UNIVERSITY OF MINNESOTA

Magnetic and nematic fluctuations in iron-based superconductors

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University of Minnesota

Riverhead, NY

Sep 05th, 2013

Collaborators:

RMF, Bohmer, Meingast, and Schmalian, *Phys. Rev. Lett. (in press)*

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(Karlsruhe)

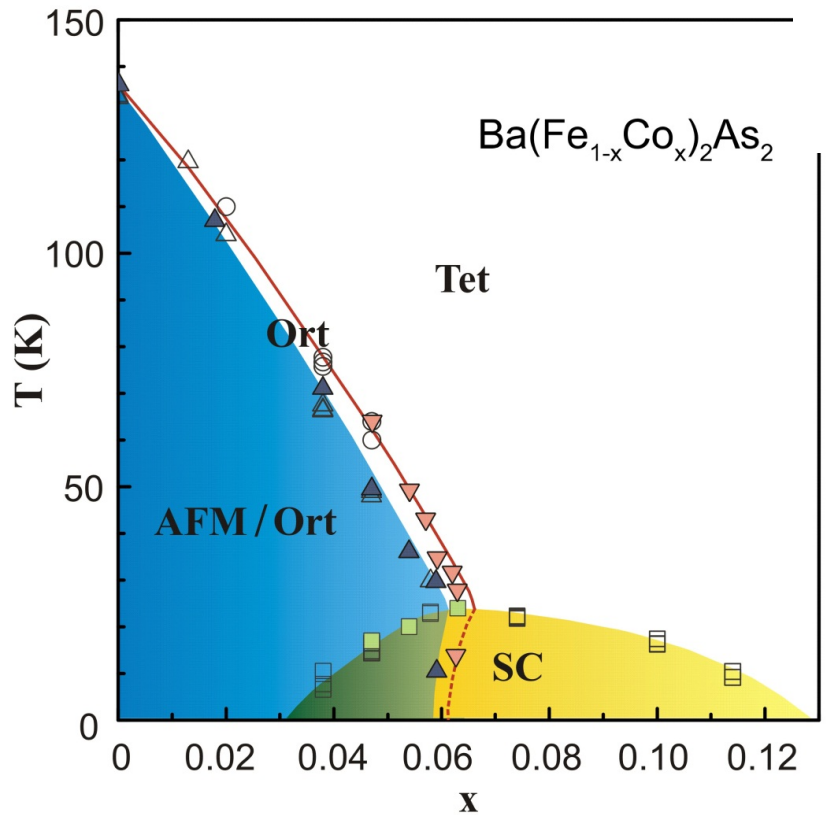
RMF, Maiti, Wölfle, and Chubukov, *Phys. Rev. Lett.* ***111***, *057001 (2013)*

Andrey Chubukov
(Madison)

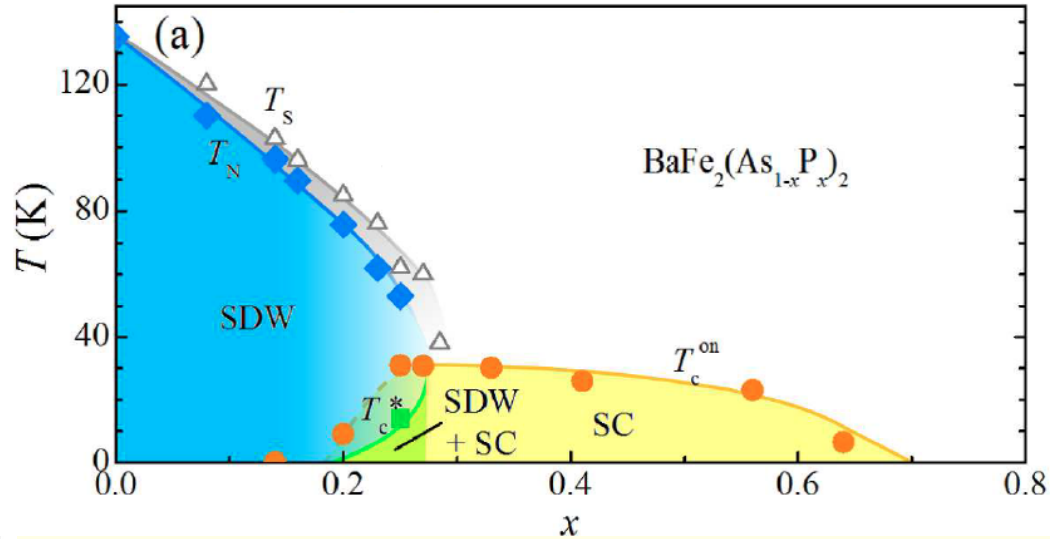
Saurabh Maiti
(Florida)

Peter Wölfle
(Karlsruhe)

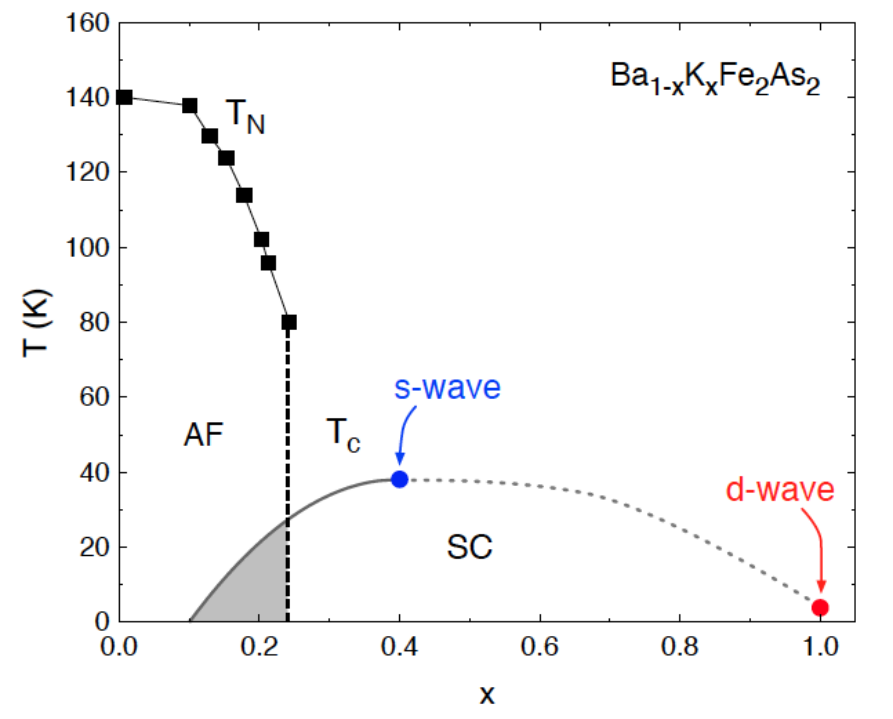
Iron pnictides: phase diagrams



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

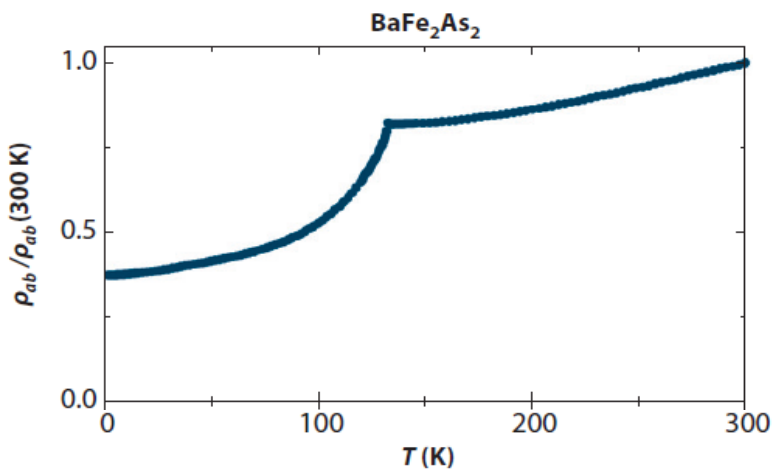


Iye et al, JPSP (2012)

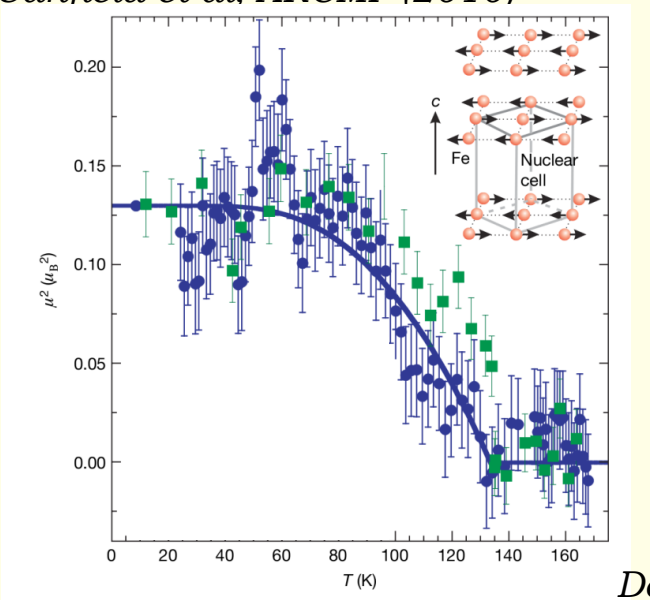


Reid et al, PRL (2012)

Iron pnictides: magnetic order



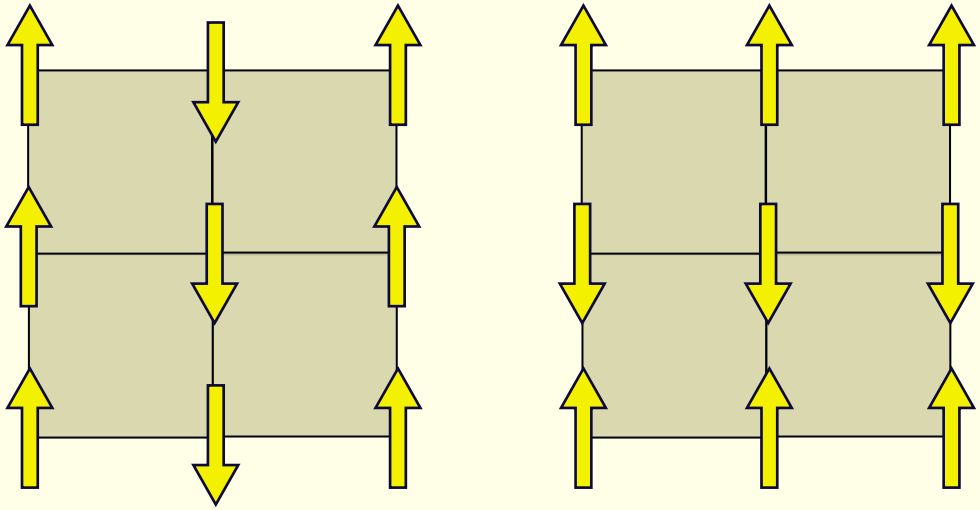
Canfield et al, ARCMP (2010)



De la Cruz et al, Nature (2008)

system remains metallic

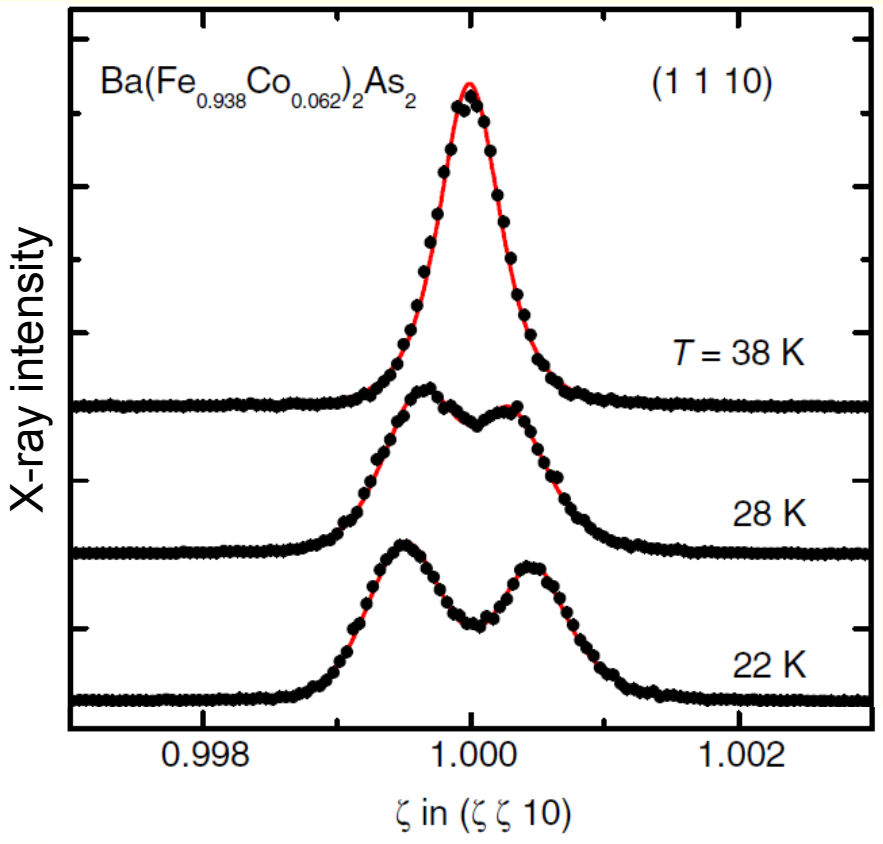
two degenerate magnetic stripe states



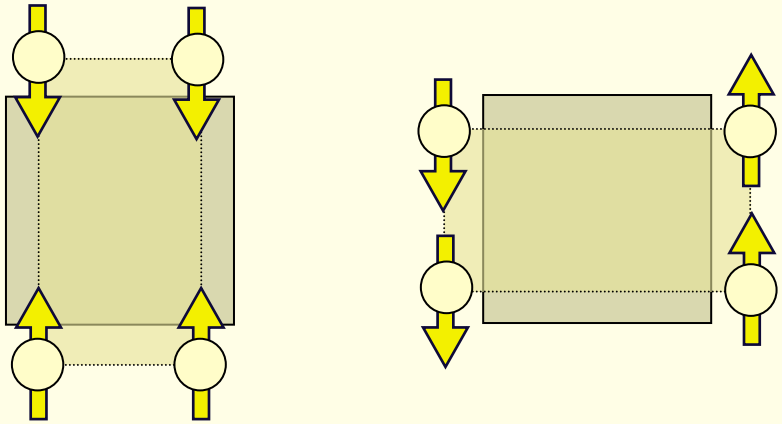
$\mathbf{Q}_1 = (\pi, 0)$ $\mathbf{Q}_2 = (0, \pi)$

Iron pnictides: structural order

tetragonal to orthorhombic transition

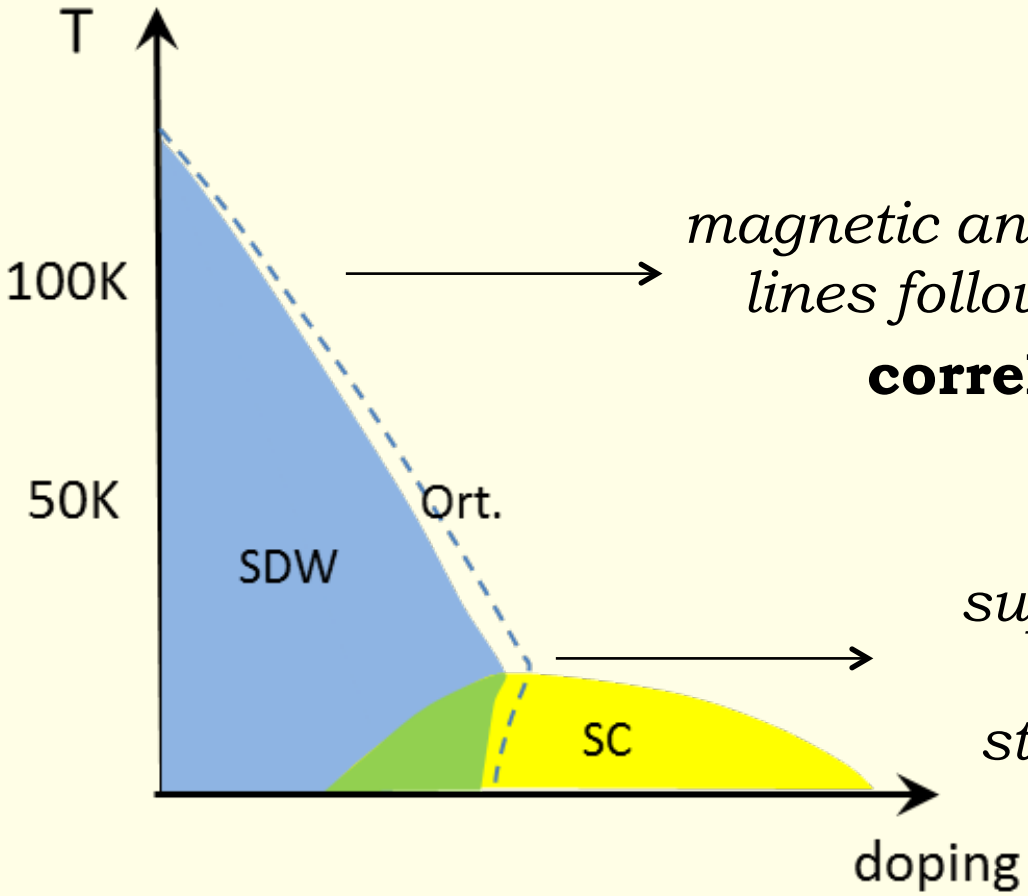


magneto-elastic coupling



Nandi et al, PRL (2010)

Iron pnictides: typical phase diagram

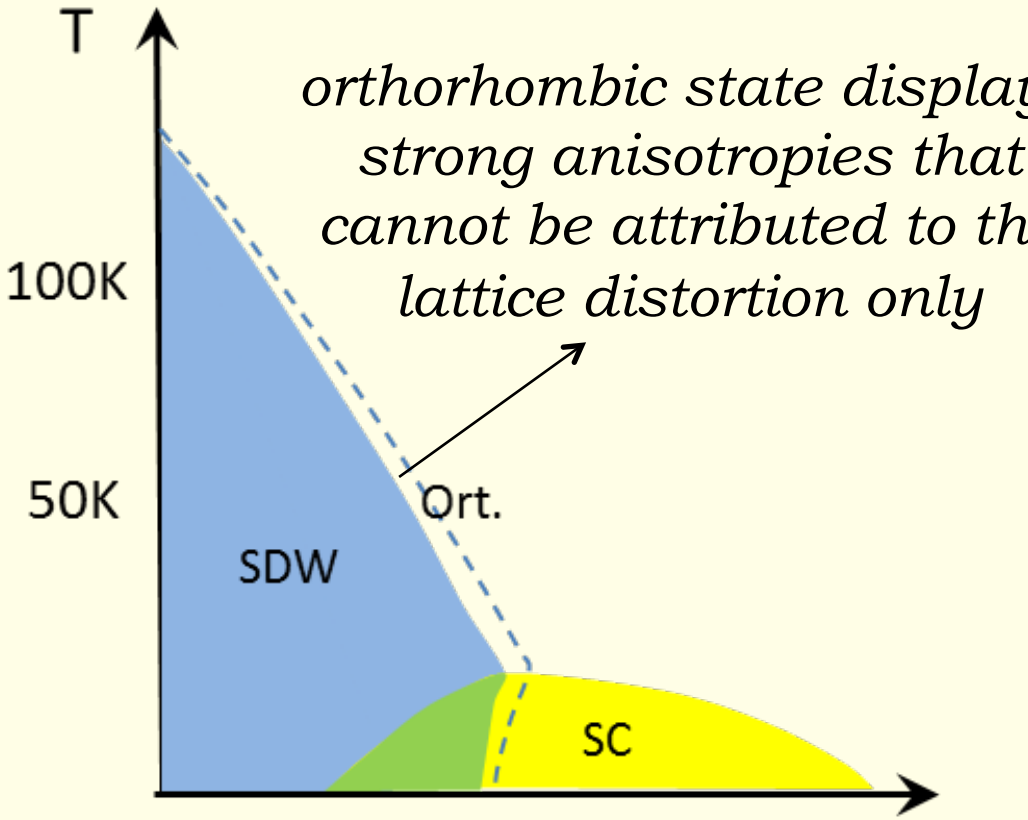


magnetic and structural transition lines follow closely each other

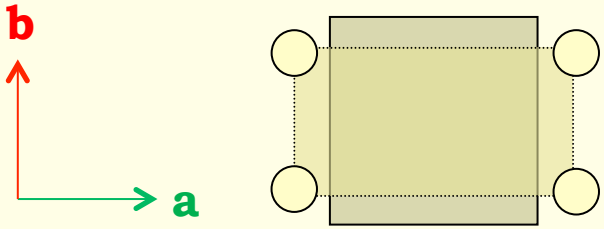
correlated phases!

