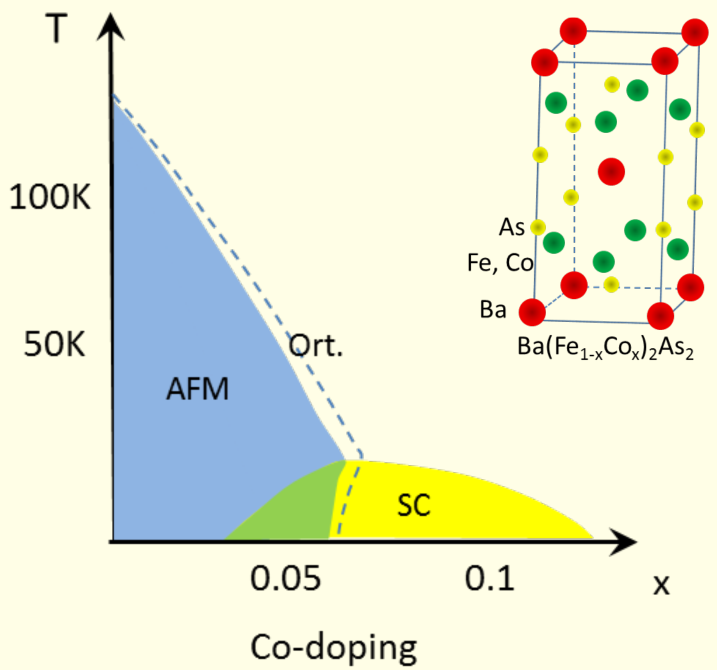


Kasahara et al, PRB (2010)

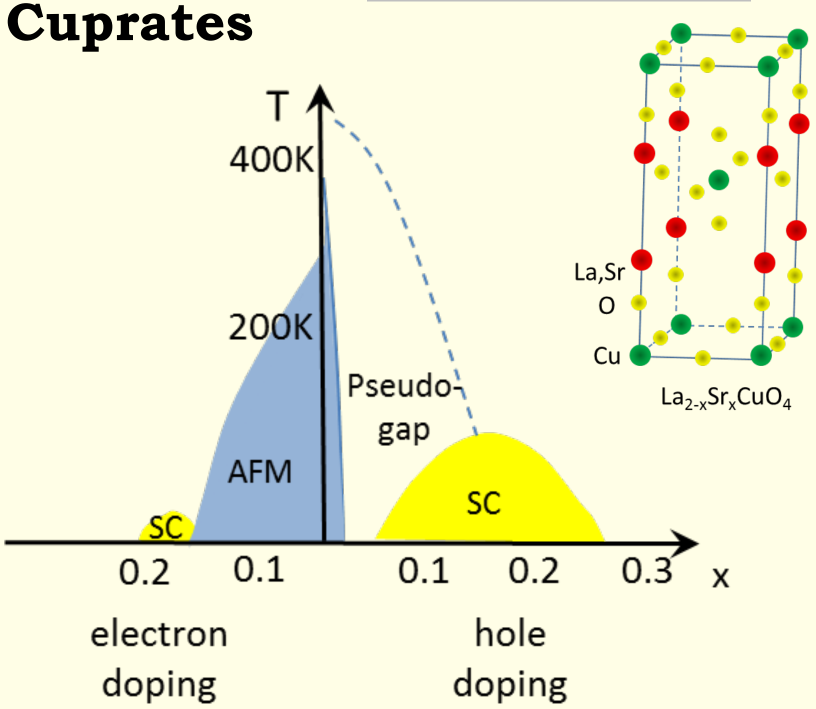
Ni et al, PRB (2008) *RMF et al, PRB (2010)*
Pratt et al, PRL (2009) *Nandi et al, PRL (2010)*

Iron arsenides *vs* cuprates

Iron arsenides



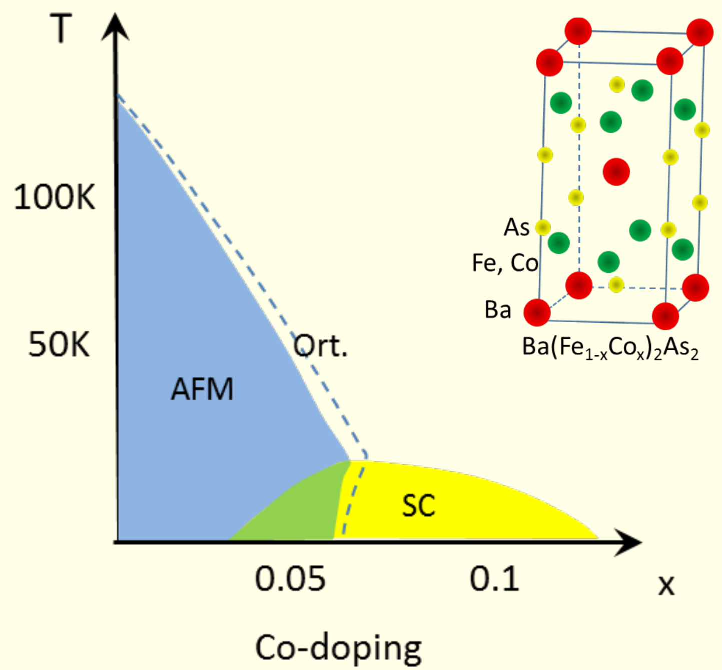
Cuprates



J Schmalian, Physik Journal

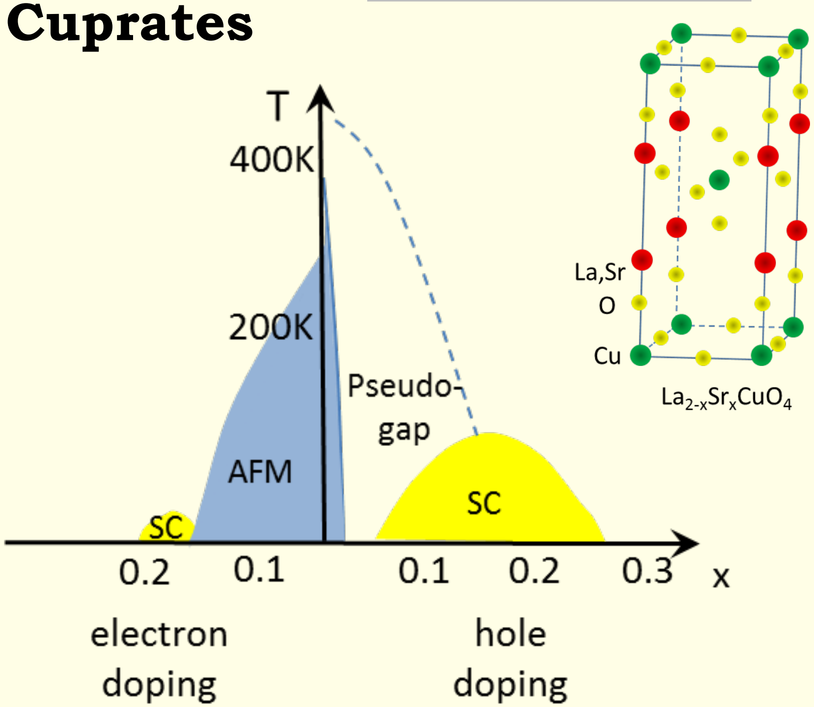
Iron arsenides *vs* cuprates

Iron arsenides



- 3d electrons
- layered materials
- high values of T_c
- unconventional SC (?) close to AFM transition

Cuprates



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Iron arsenides *vs* cuprates

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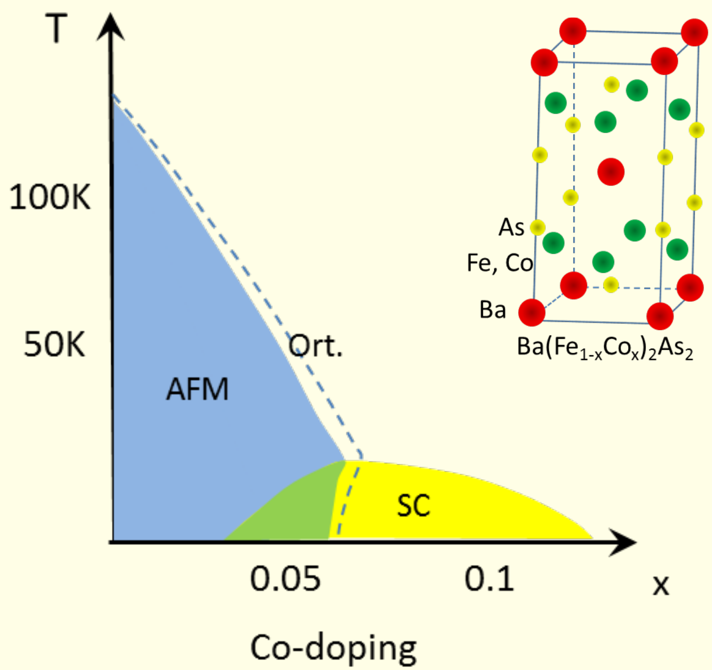
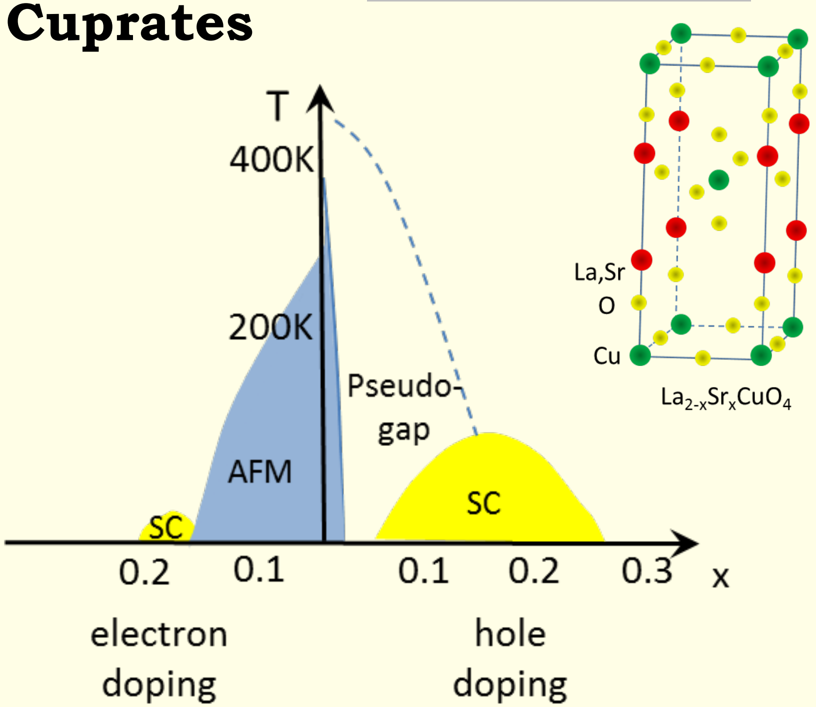


- parent compound is metallic
- five iron bands with *n = 6*
- itinerant magnetism

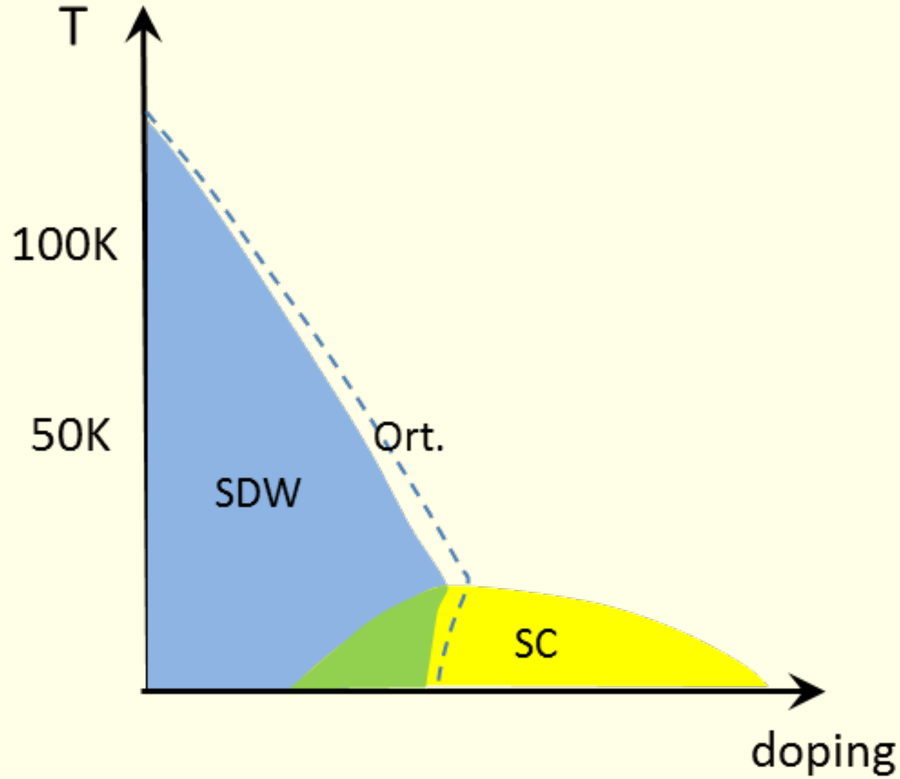
Cuprates



- parent compound is a Mott insulator
- one copper band with *n = 1*
- localized magnetism

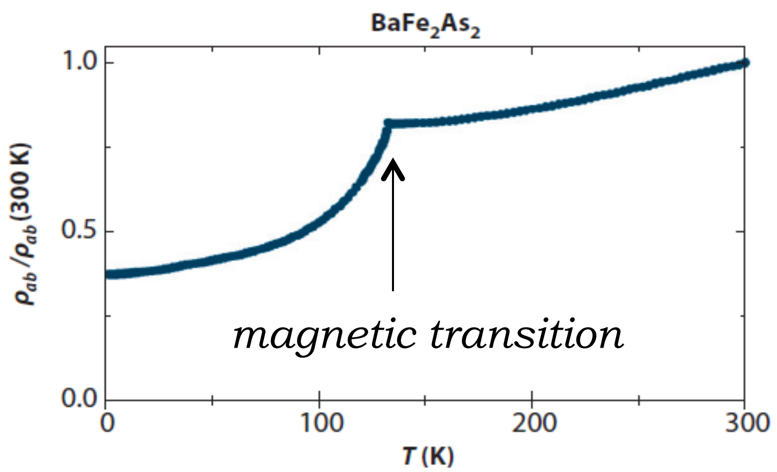
Iron pnictides: typical phase diagram

magnetic, structural, and superconducting order

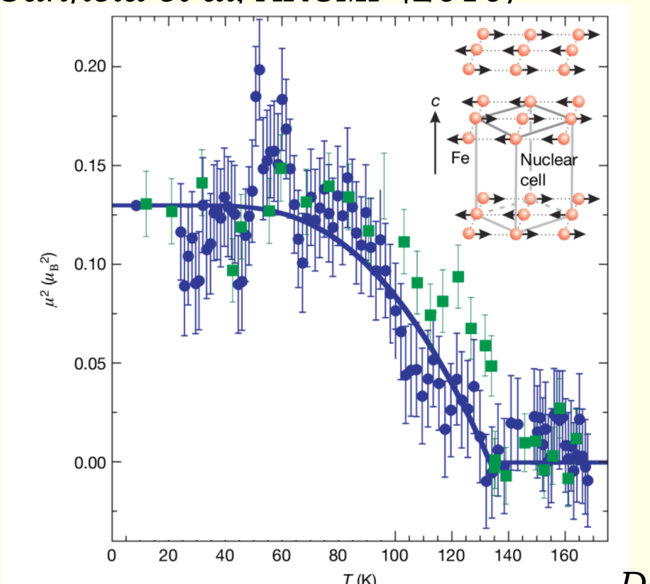


- How these different ordered states interact with each other?
- Is there a primary degree of freedom?

Iron pnictides: magnetic order



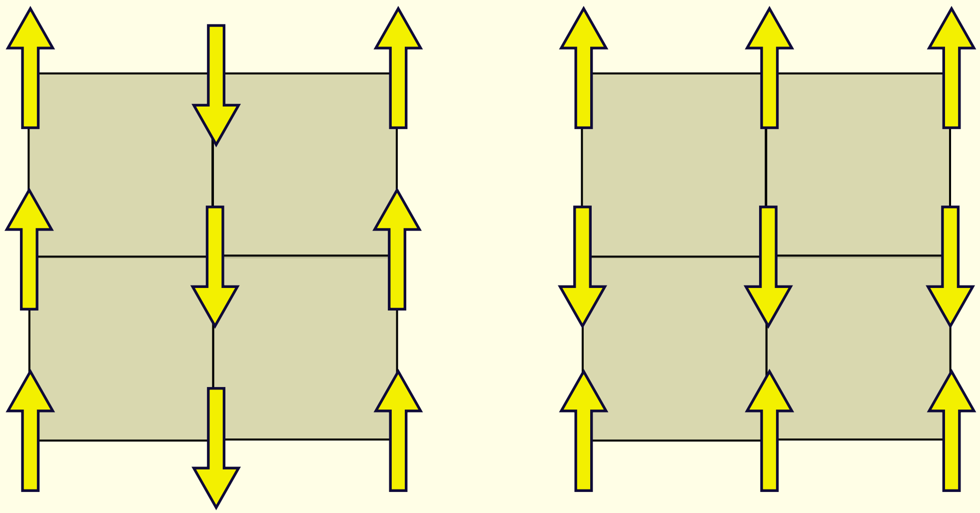
Canfield et al, ARCMP (2010)



De la Cruz et al, Nature (2008)

system remains metallic

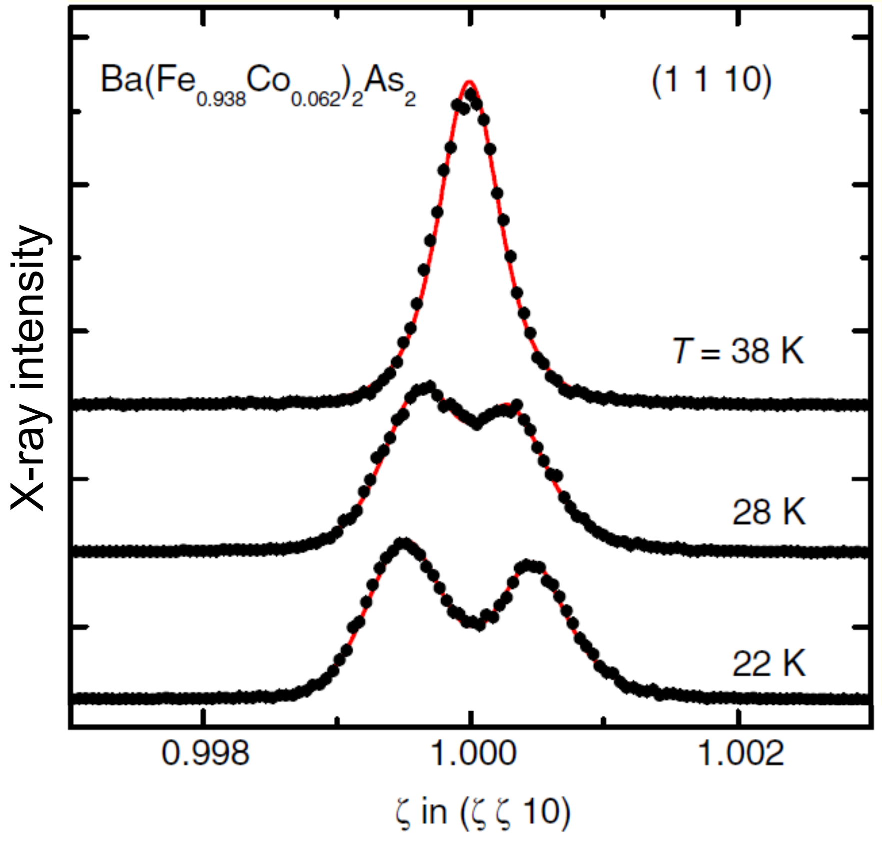
two magnetic stripe states



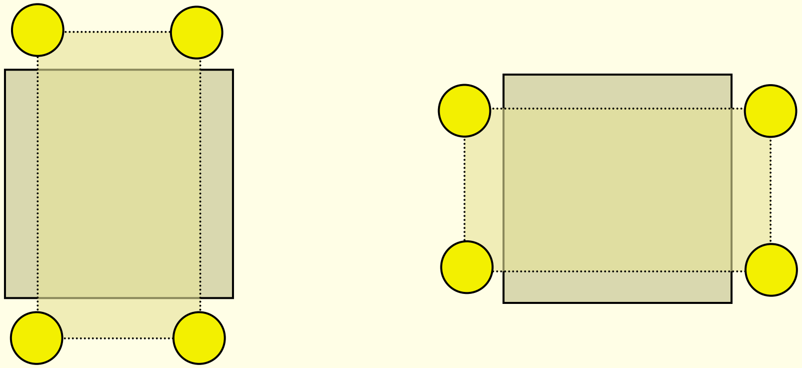
$\mathbf{Q}_1 = (\pi, 0)$ $\mathbf{Q}_2 = (0, \pi)$

Iron pnictides: structural order

tetragonal to orthorhombic transition

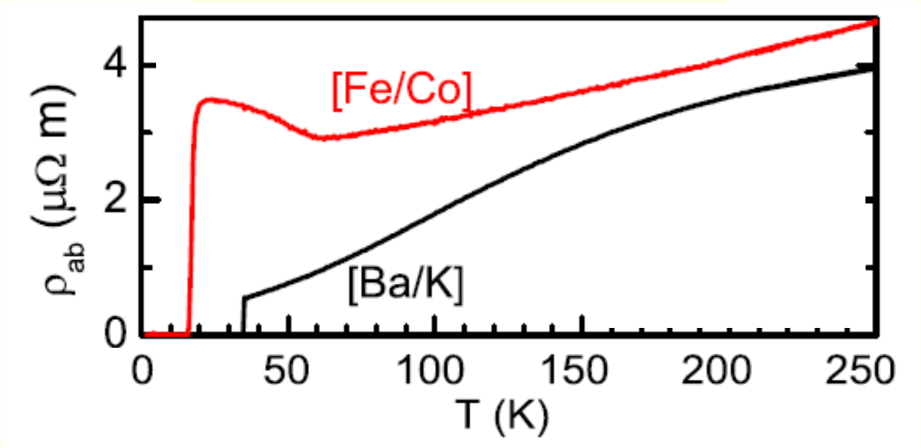


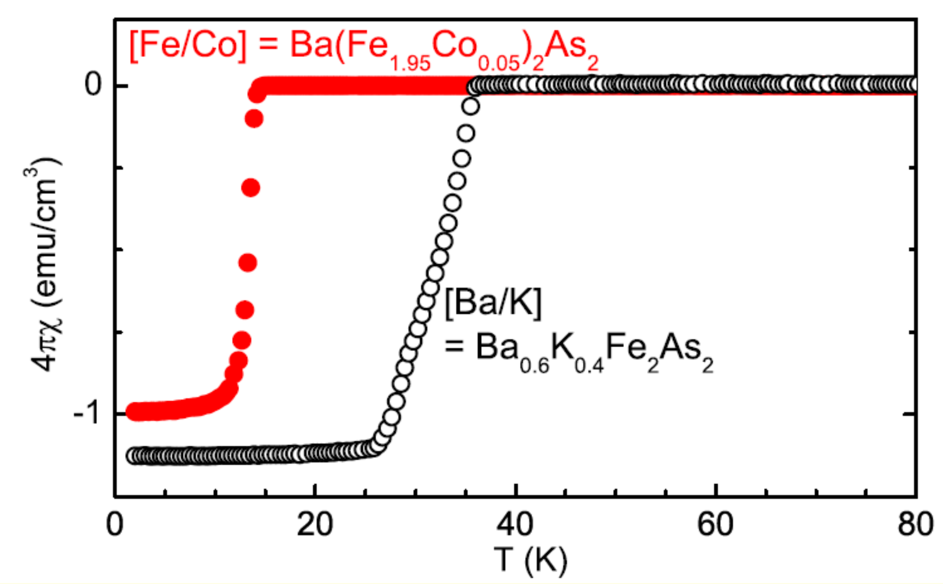
twin domains



Nandi et al, PRL (2010)

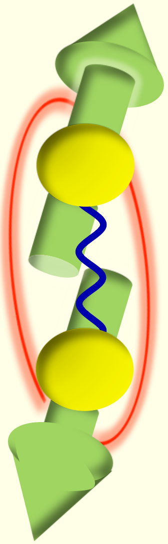
Iron pnictides: superconducting order





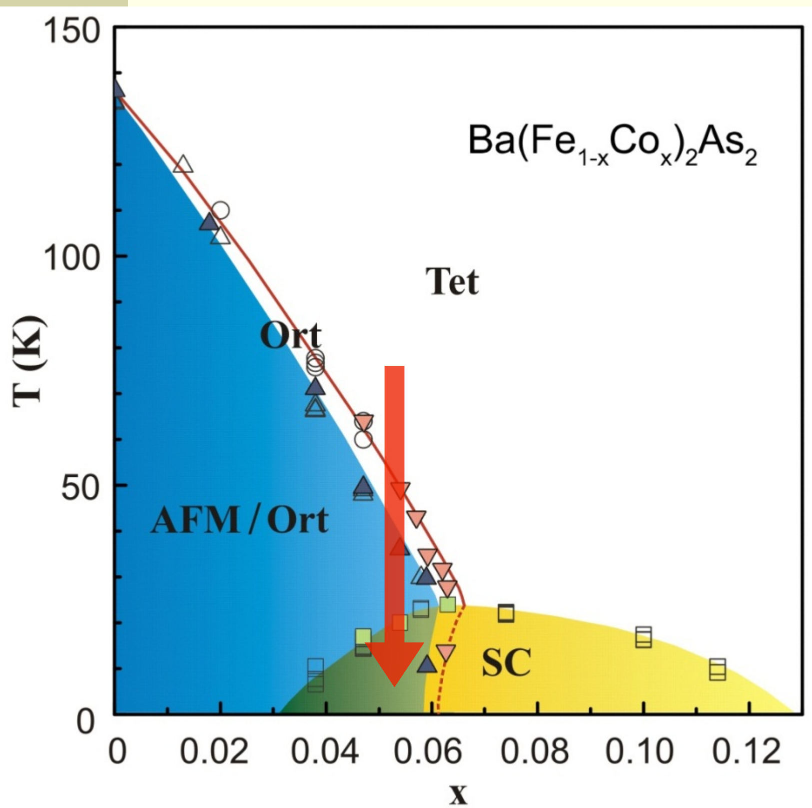
Julien et al, EPL (2009)

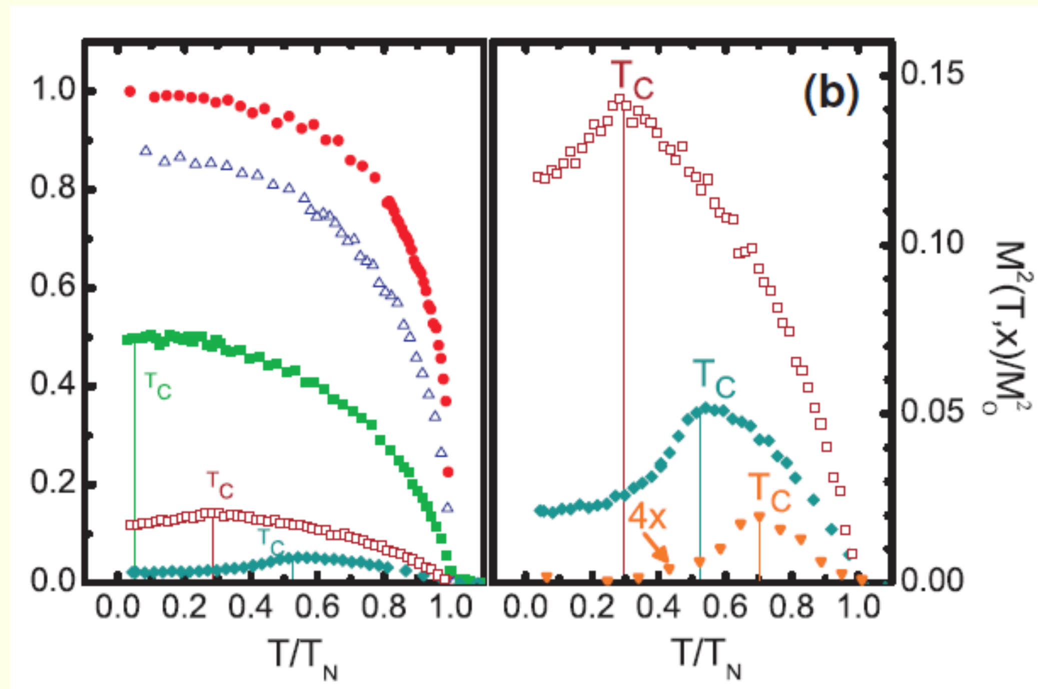
pairing: conventional (phonons) or unconventional (electronic)?



