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Interplay between superconductivity, magnetism and nematic order in the iron pnictides - Part II

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Columbia University &

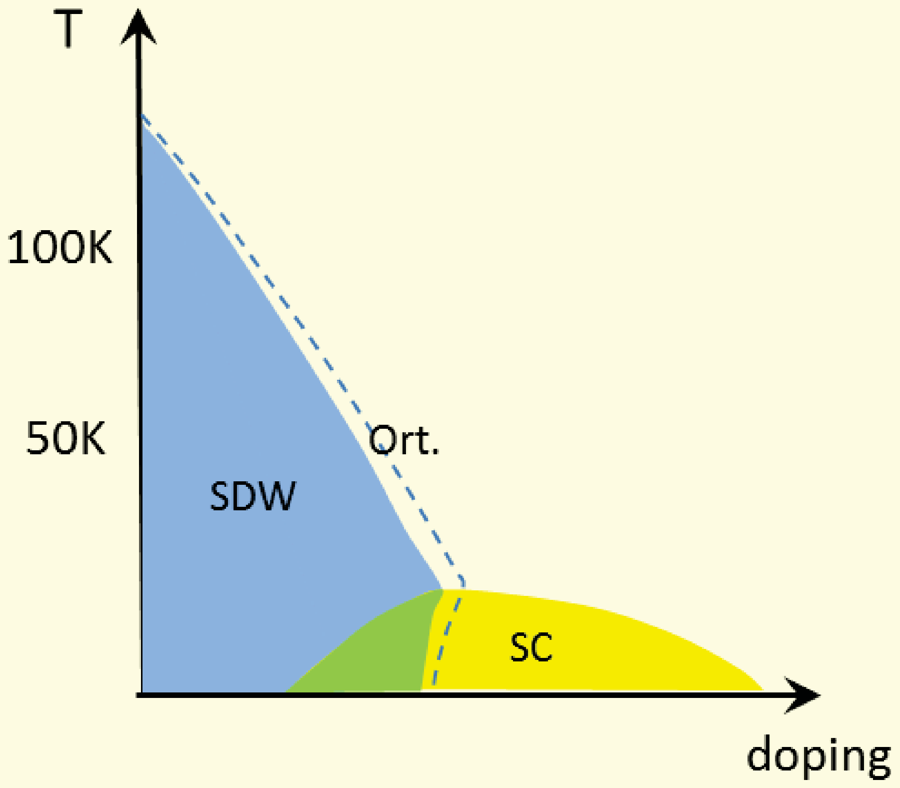
Los Alamos National Laboratory

ICTP Workshop

Aug 10th, 2012

Iron pnictides: typical phase diagram

magnetic, structural, and superconducting order



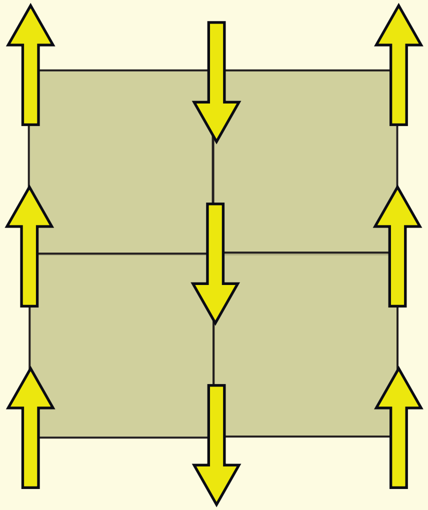
- How these different ordered states interact with each other?
- Is there a primary degree of freedom?

Outline

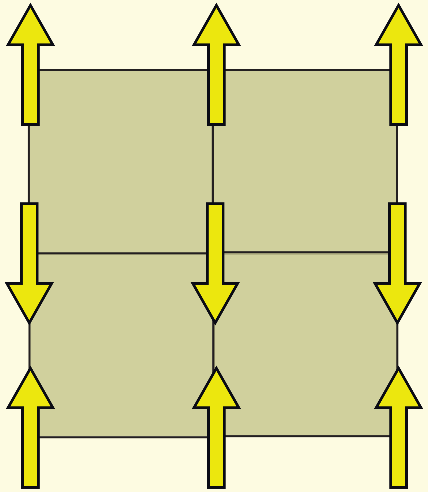
1. **The superconducting state (Lecture I)**
   - *unconventional superconductivity*
2. **The magnetic state (Lectures I & II)**
   - *itinerant or localized?*
3. **The nematic state (Lecture II)**
   - *a new electronic phase that emerges from magnetism and triggers structural and orbital order*
4. **Competing orders (Lecture II)**
   - *competition between SC, magnetism, and nematics*

Iron pnictides: magnetic order

- How to describe the magnetically ordered state?
  - *itinerant or localized picture?*