superconductivity close to magnetic and structural instabilities

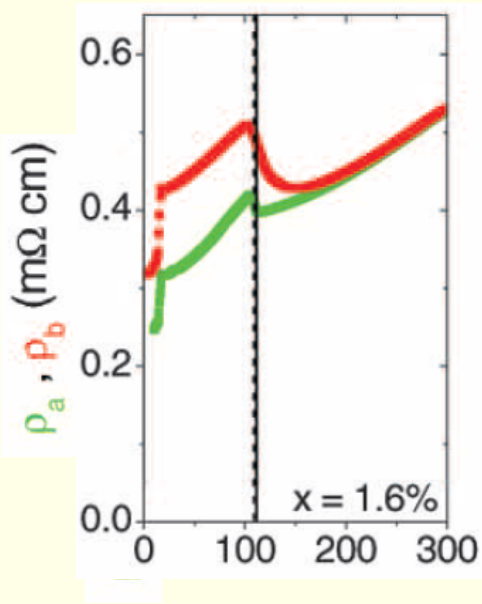
Iron pnictides: nematic order



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

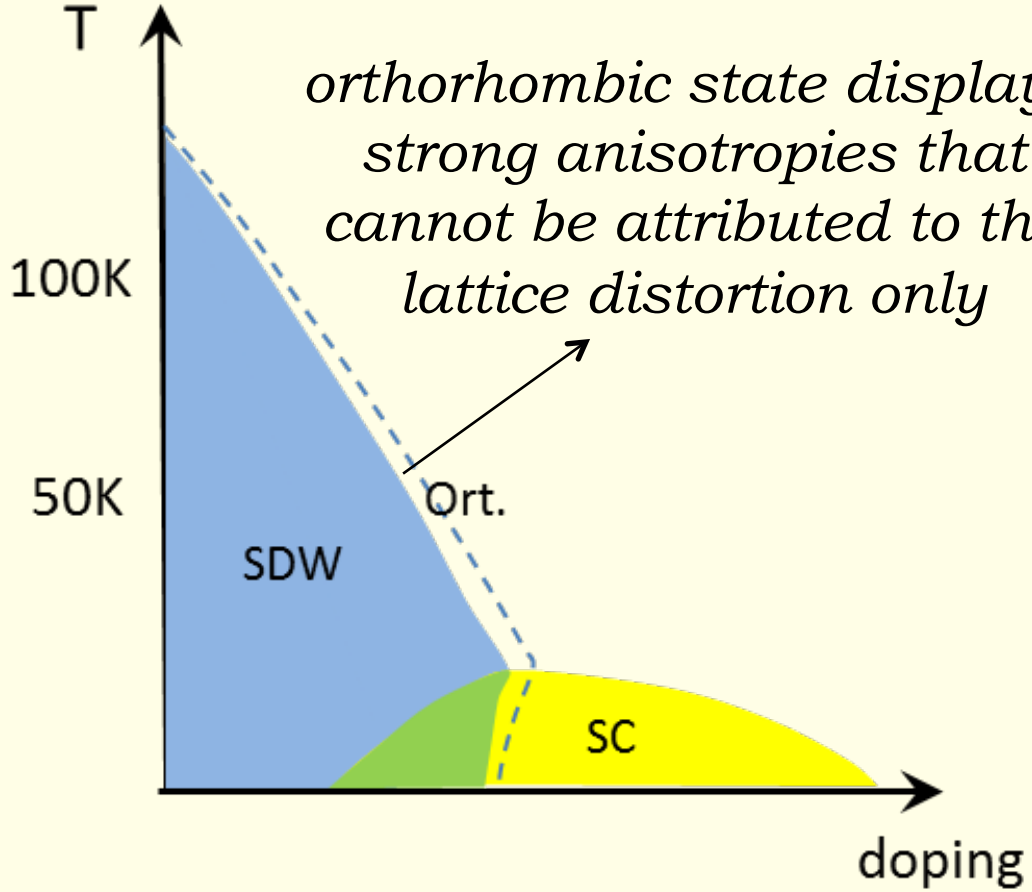


- **resistivity**



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

Iron pnictides: nematic order



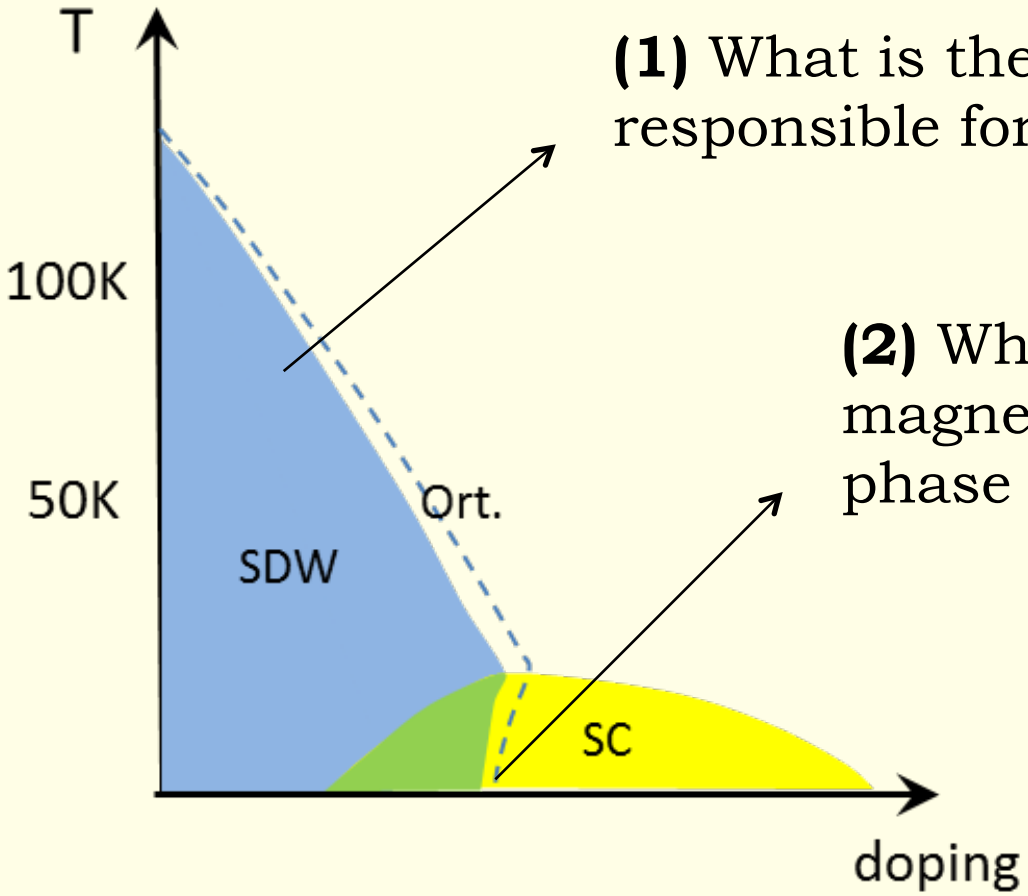
orthorhombic state displays strong anisotropies that cannot be attributed to the lattice distortion only

- **resistivity**
- **optical spectrum**
- **orbital polarization**
- **density of states**
- **magnetic suscept**

underlying electronic order that spontaneously breaks tetragonal symmetry: nematic phase

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

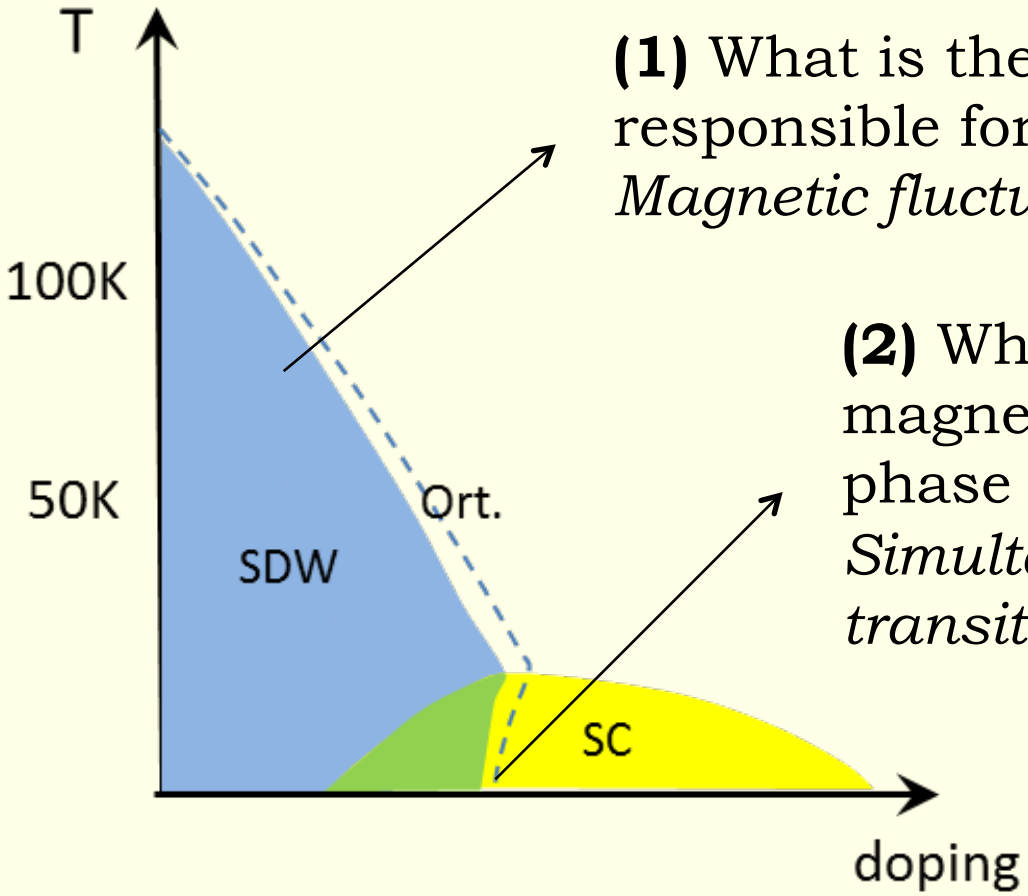
In this talk:



(1) What is the microscopic mechanism responsible for electronic nematicity?

(2) What is the nature of the magnetic and nematic quantum phase transitions?

In this talk:



(1) What is the microscopic mechanism responsible for electronic nematicity?
Magnetic fluctuations

(2) What is the nature of the magnetic and nematic quantum phase transitions?
Simultaneous weakly 1st order transition

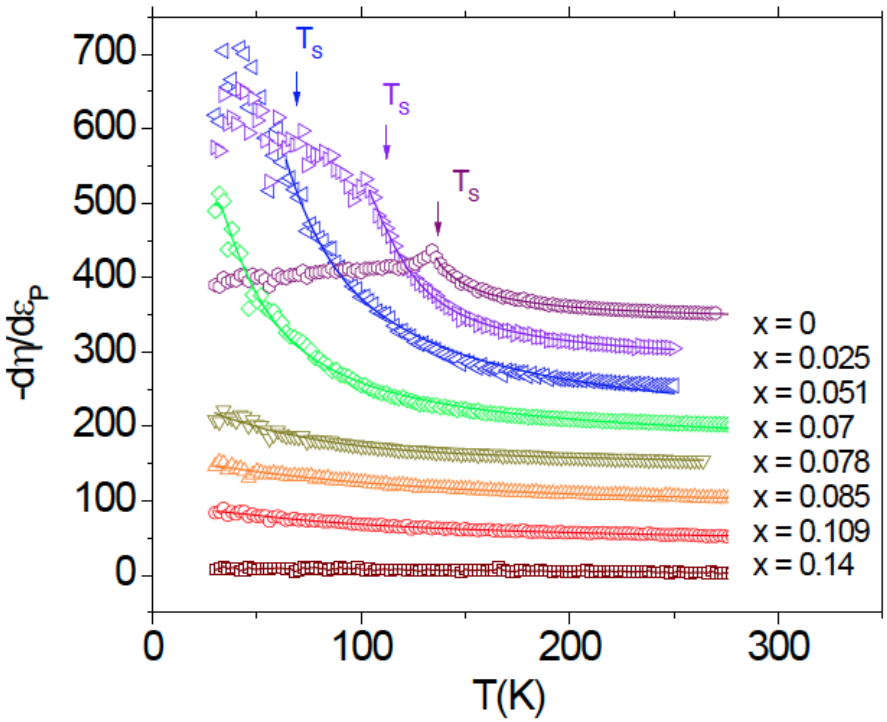
Outline

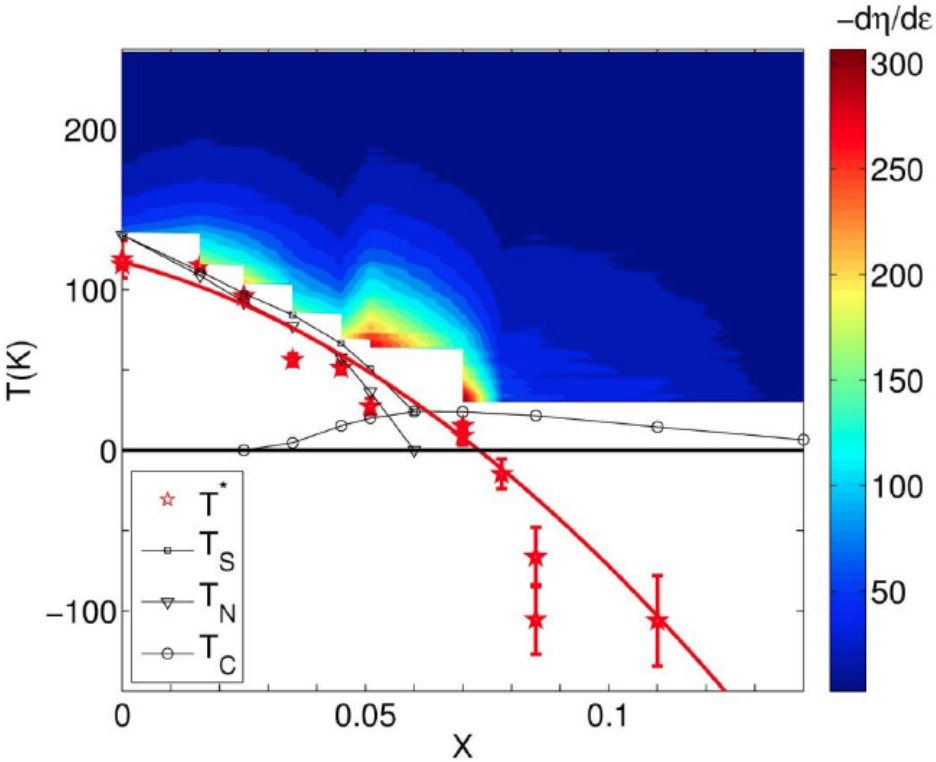
1. **Microscopic origin of the nematic state**
   - *scaling between elastic and magnetic fluctuations*
   - *evidence for magnetically-driven structural transition*

2. **Magnetic and nematic quantum phase transitions**
   - *competition between nematicity and superconductivity*
   - *single weakly first-order quantum phase transition inside the superconducting dome*

Nematic fluctuations and the shear modulus

- Transport experiments indicate that an electronic order parameter drives the structural transition





Chu et al, Science (2012)

Nematic fluctuations and the shear modulus

- Whatever the nematic order parameter is, it must couple linearly to the orthorhombic distortion

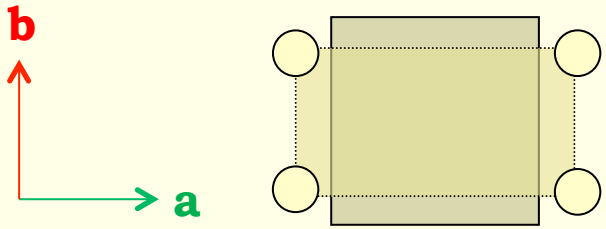
$$F[\varphi,\delta] = \frac{C_{s,0}}{2}\delta^2 - \lambda\delta\varphi + F[\varphi]$$

φ: nematic order parameter

δ: orthorhombic distortion

λ: coupling constant

$C_{s,0}$: bare shear modulus



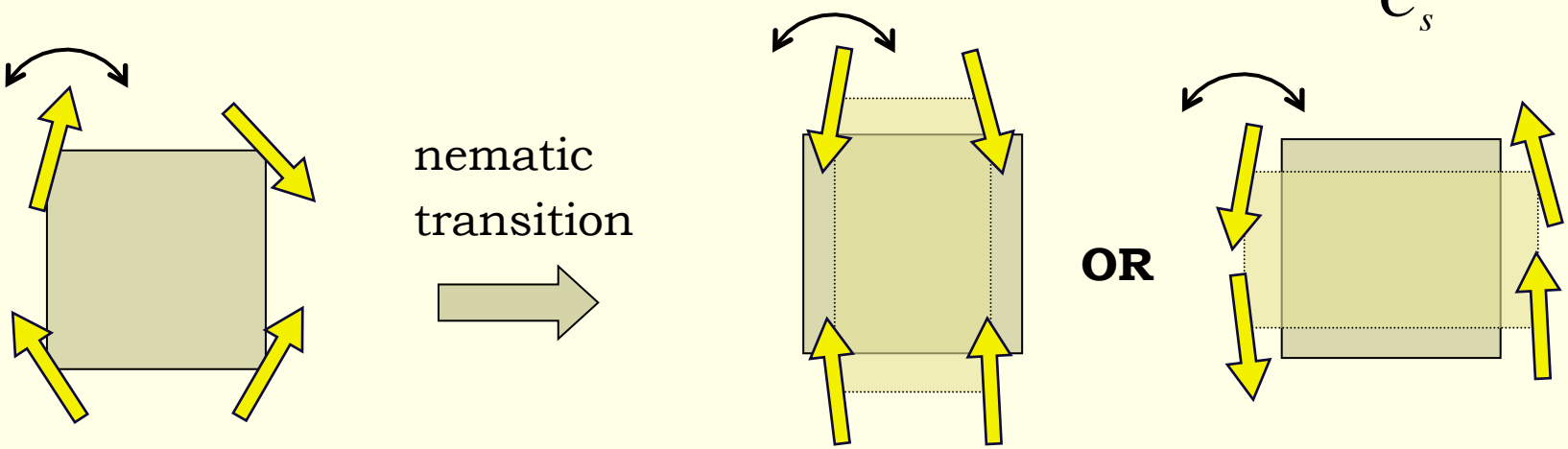
$$\delta = \frac{a-b}{a+b}$$

Nematic fluctuations and the shear modulus

- Whatever the nematic order parameter is, it must couple linearly to the orthorhombic distortion

$$F[\varphi,\delta] = \frac{C_{s,0}}{2}\delta^2 - \lambda\,\delta\varphi + F[\varphi]$$

- Nematic order leads to lattice distortion: $\langle\delta\rangle = \frac{\lambda}{C_s}\langle\varphi\rangle$



$\varphi = 0$ $\varphi > 0$ $\varphi < 0$

Nematic fluctuations and the shear modulus

- Whatever the nematic order parameter is, it must couple linearly to the orthorhombic distortion

$$F[\varphi,\delta] = \frac{C_{s,0}}{2}\delta^2 - \lambda\,\delta\varphi + F[\varphi]$$

- Nematic fluctuations reduce the energy cost of an instantaneous orthorhombic distortion $\chi_{\text{nem}} \propto \langle \varphi^2 \rangle$

$$\left(\frac{C_s}{C_{s,0}}\right)^{-1} = 1 + \left(\frac{\lambda^2}{C_{s,0}}\right)\chi_{\text{nem}}$$

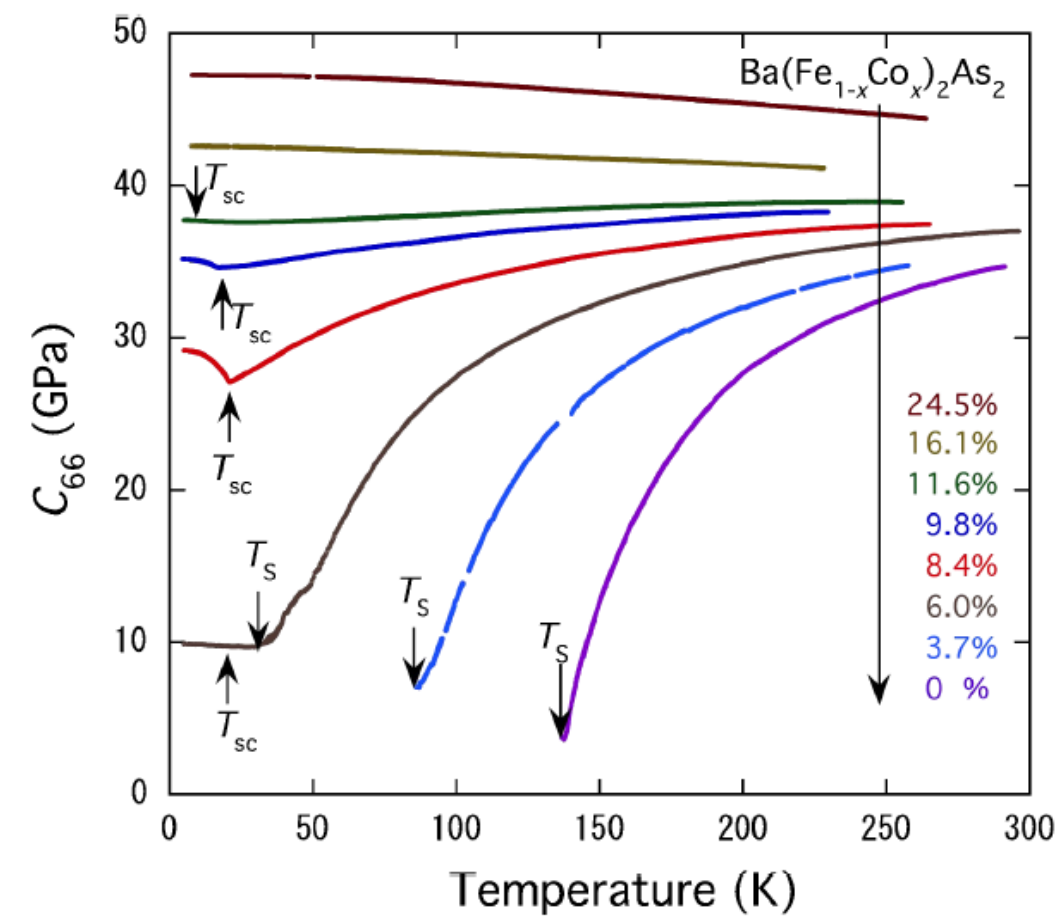
RMF *et al, Phys. Rev. Lett.* ***105****, 157003 (2010)*

Nematic fluctuations (probed via shear modulus) are strong near the SC dome!