Competing phases: experimental observations

- Neutron diffraction: suppression of the **magnetic order parameter** below T_c



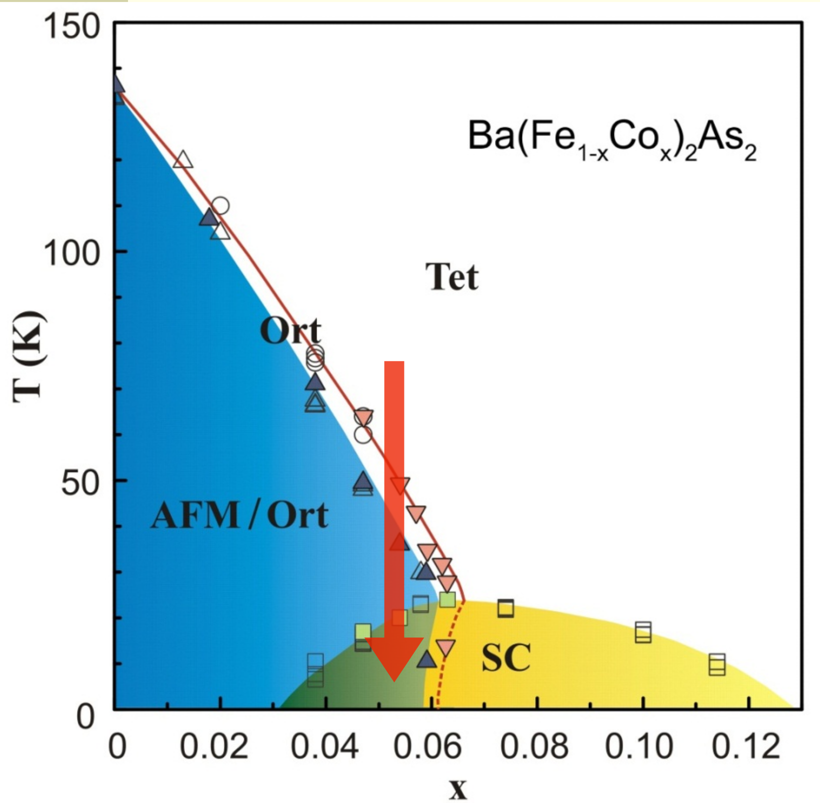


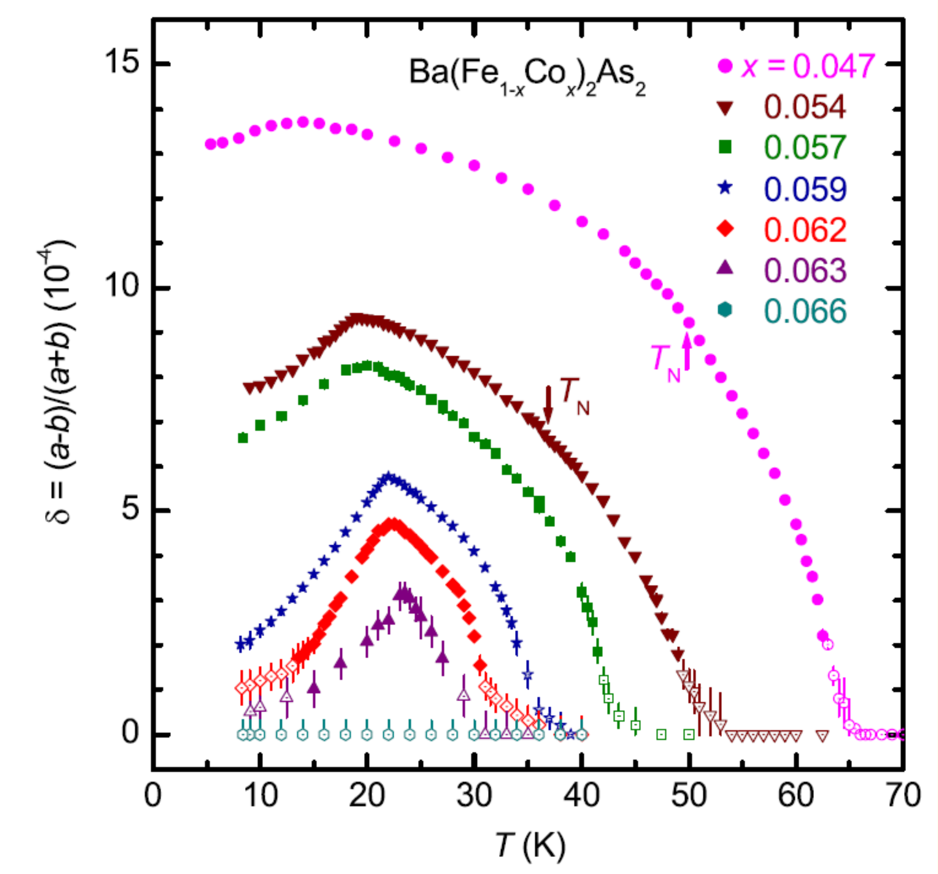
RMF et al, PRB (2010)

Pratt et al, PRL (2009) *Christianson et al, PRL (2009)*

Competing phases: experimental observations

- X-ray diffraction: suppression of the **orthorhombic order parameter** below T_c

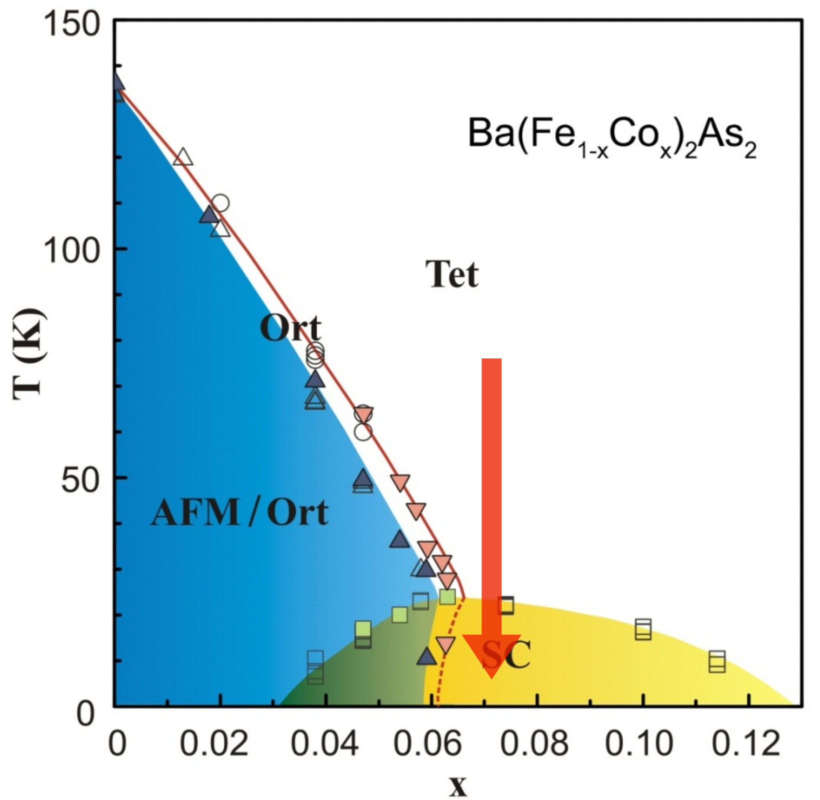


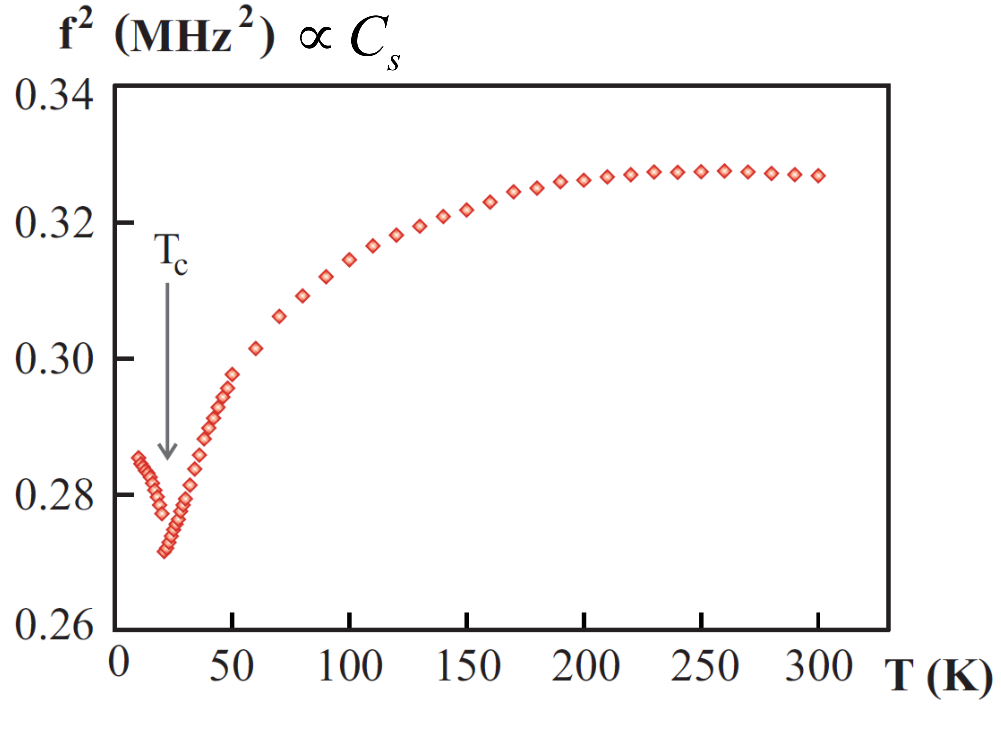


Nandi,…, RMF et al, PRL (2010)

Competing phases: experimental observations

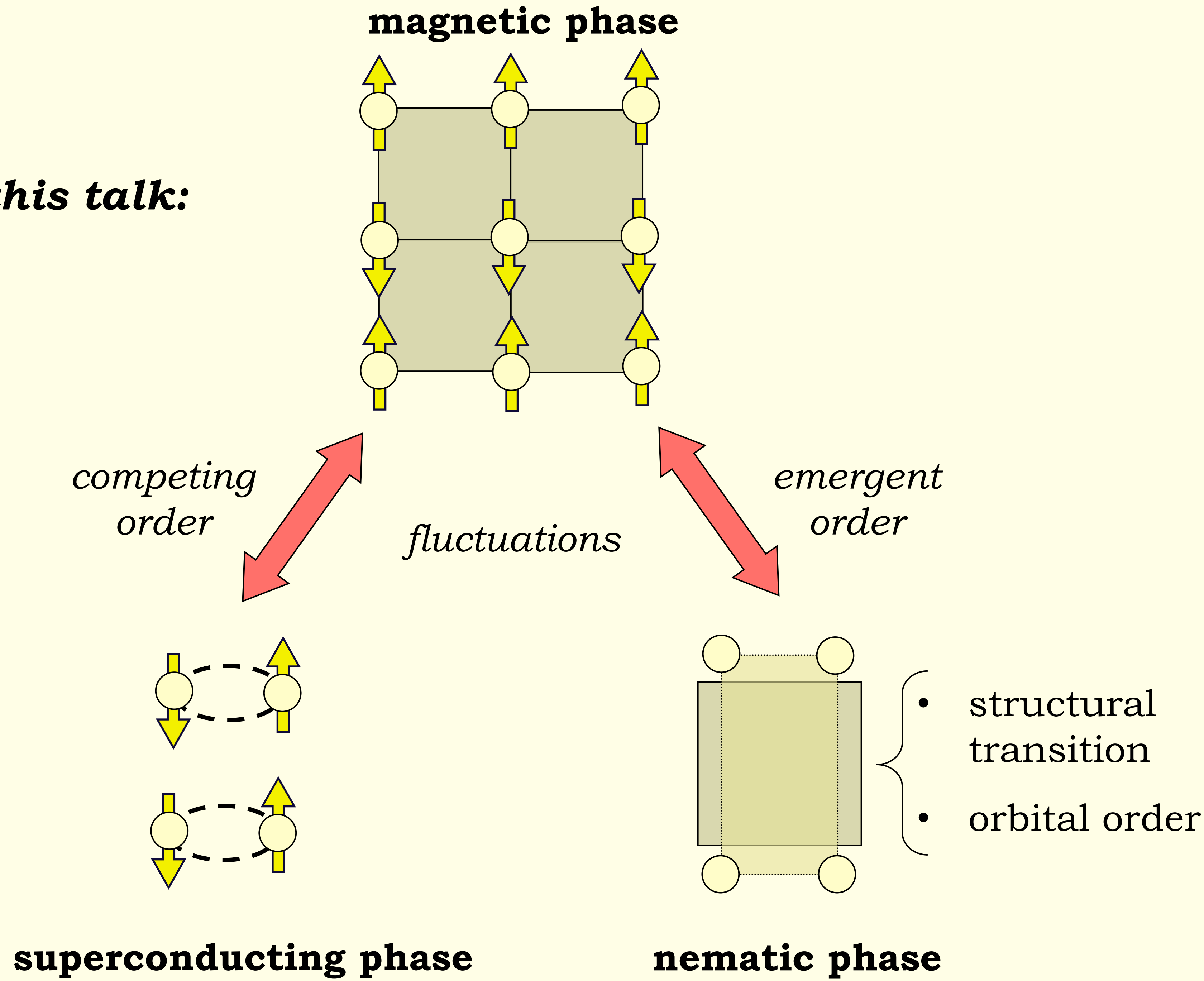
- Ultrasound spectroscopy: hardening of the **shear modulus** below T_c





RMF et al, PRL (2010)

In this talk:



magnetic phase
competing order
fluctuations
emergent order
superconducting phase
nematic phase
• structural transition
• orbital order

Outline

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  - experimental evidence for competing phases
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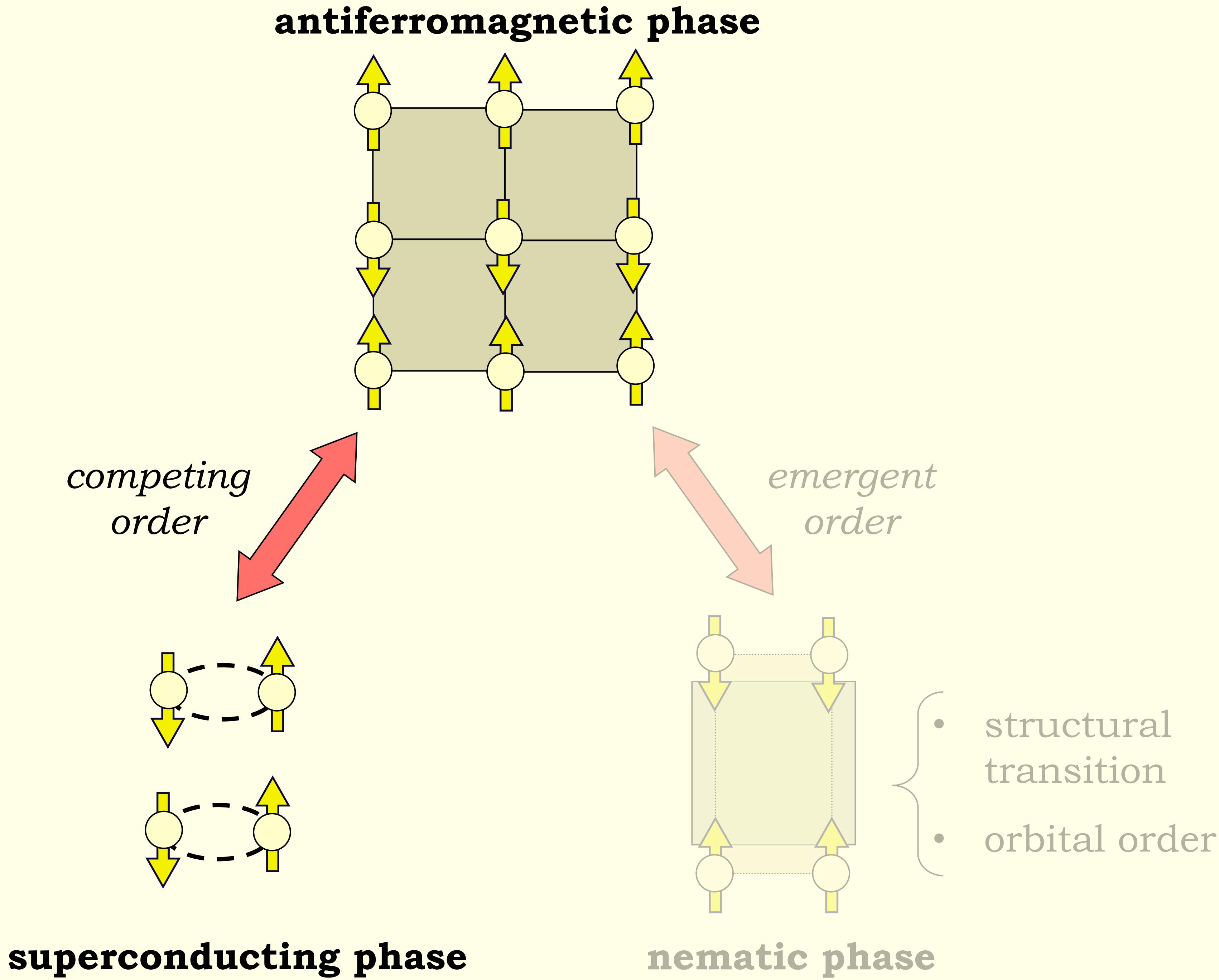
antiferromagnetic phase
competing order
emergent order
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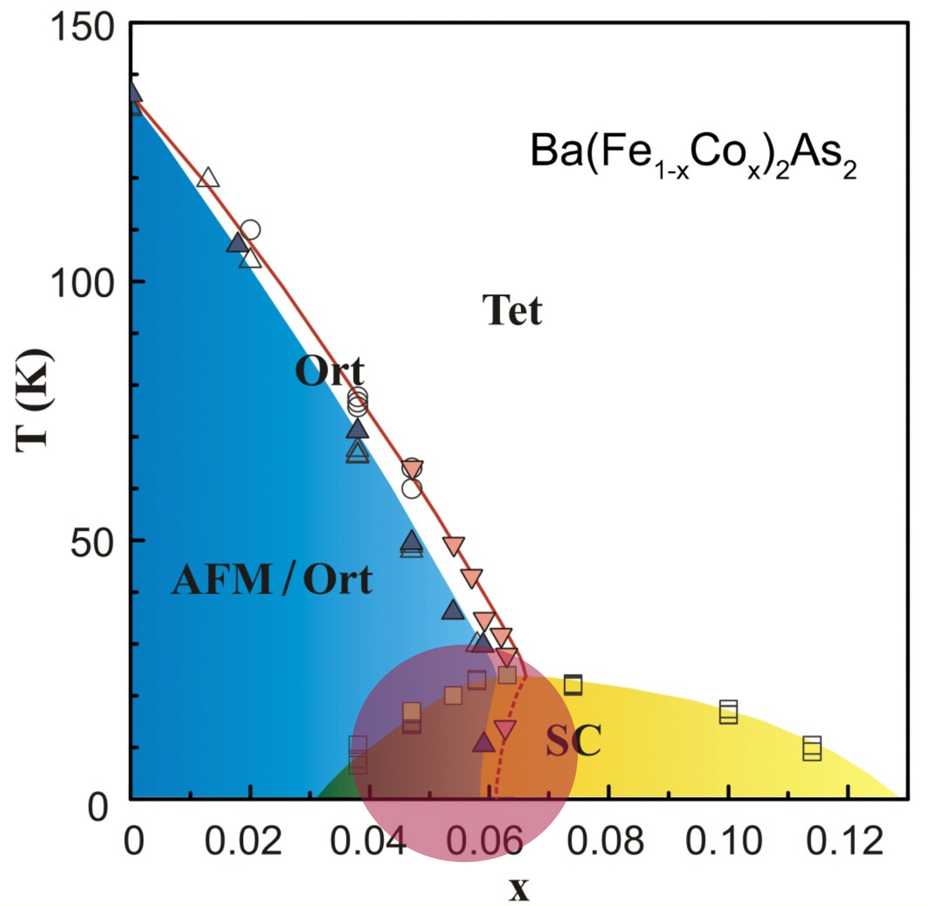
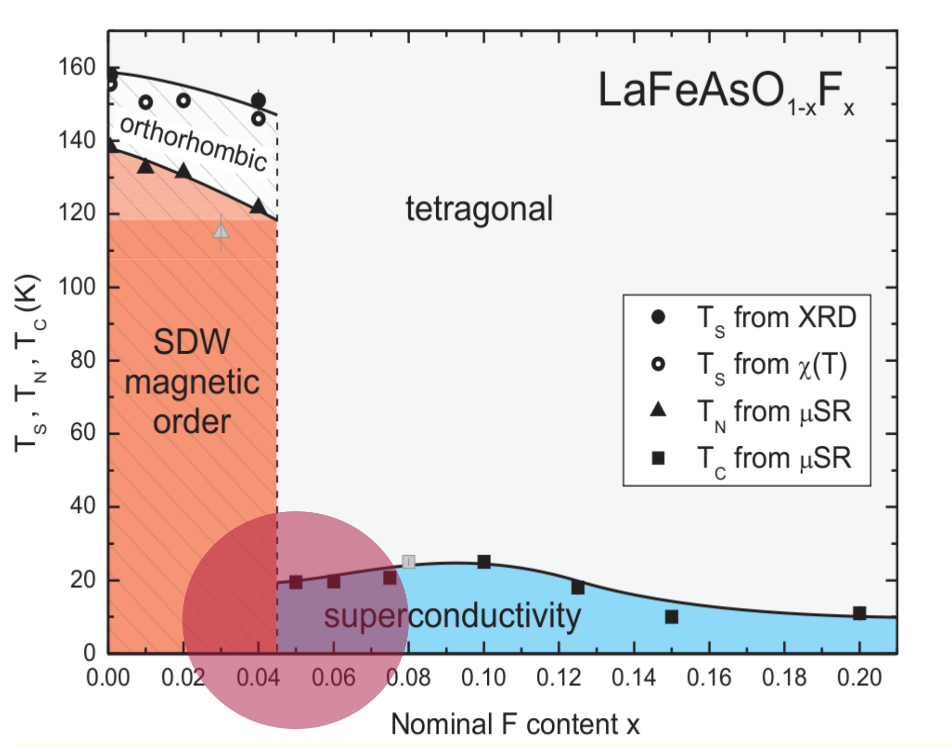
nematic phase
• structural transition
• orbital order

Competition between SDW and SC: coexistence or phase separation?