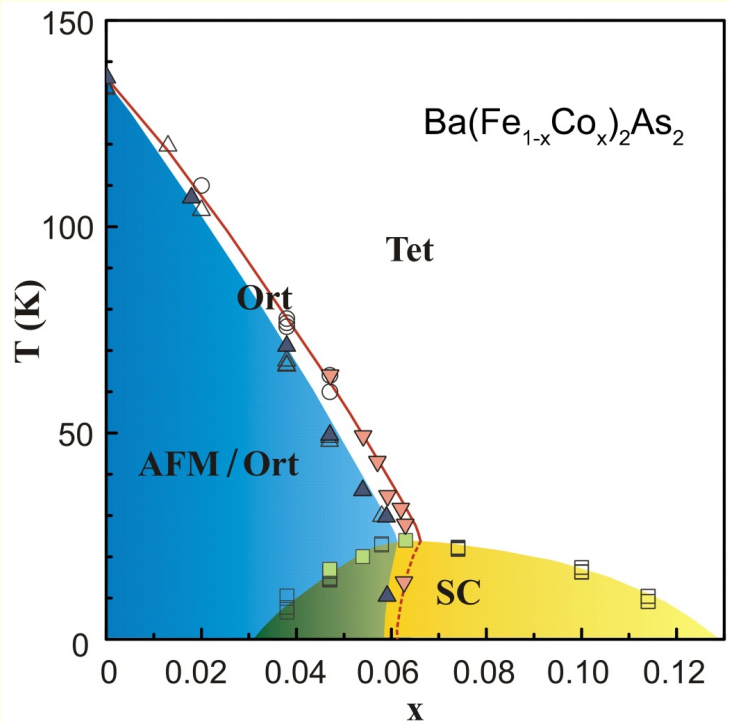
Journal of the Physical Society of Japan **81** (2012) 024604 FULL PAPERS
DOI: 10.1143/JPSJ.81.024604

Structural Quantum Criticality and Superconductivity in Iron-Based Superconductor $Ba(Fe_{1-x}Co_x)_2As_2$

Masahito YOSHIZAWA[1,4*], Daichi KIMURA[1], Taiji CHIBA[1], Shalamujiang SIMAYI[1,4], Yoshiki NAKANISHI[1,4], Kunihiro KIHOU[2,4], Chul-Ho LEE[2,4], Akira IYO[2,4], Hiroshi EISAKI[2,4], Masamichi NAKAJIMA[3,4], and Shin-ichi UCHIDA[3,4]



$$C_s^{-1} \to \infty \text{ at } T_s$$

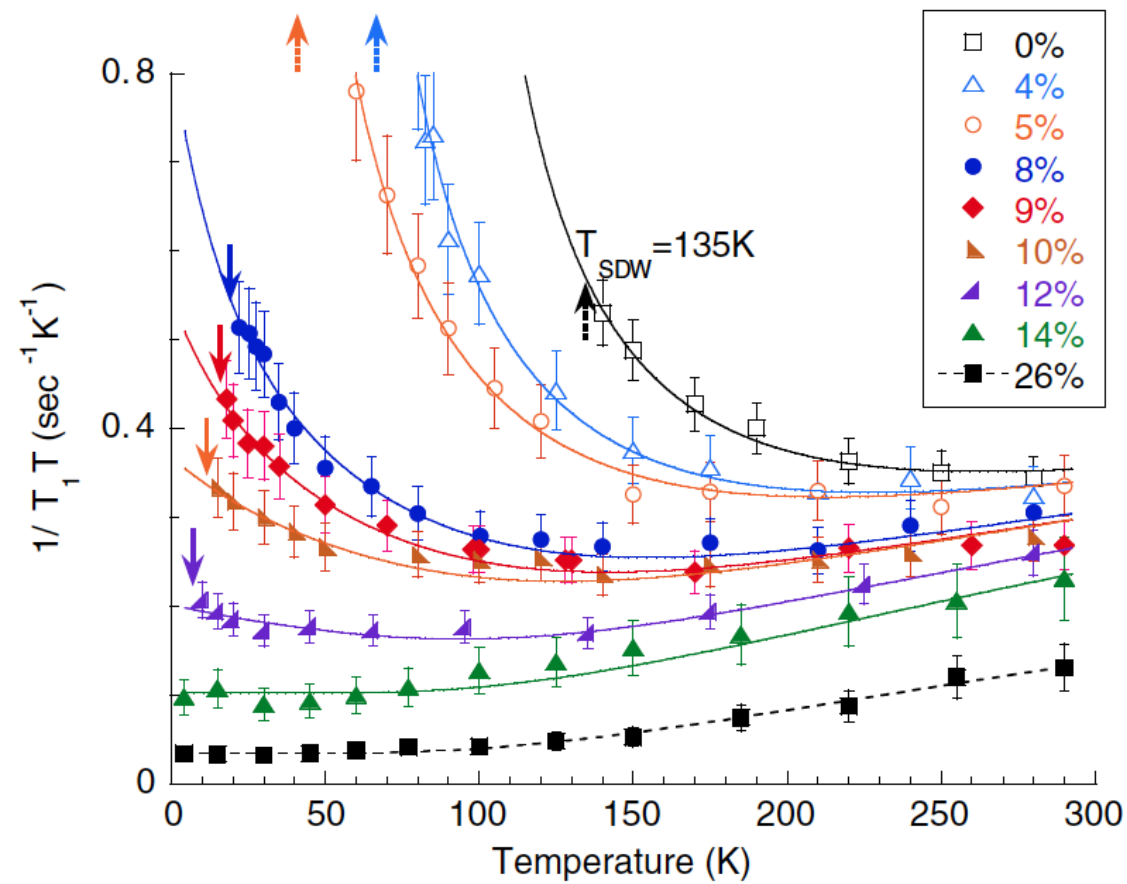


Magnetic fluctuations (probed via NMR) are also strong near the SC dome!

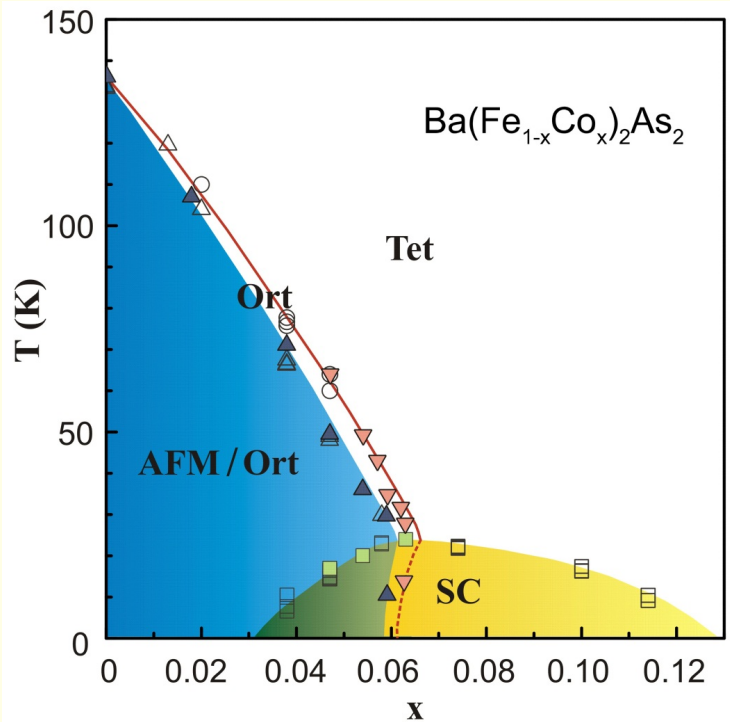
PRL **104,** 037001 (2010) PHYSICAL REVIEW LETTERS week ending 22 JANUARY 2010

Contrasting Spin Dynamics between Underdoped and Overdoped $Ba(Fe_{1-x}Co_x)_2As_2$

F. L. Ning,[1] K. Ahilan,[1] T. Imai,[1,2] A. S. Sefat,[3] M. A. McGuire,[3] B. C. Sales,[3] D. Mandrus,[3] P. Cheng,[4] B. Shen,[4] and H.-H Wen[4]

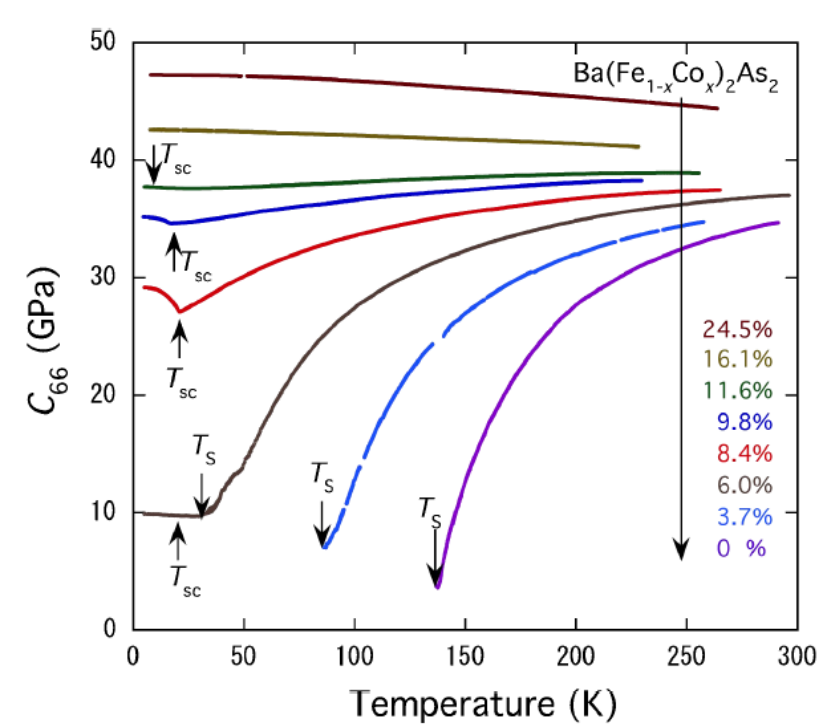


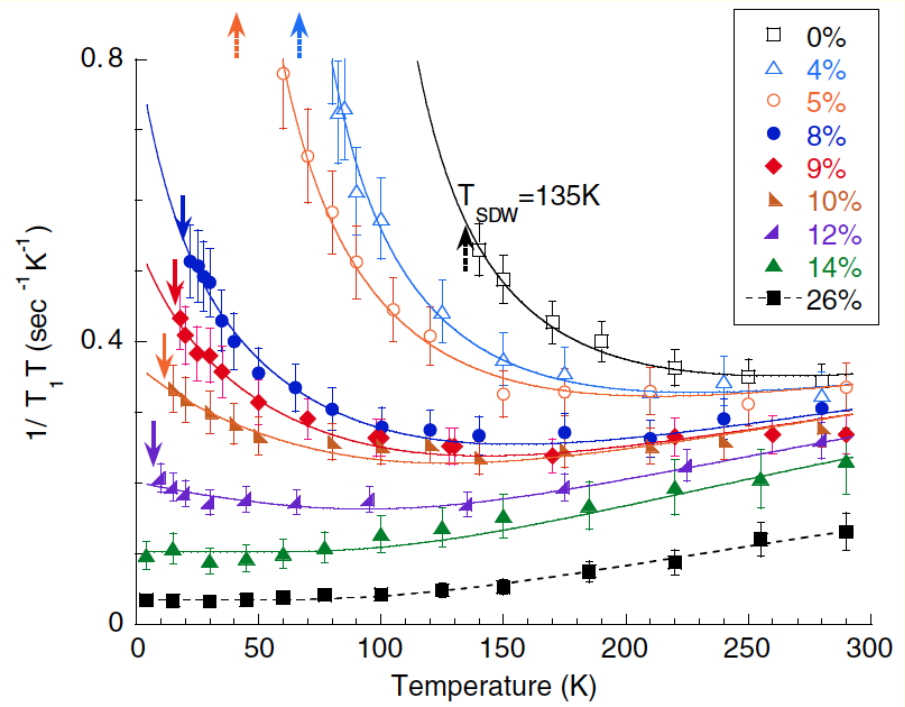
$$(T_1T)^{-1} \rightarrow \infty \text{ at } T_m$$



Relationship between magnetic and nematic fluctuations?

- Is there a relationship between magnetic and nematic fluctuations?

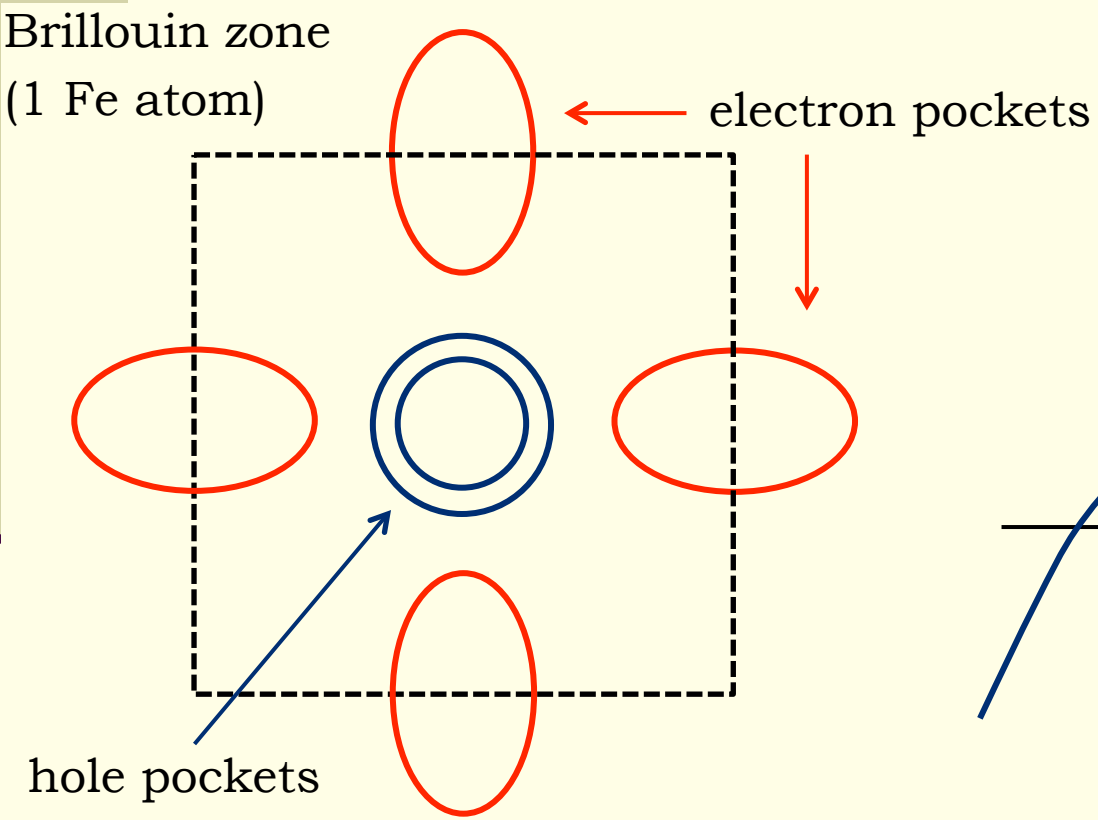


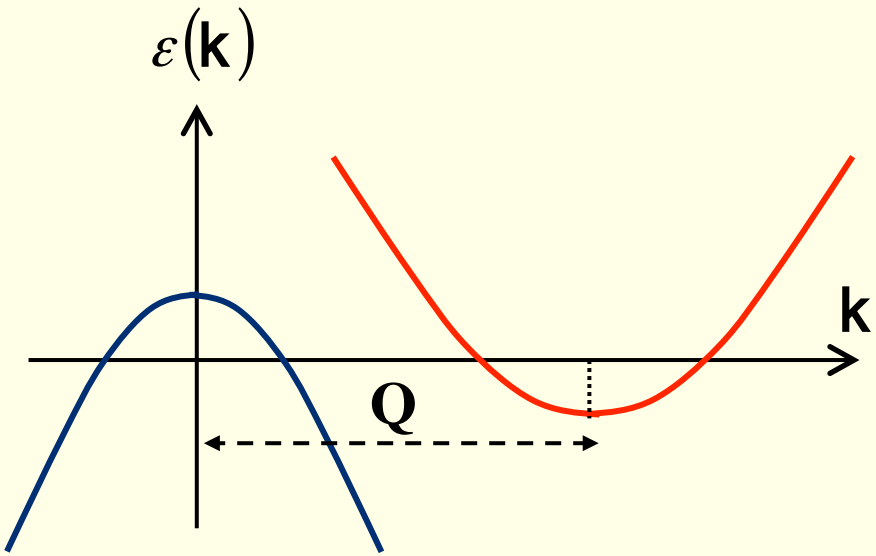


$$\left(\frac{C_s}{C_{s,0}}\right)^{-1} = 1 + \left(\frac{\lambda^2}{C_{s,0}}\right)\chi_{\text{nem}} \quad ?$$

Nematic order: magnetic mechanism

- Fermi surface of the iron pnictides:

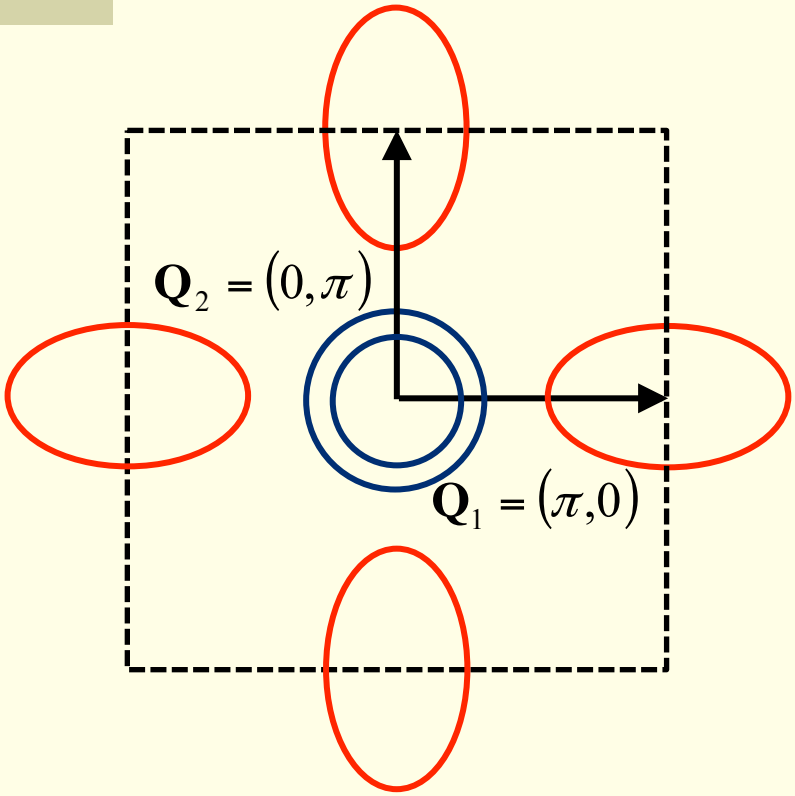


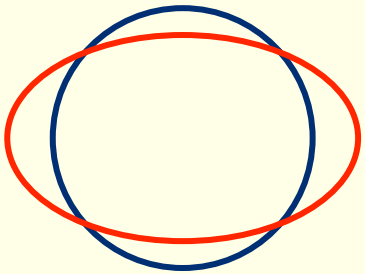


RMF, Chubukov, Eremin, Knolle, Schmalian, PRB (2012)

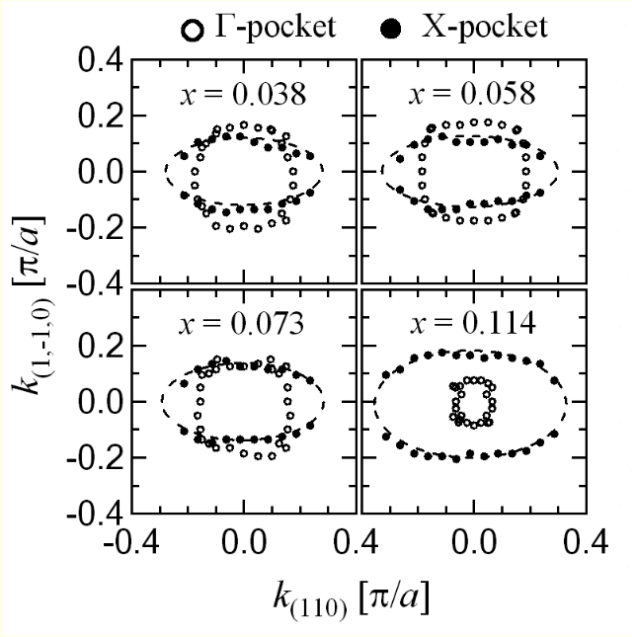
Nematic order: magnetic mechanism

- Bands have good nesting features: Stoner magnetism





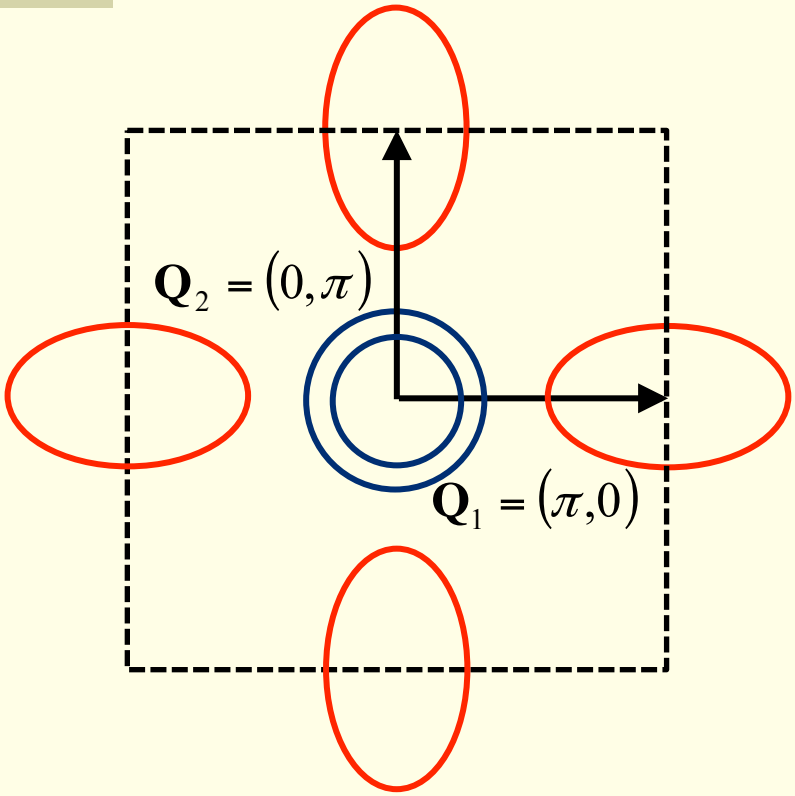
$$\chi_0(Q) \approx \log \frac{E_F}{T}$$



ARPES data

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

Nematic order: magnetic mechanism



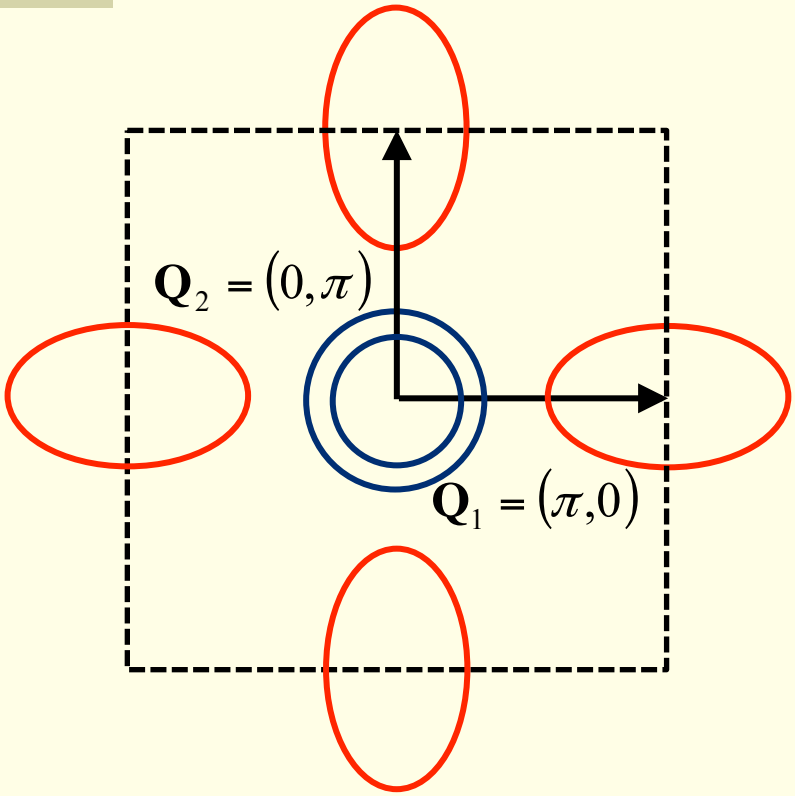
Two competing spin-density wave instabilities driven by nesting:

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

what is the ground state?