Local probe experiments:



microscopic coexistence



phase separation

Competition between SDW and SC: coexistence or phase separation?

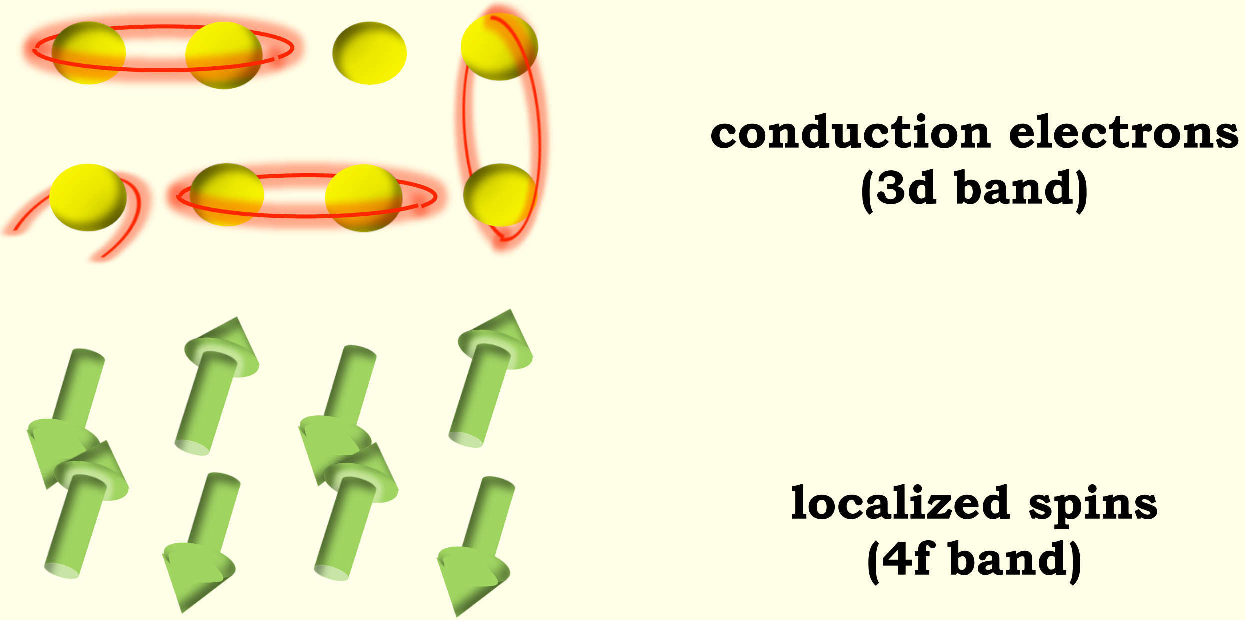
- Bulk measurements and local probes: in some FeAs compounds there is microscopic coexistence and in others, mutual exclusion.

Microscopic coexistence: $Ba(Fe_{1-x}Co_x)_2As_2$; $BaFe_2(As_{1-x}P_x)_2$; $(Ba_{1-x}K_x)Fe_2As_2$; $SmFeAs(O_{1-x}F_x)$ ⟶ unsettled

Phase separation: $LaFeAs(O_{1-x}F_x)$; $PrFeAs(O_{1-x}F_x)$; $(Sr_{1-x}Na_x)Fe_2As_2$; $CaFe_2As_2$ (pressure)

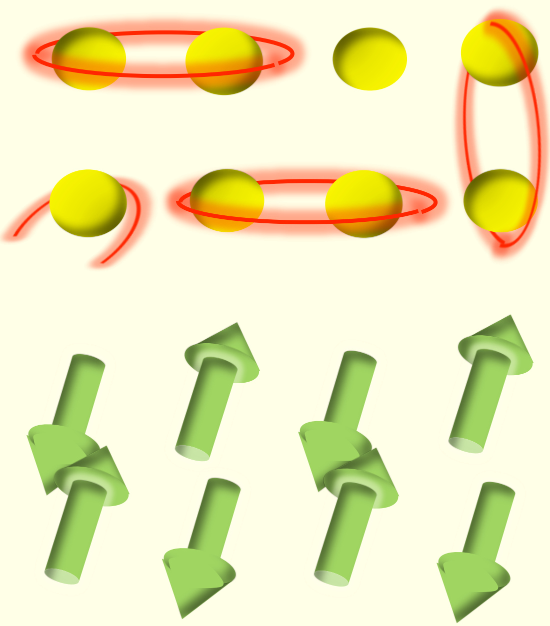
Competition between SDW and SC: coexistence or phase separation?

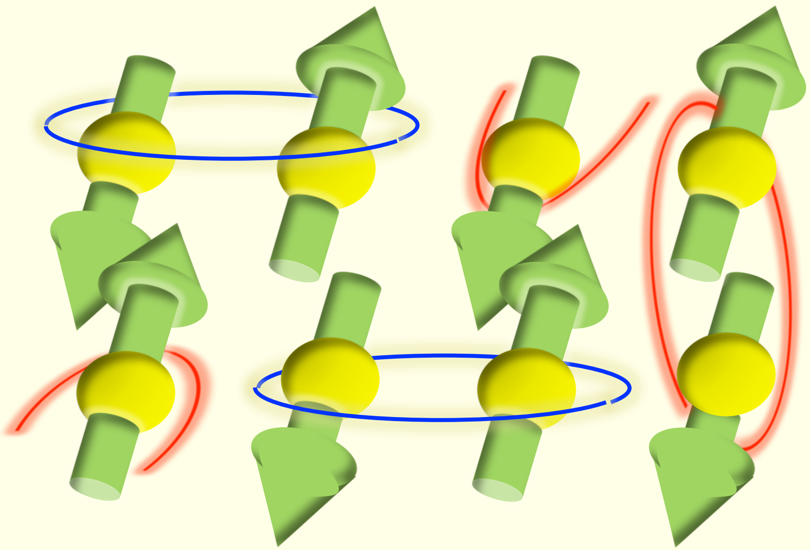
- In some conventional superconductors, magnetism can only coexist with superconductivity when the two phenomena involve *different* electrons



Competition between SDW and SC: coexistence or phase separation?

- In some conventional superconductors, magnetism can only coexist with superconductivity when the two phenomena involve *different* electrons
  - here, the electrons that cause magnetism are the *same* that cause superconductivity





J Schmalian, Physik Journal

Competition between SDW and SC: phenomenological model

$$F\left[M,\Delta\right]=\frac{a_m}{2}M^2+\frac{u_m}{4}M^4+\frac{a_s}{2}\left|\Delta\right|^2+\frac{u_s}{4}\left|\Delta\right|^4+\frac{\gamma}{2}\left|\Delta\right|^2M^2$$

Competition between SDW and SC: phenomenological model

$$F[M,\Delta]=\frac{a_m}{2}M^2+\frac{u_m}{4}M^4+\frac{a_s}{2}|\Delta|^2+\frac{u_s}{4}|\Delta|^4+\frac{\gamma}{2}|\Delta|^2M^2$$

- Minimization with respect to M leads to

$$a_m+u_mM^2=-\gamma|\Delta|^2$$

and we obtain the effective free energy

<0 : first-order

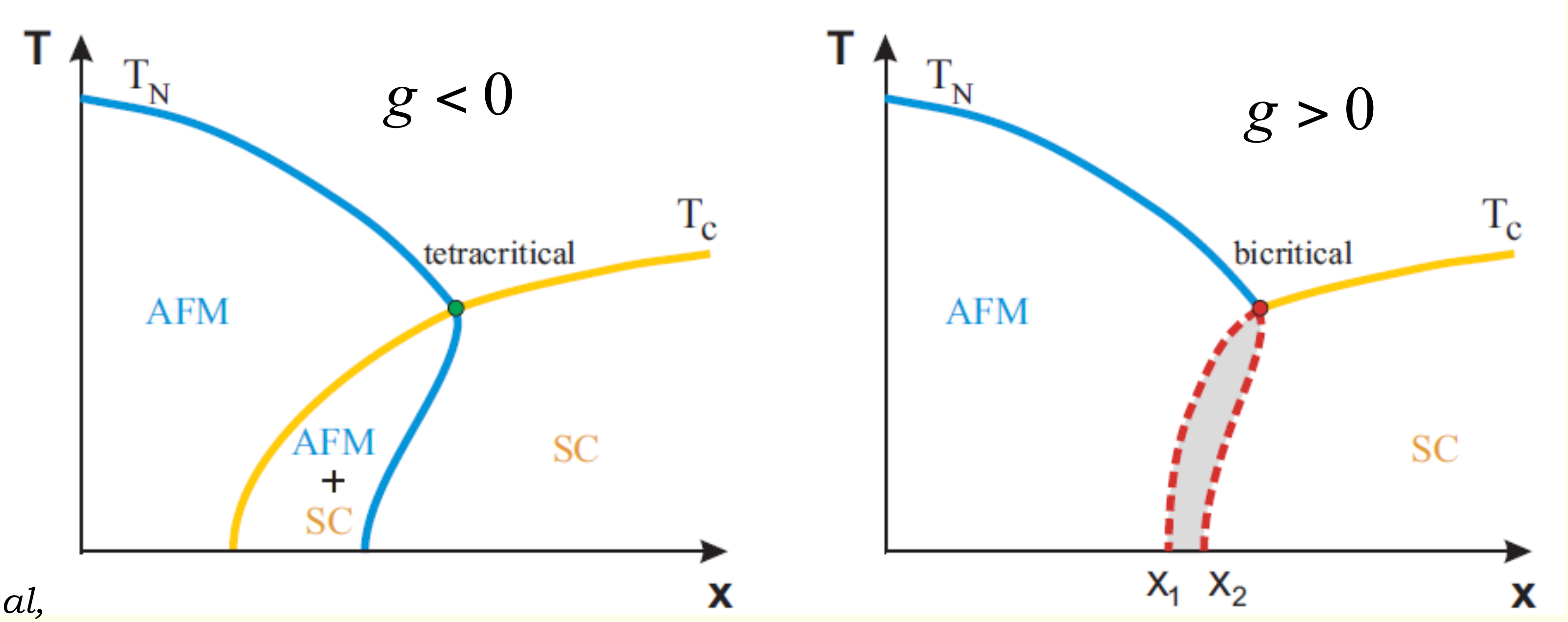
$$F[\Delta]=-\frac{a_m^2}{4u_m}+\frac{a_s}{2}\left(1-\frac{a_m\gamma}{a_su_m}\right)|\Delta|^2+\frac{u_s}{4}\left(\underbrace{1-\frac{\gamma^2}{u_su_m}}\right)|\Delta|^4$$

>0 : second-order

Competition between SDW and SC: phenomenological model

$$F[M,\Delta] = \frac{a_m}{2}M^2 + \frac{u_m}{4}M^4 + \frac{a_s}{2}|\Delta|^2 + \frac{u_s}{4}|\Delta|^4 + \frac{\gamma}{2}|\Delta|^2 M^2$$

$$g = \frac{\gamma}{\sqrt{u_m u_s}} - 1$$



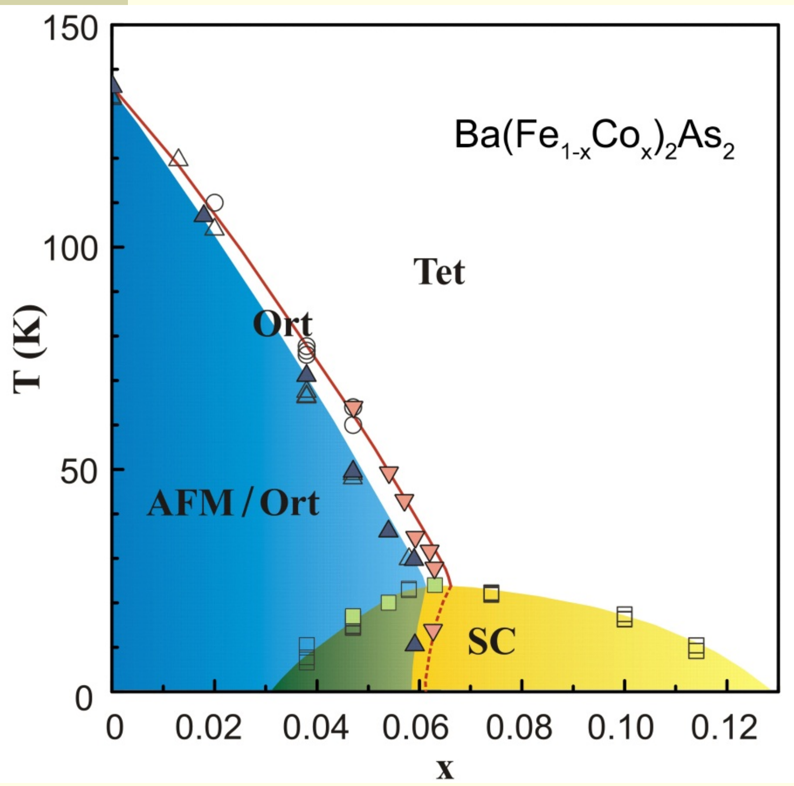
Kosterlitz et al, PRB (1976)

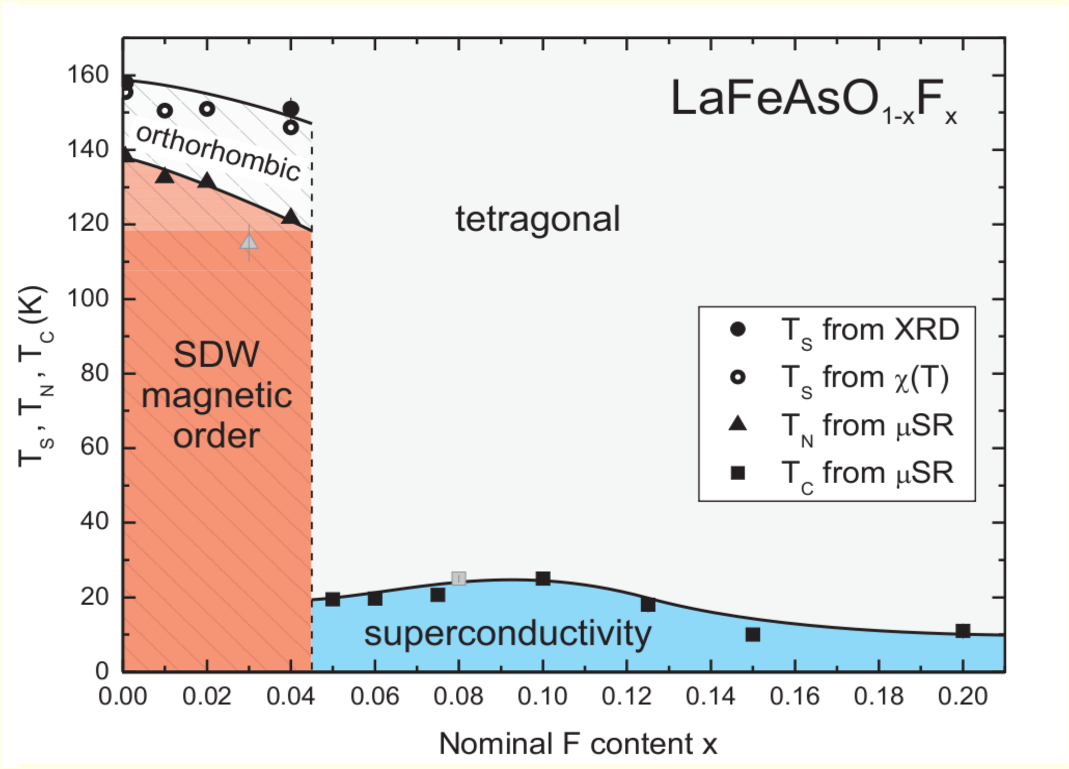
coexistence **phase separation**

Competition between SDW and SC: phenomenological model

$$F[M,\Delta]=\frac{a_m}{2}M^2+\frac{u_m}{4}M^4+\frac{a_s}{2}|\Delta|^2+\frac{u_s}{4}|\Delta|^4+\frac{\gamma}{2}|\Delta|^2M^2$$

$g<0$ $g>0$

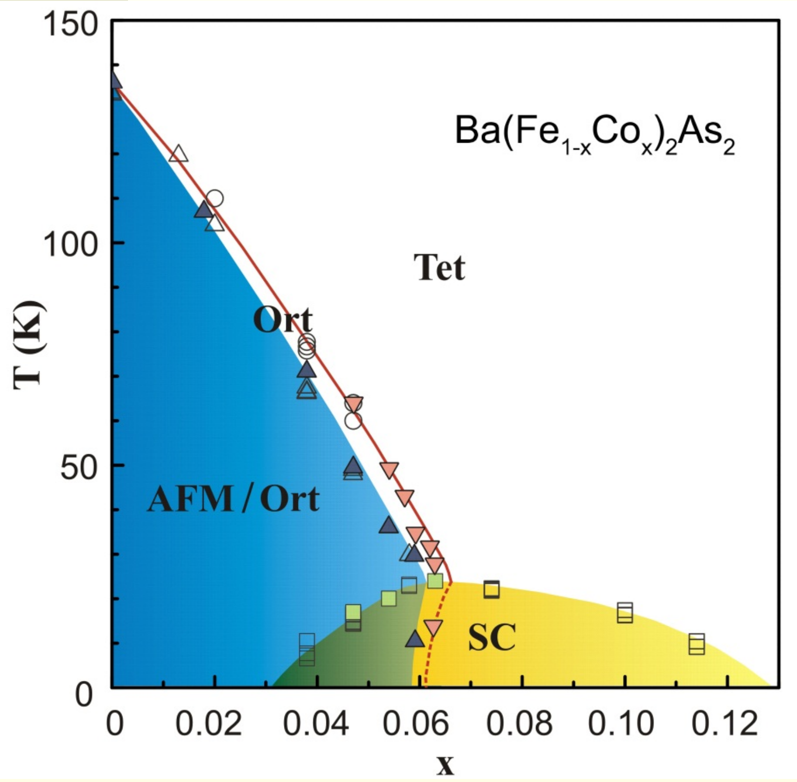


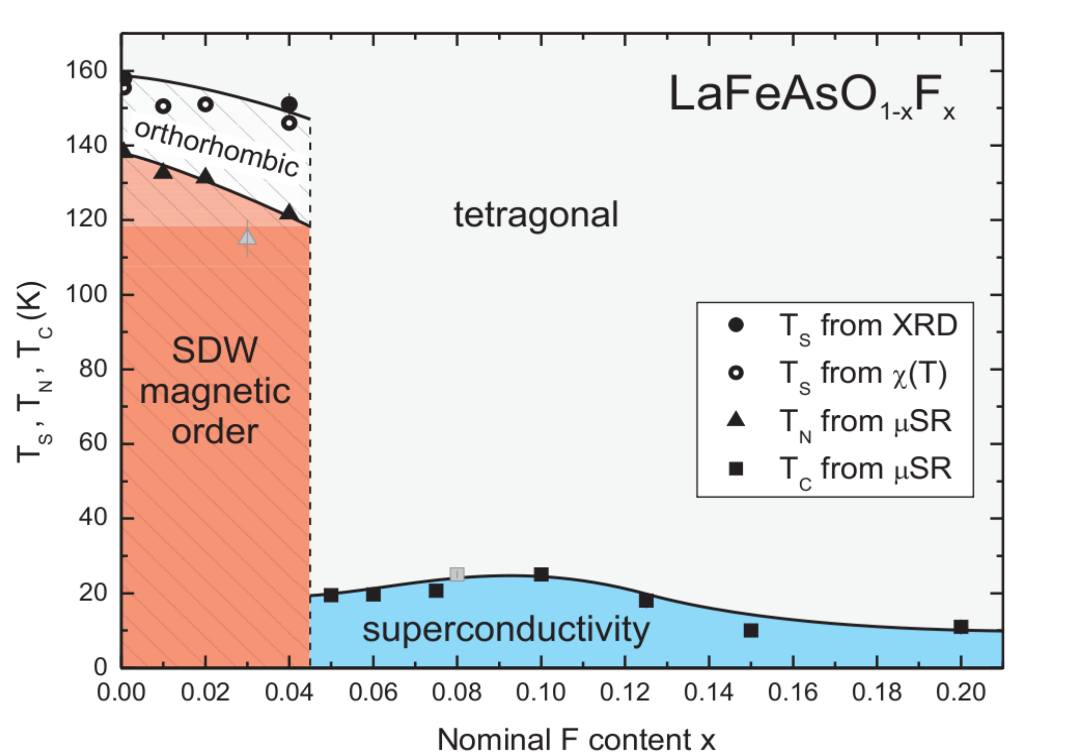


Competition between SDW and SC: phenomenological model

How to describe this competition from a microscopic model?

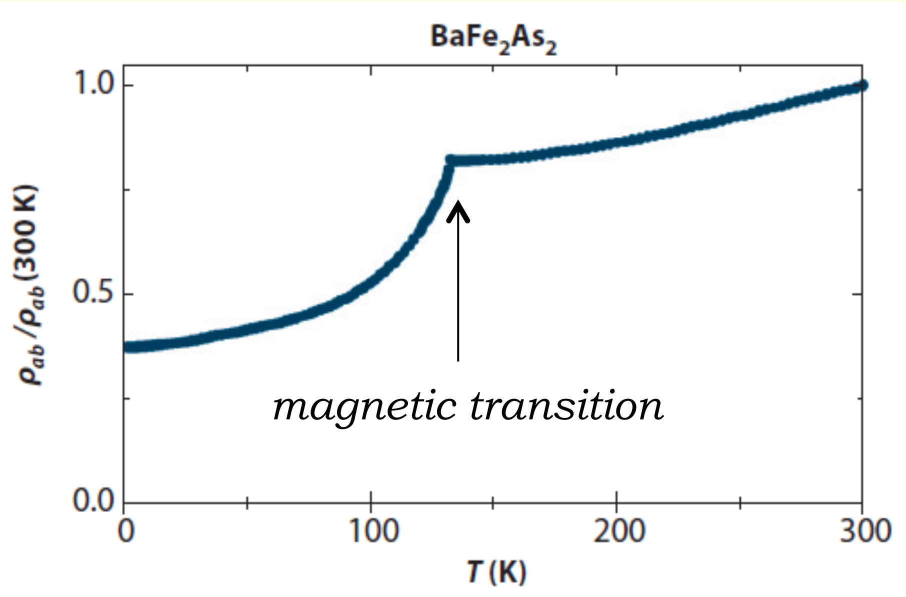
$g < 0$ $g > 0$



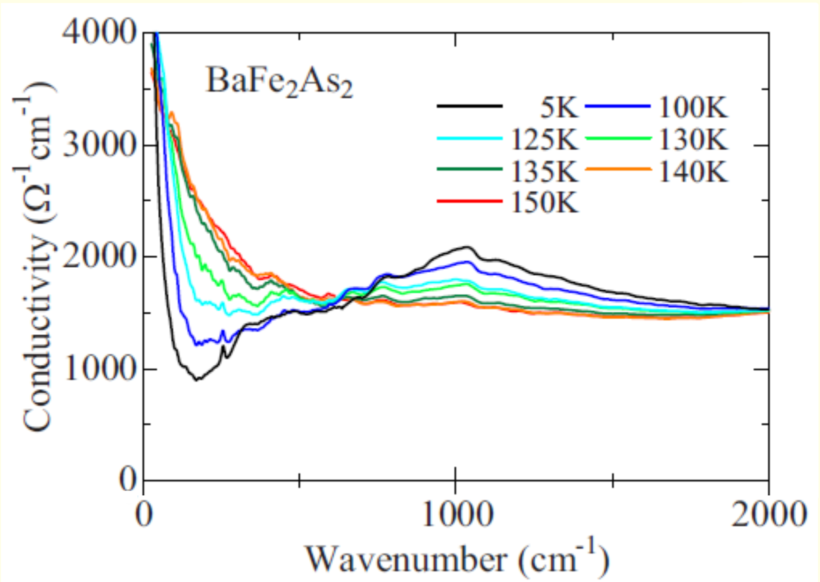


Magnetic state: itinerant approach

- Experiments reveal that these systems are better described as metallic itinerant magnets



Canfield et al, ARCMP (2010)

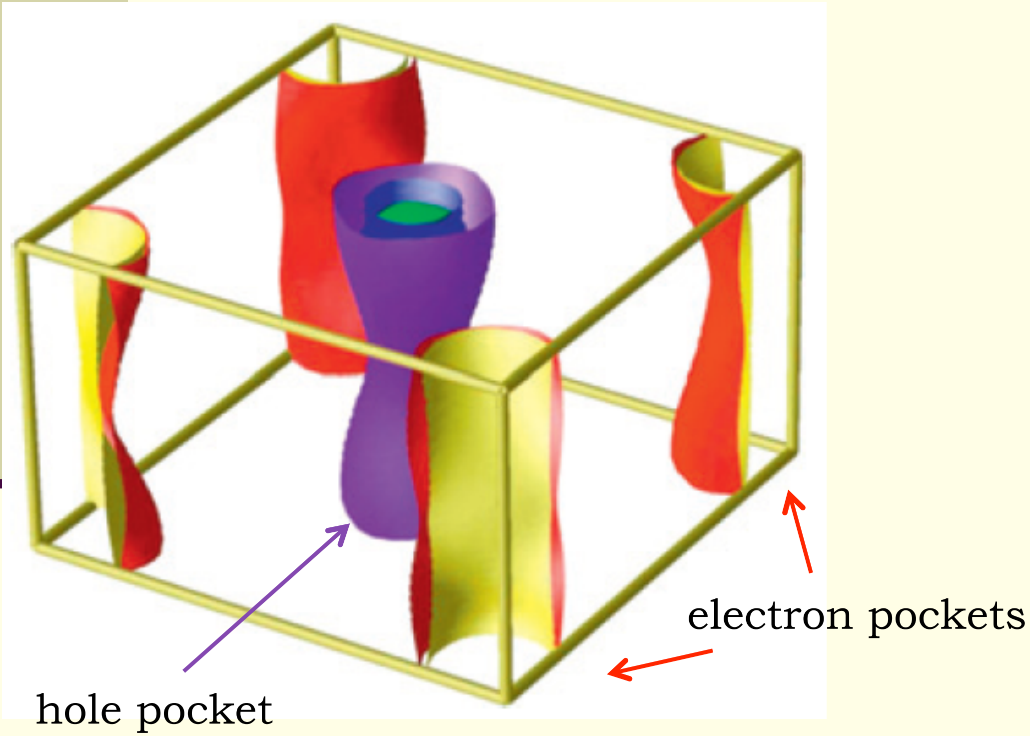


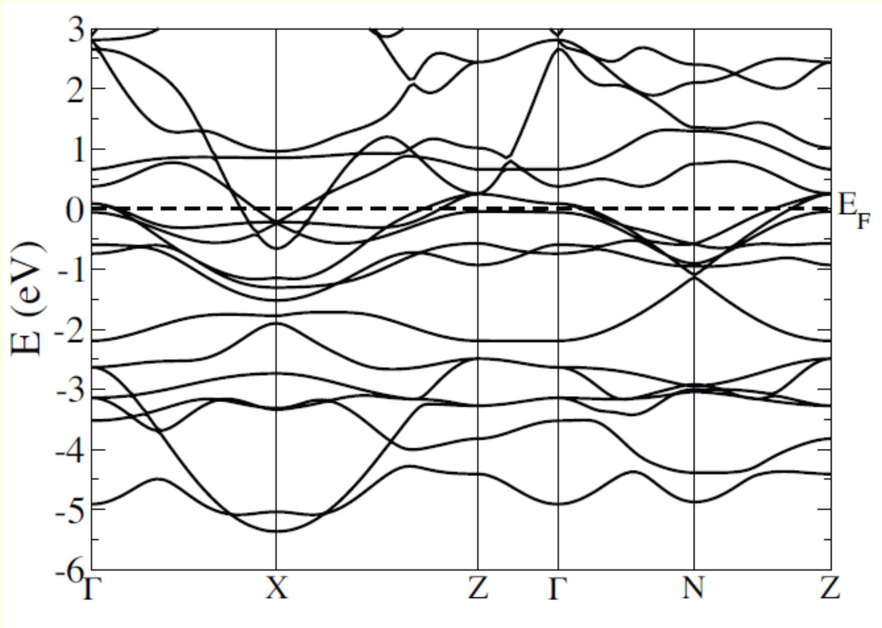
Nakajima et al, PRB (2010)

- ➢ conduction electrons are responsible for the magnetism

Iron pnictides: band structure

- DFT calculations: Fermi surface has multiple sheets
  - $3d^6$ configuration: several orbitals cross the Fermi level



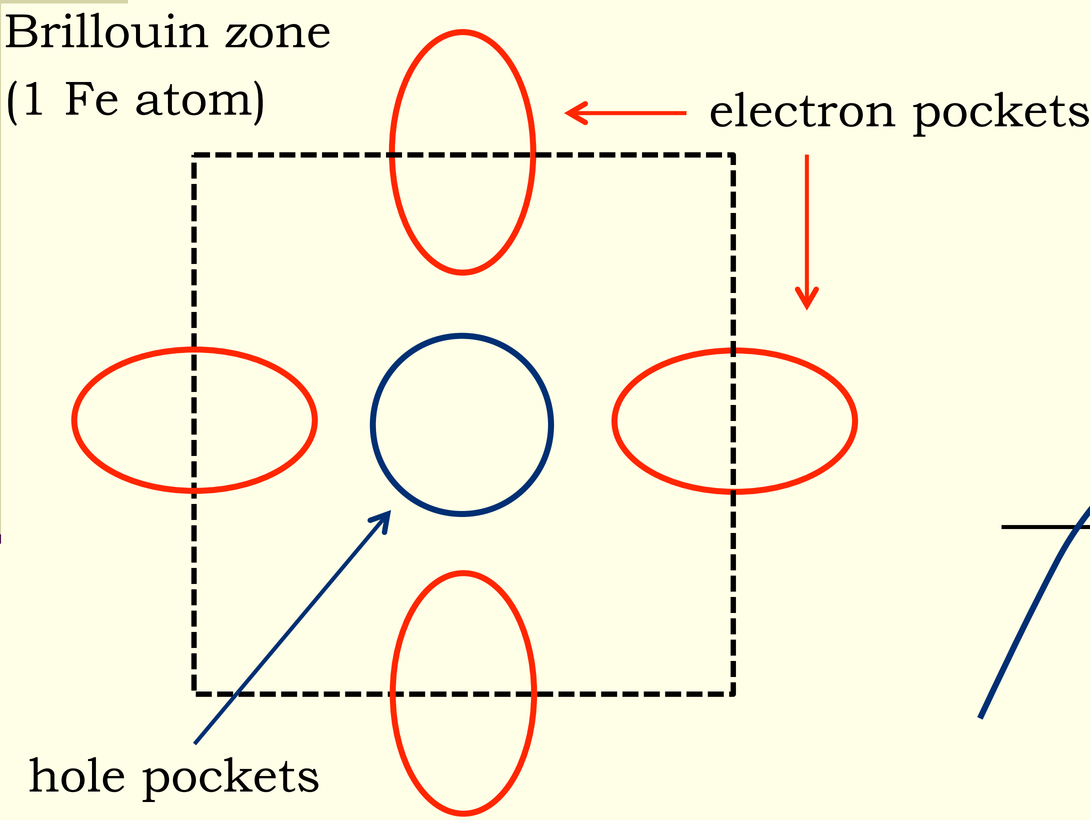


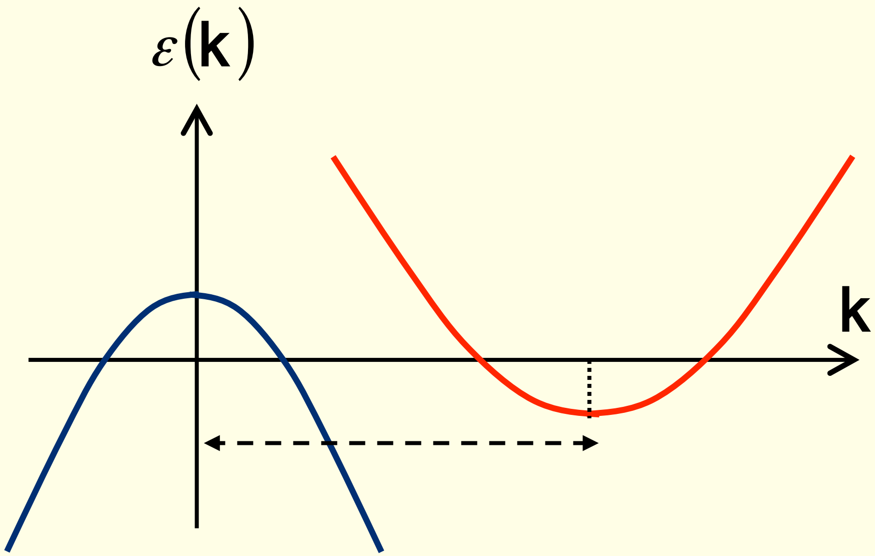
Paglione and Greene, Nature Phys (2010)

Zhang and Singh, PRB (2009)

Iron pnictides: band structure

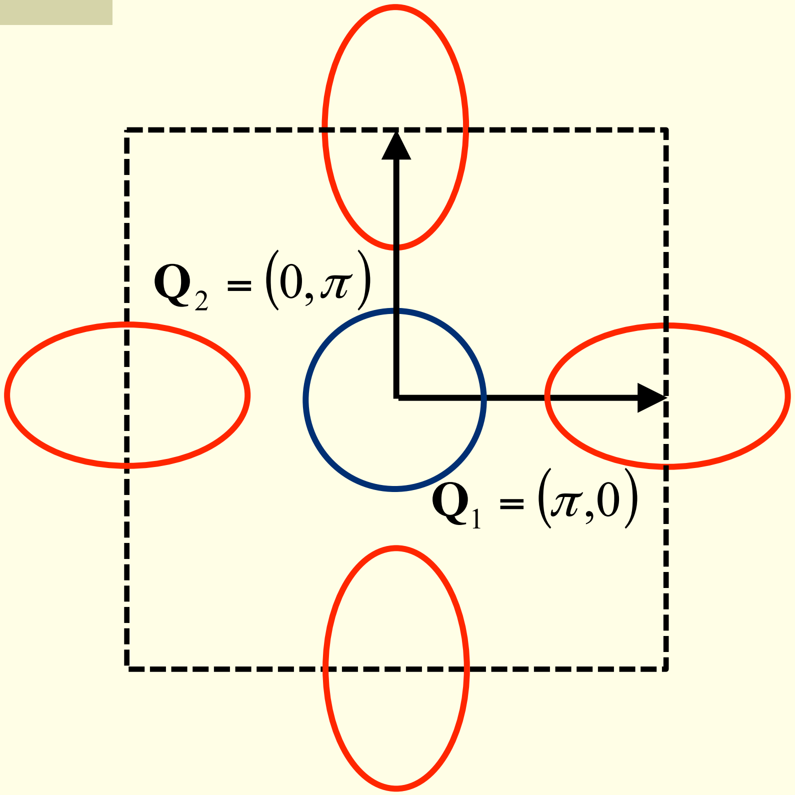
- Fermi surface of the iron pnictides (theorist view):

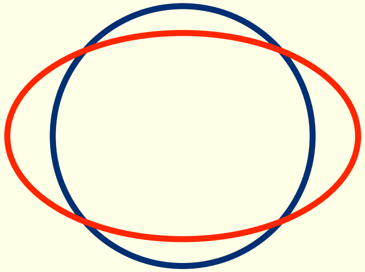




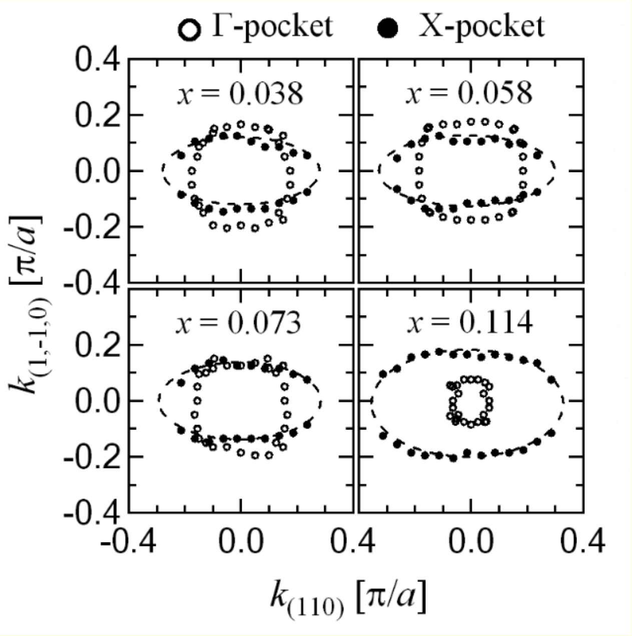
Iron pnictides: itinerant magnetism

- Bands have good nesting features: Stoner magnetism





$$\chi_0(Q) \approx \log \frac{E_F}{T}$$

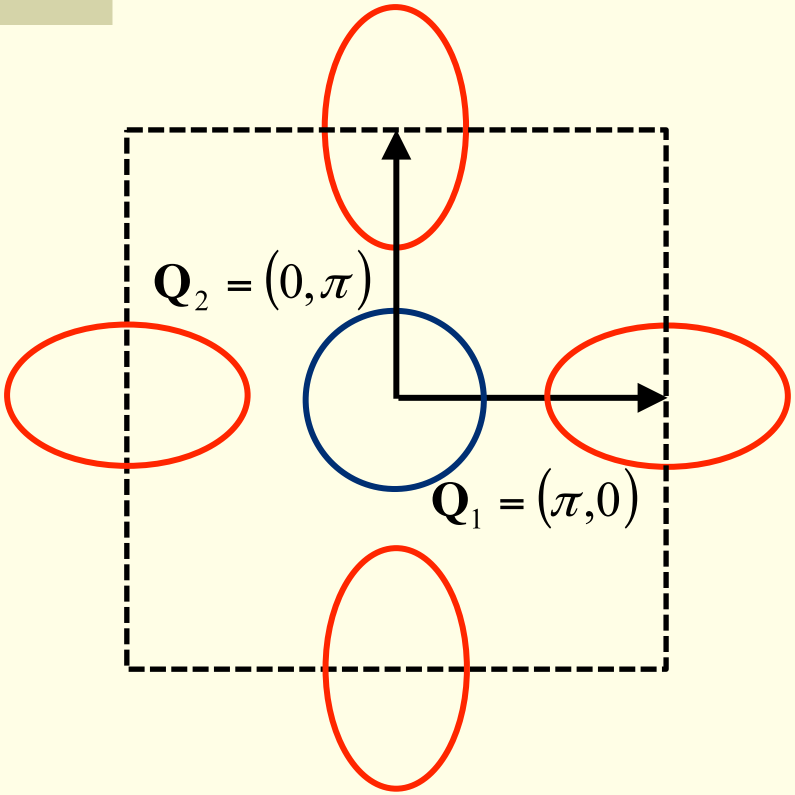


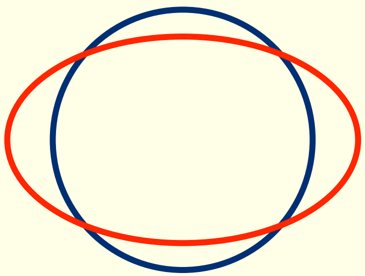
ARPES data

Liu, Kondo, RMF *et al, Nature Phys.* ***6****, 419 (2010)*

Iron pnictides: itinerant magnetism

- Bands have good nesting features: Stoner magnetism





$$\chi_0(Q) \approx \log \frac{E_F}{T}$$

include interaction:

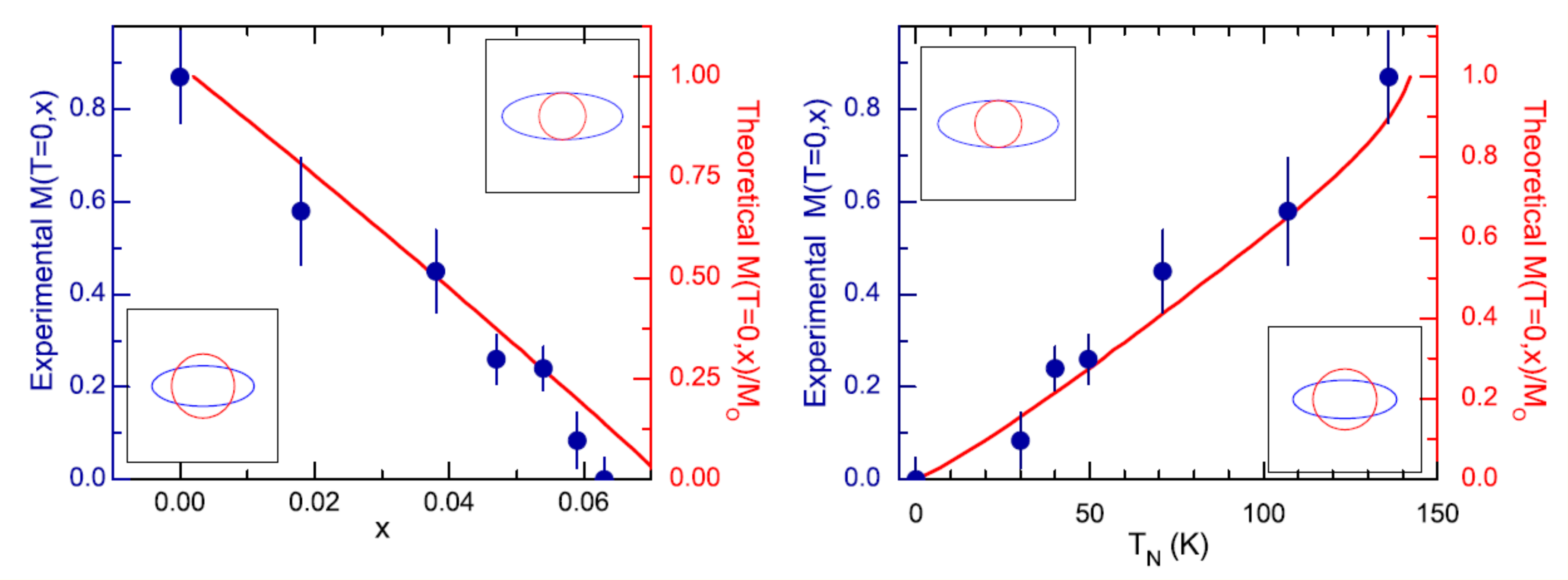
$$\chi(Q) = \frac{\chi_0(Q)}{1 - U\,\chi_0(Q)}$$

small electronic interaction can lead to a magnetically ordered state (SDW) with ordering vector *Q_i*

Iron pnictides: itinerant magnetism

- Quantitative agreement with experimental data

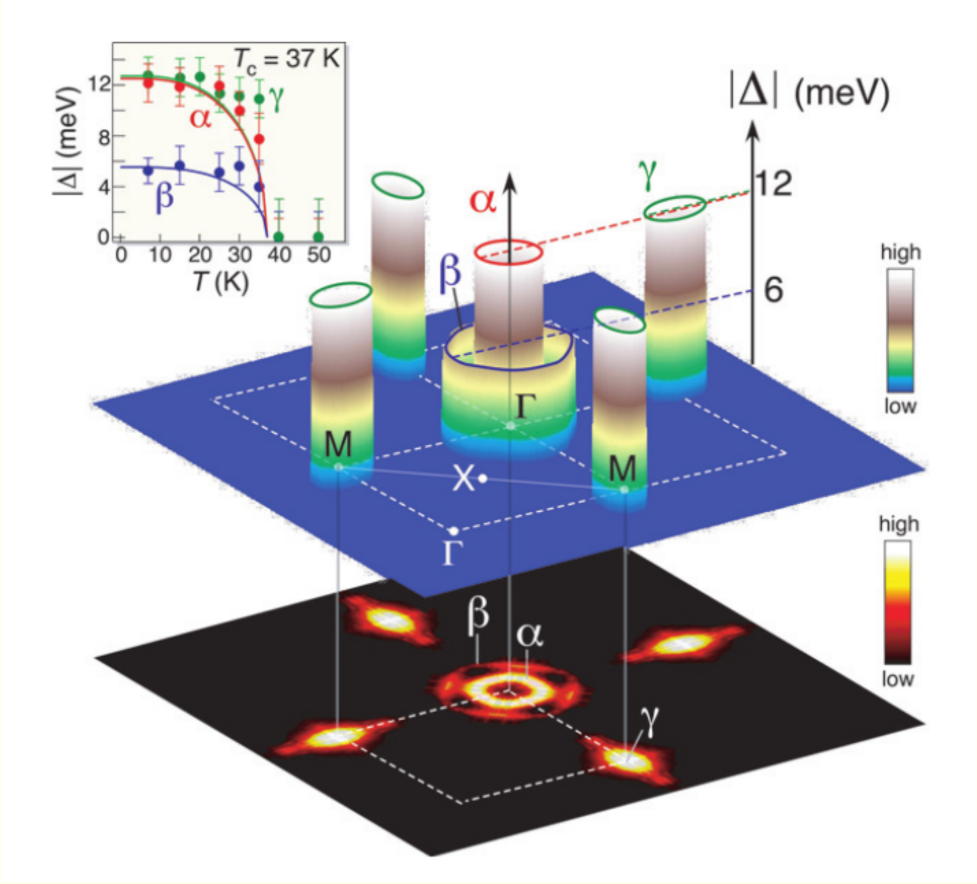
$$H_{\rm SDW} = -\sum_{\mathbf{k},\sigma} \sigma \mathrm{M}\left(c^{+}_{\mathbf{k}+\mathbf{q}\sigma} d_{\mathbf{k}\sigma} + d^{+}_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma}\right)$$

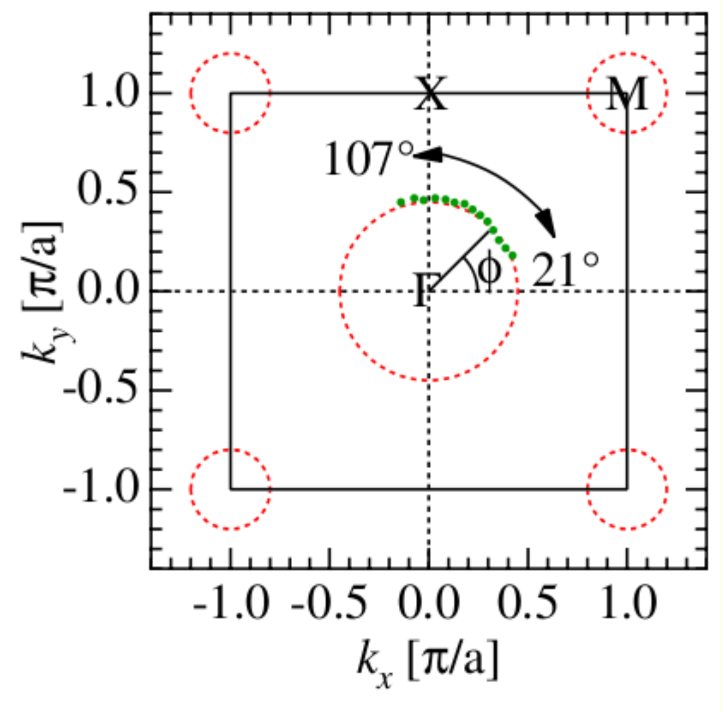


RMF *et al, Phys. Rev. B* ***81****, 140501(R) (2010)*

Iron pnictides: superconducting state

- ARPES: amplitude of the gaps, but not their relative sign





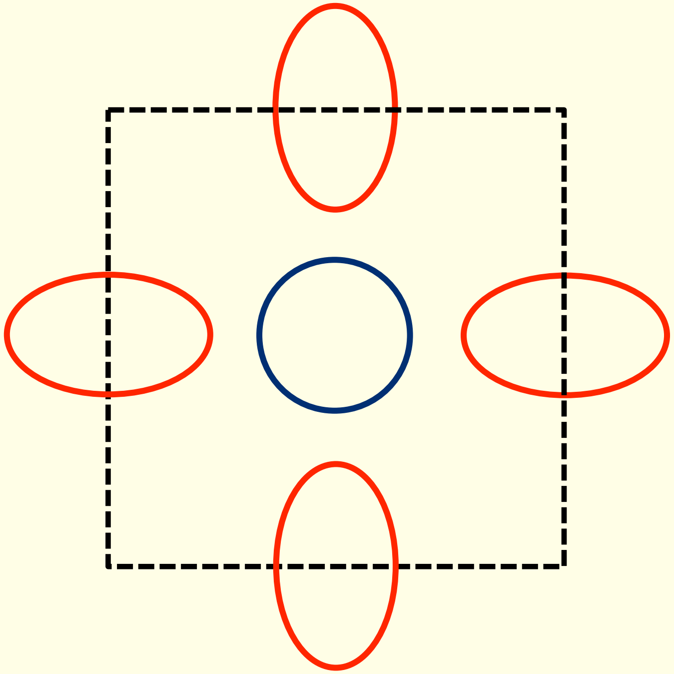
Kondo et al, PRL (2008)

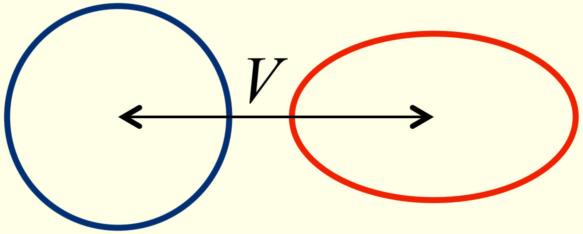
Ding et al, EPL (2008)

Iron pnictides: candidates for the SC state

- Pairing problem in a simplified two-band model

$$H_{\mathrm{SC}} = -\sum_{\mathbf{k}+\mathbf{Q}} \Delta_1 \left(c^+_{\mathbf{k}\uparrow} c^+_{-\mathbf{k}\downarrow} + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \right) - \sum_{\mathbf{k}} \Delta_2 \left(d^+_{\mathbf{k}\uparrow} d^+_{-\mathbf{k}\downarrow} + d_{-\mathbf{k}\downarrow} d_{\mathbf{k}\uparrow} \right)$$





$$\begin{cases} \Delta_1 = -V N_2 \Delta_2 \ln\left(\dfrac{\Lambda}{T_c} \right) \\ \Delta_2 = -V N_1 \Delta_1 \ln\left(\dfrac{\Lambda}{T_c} \right) \end{cases}$$

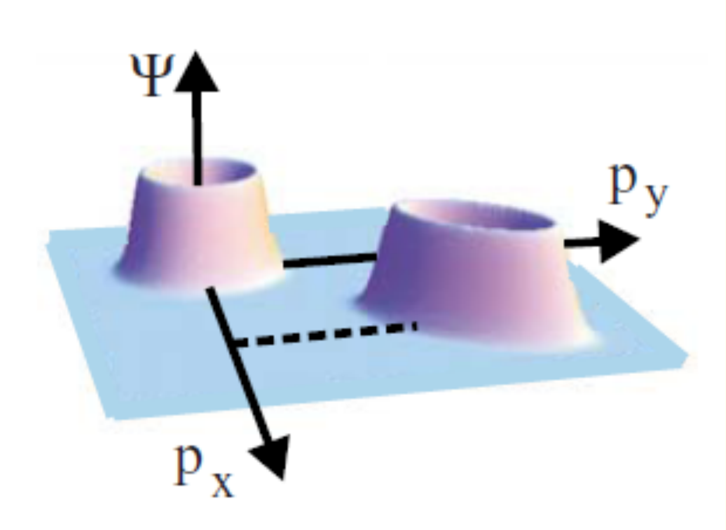
Iron pnictides: candidates for the SC state