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

Nematic order: magnetic mechanism



Hamiltonian

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{(\mathrm{h})} d_{\mathbf{k}\alpha}^{+} d_{\mathbf{k}\alpha} + \sum_{\mathrm{j},\mathbf{k}} \varepsilon_{\mathrm{j},\mathbf{k}}^{(\mathrm{e})} c_{\mathrm{j},\mathbf{k}\alpha}^{+} c_{\mathrm{j},\mathbf{k}\alpha}$$

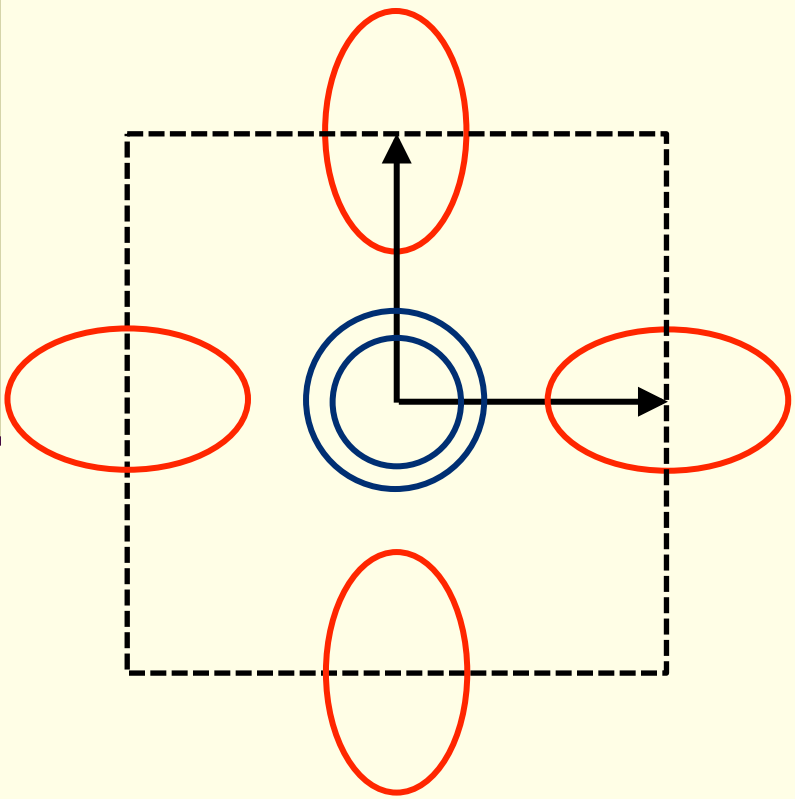
$$+I \sum_{\mathrm{j},\mathbf{k},\mathbf{k}'} \left(c_{\mathrm{j},\mathbf{k}\alpha}^{+} \sigma_{\alpha\beta} d_{\mathbf{k}\beta} \right) \cdot \left(d_{\mathbf{k}'\gamma}^{+} \sigma_{\gamma\delta} c_{\mathrm{j},\mathbf{k}'\delta} \right)$$

calculate the free energy of the electronic system (Hertz-Millis approach)

we skip the details and present the main results

Nematic order: magnetic mechanism

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



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

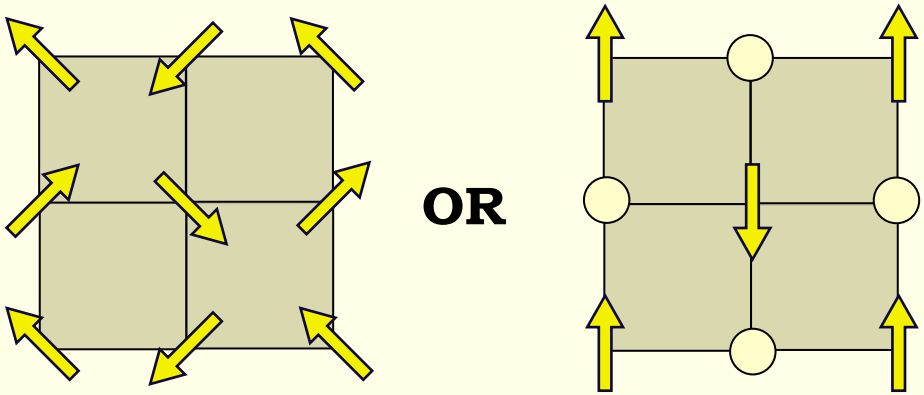
$$G_{i,k}^{-1} = i\omega_n - \varepsilon_{\mathbf{k}}$$

Nematic order: magnetic mechanism

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

competing order paramaters:

$g < 0$: "coexistence" (C_4 symmetric SDW) $M_1^2 = M_2^2$



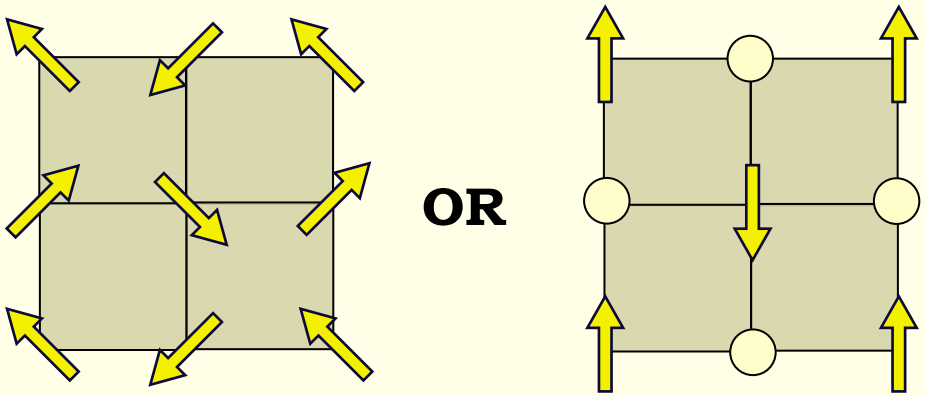
$\mathbf{M}_1 \perp \mathbf{M}_2$ $\mathbf{M}_1 \parallel \mathbf{M}_2$

Nematic order: magnetic mechanism

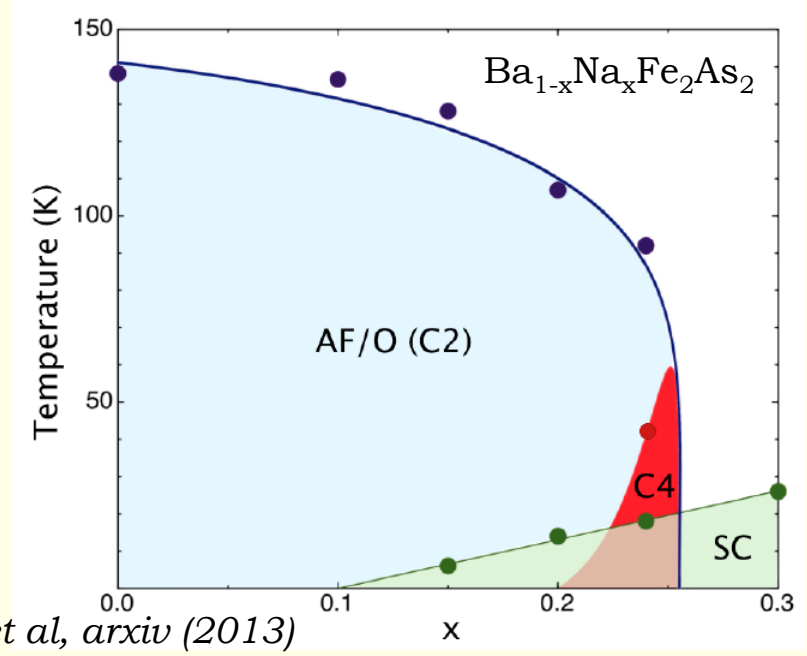
$$F_{\text{mag}} = \frac{a}{2}\left(M_1^2 + M_2^2\right) + \frac{u}{4}\left(M_1^2 + M_2^2\right)^2 - \frac{g}{4}\left(M_1^2 - M_2^2\right)^2$$

competing order paramaters:

$g < 0$: "coexistence" (C_4 symmetric SDW)



$$M_1^2 = M_2^2$$



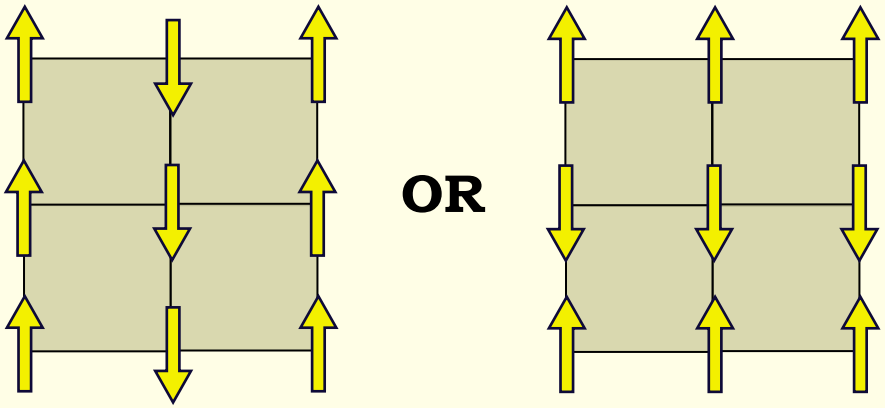
Avci et al, arxiv (2013)

Nematic order: magnetic mechanism

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

competing order paramaters:

$g > 0$: no "coexistence" (magnetic stripes) $M_1^2 M_2^2 = 0$



$M_1 \neq 0$ $\quad$ $M_1 = 0$

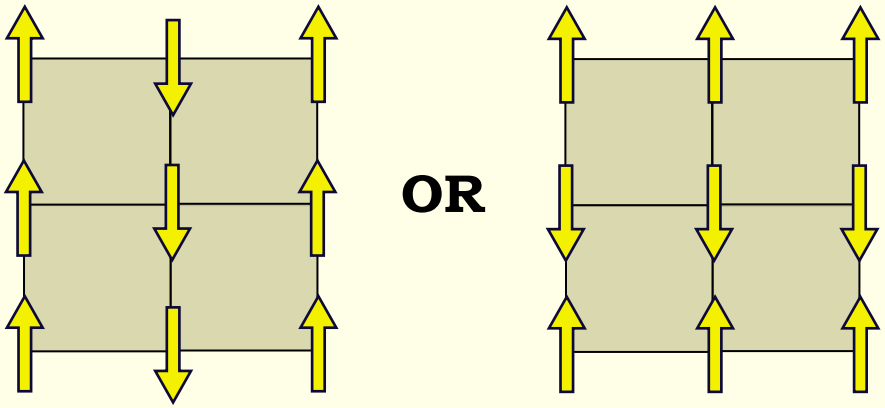
$M_2 = 0$ $\quad$ $M_2 \neq 0$

Nematic order: magnetic mechanism

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

competing order paramaters:

$g > 0$: symmetry-breaking: ***O(3)*** x $\boldsymbol{Z_2}$



Emergent Z_2 (Ising) nematic order parameter: $\varphi = \left\langle M_1^2 \right\rangle - \left\langle M_2^2 \right\rangle$

Nematic order: magnetic mechanism

Equation of state for the nematic order parameter:

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

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

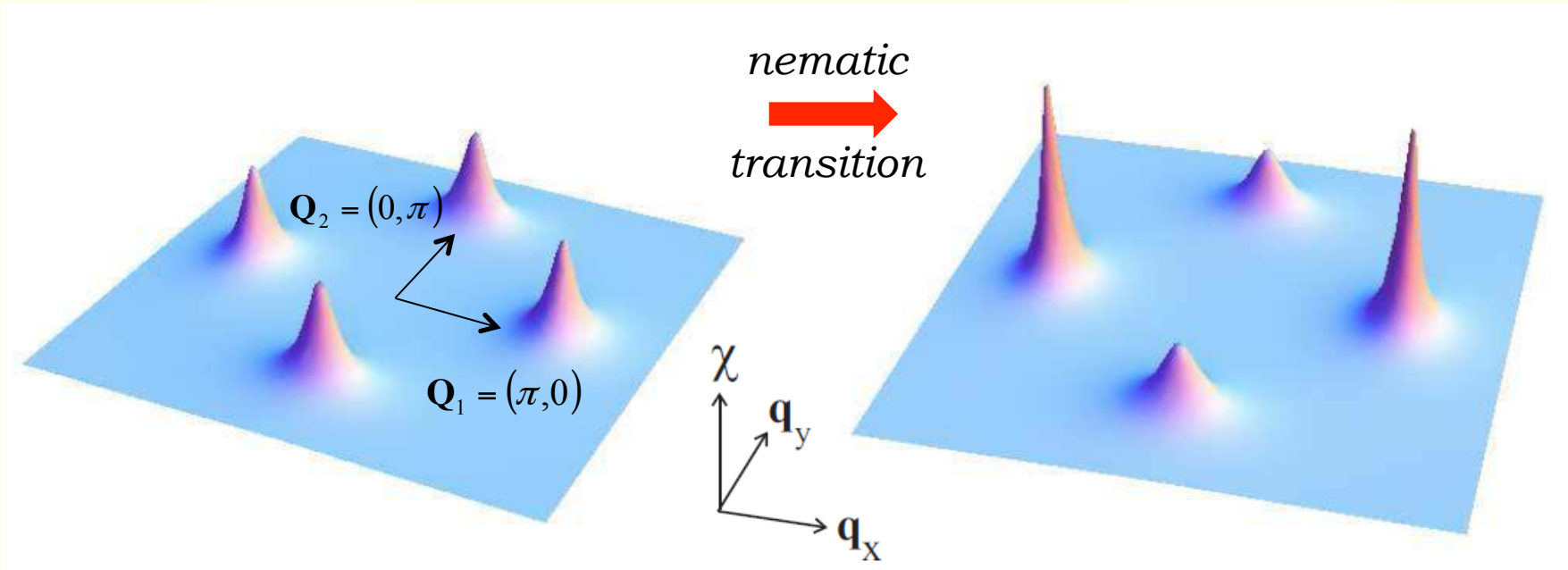
$$\left\langle M_1^2 \right\rangle \neq \left\langle M_2^2 \right\rangle$$

magnetic fluctuations → **nematic order**

for a localized-spin model, cf. Fang et al (2008) & Xu et al (2008)

Nematic order: magnetic mechanism

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



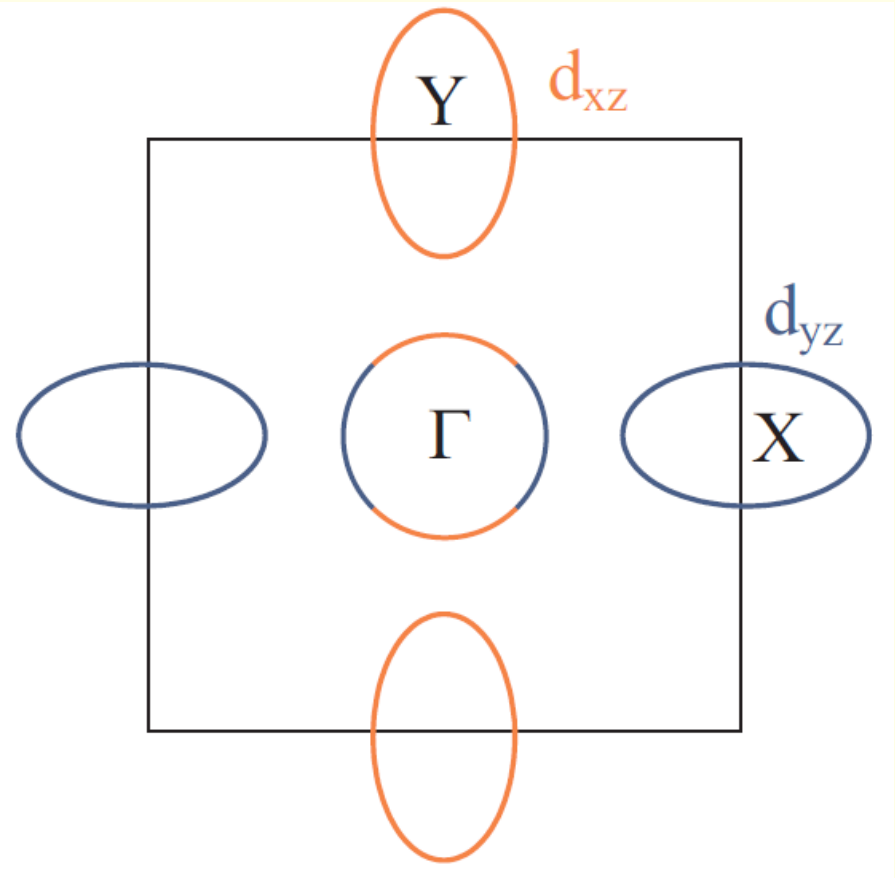
x and ***y*** directions become inequivalent:
Z_2 (tetragonal) symmetry breaking

$$\varphi = \langle M_1^2 \rangle - \langle M_2^2 \rangle$$

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

Nematic order: magnetic mechanism

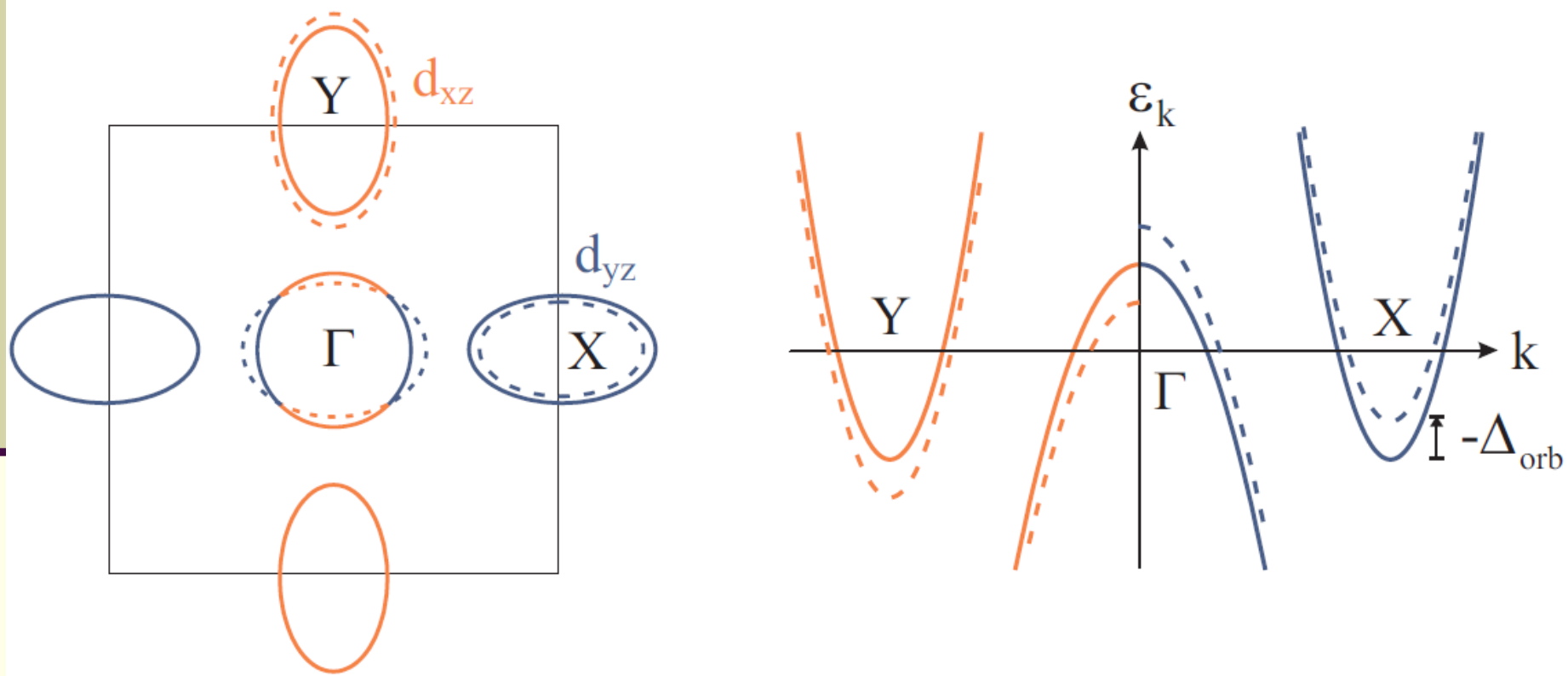
- Distinct Fermi pockets have different orbital content



Fe configuration: $3d^6$

Nematic order: magnetic mechanism

- Nematic order induces unequal occupations of d_{xz} and d_{yz} orbitals: *ferro-orbital order*

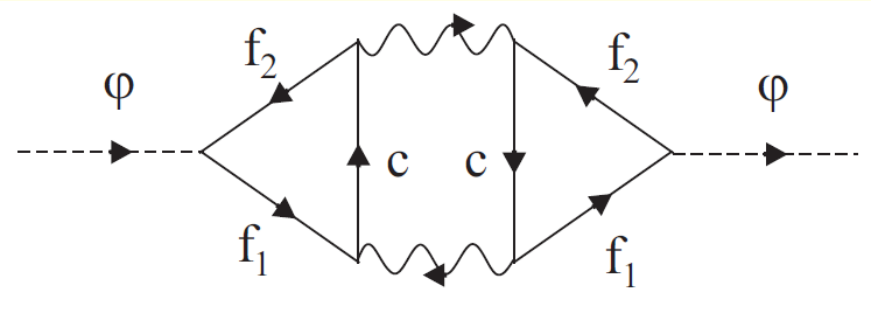


$$\langle n_{xz} \rangle - \langle n_{yz} \rangle \propto \varphi$$

cf. also Ku et al, PRL (2009); Phillips et al, PRB (2009); Devereaux et al, PRB (2009); WC Lee et al, PRB (2011)

Nematic susceptibility due to magnetic fluctuations

- Contribution of the magnetic fluctuations to the nematic susceptibility is given by the Aslamazov-Larkin diagram



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

(for a finite temperature phase transition)

RMF *et al, Phys. Rev. Lett.* ***105****, 157003 (2010)*

Nematic susceptibility due to magnetic fluctuations

- Contribution of the magnetic fluctuations to the nematic susceptibility:

$$\chi_{\text{nem}} = \frac{\sum_{\mathbf{q}} \chi_{\text{mag}}^{2}(\mathbf{q})}{1 - g\sum_{\mathbf{q}} \chi_{\text{mag}}^{2}(\mathbf{q})}$$

  - *But NMR spin-lattice relaxation rate is also proportional to this quantity* $\chi_{\text{mag}}^{-1}(\mathbf{q},\omega) = \chi_{\text{mag}}^{-1}(\mathbf{q}) - i\omega$

$$\frac{1}{T_1 T} \propto \lim_{\omega \to 0} \sum_{\mathbf{q}} \frac{\chi''_{\text{mag}}(\mathbf{q},\omega)}{\omega} \propto \sum_{\mathbf{q}} \chi_{\text{mag}}^{2}(\mathbf{q})$$

Relationship between magnetic and nematic fluctuations?