- Pairing due to conventional attractive electron-phonon interaction (enhanced by charge/orbital fluctuations)

$$V < 0$$

Kontani & Onari, PRL (2010)

s^{++} **state**



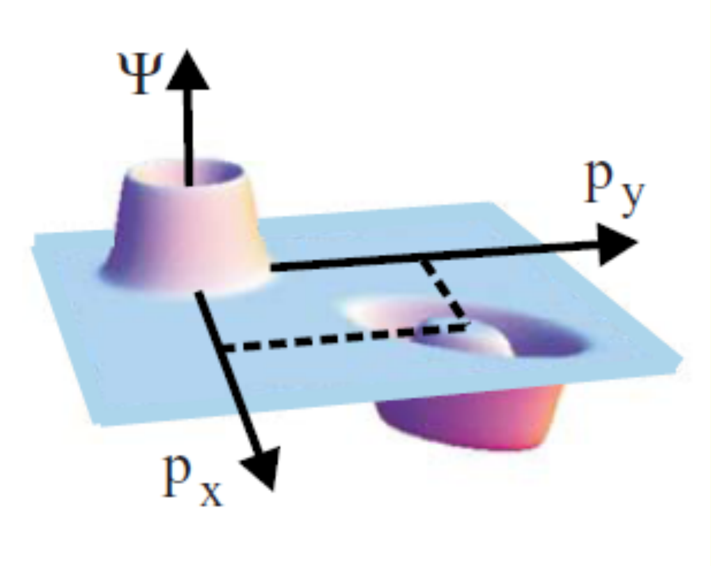
$$\begin{cases} \Delta_1 > 0 \\ \Delta_2 > 0 \end{cases}$$

Iron pnictides: candidates for the SC state

- Pairing due to purely repulsive electronic interaction (enhanced by spin fluctuations)

$$V > 0$$

s^{+-} state

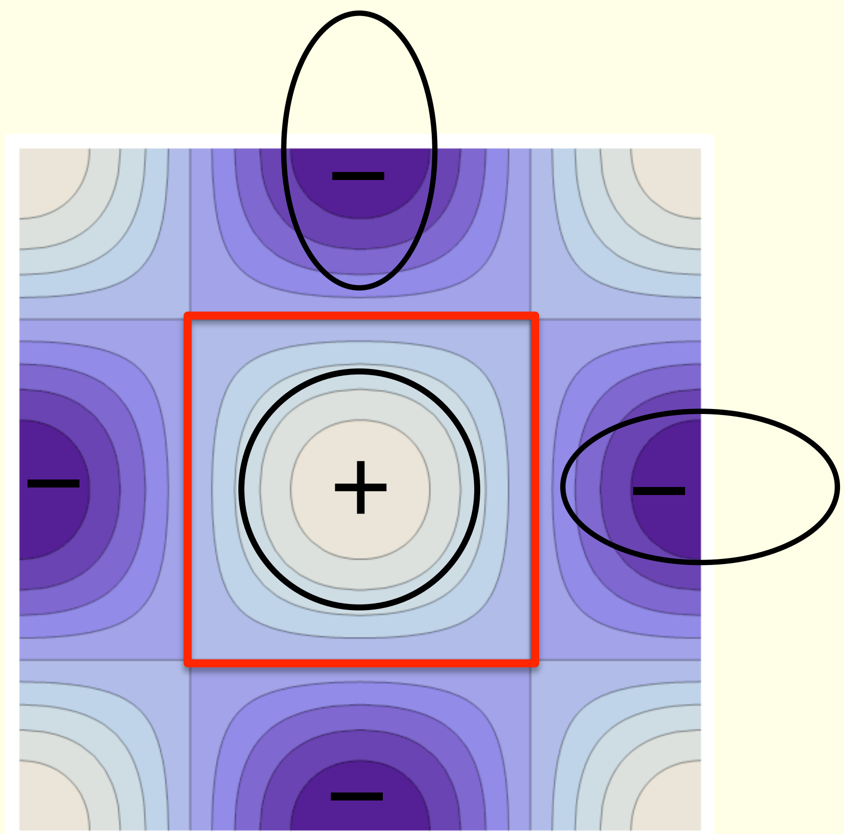


$$\begin{cases} \Delta_1 > 0 \\ \Delta_2 < 0 \end{cases}$$

Mazin et al, PRL (2008)
Kuroki et al, PRL (2008)
Chubukov et al, PRB (2008)
Cvetkovic et al, EPL (2009)
Wang et al, PRL (2009)
Sknepnek et al, PRB (2009)
Graser et al, NJP (2009)

Iron pnictides: candidates for the SC state

- In the s^{+-} state, the position of the gap function zeros is not enforced by symmetry



Competition between SDW and SC: microscopic model

- Hertz-Millis approach to the two-band model

$$H = H_0 + H_{\mathrm{SDW}} + H_{\mathrm{SC}}$$

$$\begin{cases} H_0 = \sum_{\mathbf{k},\sigma} \left(\varepsilon_{1,\mathbf{k+Q}} - \mu\right) c^+_{\mathbf{k+Q}\sigma} c_{\mathbf{k+Q}\sigma} + \sum_{\mathbf{k},\sigma} \left(\varepsilon_{2,\mathbf{k}} - \mu\right) d^+_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma} \\ H_{\mathrm{SDW}} = -\sum_{\mathbf{k},\sigma} \sigma \mathrm{M} \left(c^+_{\mathbf{k+q}\sigma} d_{\mathbf{k}\sigma} + d^+_{\mathbf{k}\sigma} c_{\mathbf{k+q}\sigma} \right) \\ H_{\mathrm{SC}} = -\sum_{\mathbf{k+Q}} \Delta_1 \left(c^+_{\mathbf{k}\uparrow} c^+_{\mathbf{-k}\downarrow} + c_{\mathbf{-k}\downarrow} c_{\mathbf{k}\uparrow} \right) - \sum_{\mathbf{k}} \Delta_2 \left(d^+_{\mathbf{k}\uparrow} d^+_{\mathbf{-k}\downarrow} + d_{\mathbf{-k}\downarrow} d_{\mathbf{k}\uparrow} \right) \end{cases}$$

Competition between SDW and SC: microscopic model

- We can then **derive** the Ginzburg-Landau coefficients

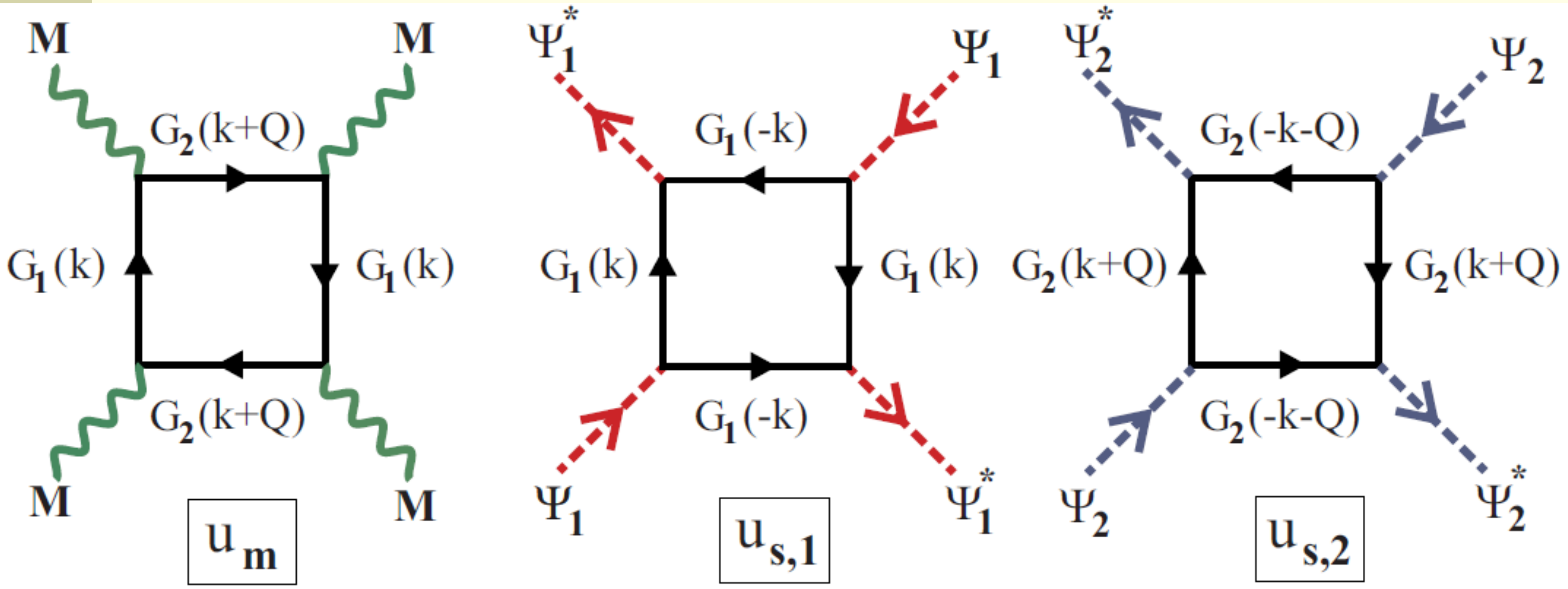
$$F[M,\Delta] = \frac{a_m}{2} M^2 + \frac{u_m}{4} M^4 + \frac{a_s}{2} |\Delta|^2 + \frac{u_s}{4} |\Delta|^4 + \frac{\gamma}{2} |\Delta|^2 M^2$$

$$g = \frac{\gamma}{\sqrt{u_m u_s}} - 1$$

Competition between SDW and SC: microscopic model

- We can then **derive** the Ginzburg-Landau coefficients

$$\longrightarrow \equiv G_i(\mathbf{k},\omega_n) = \frac{1}{i\omega_n - \xi_{i,\mathbf{k}}}$$



Competition between SDW and SC: microscopic model

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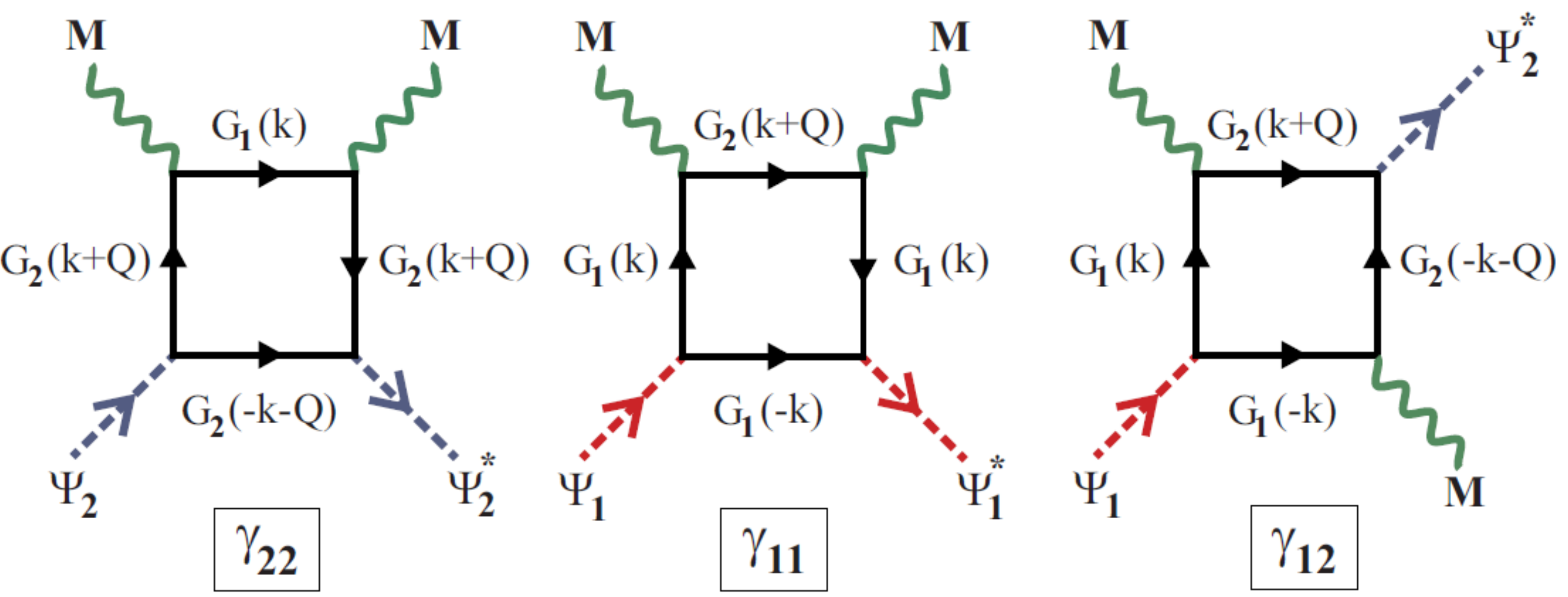
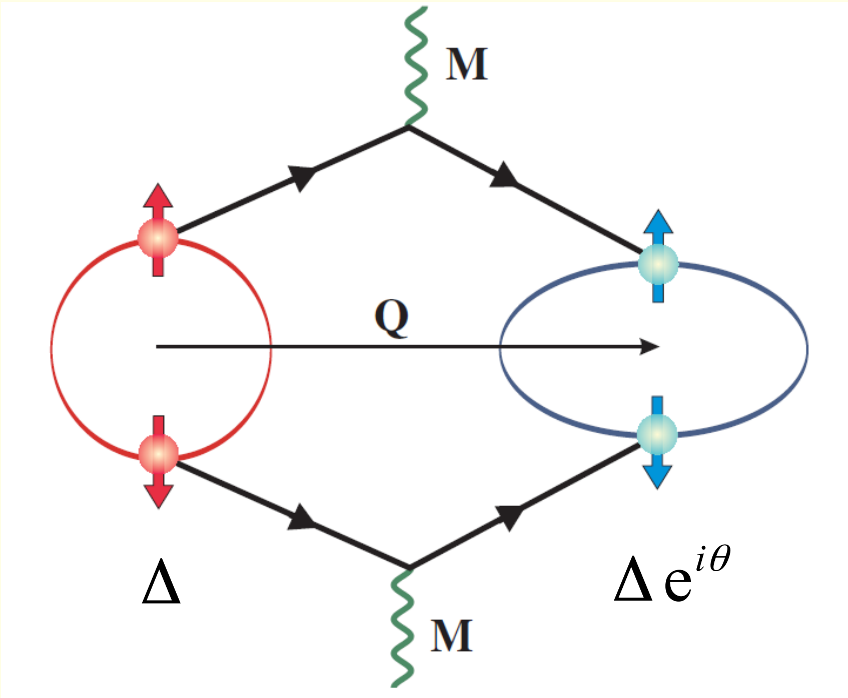


Competition between SDW and SC: microscopic model

- Strength of the competition term depends on the symmetry of the superconducting state



$$\gamma_{12} \propto M^2 |\Delta|^2 \cos\theta \quad \begin{cases} \theta = 0 & s^{++} \text{ state} \\ \theta = \pi & s^{+-} \text{ state} \end{cases}$$

RMF and Schmalian, PRB (2010)
Vorontsov, Vavilov, and Chubukov, PRB (2010)

Coexistence between SDW and SC: perfect nesting

- For perfect nesting:

$$F = \frac{a}{2}\left(|\Delta|^2 + M^2\right) + \frac{u}{4}\left(|\Delta|^2 + M^2\right)^2 + g\,u|\Delta|^2 M^2$$

$$g = \frac{1+\cos\theta}{2}$$

s^{+-} state: $g = 0$
borderline

s^{++} state: $g = 1$
phase separation

Coexistence between SDW and SC: perfect nesting

- For perfect nesting:

$$F = \frac{a}{2}\left(|\Delta|^2 + M^2\right) + \frac{u}{4}\left(|\Delta|^2 + M^2\right)^2 + g\,u|\Delta|^2 M^2$$

s^{+-} state: $g = 0$

borderline

s^{++} state: $g = 1$

phase separation

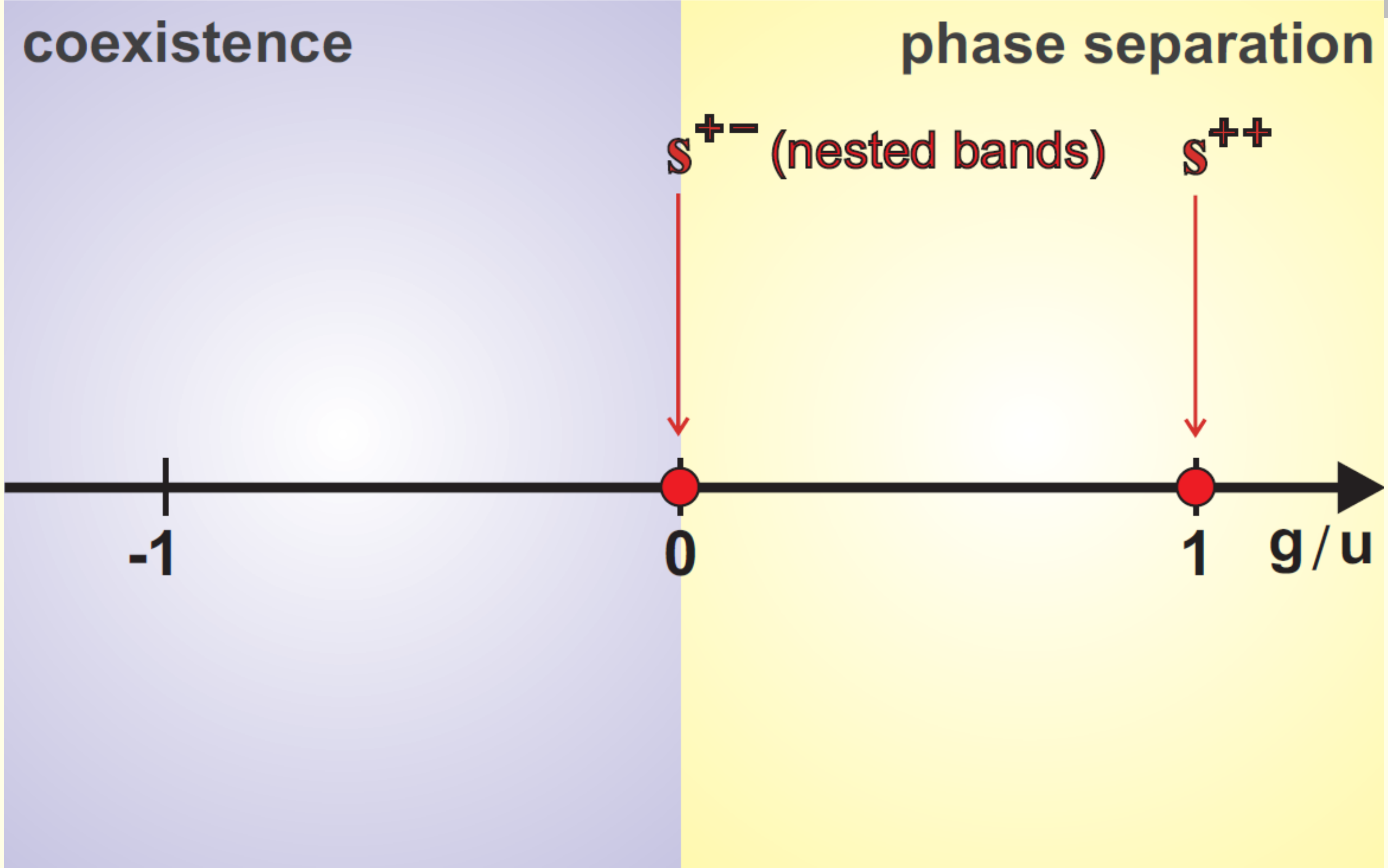
Note that $g = 0 \Rightarrow$ emergent SO(5) symmetry

$$\vec{\mathbf{N}} = \left(\mathrm{Re}\,\Delta, \mathrm{Im}\,\Delta, \mathbf{M}\right)$$

Podolsky et al, EPL (2009)

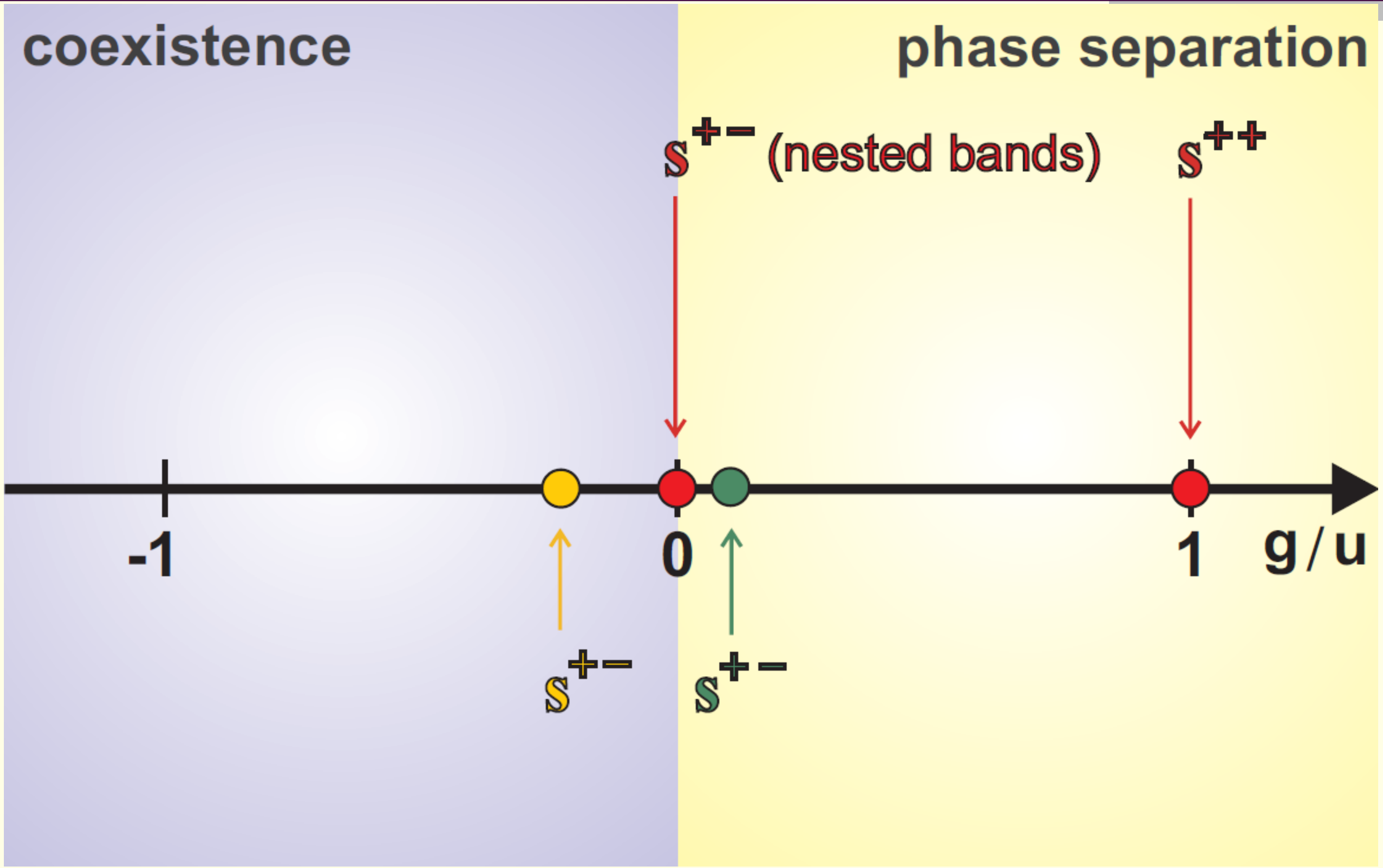
Chubukov, Physica C (2008)

Competition between SDW and SC: coexistence



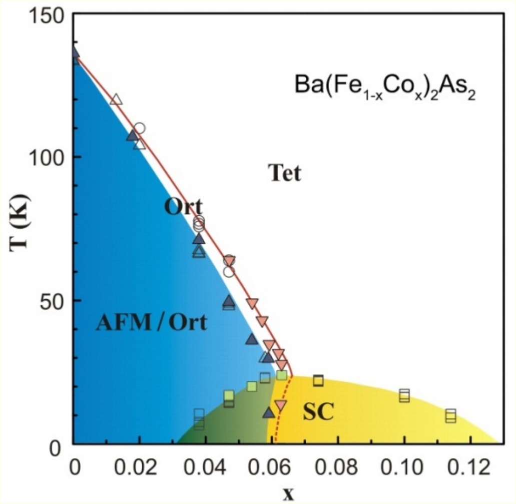
perfect nesting: $g = \dfrac{1+\cos\theta}{2}$

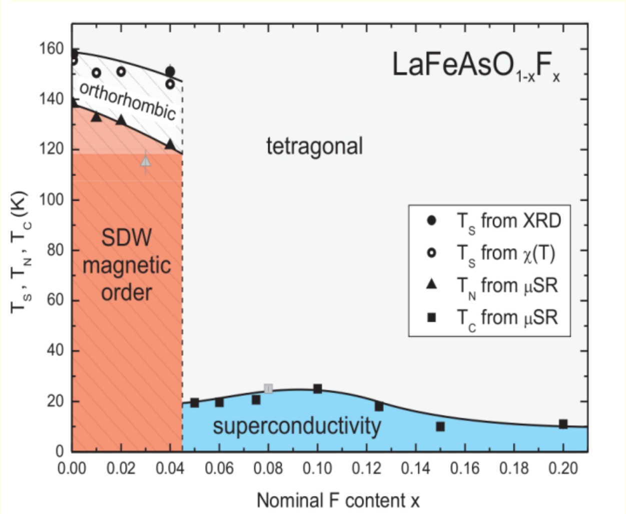
Competition between SDW and SC: coexistence



- s^{++} cannot coexist with magnetism
- s^{+-} may or may not coexist

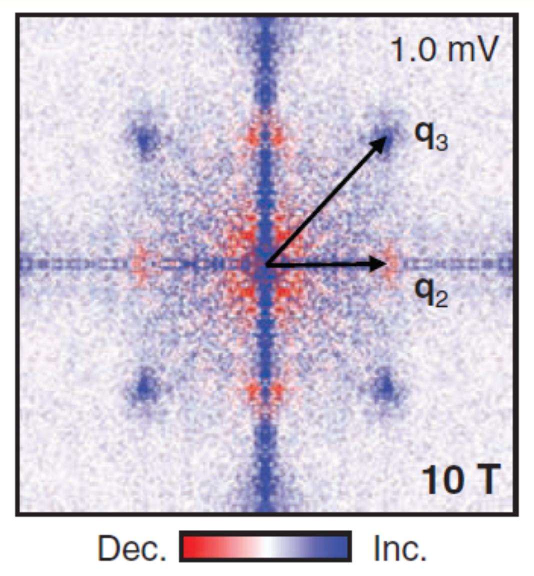
RMF et al, PRB (2010)
RMF & Schmalian, PRB (2010)





Observation of microscopic coexistence in some iron arsenides rules out the possibility of an s^{++} state

Phase sensitive STM measurements confirm that the SC state is s^{+-}



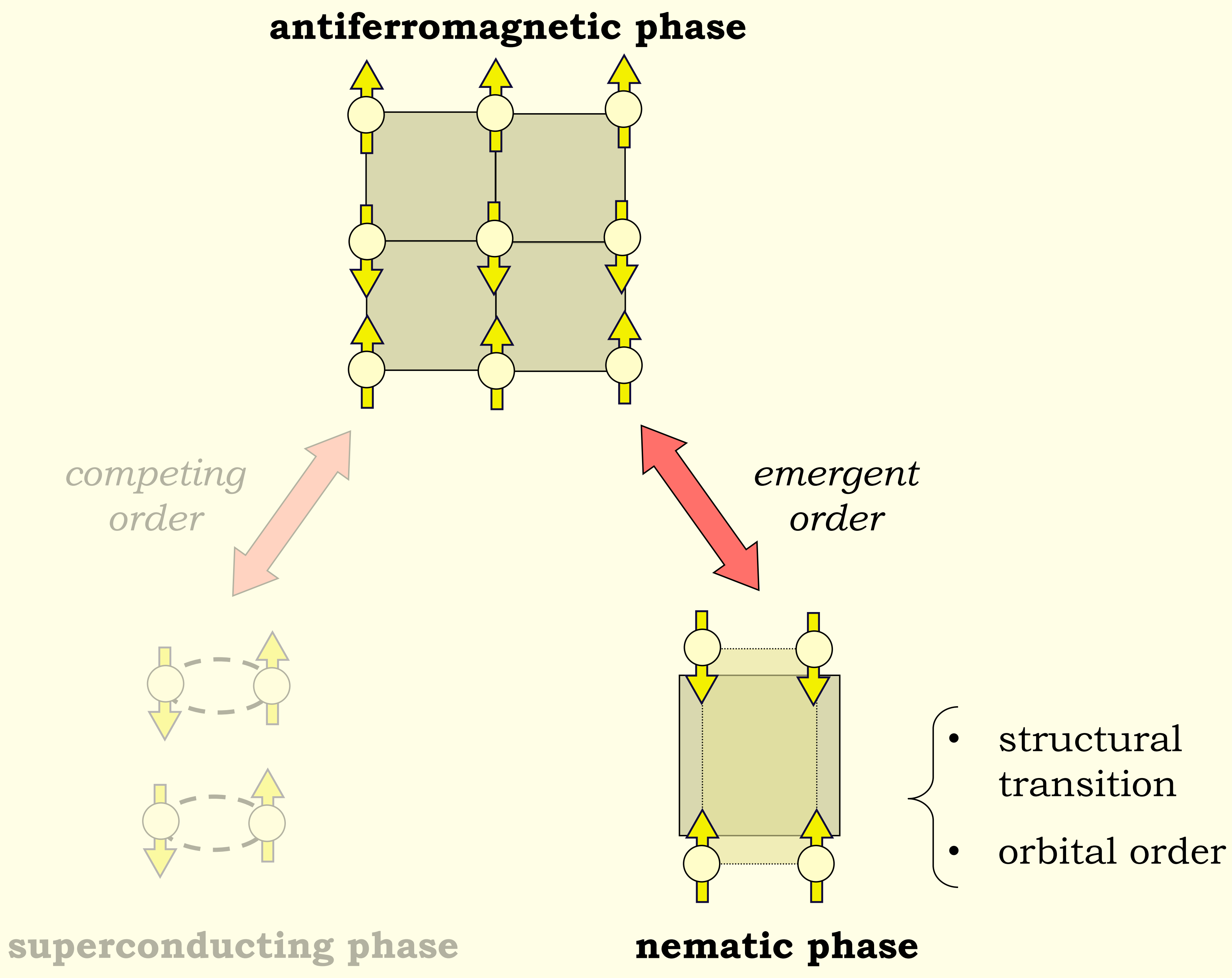
Hanaguri et al, Science (2010)

Outline

- **Brief introduction to the iron pnictides**
  - experimental evidence for competing phases

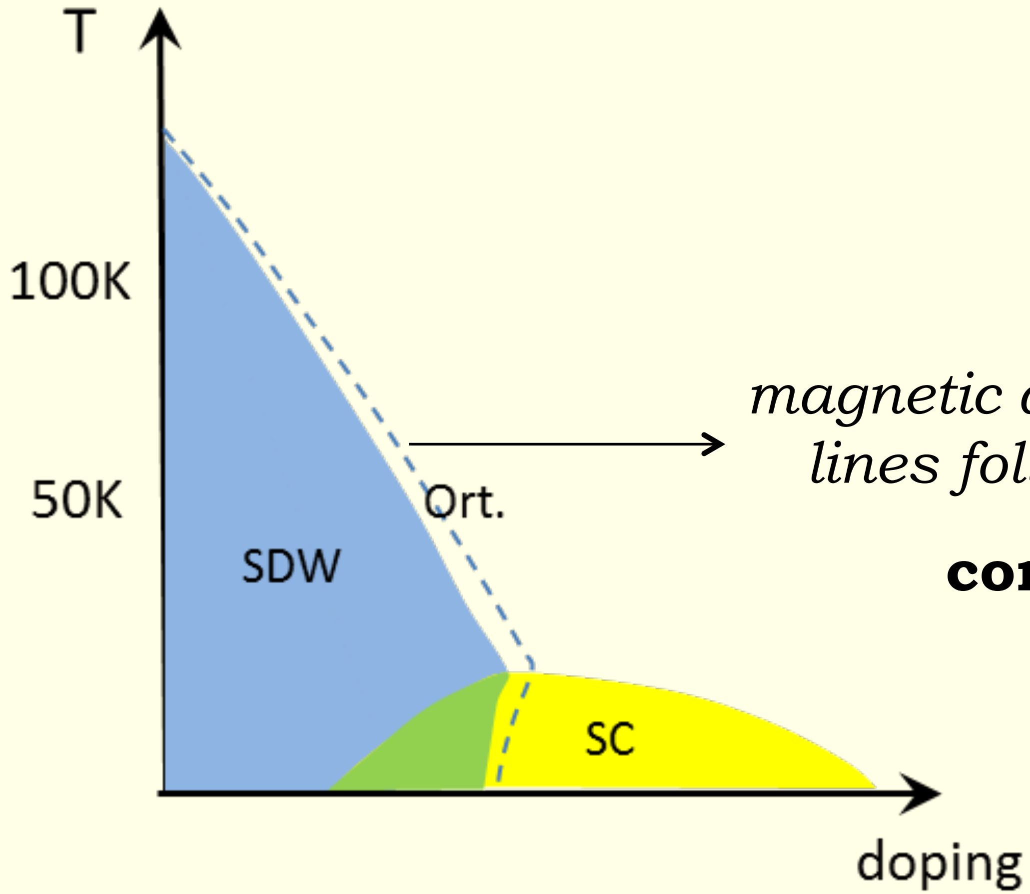
- **Competition between magnetism and superconductivity**
  - symmetry of the Cooper pair wave function

- **Competition between nematicity and superconductivity**
  - indirect competition mediated by magnetism


antiferromagnetic phase
competing order
emergent order
• structural transition
• orbital order
superconducting phase
nematic phase

Why nematics???

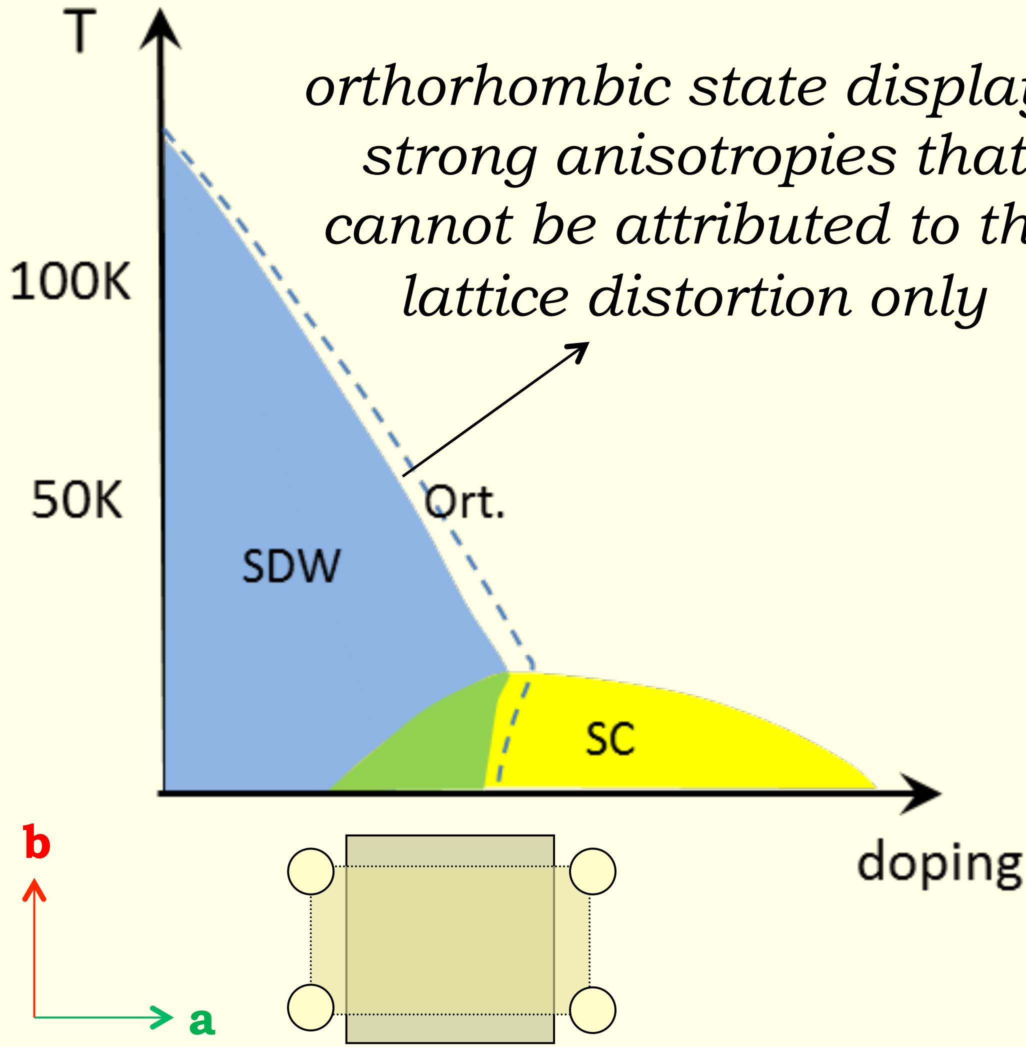
Iron pnictides: normal state properties



magnetic and structural transition lines follow closely each other

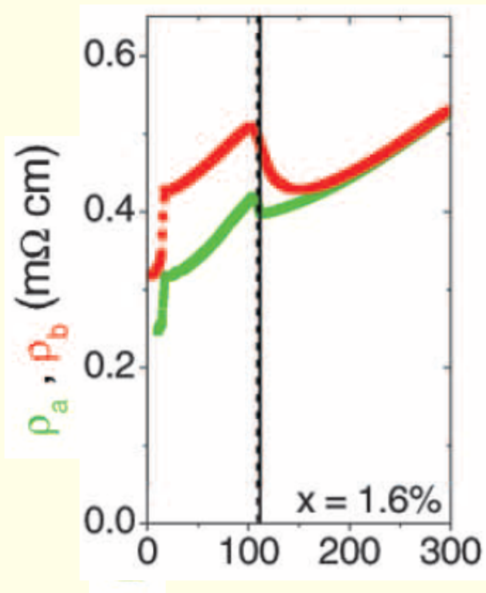
correlated phases!

Iron pnictides: normal state properties

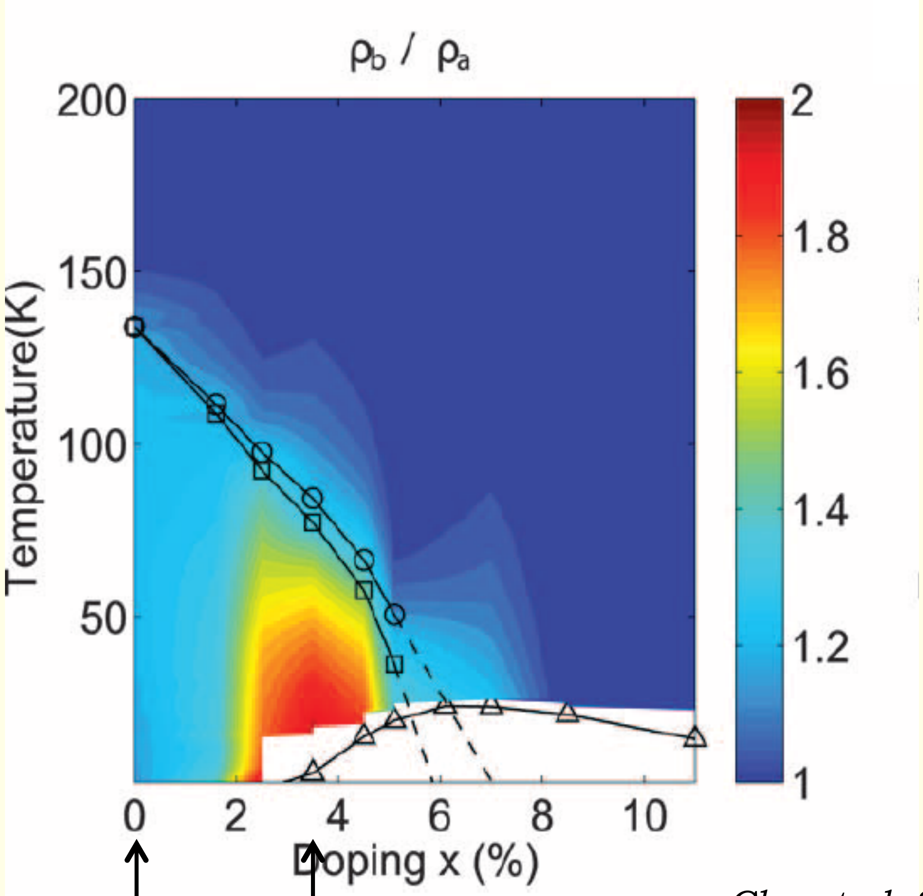


orthorhombic state displays strong anisotropies that cannot be attributed to the lattice distortion only

- **resistivity**



Chu et al, Science (2010)
Tanatar et al, PRB (2010)



Chu et al, Science (2010)

$$\frac{a-b}{a+b} \approx 0.01$$

maximum orthorhombic distortion

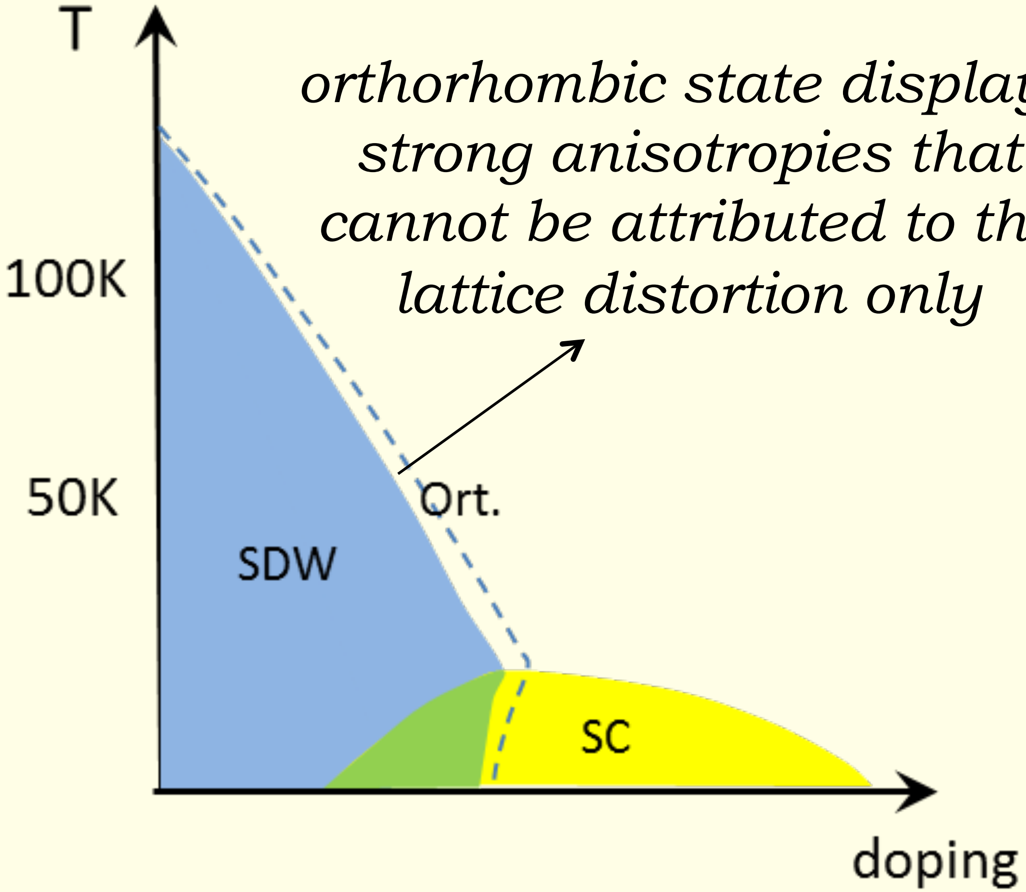
maximum resistivity anisotropy

$$\frac{\rho_b}{\rho_a} \approx 2$$

resistivity anisotropy cannot be attributed only to the orthorhombic distortion

Iron pnictides: normal state properties

orthorhombic state displays strong anisotropies that cannot be attributed to the lattice distortion only



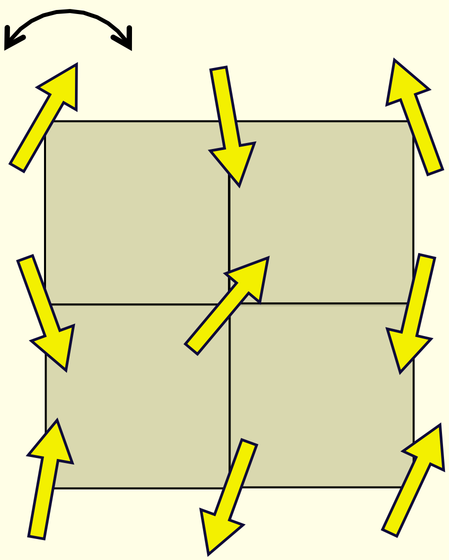
- **resistivity**
- **optical spectrum**
- **orbital polarization**
- **density of states...**

underlying electronic order that spontaneously breaks tetragonal symmetry: nematic phase

cf. Kivelson, Fradkin & Emery, Nature (1998)

Iron pnictides: nematic order

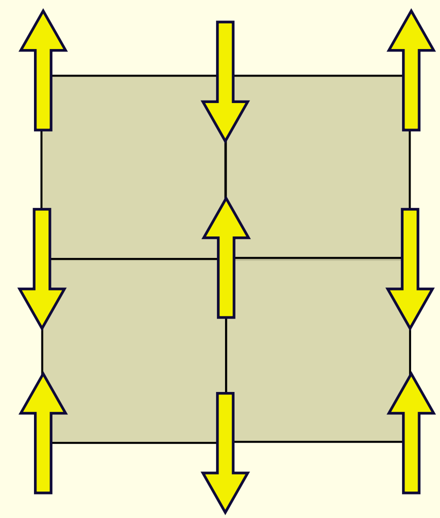
- Symmetry breaking in a regular antiferromagnet:



disordered state

O(3)

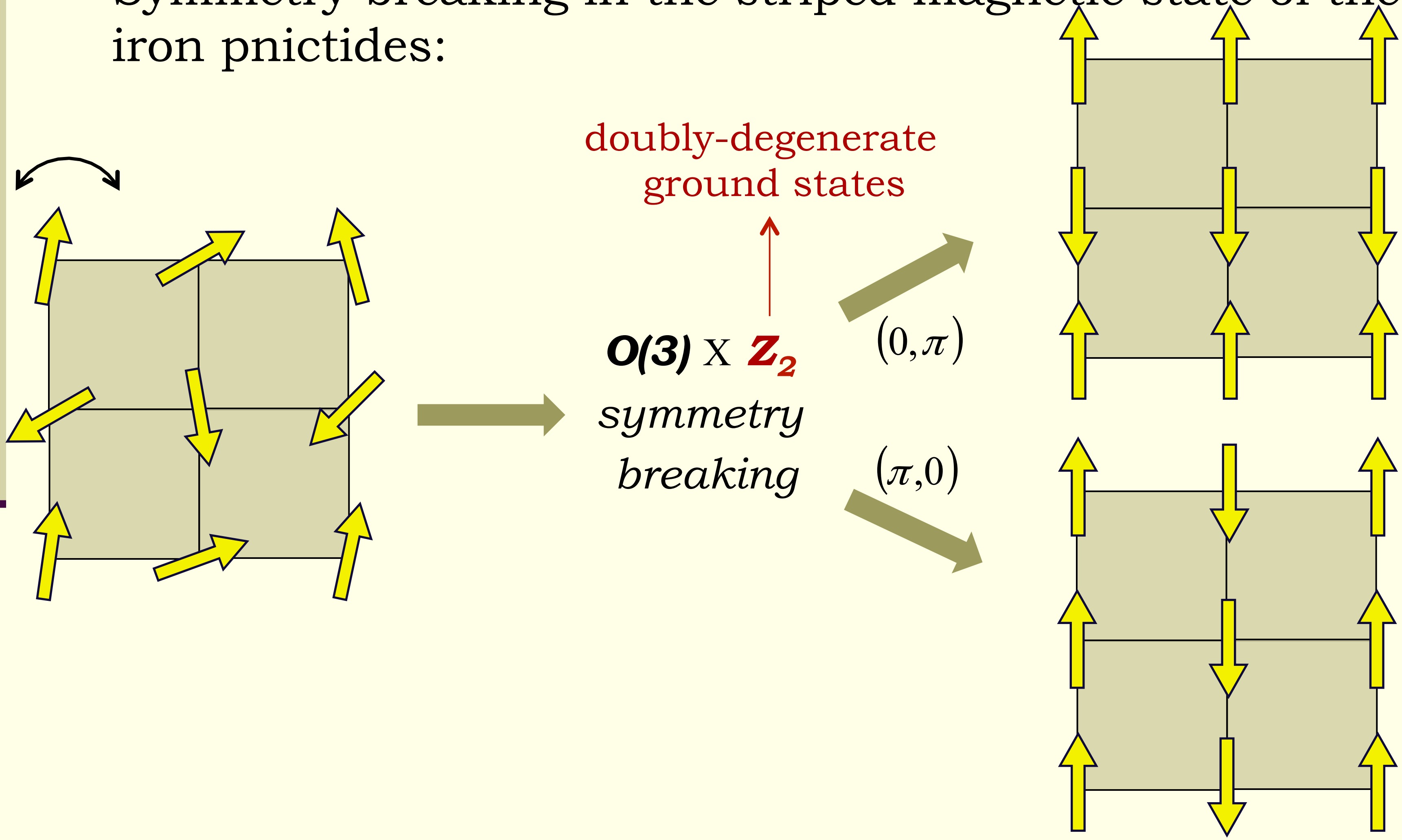
(spin-rotational) symmetry breaking



magnetic state

Iron pnictides: nematic order

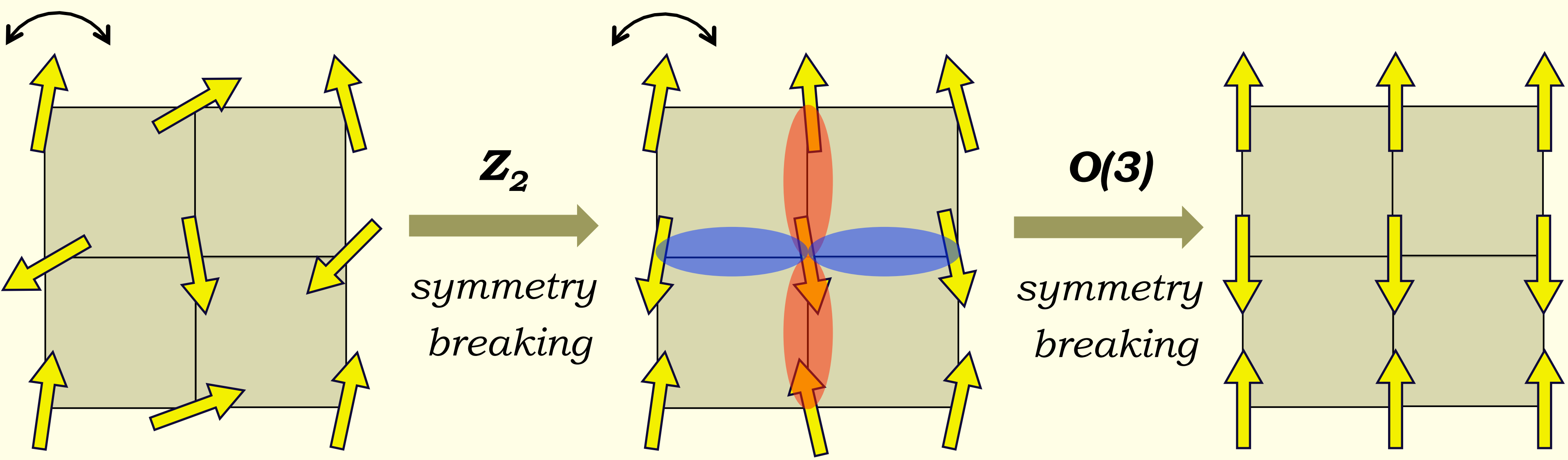
- Symmetry breaking in the striped magnetic state of the iron pnictides:



Iron pnictides: nematic order

- A state that breaks Z_2 symmetry but remains paramagnetic

spontaneous tetragonal symmetry breaking



disordered state

nematic state

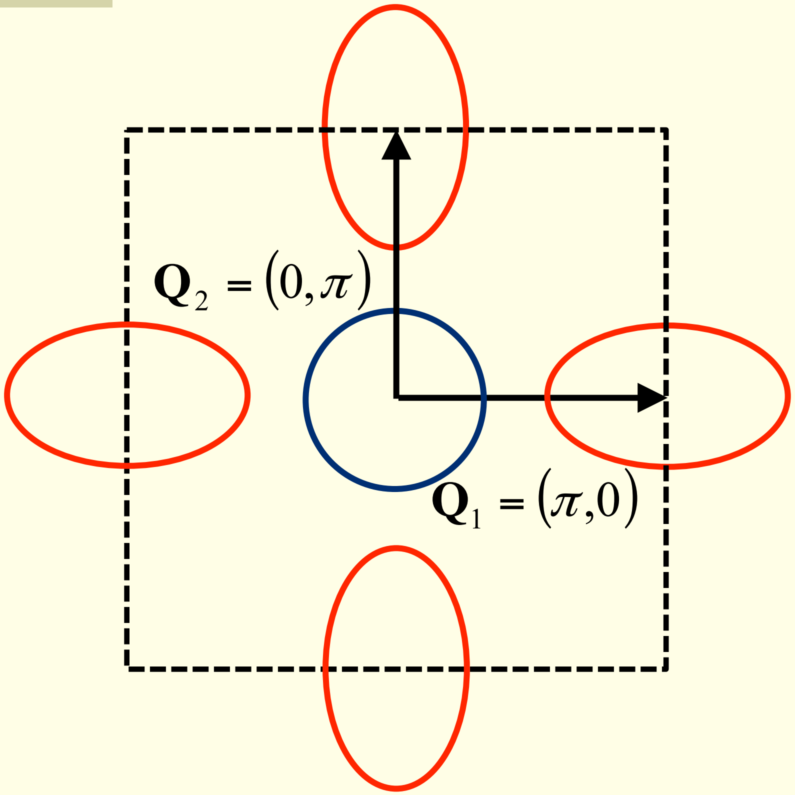
$\langle \mathbf{S}_i \cdot \mathbf{S}_{i+x} \rangle = -\langle \mathbf{S}_i \cdot \mathbf{S}_{i+y} \rangle$

magnetic state

$\langle \mathbf{S}_i \rangle \neq 0$

Chandra et al (1990)
Fang et al (2008)
Xu et al (2008)

Itinerant approach to the nematic state



Two spin-density wave instabilities driven by nesting:

$$\mathbf{S} = \mathbf{M}_1 \, e^{i\mathbf{Q}_1 \cdot \mathbf{r}} + \mathbf{M}_2 \, e^{i\mathbf{Q}_2 \cdot \mathbf{r}}$$

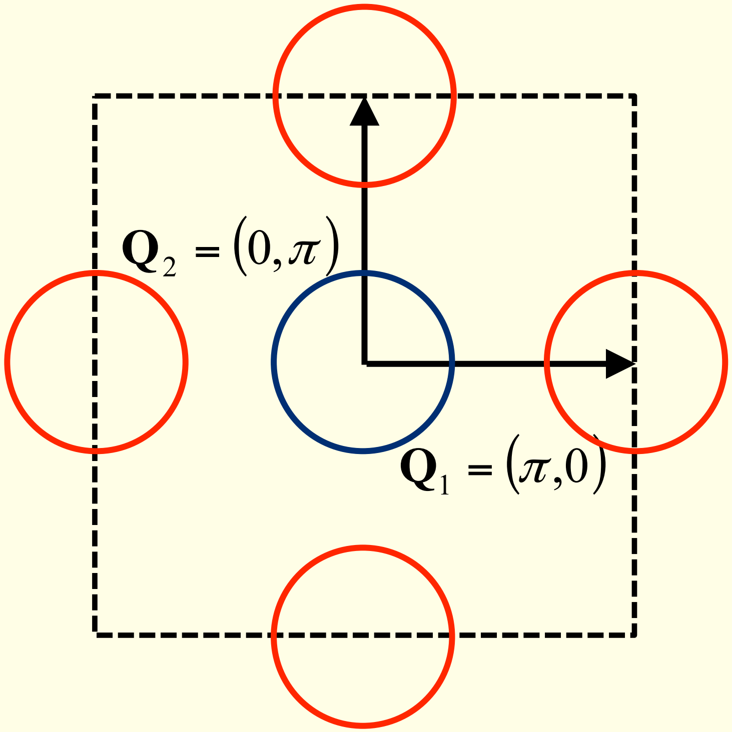
Microscopic calculation of the free energy (Hertz-Millis approach)

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{(\mathrm{h})} d_{\mathbf{k}\alpha}^{+} d_{\mathbf{k}\alpha} + \sum_{\mathrm{j},\mathbf{k}} \varepsilon_{\mathrm{j},\mathbf{k}}^{(\mathrm{e})} c_{\mathrm{j},\mathbf{k}\alpha}^{+} c_{\mathrm{j},\mathbf{k}\alpha}$$
$$+ I \sum_{\mathrm{j},\mathbf{k},\mathbf{k}',\mathbf{q}} \left(c_{\mathrm{j},\mathbf{k}\alpha}^{+} \sigma_{\alpha\beta} d_{\mathbf{k}+\mathbf{q}\beta} \right) \left(d_{\mathbf{k}'\gamma}^{+} \sigma_{\gamma\delta} c_{\mathrm{j},\mathbf{k}'-\mathbf{q}\delta} \right)$$

RMF, Chubukov, Knolle, Eremin, and Schmalian, *Phys. Rev. B* ***85****, 024534 (2012)*

Itinerant approach to the nematic state

For perfect nesting: $F_{\text{mag}} = \frac{a}{2}\left(M_1^2 + M_2^2\right) + \frac{u}{4}\left(M_1^2 + M_2^2\right)^2$

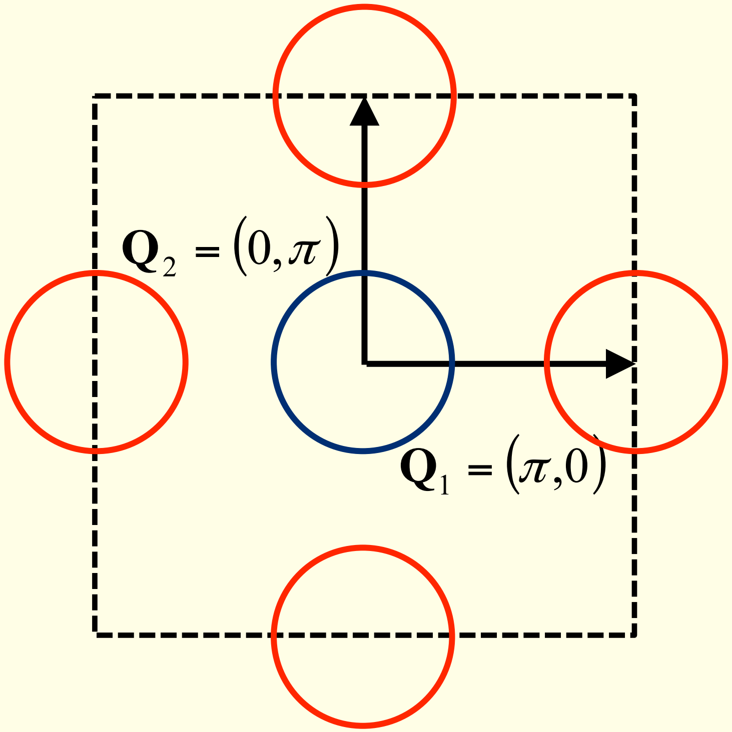


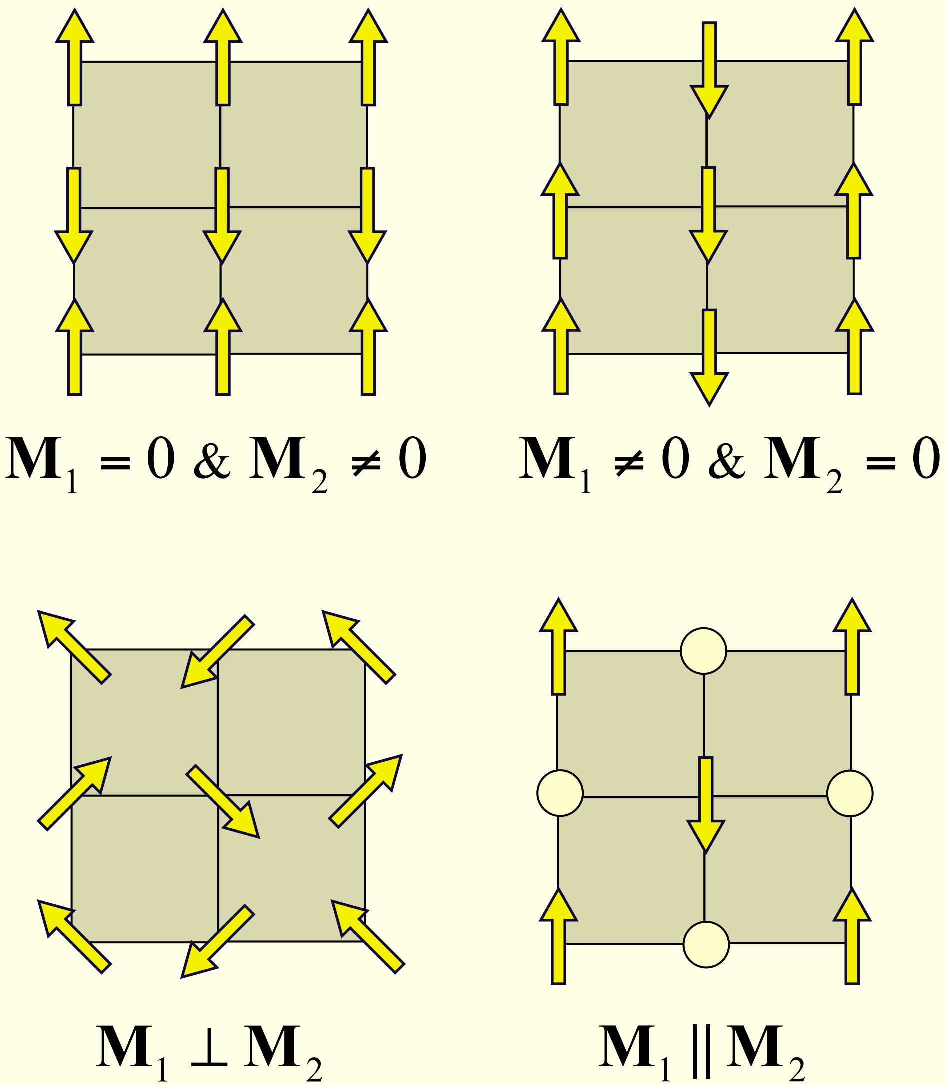
mean-field solution: $\frac{\partial F_{\text{mag}}}{\partial M_i} = 0$

$$M_1^2 + M_2^2 = \text{constant}$$

Itinerant approach to the nematic state

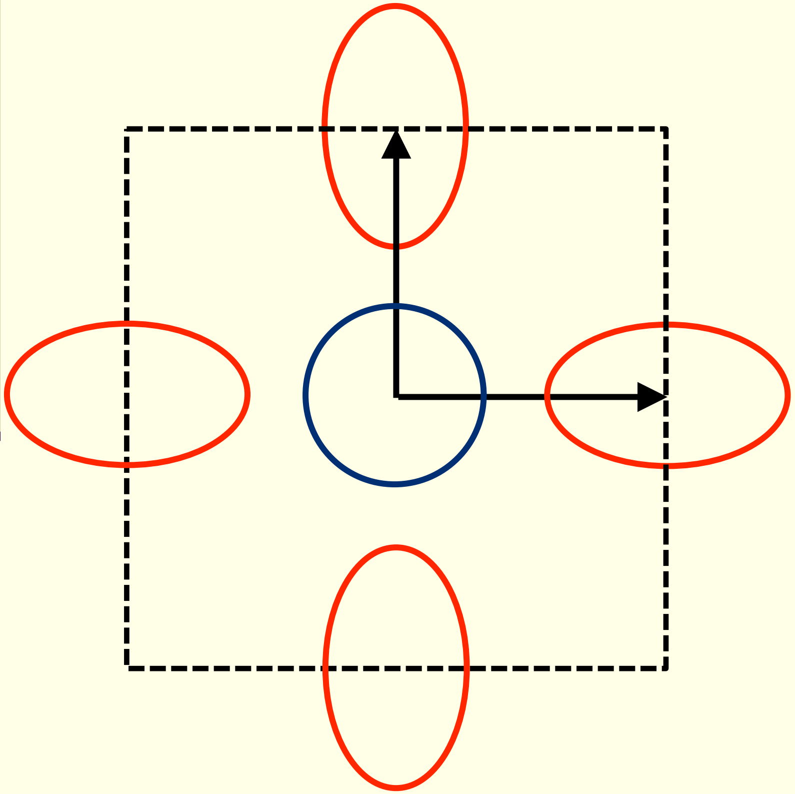
For perfect nesting:





Itinerant approach to the nematic state

Away from perfect nesting: $F_{\text{mag}} = \frac{a}{2}\left(M_1^2 + M_2^2\right) + \frac{u}{4}\left(M_1^2 + M_2^2\right)^2 - \frac{g}{4}\left(M_1^2 - M_2^2\right)^2$



$$\begin{cases} a = \dfrac{2}{U_{\text{spin}}} + 2\int_k G_{\Gamma,k} G_{X,k} \\ u = \dfrac{1}{2}\int_k G_{\Gamma,k}^2 \left(G_{X,k} + G_{Y,k}\right)^2 \\ g = -\dfrac{1}{2}\int_k G_{\Gamma,k}^2 \left(G_{X,k} - G_{Y,k}\right)^2 > 0 \end{cases}$$

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

Itinerant approach to the nematic state

mean-field solution: $\frac{\partial F_{\text{mag}}}{\partial M_i} = 0$

$$+ g\, M_1^2 M_2^2$$

$$F_{\text{mag}} = \frac{a}{2}\left(M_1^2 + M_2^2\right) + \frac{u}{4}\left(M_1^2 + M_2^2\right)^2 - \frac{g}{4}\left(M_1^2 - M_2^2\right)^2$$

Itinerant approach to the nematic state

mean-field solution: $\frac{\partial F_{\text{mag}}}{\partial M_i} = 0$

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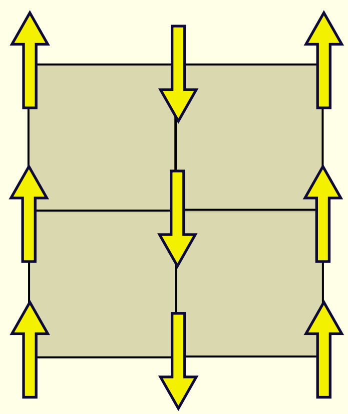
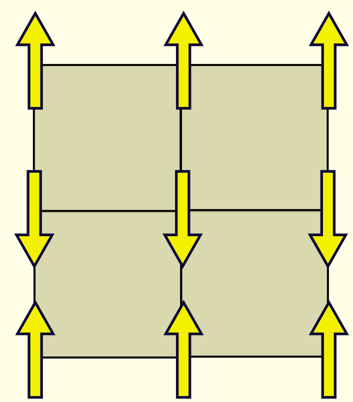
$$F_{\text{mag}} = \frac{a}{2}\left(M_1^2 + M_2^2\right) + \frac{u}{4}\left(M_1^2 + M_2^2\right)^2 - \frac{g}{4}\left(M_1^2 - M_2^2\right)^2$$



OR



$M_1 \neq 0$, $M_2 = 0$ OR $M_1 = 0$, $M_2 \neq 0$

Itinerant approach to the nematic state

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

$$F_{\mathrm{mag}} = \chi_{\mathrm{mag}}^{-1}(\mathbf{q})\left(M_1^2 + M_2^2\right) + \frac{u}{4}\underbrace{\left(M_1^2 + M_2^2\right)^2}_{\psi \propto M_1^2 + M_2^2} - \frac{g}{4}\underbrace{\left(M_1^2 - M_2^2\right)^2}_{\varphi \propto M_1^2 - M_2^2}$$

nematic order parameter

Itinerant approach to the nematic state

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

$$F_{\text{mag}} = \chi_{\text{mag}}^{-1}(\mathbf{q})\left(M_1^2 + M_2^2\right) + \frac{u}{4}\underbrace{\left(M_1^2 + M_2^2\right)^2}_{\psi \propto M_1^2 + M_2^2} - \frac{g}{4}\underbrace{\left(M_1^2 - M_2^2\right)^2}_{\varphi \propto M_1^2 - M_2^2}$$

nematic order parameter

- By integrating out the magnetic fluctuations, we obtain the free energy for the nematic degrees of freedom

$$F_{\text{nem}} = \frac{a_n}{2}\varphi^2 + \frac{u_n}{4}\varphi^4$$

Itinerant approach to the nematic state

Equation of state for the nematic order parameter:

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

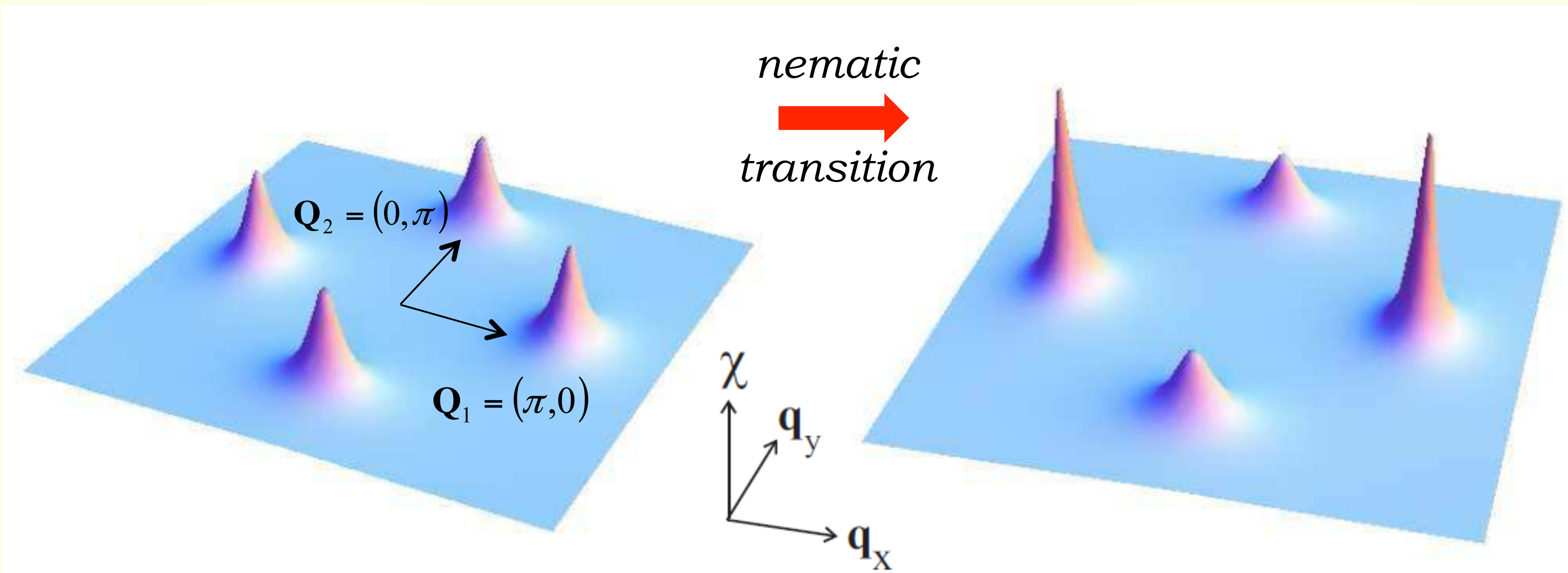
$\varphi \neq 0$ **solution already in the paramagnetic phase, when the magnetic susceptibility is large enough**

$$\left\langle M_1^2 \right\rangle \neq \left\langle M_2^2 \right\rangle$$

magnetic fluctuations → **nematic order**

Itinerant approach to the nematic state

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



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

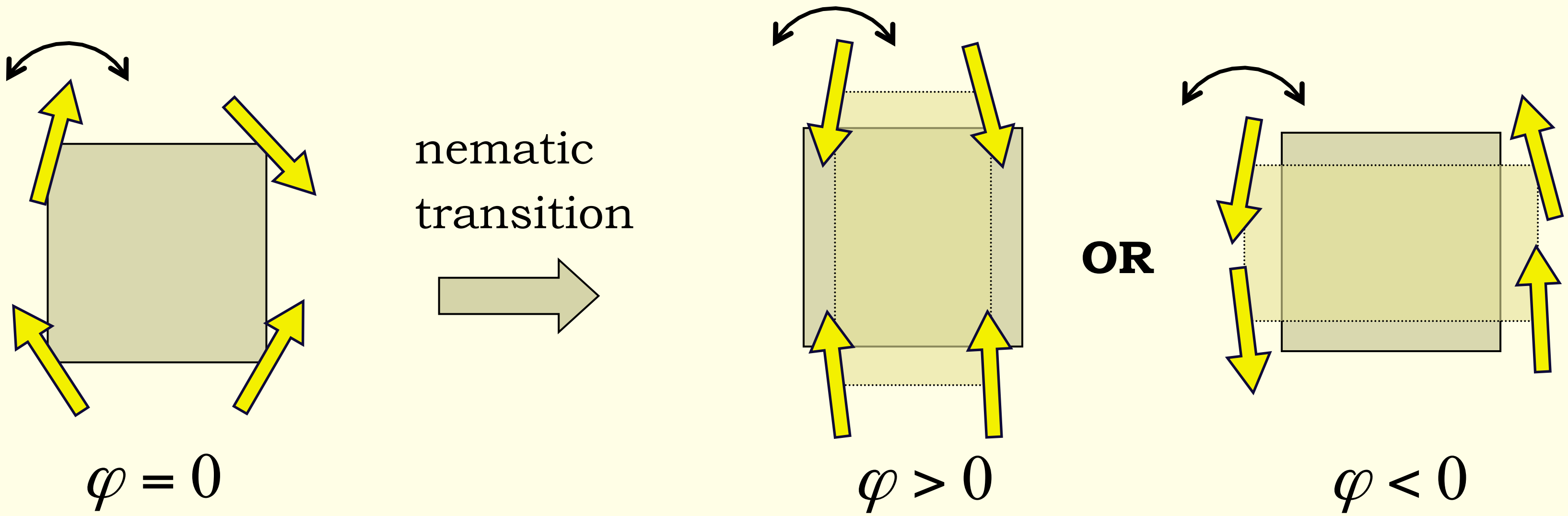
RMF, Chubukov, Eremin, Knolle, Schmalian, PRB (2012)