- A scaling relation between elastic and magnetic fluctuations

$$\left(\frac{C_s}{C_{s,0}}\right)^{-1} = 1 + \left(\frac{\lambda^2}{C_{s,0}}\right)\chi_{\text{nem}}$$

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

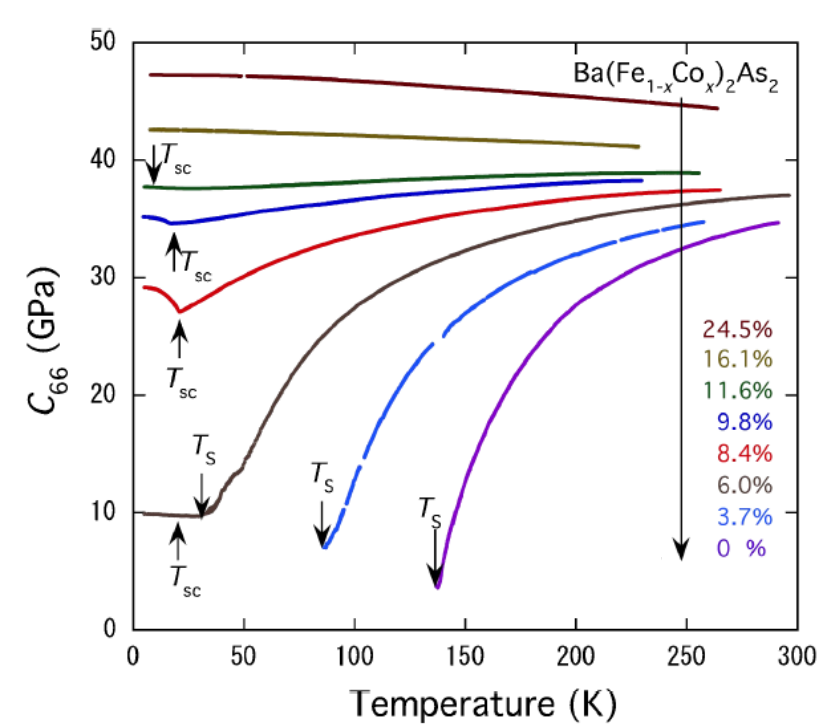
$$\left(\frac{C_s}{C_{s,0}}\right)^{-1} = 1 + \left[a\left(T_1 T\right) - b\right]^{-1}$$

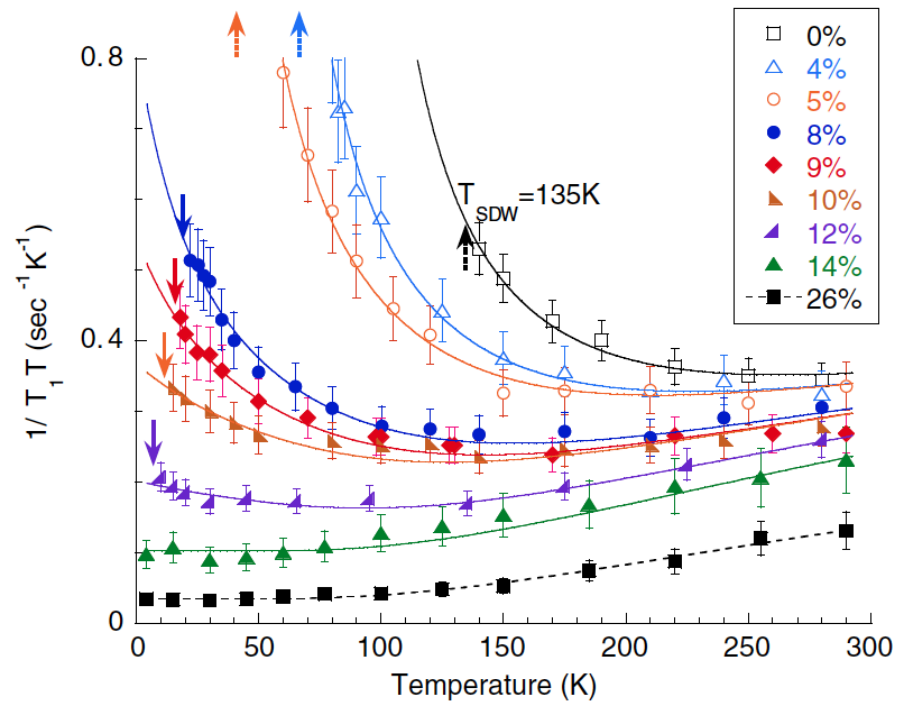
$$b = \frac{g}{\left(\lambda^2 / C_{s,0}\right)}$$

Relationship between magnetic and nematic fluctuations?

- A scaling relation between elastic and magnetic fluctuations

$$\left(\frac{C_s}{C_{s,0}}\right)^{-1} = 1 + \left[a(T_1T) - b\right]^{-1}$$





Relationship between magnetic and nematic fluctuations?

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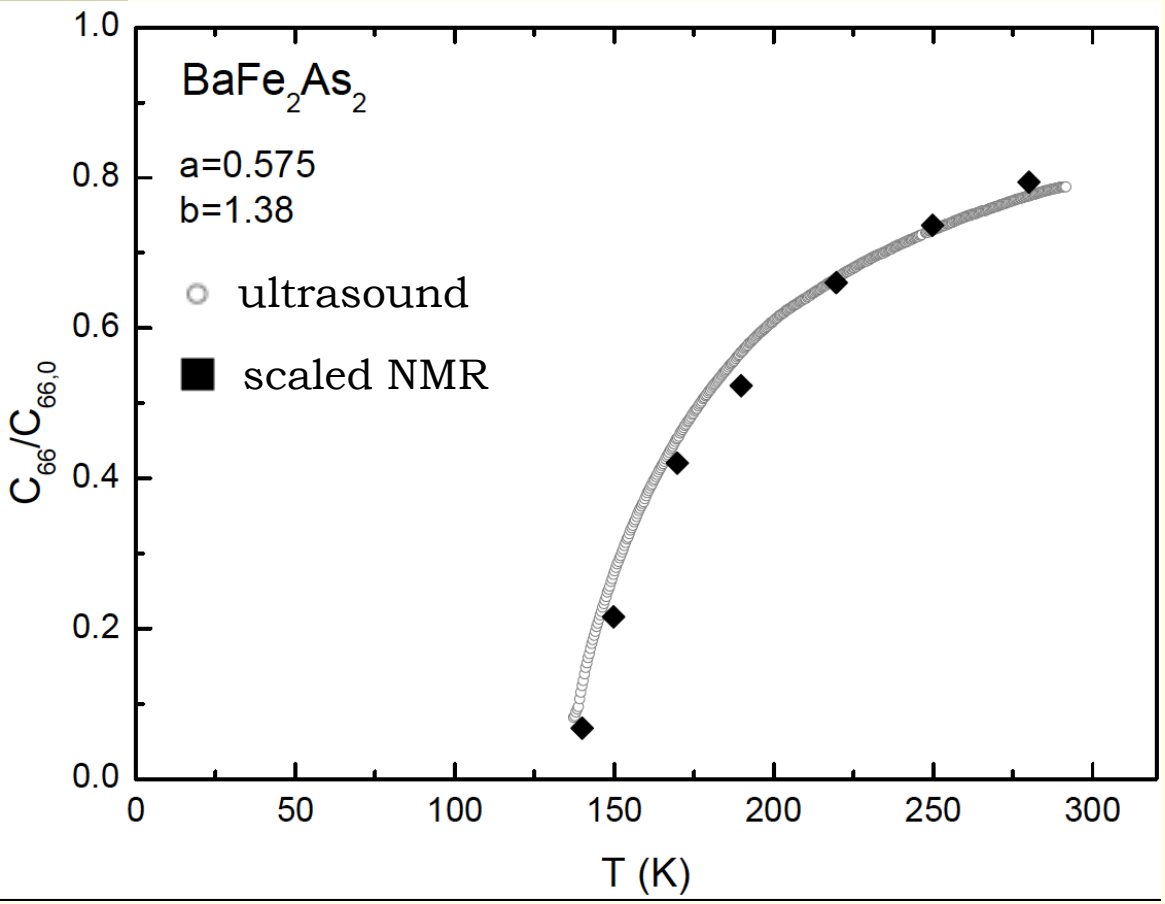


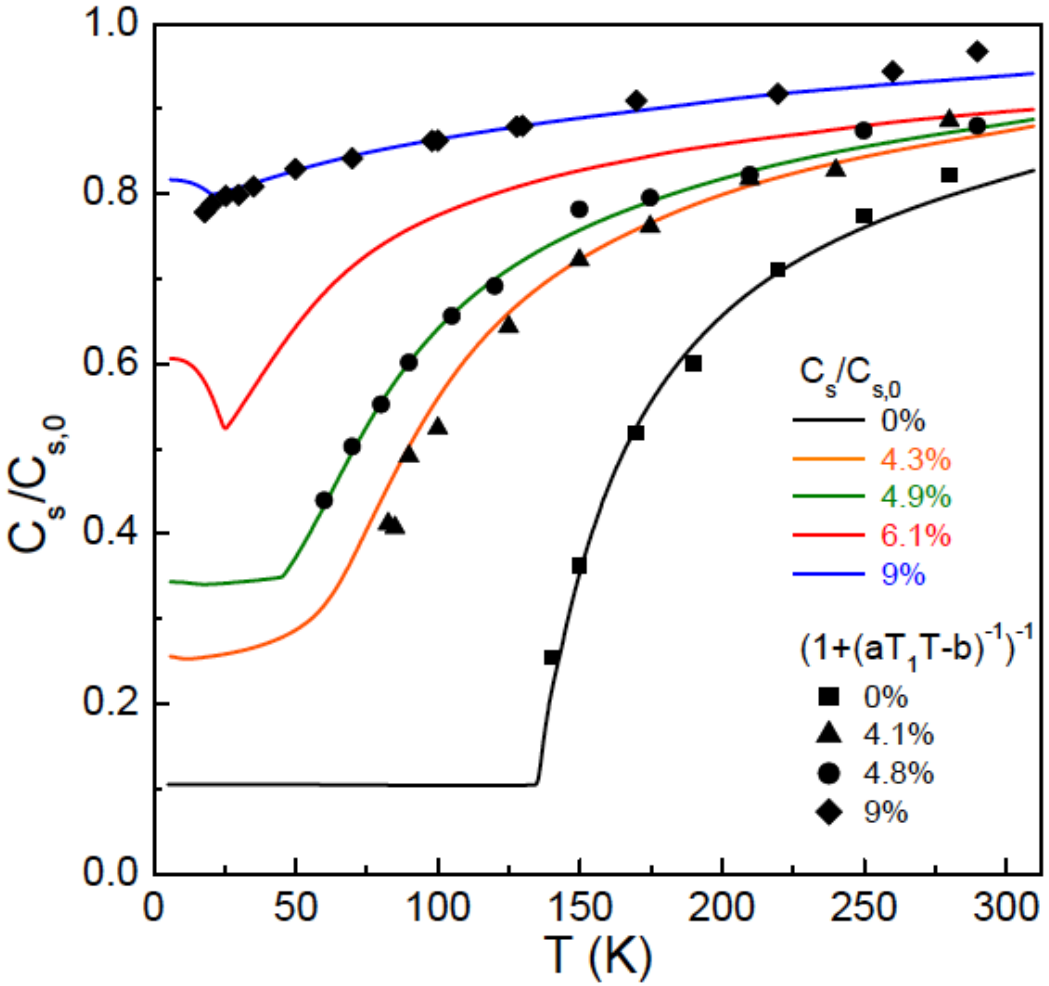
$$\left(\frac{C_s}{C_{s,0}}\right)^{-1} = 1 + \left[a\left(T_1T\right) - b\right]^{-1}$$

evidence for a magnetically driven structural transition

RMF, Bohmer, Meingast, Schmalian, *PRL (in press)*

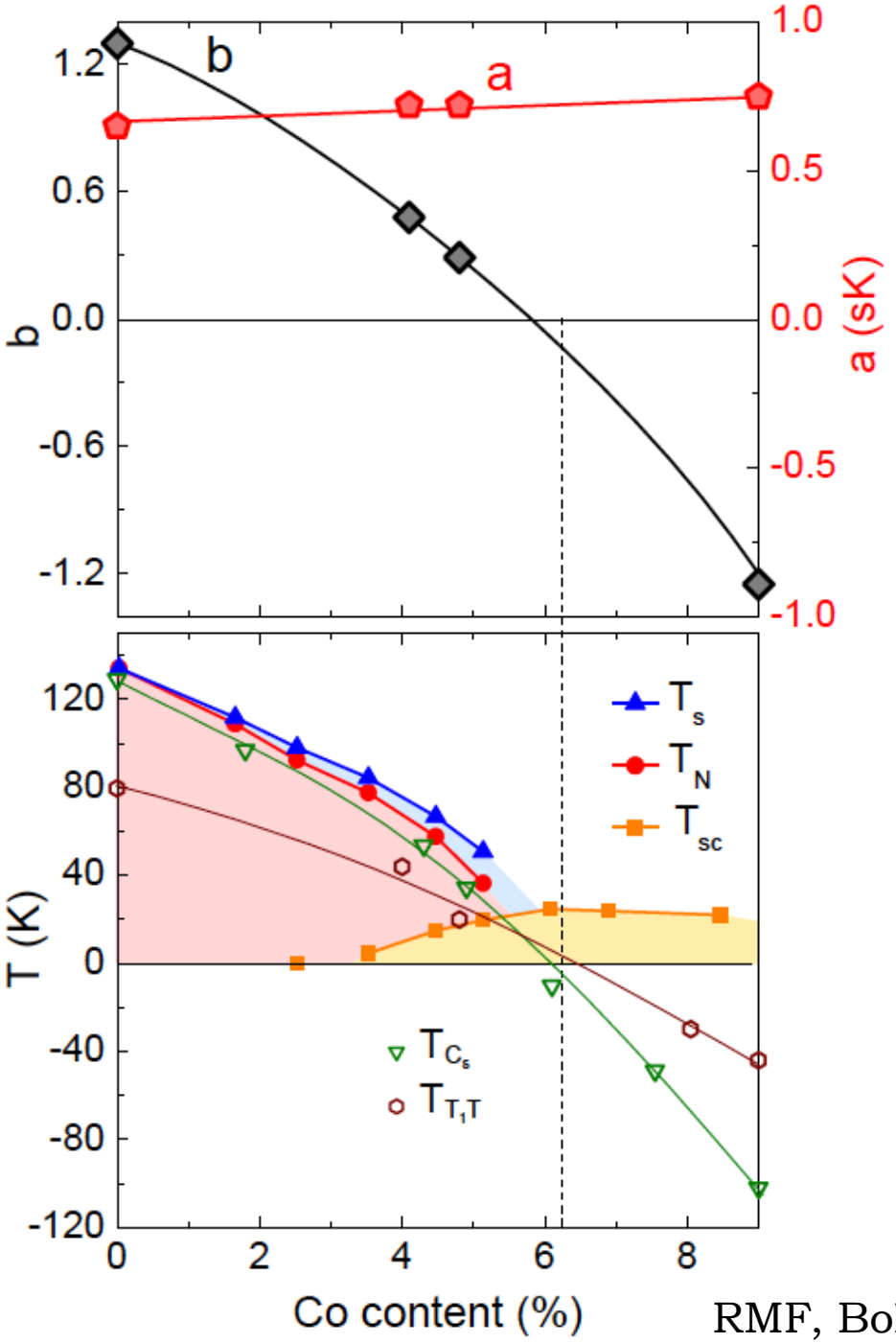
Relationship between magnetic and nematic fluctuations?

- A scaling relation between elastic and magnetic fluctuations



$$\left(\frac{C_s}{C_{s,0}}\right)^{-1} = 1 + \left[a(T_1T) - b\right]^{-1}$$

scaling observed for several doping levels



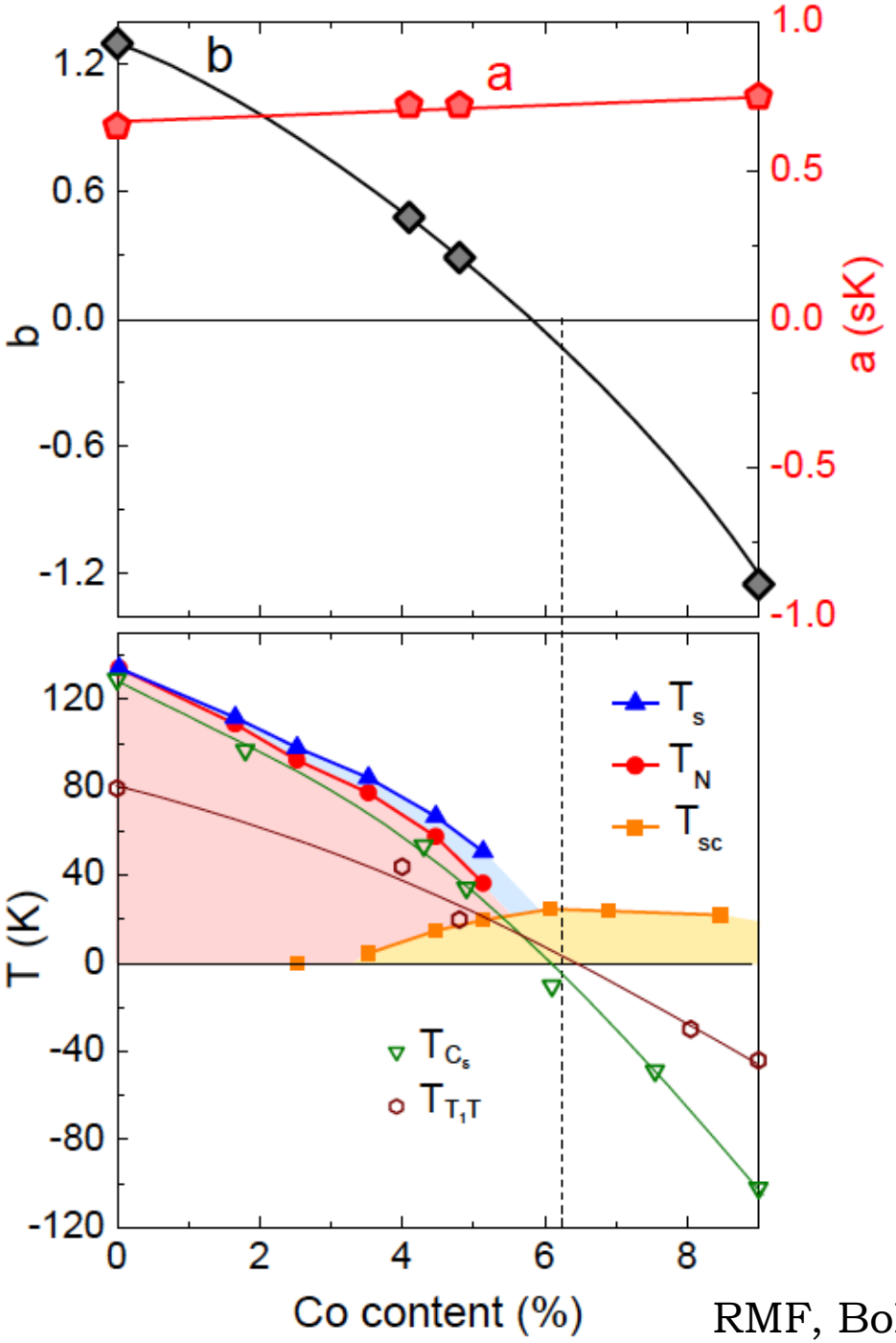
$$\left(\frac{C_s}{C_{s,0}}\right)^{-1} = 1 + \left[a(T_1T) - b\right]^{-1}$$

$$b = \frac{g}{\left(\lambda^2 / C_{s,0}\right)}$$

$b \sim 1$: ***strong contribution of the magneto-elastic coupling***

cf. Dagotto et al, PRL (2013)

RMF, Bohmer, Meingast, Schmalian, *PRL (in press)*



$$\left(\frac{C_s}{C_{s,0}}\right)^{-1} = 1 + \left[a(T_1T) - b\right]^{-1}$$

$$b = \frac{g}{\left(\lambda^2 / C_{s,0}\right)}$$

$g \rightarrow 0$ near optimal doping: critical fluctuations with enhanced $O(6)$ symmetry

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

impact on Cooper-pair formation?