Nematic transition triggers structural transition

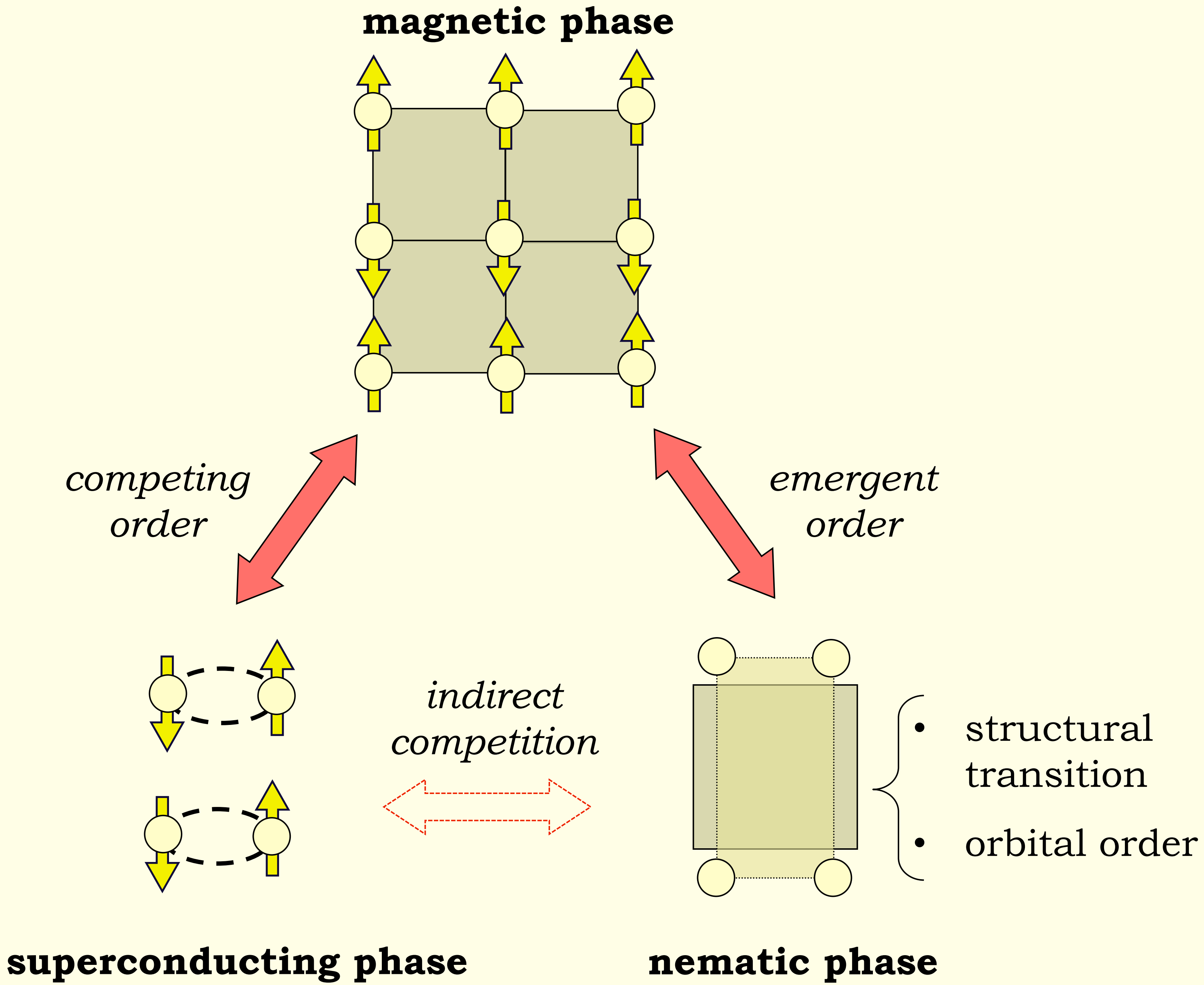
magneto-elastic coupling: $H_{\text{mag-el}} = \lambda \sum_{\mathbf{k}} \delta \left(c^{+}_{X,\mathbf{k}\alpha} c_{X,\mathbf{k}\alpha} - c^{+}_{Y,\mathbf{k}\alpha} c_{Y,\mathbf{k}\alpha} \right)$

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

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



Structural transition driven by magnetic fluctuations

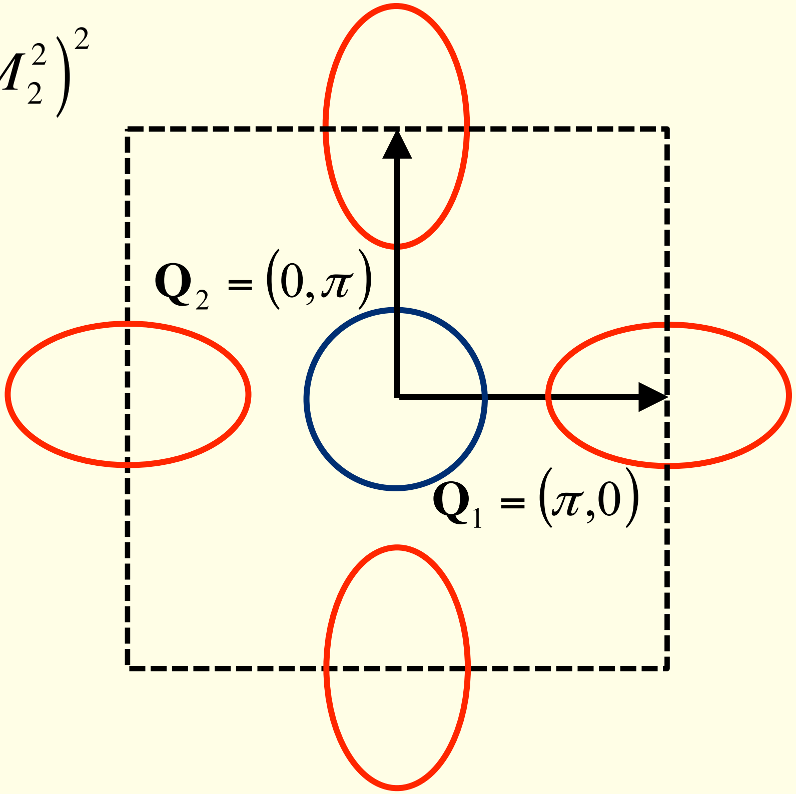

magnetic phase
competing order
emergent order
indirect competition
• structural transition
• orbital order
superconducting phase
nematic phase

Competition between superconductivity and nematicity

- Nematicity is a consequence of magnetic fluctuations

Free energy (without SC)

$$F = \frac{a_m}{2}\left(M_1^2 + M_2^2\right) + \frac{u_m}{4}\left(M_1^2 + M_2^2\right)^2 - \frac{g_m}{4}\left(M_1^2 - M_2^2\right)^2$$



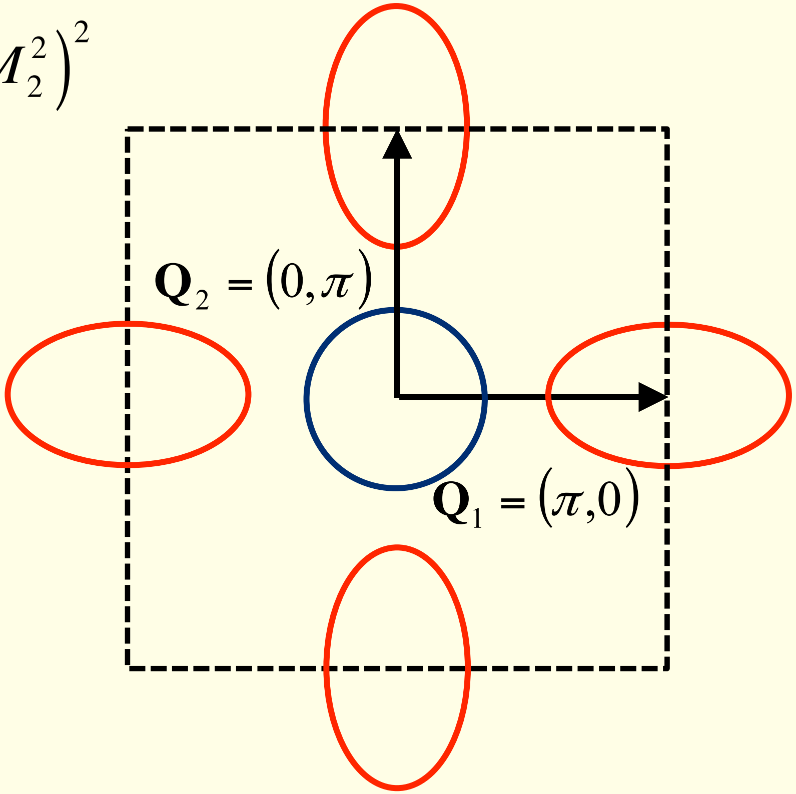
Competition between superconductivity and nematicity

- But magnetism competes with SC

Free energy (with SC)

$$F = \frac{a_m}{2}\left(M_1^2 + M_2^2\right) + \frac{u_m}{4}\left(M_1^2 + M_2^2\right)^2 - \frac{g_m}{4}\left(M_1^2 - M_2^2\right)^2$$
$$+\frac{a_s}{2}|\Delta|^2 + \frac{u_s}{4}|\Delta|^4 + \frac{\gamma_{ms}}{2}\left(M_1^2 + M_2^2\right)|\Delta|^2$$

competition between magnetism and SC



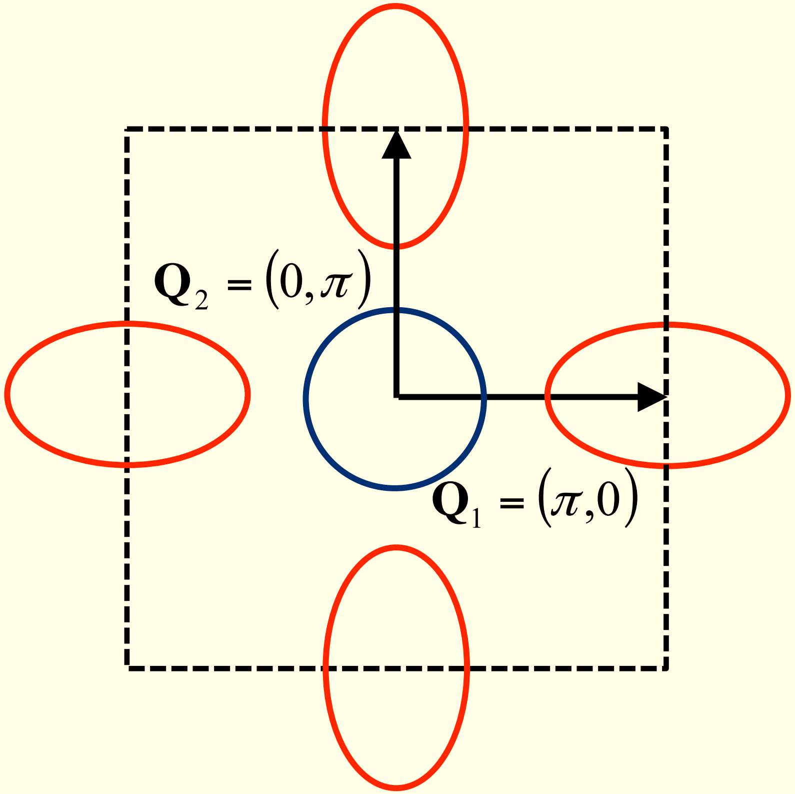
Competition between superconductivity and nematicity

- By integrating out the magnetic fluctuations, we obtain an indirect competition between nematicity and SC

$$F = \frac{a_n}{2}\varphi^2 + \frac{u_n}{4}\varphi^4 + \frac{a_s}{2}|\Delta|^2 + \frac{u_s}{4}|\Delta|^4 + \frac{\gamma_{ns}}{2}\varphi^2|\Delta|^2$$

competition between nematicity and SC

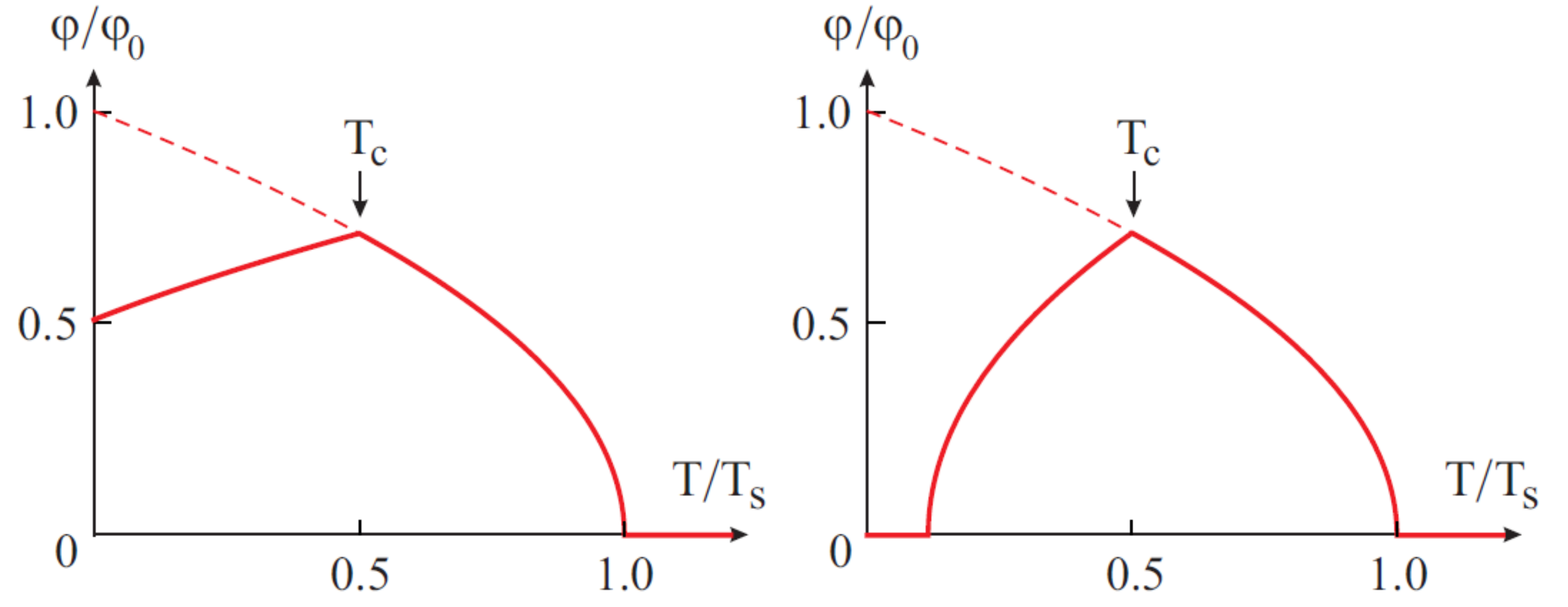
$$\gamma_{ns} \propto \gamma_{ms}$$



RMF, Maiti,Wolfle & Chubukov *(2013)*

Competition between superconductivity and nematicity

- Due to its magnetic origin, nematicity also competes with superconductivity
  - *even in the absence of long-range magnetic order*

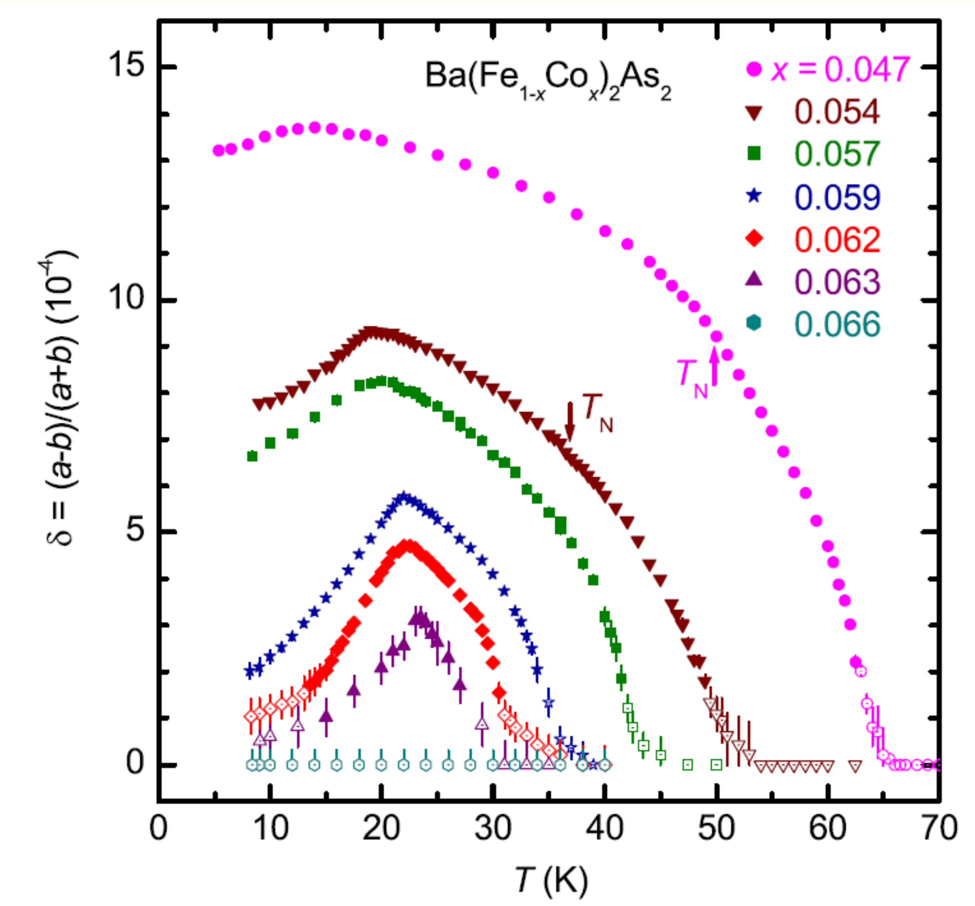


RMF & Schmalian, SUST (2012)

Competition between superconductivity and nematicity

- X-ray diffraction: experimental observation of the suppression of the orthorhombic distortion below T_c

competition
& coexistence



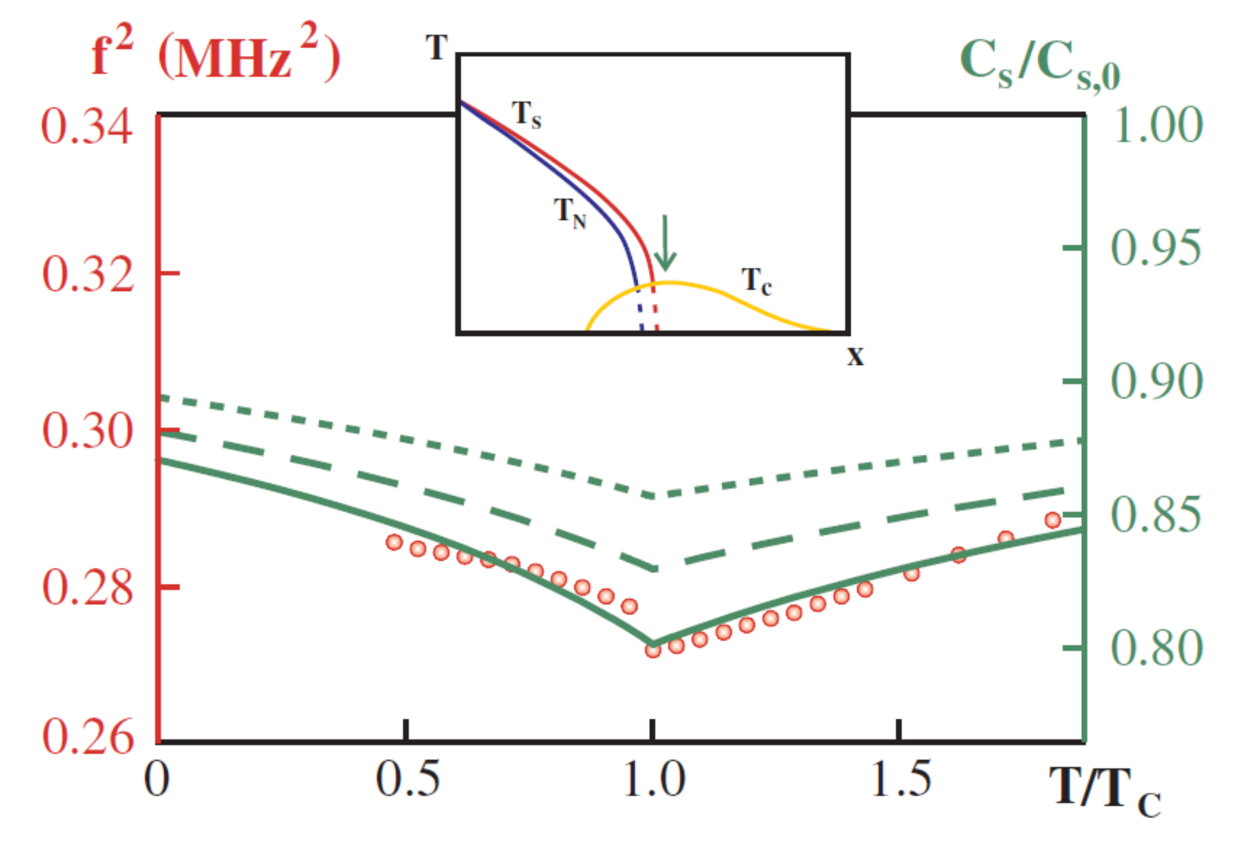
Nandi,..., RMF et al, PRL (2010)

Competition between superconductivity and nematicity

- The same model explains the hardening of the shear modulus below the SC transition temperature.

$$\left(\frac{C_s}{C_{s,0}}\right)^{-1} = 1 + \left(\frac{\lambda}{C_{s,0}}\right)\chi_{\mathrm{nem}}$$

$$\chi_{\mathrm{nem}} = \frac{\sum_{\mathbf{k}} \chi^2_{\mathrm{mag}}(\mathbf{k})}{1 - g\sum_{\mathbf{k}} \chi^2_{\mathrm{mag}}(\mathbf{k})}$$

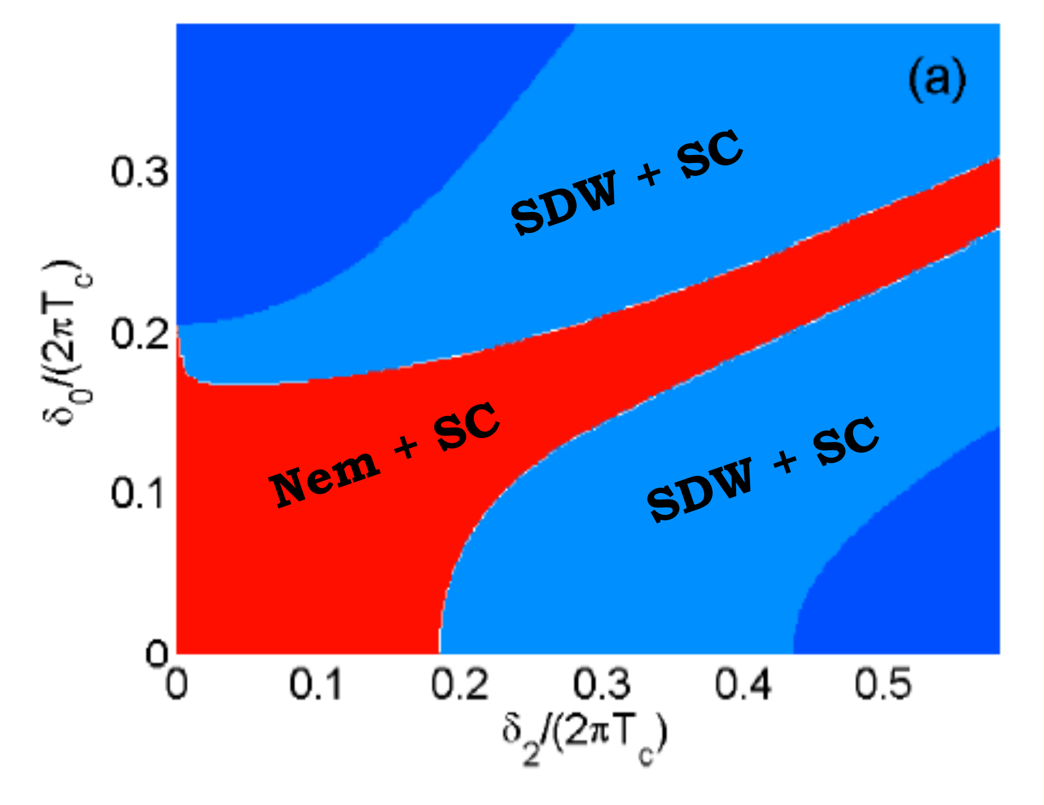


RMF et al, PRL (2010)

Competition between superconductivity and nematicity

- Nematicity and superconductivity compete, but can coexist!

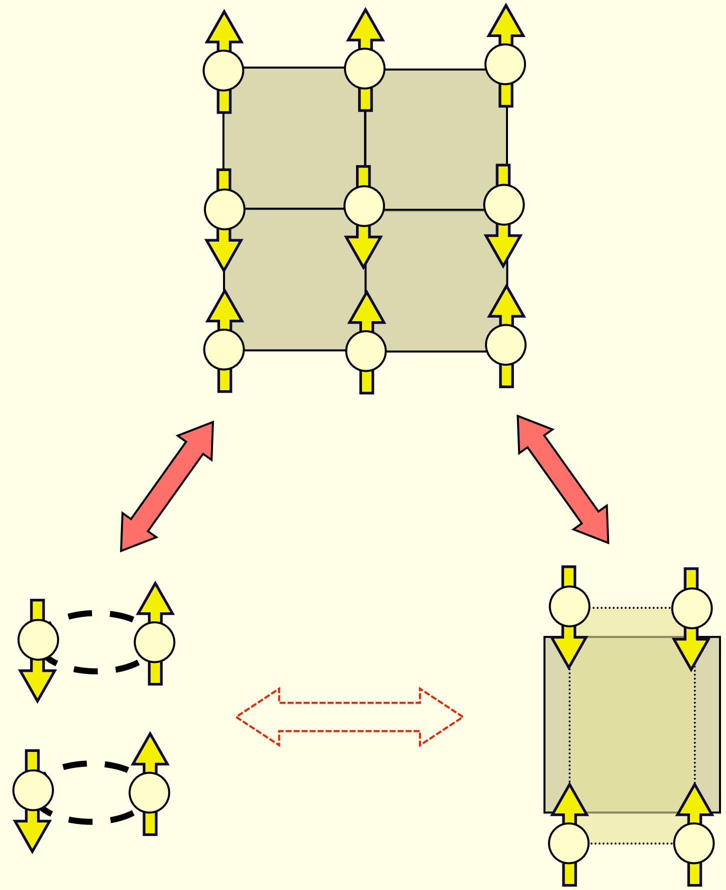
band ellipticity (pressure)



carrier concentration (doping)

RMF, Maiti,Wolfle & Chubukov *(2013)*

Conclusions



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