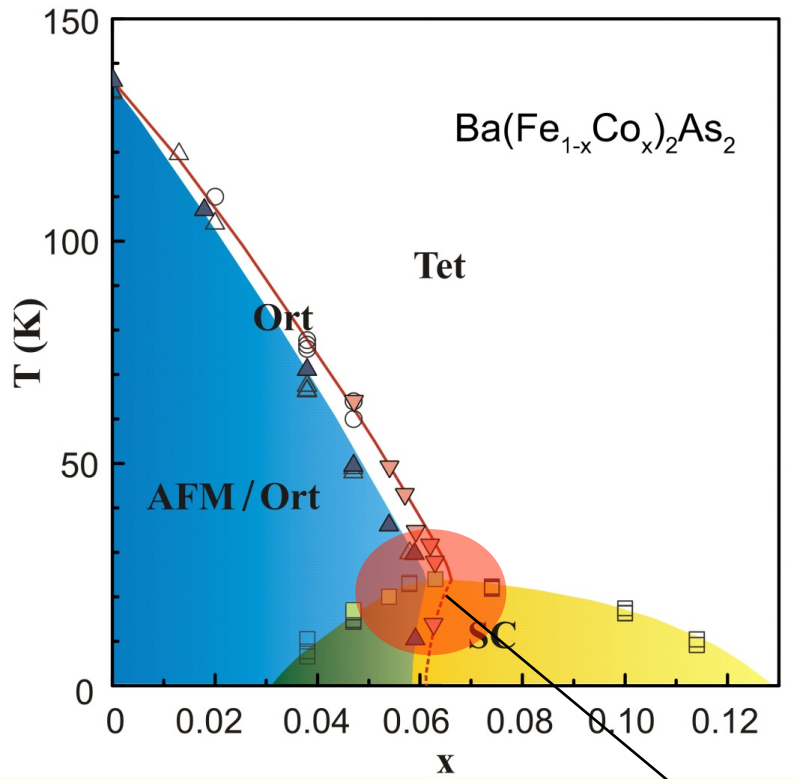
RMF, Bohmer, Meingast, Schmalian, *PRL (in press)*

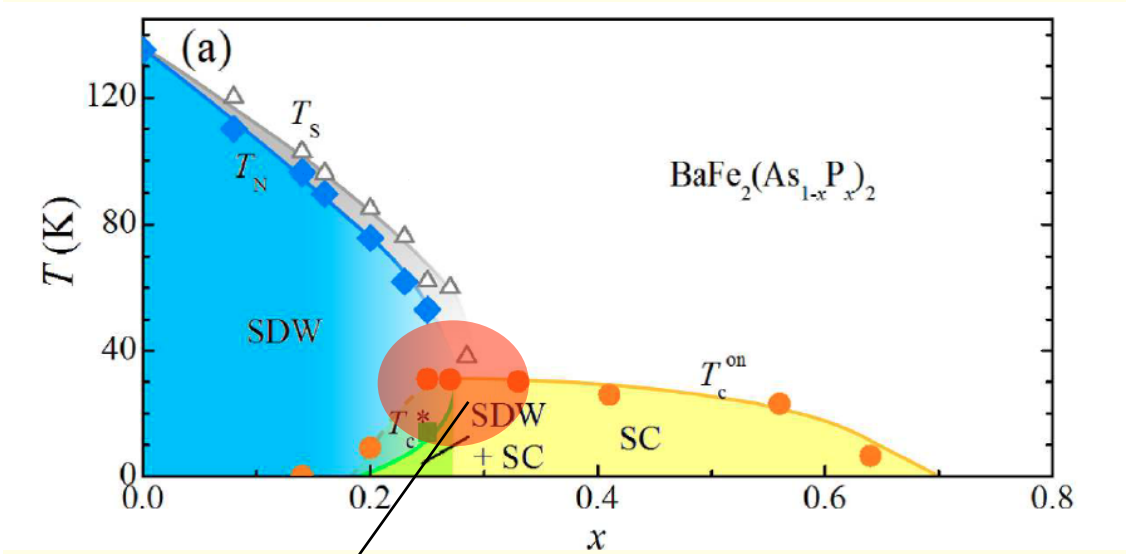
Outline

1. **Microscopic origin of the nematic state**
   - *scaling between elastic and magnetic fluctuations*
   - *evidence for magnetically-driven structural transition*

2. **Magnetic and nematic quantum phase transitions**
   - *competition between nematicity and superconductivity*
   - *single weakly first-order quantum phase transition inside the superconducting dome*

What is the fate of the magnetic and nematic transitions?



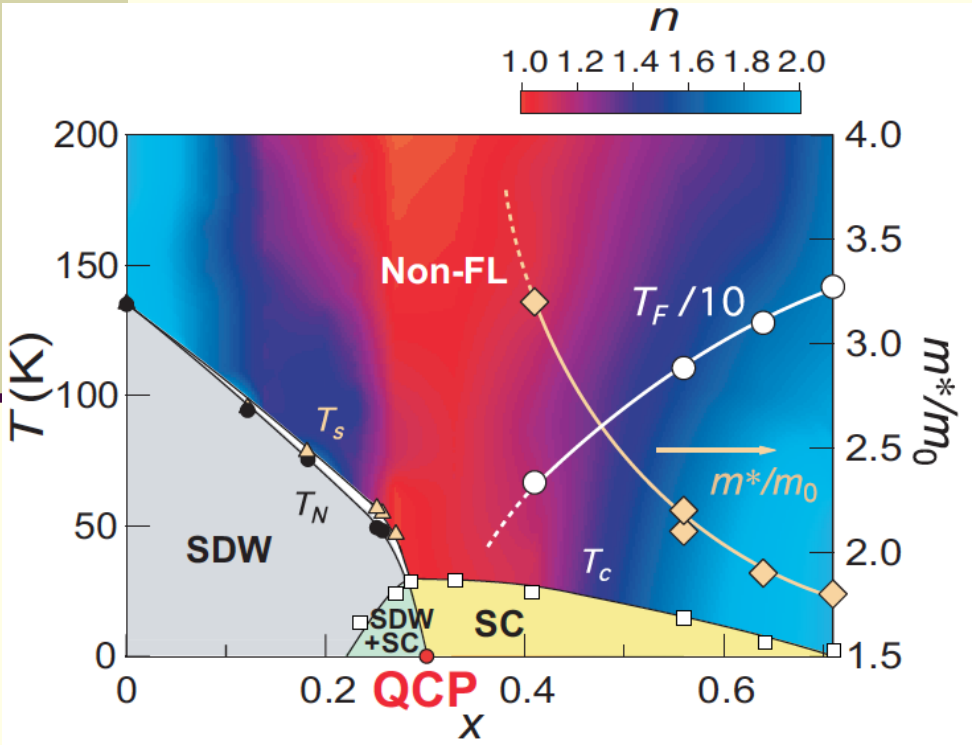


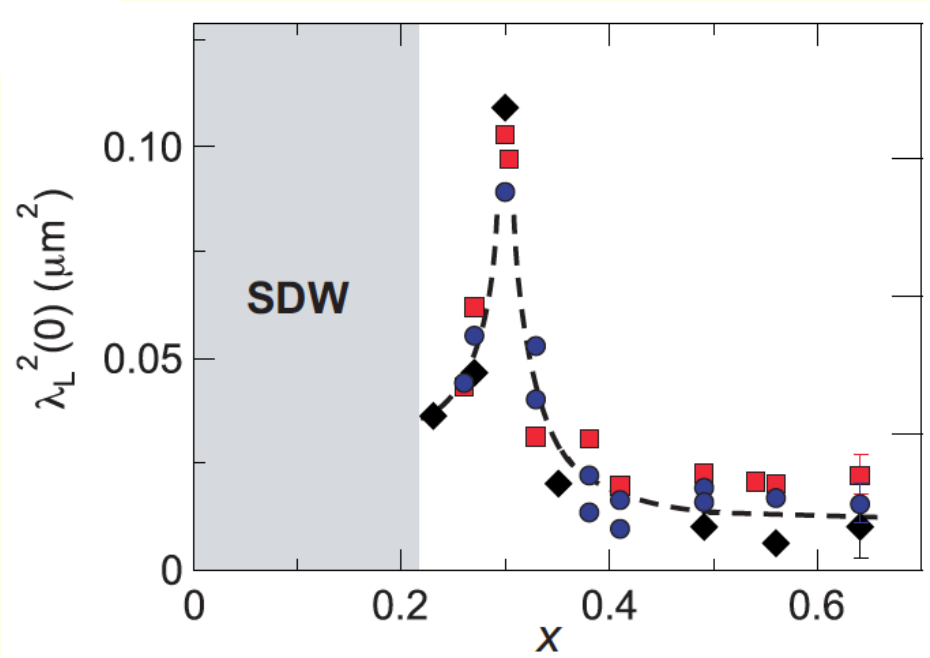
two separate transitions meet the SC dome

- Can both orders coexist with SC?
- If yes, what is their fate at *T=0*?

What is the fate of the magnetic and nematic transitions?

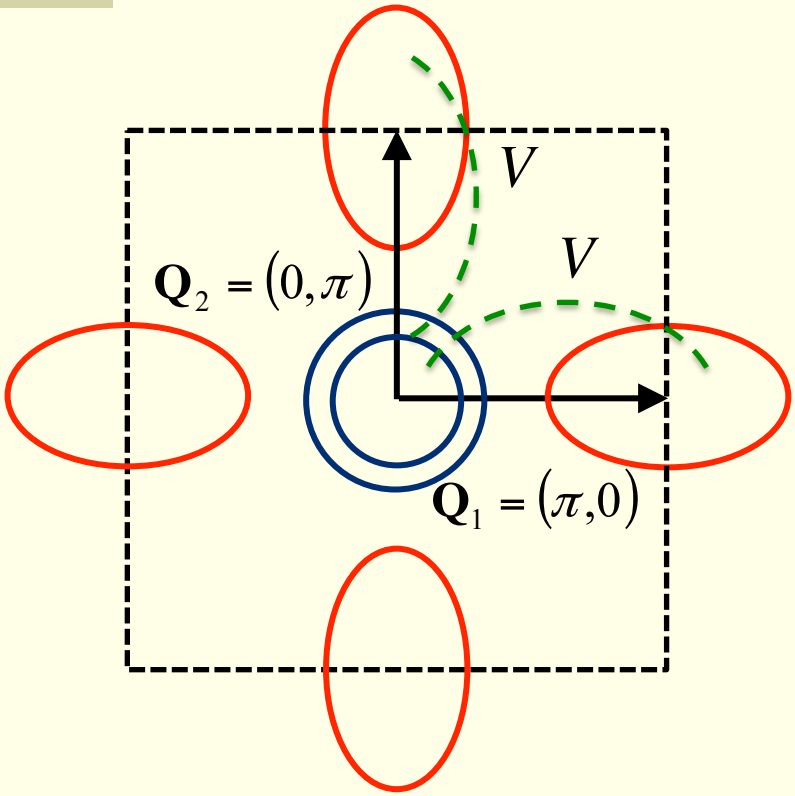
- Penetration depth shows a single quantum transition and non-Fermi liquid behavior
  - What is the nature of this T=0 transition?





Hashimoto et al, Science (2012)

Microscopic model for magnetism, nematicity, and SC



Magnetism: two competing SDW instabilities

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

Nematicity: induced by SDW fluctuations

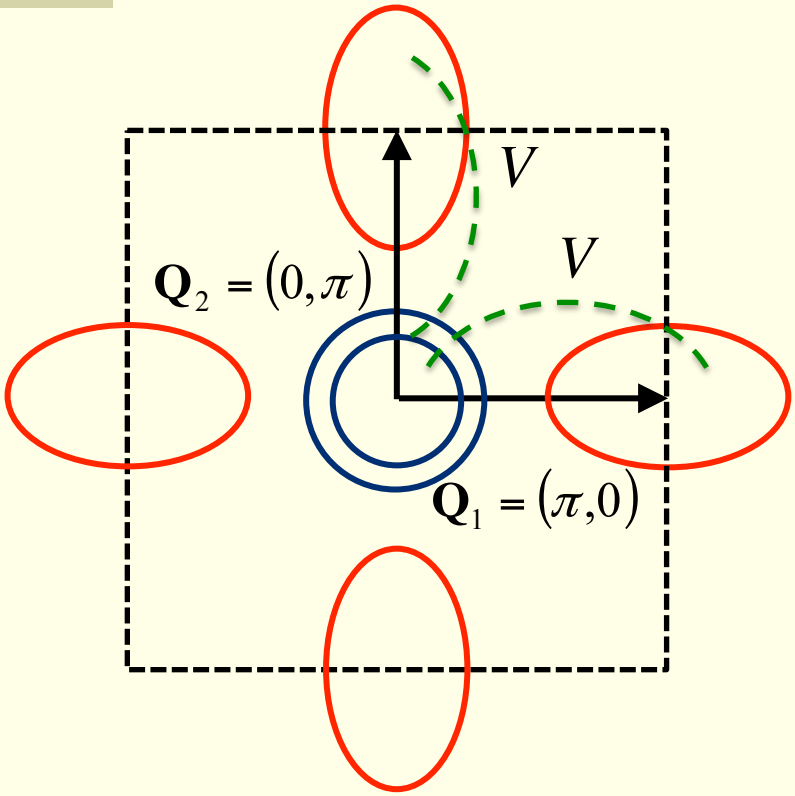
$$\varphi \propto \langle M_1^2 \rangle - \langle M_2^2 \rangle$$

Superconductivity: repulsive electronic interaction enhanced by spin fluctuations

$$\Delta_\Gamma \propto -\Delta_{X/Y}$$

RMF, Maiti, Wölfle, Chubukov, *Phys. Rev. Lett.* ***111***, *057001 (2013)*

Microscopic model for magnetism, nematicity, and SC



Hamiltonian

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{(\mathrm{h})} d_{\mathbf{k}\alpha}^{+} d_{\mathbf{k}\alpha} + \sum_{\mathrm{j},\mathbf{k}} \varepsilon_{\mathrm{j},\mathbf{k}}^{(\mathrm{e})} c_{\mathrm{j},\mathbf{k}\alpha}^{+} c_{\mathrm{j},\mathbf{k}\alpha}$$

$$+I \sum_{\mathrm{j},\mathbf{k},\mathbf{k}'} \left(c_{\mathrm{j},\mathbf{k}\alpha}^{+} \sigma_{\alpha\beta} d_{\mathbf{k}\beta} \right) \cdot \left(d_{\mathbf{k}'\gamma}^{+} \sigma_{\gamma\delta} c_{\mathrm{j},\mathbf{k}'\delta} \right)$$

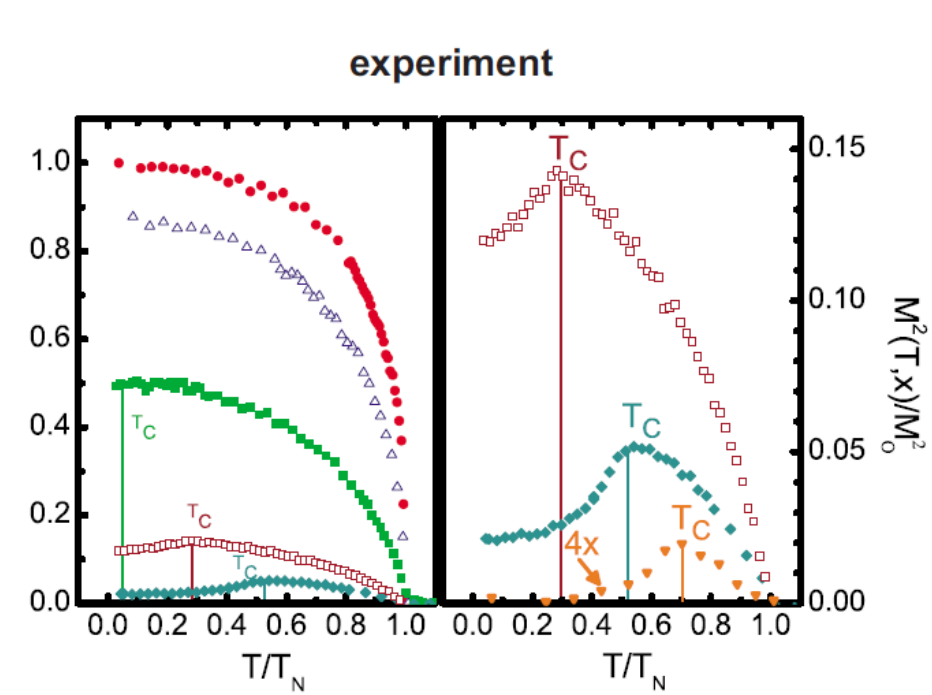
$$+V \sum_{\mathrm{j},\mathbf{k},\mathbf{k}'} \left(c_{\mathrm{j},\mathbf{k}\alpha}^{+} c_{j,-\mathbf{k}\bar{\alpha}}^{+} \right) \left(d_{\mathbf{k}'\beta} d_{\mathrm{j},-\mathbf{k}'\bar{\beta}} \right)$$

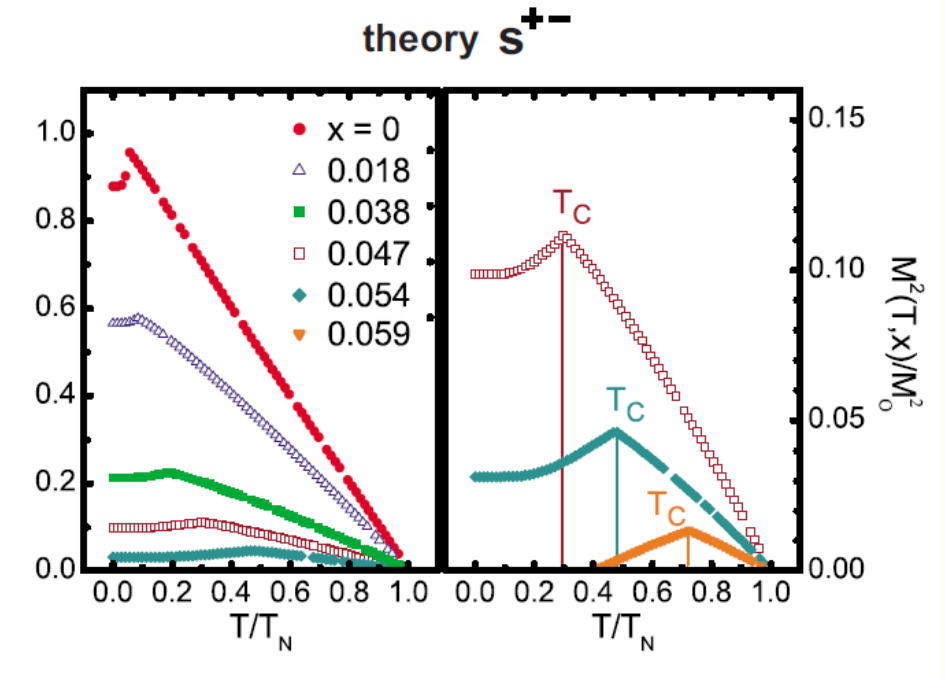
calculate the free energy of the coupled system (three ordered states)

we skip the details and present the main results

Competition between superconductivity and magnetism

- Competition between magnetism and superconductivity: the same electrons are responsible for both orders





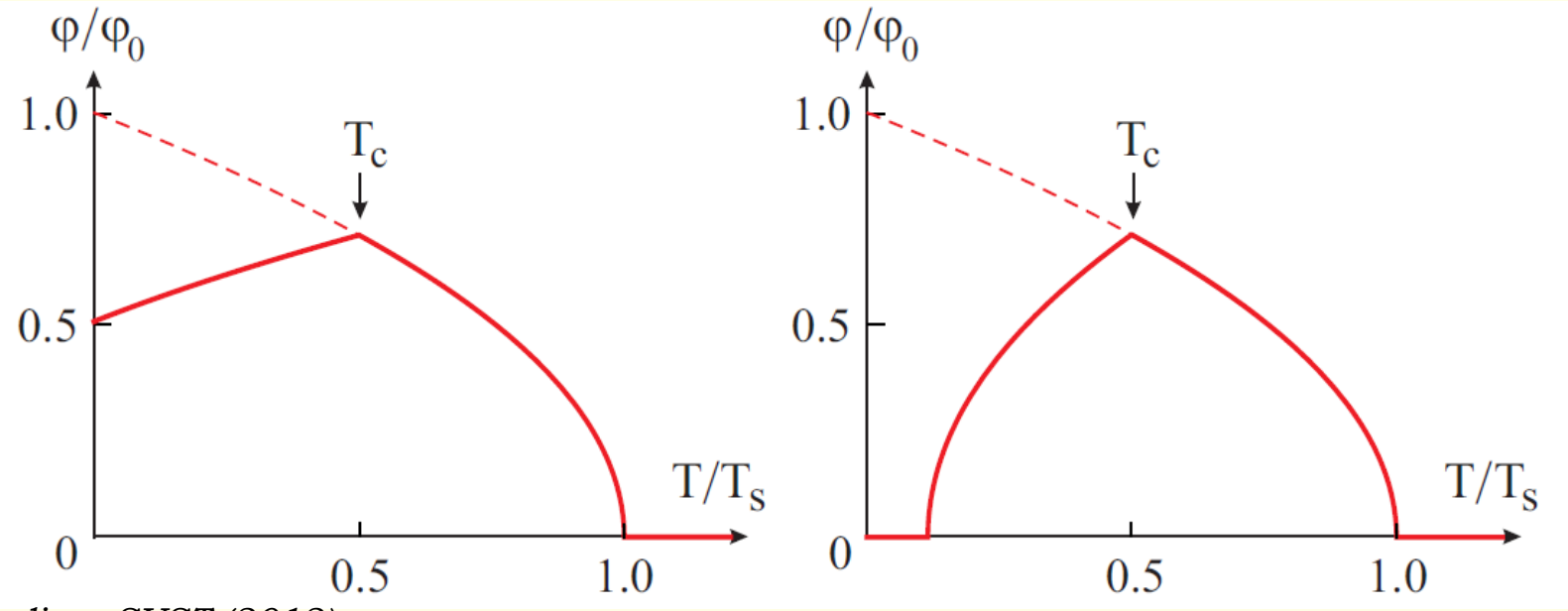
RMF et al, PRB (2010)
RMF & Schmalian, PRB (2010)
Vorontsov et al, PRB (2010)

Competition between superconductivity and nematicity

- Due to its magnetic origin, nematicity also competes (indirectly) with superconductivity

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

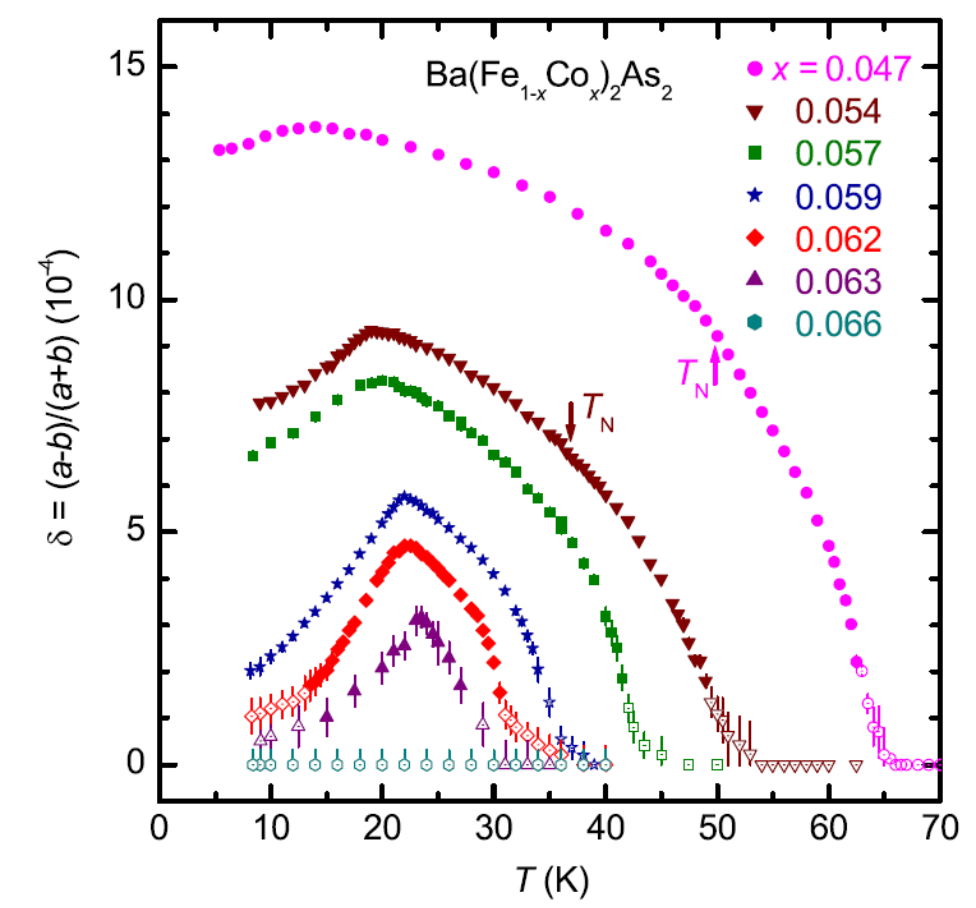
  - *even in the absence of long-range magnetic order*



RMF & Schmalian, SUST (2012)

Competition between superconductivity and nematicity

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

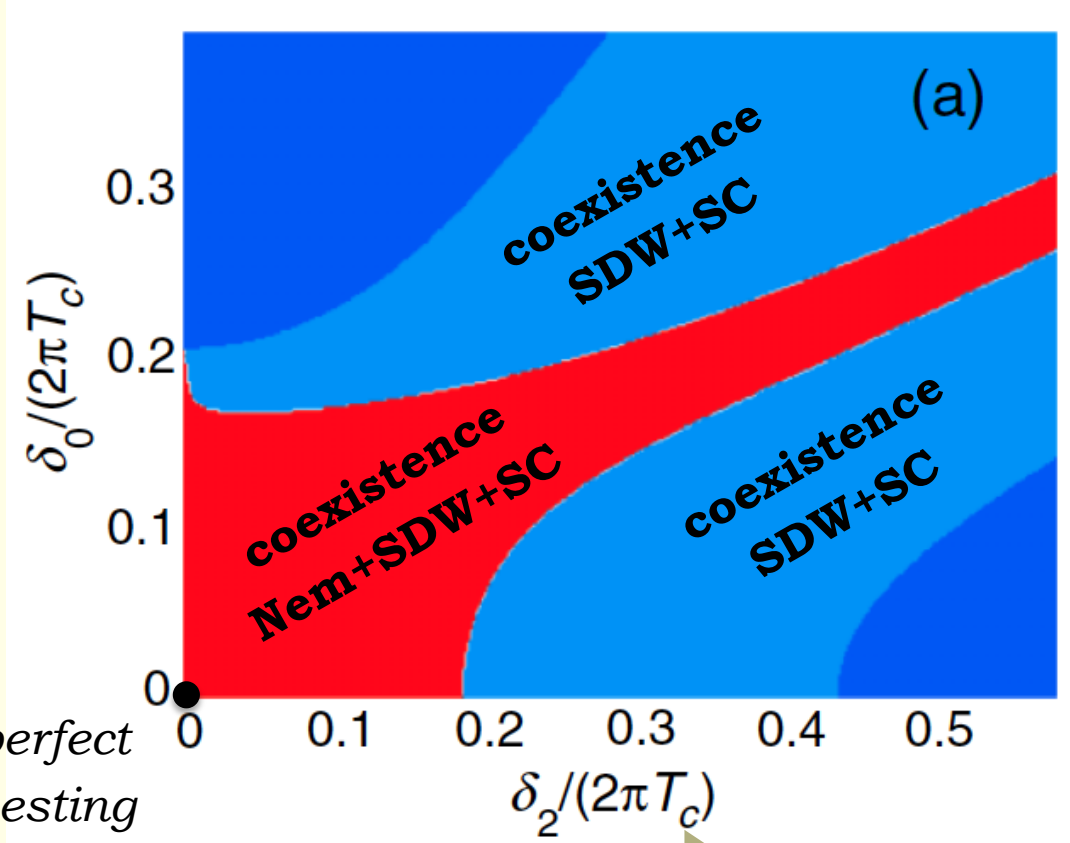


Nandi,..., RMF et al, PRL (2010)

Coexistence between magnetism, nematicity, and SC

- Due to its magnetic origin, nematicity coexists microscopically with SC for a wide range of parameters

carrier concentration (doping)



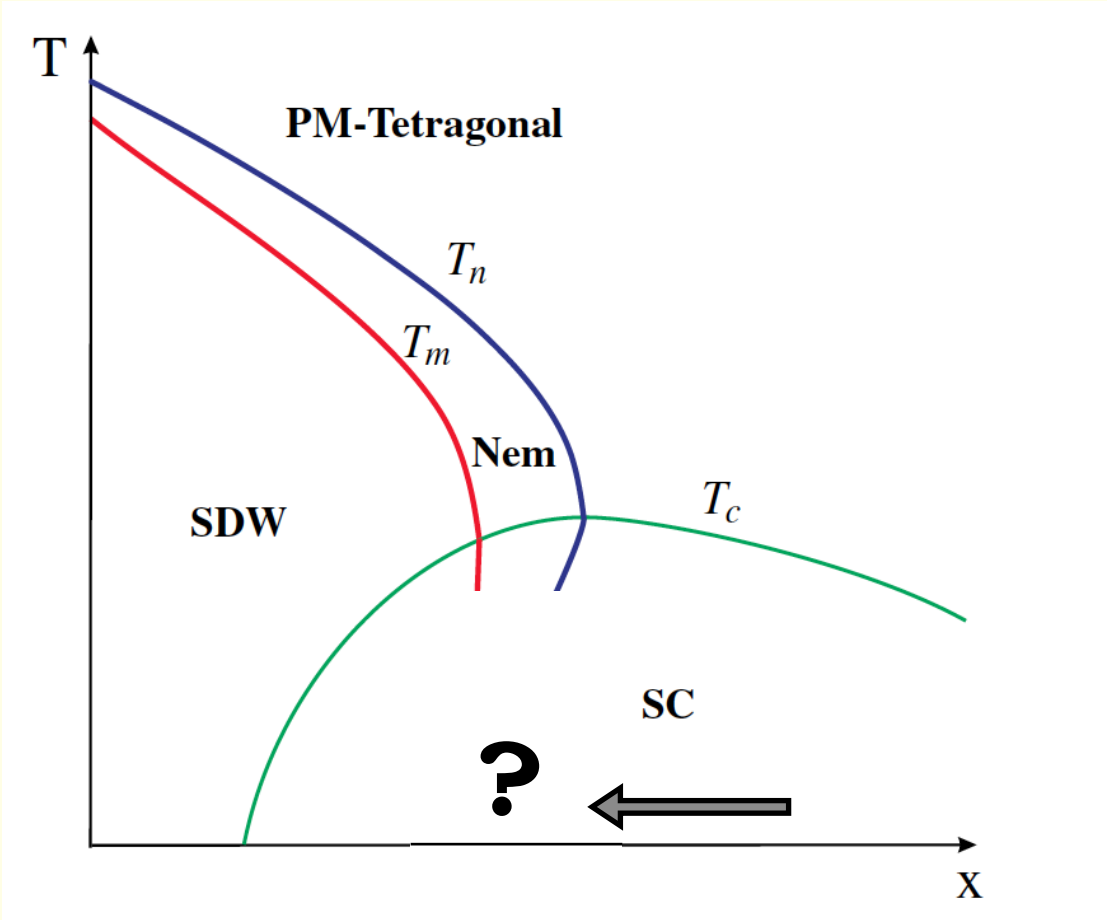
perfect nesting

band ellipticity (pressure)

RMF, Maiti, Wölfle, Chubukov, PRL (2013)

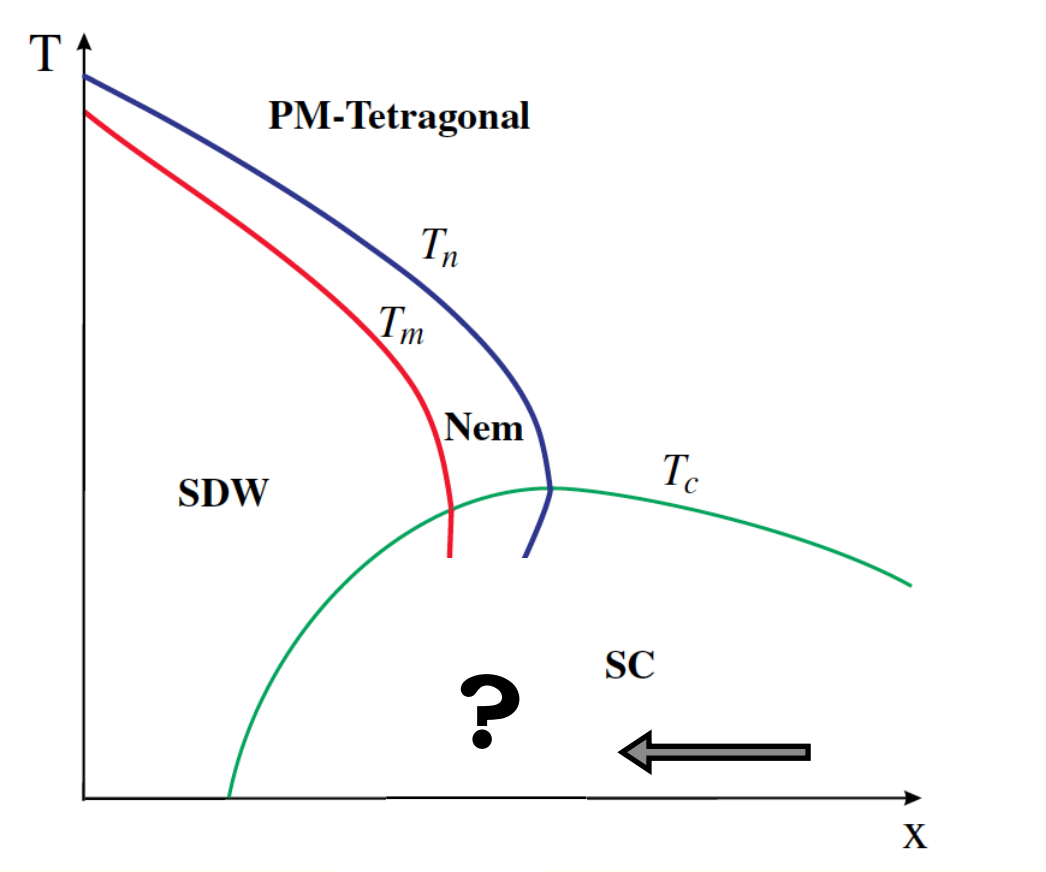
Coexistence between magnetism, nematicity, and SC

- What is the fate of the magnetic and nematic transitions deep inside the SC dome?



Coexistence between magnetism, nematicity, and SC

- Main effect of the coexistence with SC: change of the magnetic excitations from overdamped to propagating



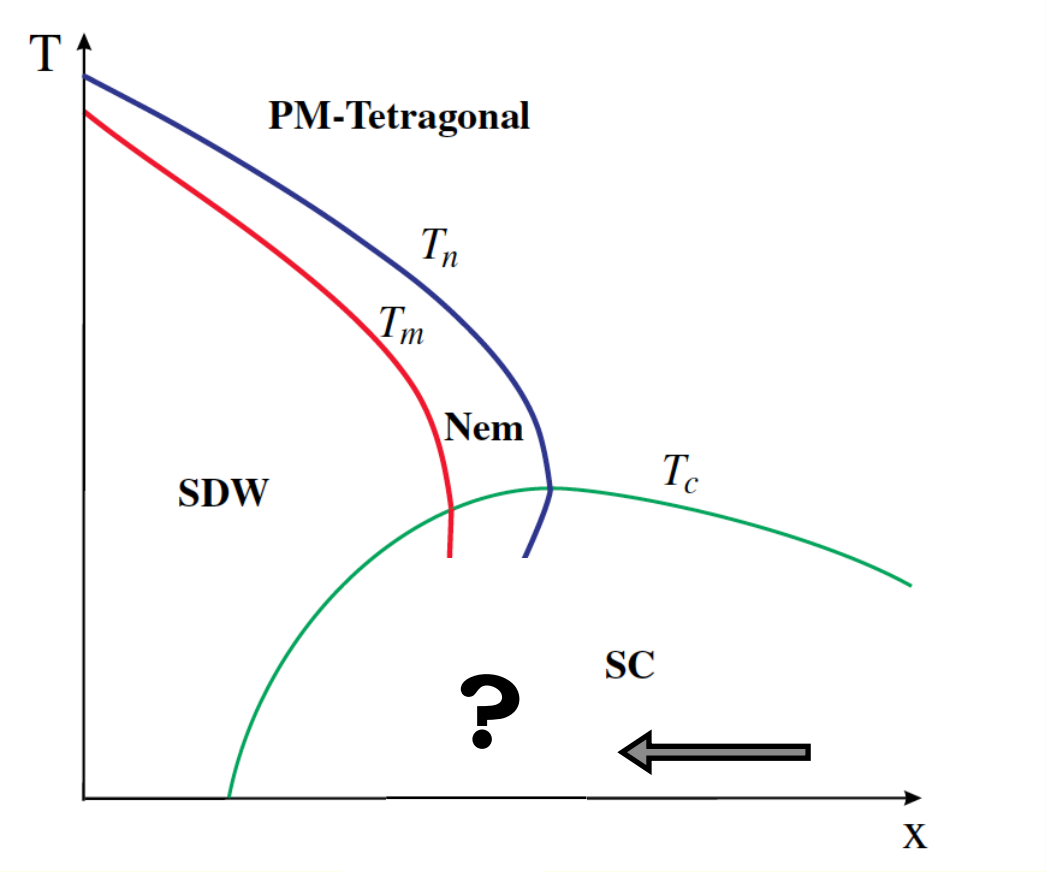
without SC: overdamped

$$\chi_{\text{mag}}^{-1}(\mathbf{q},\omega) = \chi_{\text{mag}}^{-1}(\mathbf{q}) - i\omega$$

$$d_{\text{eff}} = d + 2$$

Coexistence between magnetism, nematicity, and SC

- Main effect of the coexistence with SC: change of the magnetic excitations from overdamped to propagating



without SC: overdamped

$$\chi_{\text{mag}}^{-1}(\mathbf{q},\omega) = \chi_{\text{mag}}^{-1}(\mathbf{q}) - i\omega$$

$$d_{\text{eff}} = d + 2$$

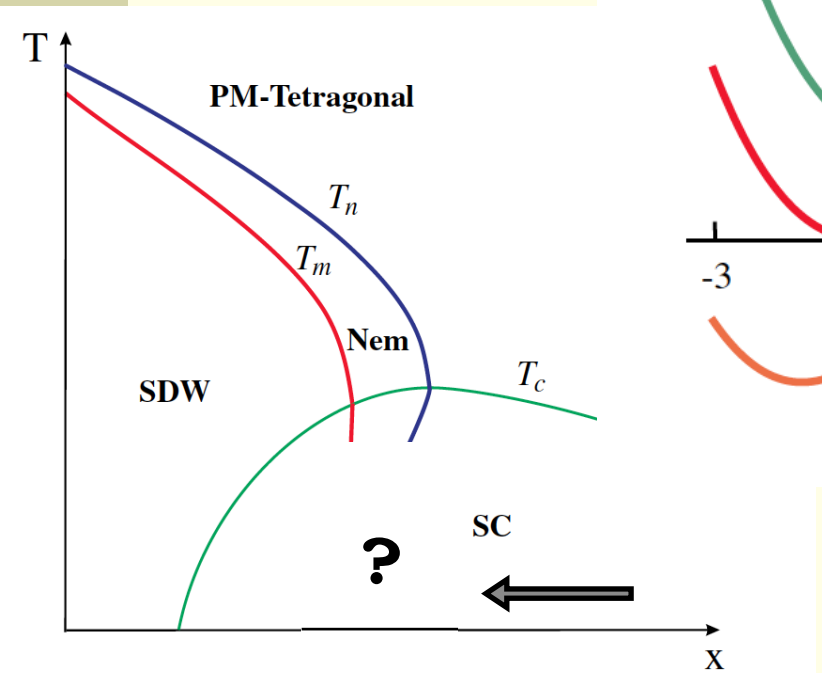
with SC: propagating

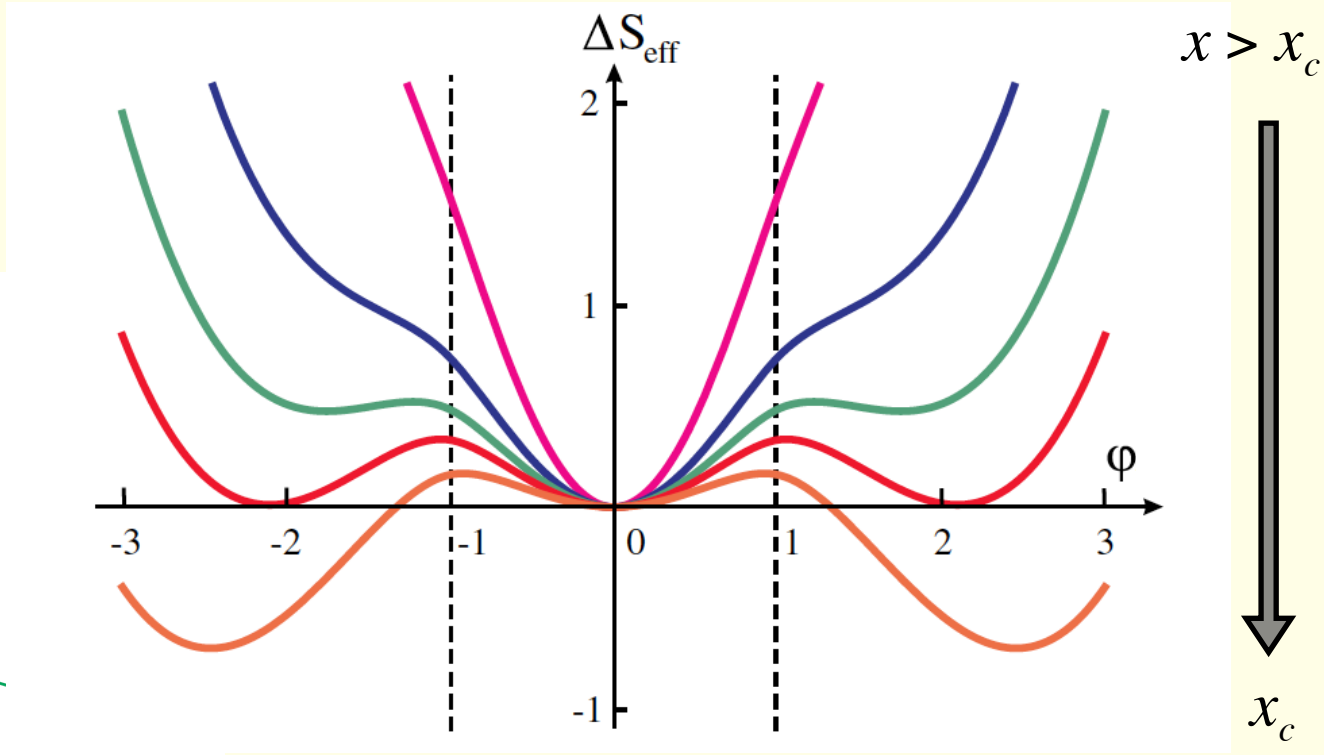
$$\chi_{\text{mag}}^{-1}(\mathbf{q},\omega) = \chi_{\text{mag}}^{-1}(\mathbf{q}) - \omega^2$$

$$d_{\text{eff}} = d + 1$$

Magnetic and nematic transitions inside the SC dome

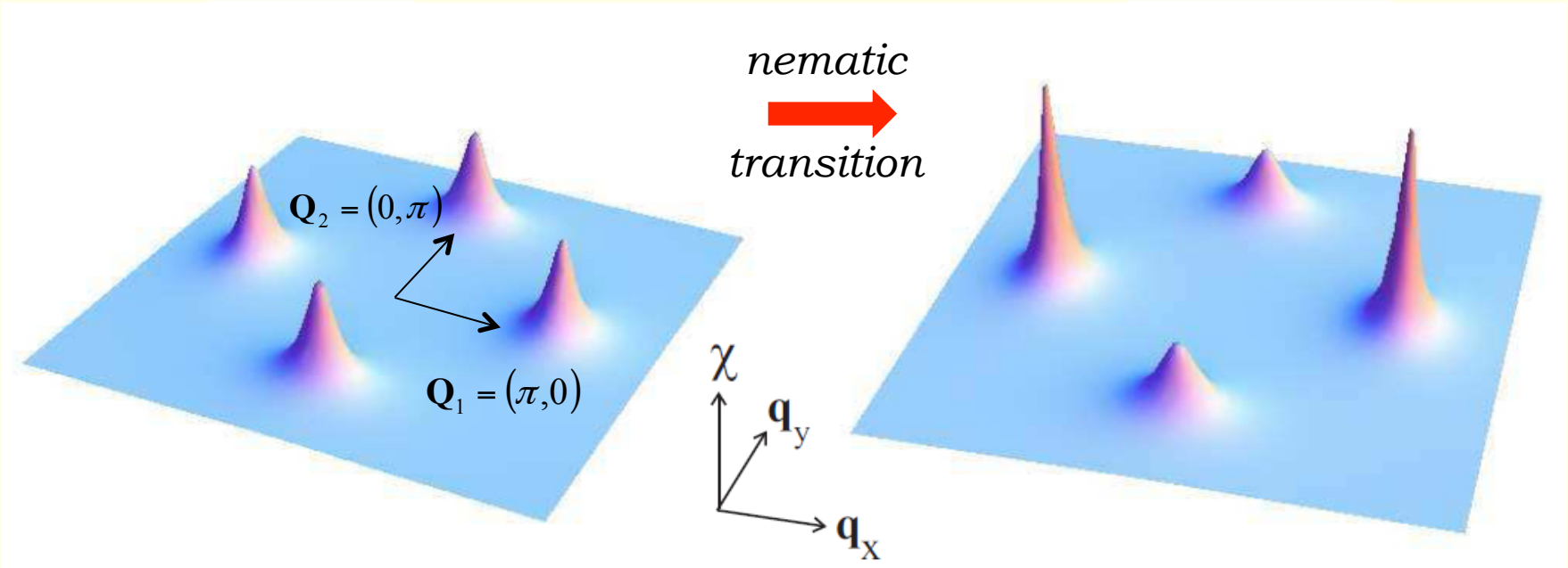
- Nematic action at *T=0*: first-order nematic transition





Magnetic and nematic transitions inside the SC dome

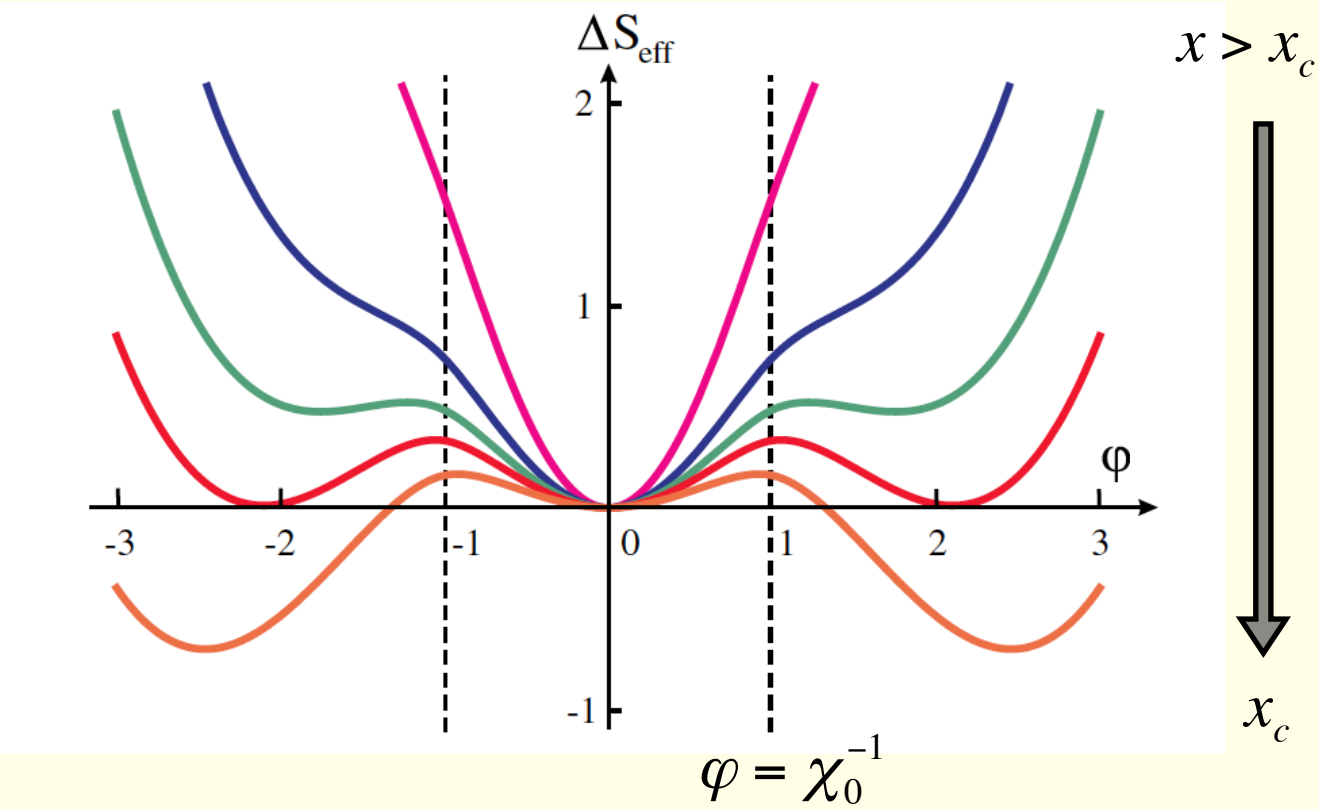
- Feedback effect: nematic order renormalizes the magnetic spectrum



$$\begin{cases} \chi_{\text{mag}}^{-1}(\mathbf{Q}_1) = \chi_0^{-1} - \varphi \\ \chi_{\text{mag}}^{-1}(\mathbf{Q}_2) = \chi_0^{-1} + \varphi \end{cases}$$

Magnetic and nematic transitions inside the SC dome

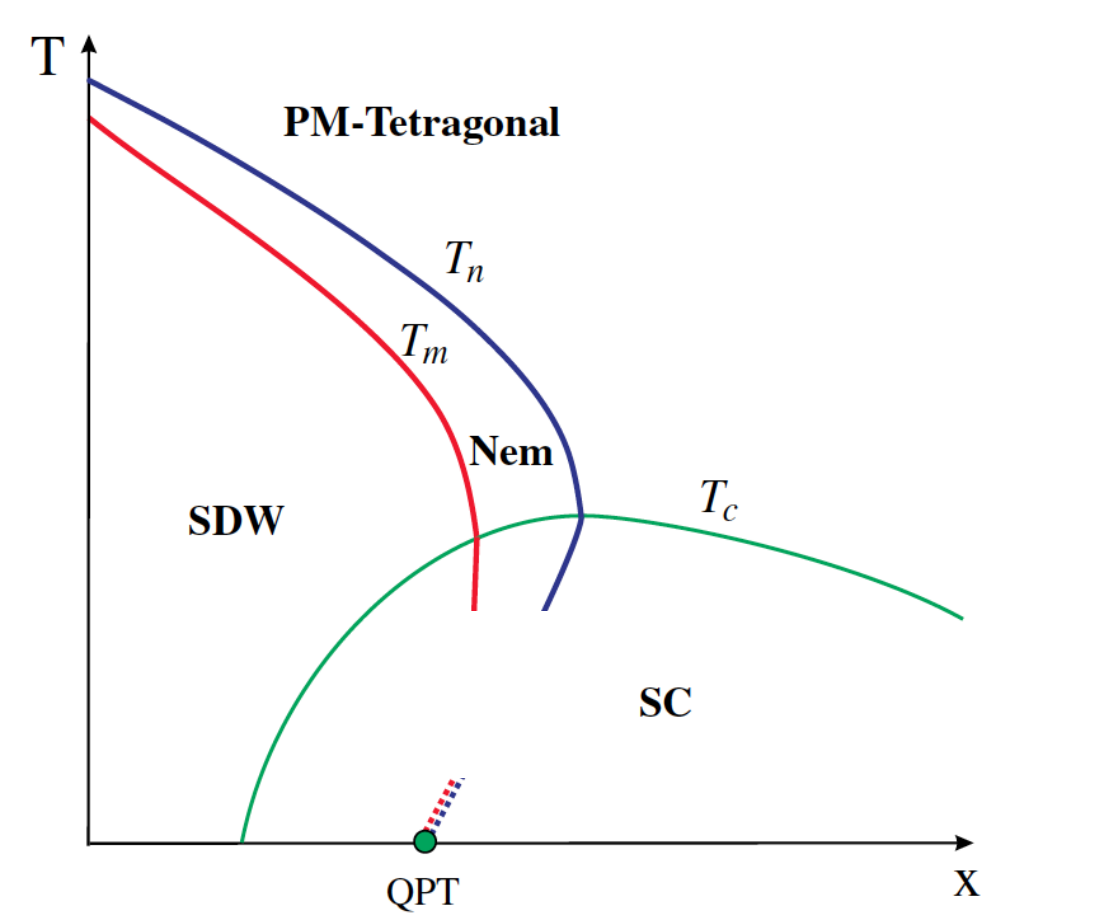
- Nematic action at *T=0*: first-order nematic transition



$\chi_{mag}^{-1}(\mathbf{Q}_1) = \chi_0^{-1} - \varphi$: **jump of the nematic order parameter is large enough to induce a simultaneous first-order magnetic transition**

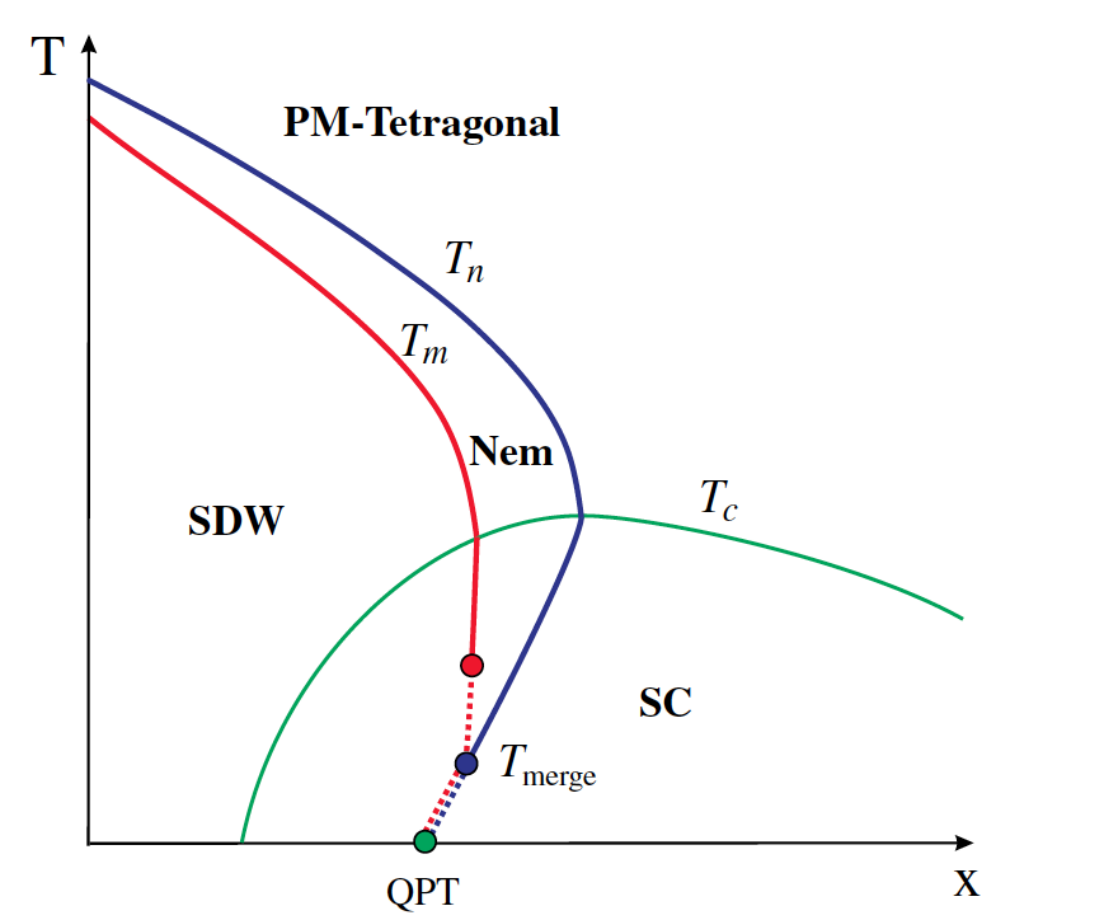
Magnetic and nematic transitions inside the SC dome

- Single and simultaneous magnetic-nematic quantum phase transition



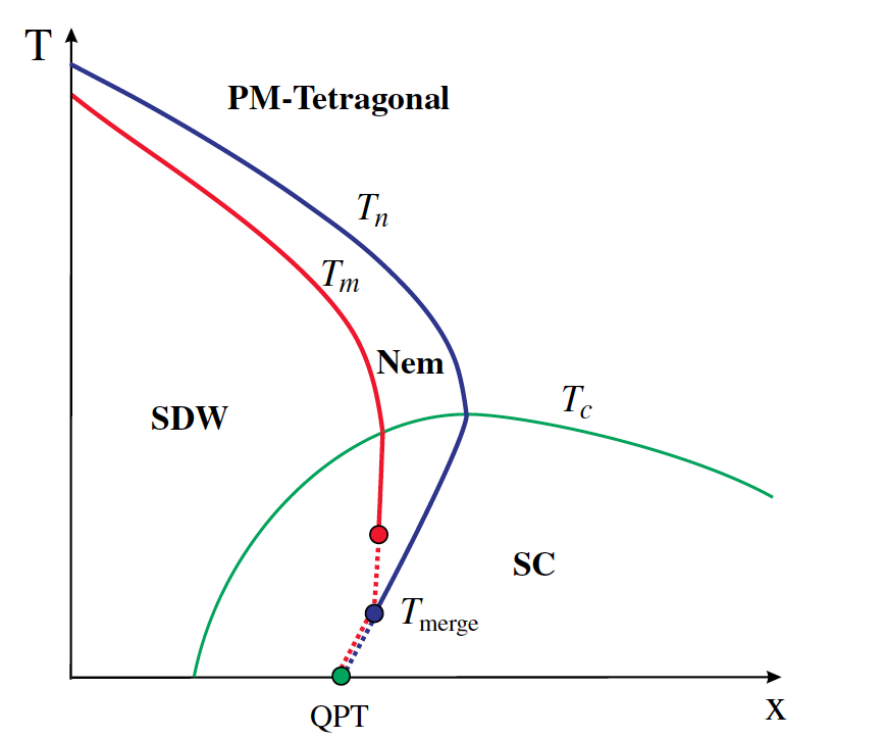
Magnetic and nematic transitions inside the SC dome

- Single and simultaneous magnetic-nematic quantum phase transition

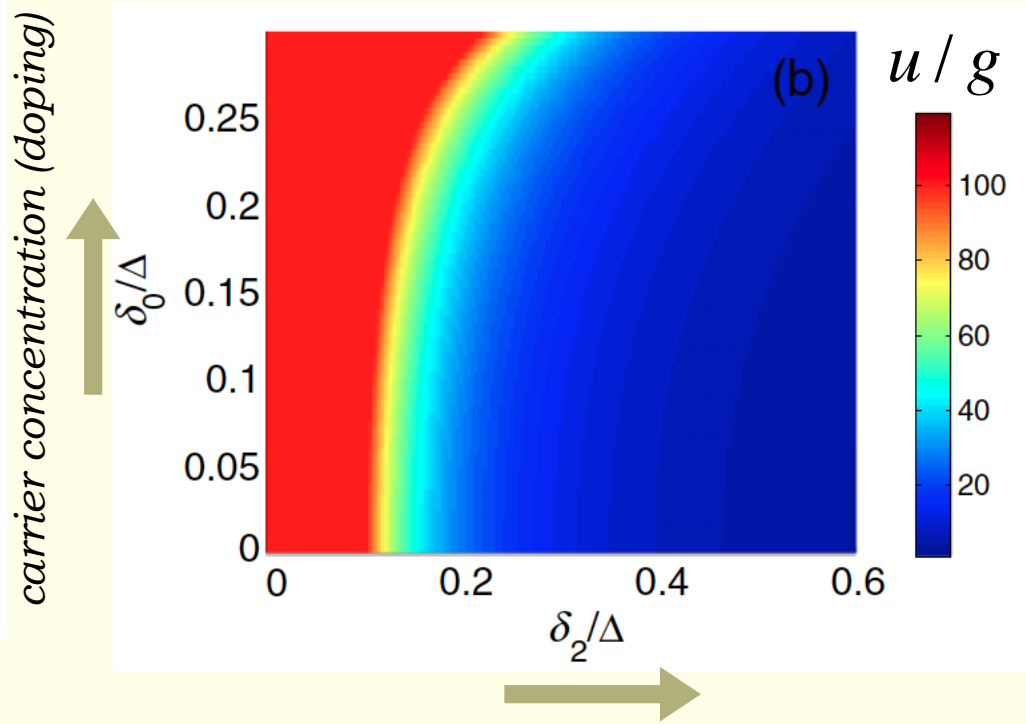


Magnetic and nematic transitions inside the SC dome

- reduced effective dimensionality (*d+1*) places the system in the borderline between split and simultaneous transitions
- coexistence with SC makes it a very weak first-order transition



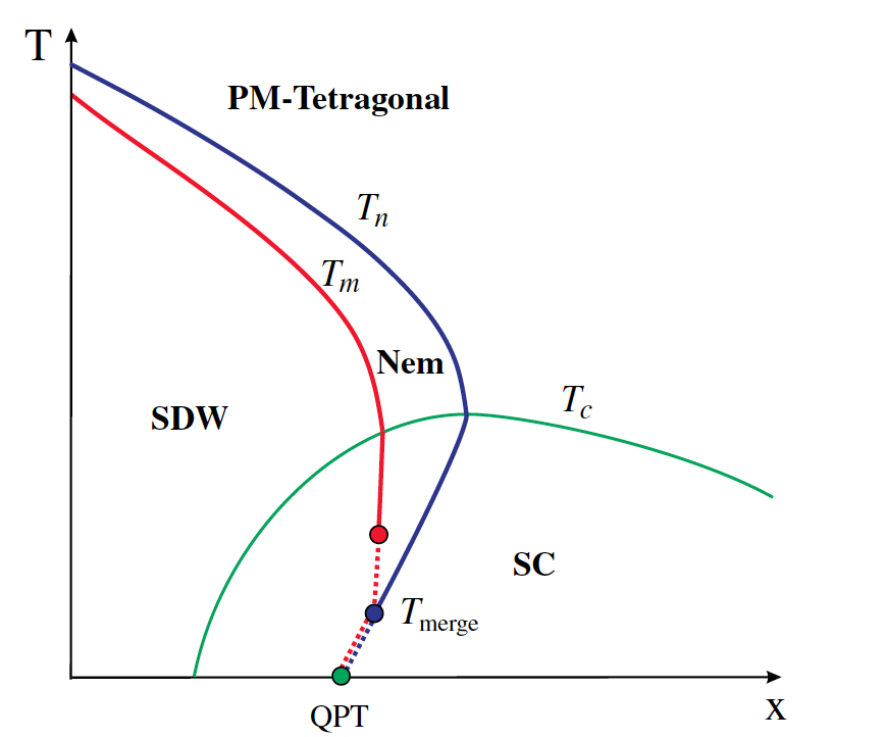
$$\sqrt{\Delta\varphi}\,,\, T_{\text{merge}} \propto g/u$$

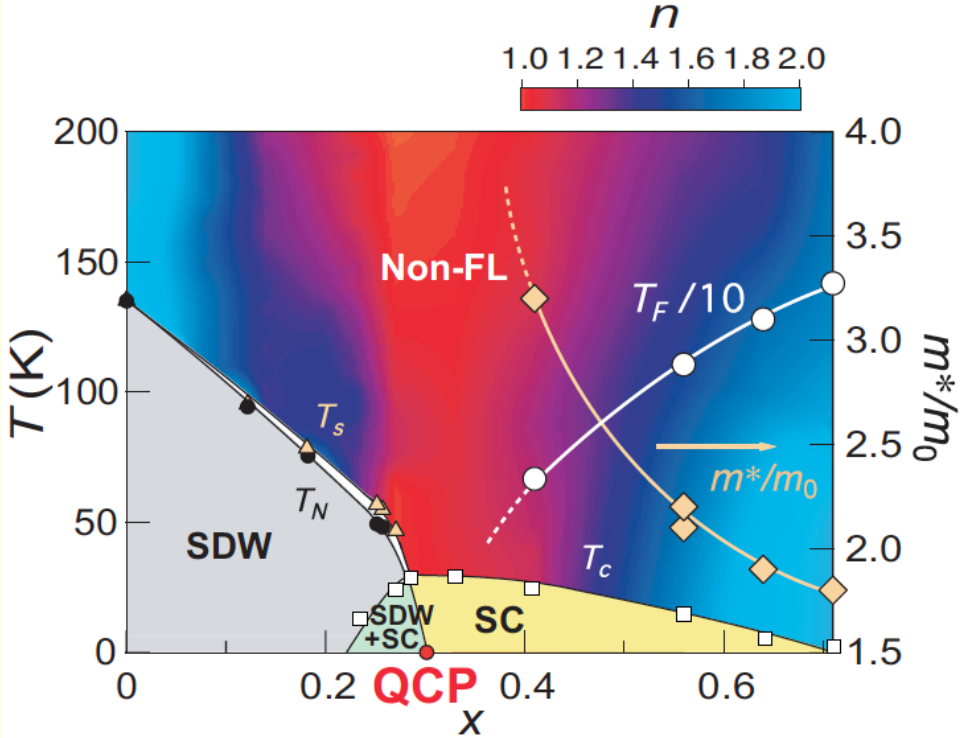


RMF, Maiti, Wölfle, Chubukov, PRL (2013)

Magnetic and nematic transitions inside the SC dome

- Single weakly first-order quantum phase transition is consistent with the experimental observations (non-Fermi liquid behavior + penetration depth)

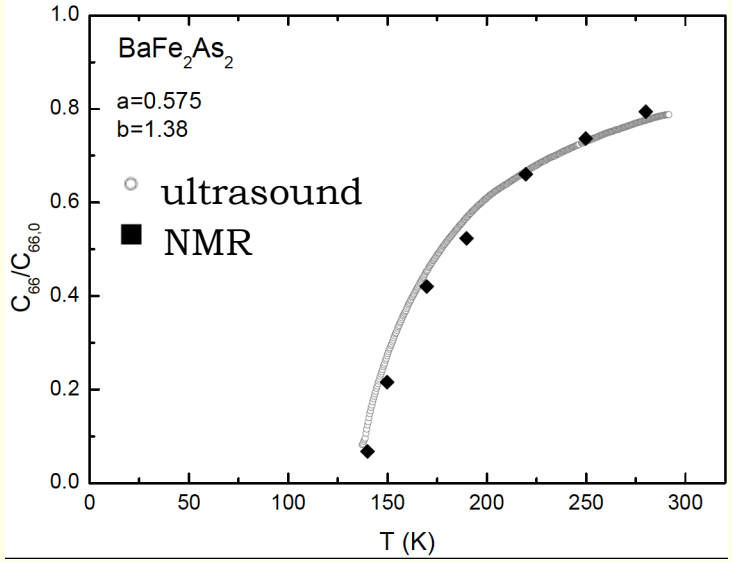


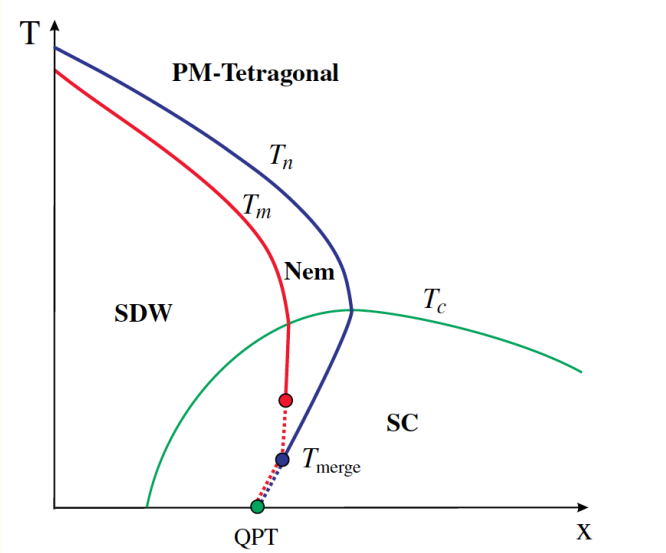


RMF, Maiti, Wölfle, Chubukov, PRL (2013)

Hashimoto et al, Science (2012)

Conclusions:





- Scaling between shear modulus and NMR spin-lattice relaxation rate provides strong evidence for a magnetically-driven structural transition and for a nematic instability promoted by magnetic fluctuations

- Magnetism and nematicity compete but coexist with SC, giving rise to a simultaneous, weakly first-order quantum phase transition deep inside the SC dome.

RMF *et al, Phys. Rev. Lett.* ***105****, 157003 (2010)*

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

RMF, Maiti, Wölfle, and Chubukov, *Phys. Rev. Lett.* ***111****, 057001 (2013)*

RMF, Bohmer, Meingast, and Schmalian, *Phys. Rev. Lett. (in press)*