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



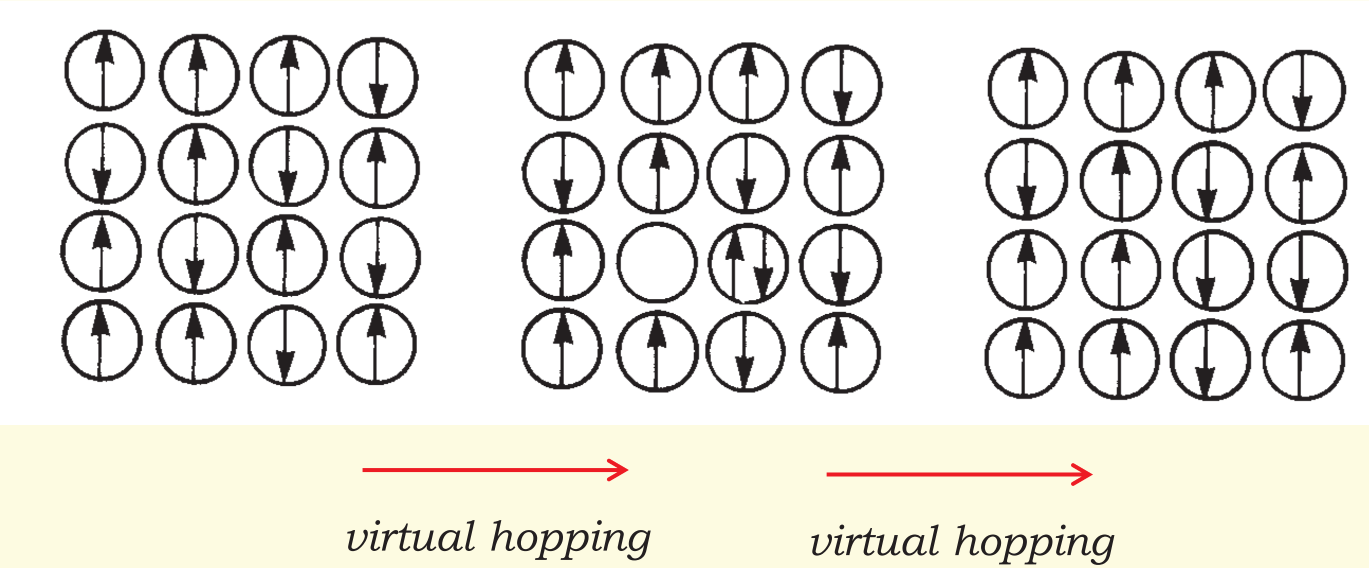
$\mathbf{Q}_2 = (0, \pi)$

Digression: localized and itinerant magnetism

- *Localized limit*: strong Coulomb repulsion
  - Hubbard model at half-filling

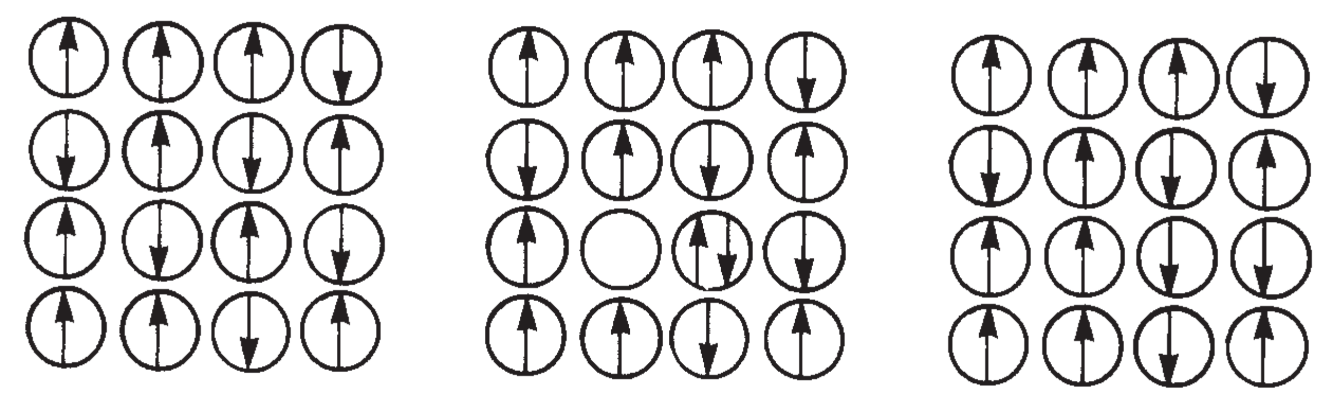
$$H = -t \sum_{\langle ij \rangle,\sigma} \left(c_{i\sigma}^{+} c_{j\sigma} + c_{j\sigma}^{+} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad t << U$$

  - perturbation theory: energy gain due to virtual hopping



Digression: localized and itinerant magnetism

- *Localized limit*: strong Coulomb repulsion



  - effective Heisenberg Hamiltonian

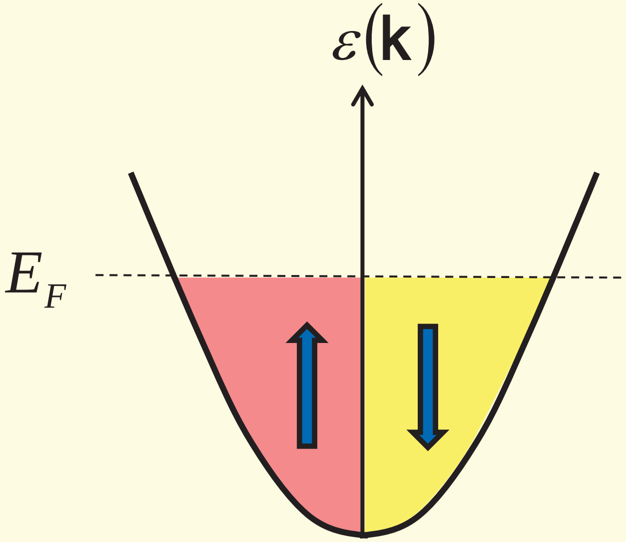
$$H = J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j \qquad J = \frac{t^2}{U}$$

energy gain comes from the kinect term

Digression: localized and itinerant magnetism

- *Itinerant limit*: to simplify, first consider the case of a ferromagnet (Stoner model)

the ground state of non-interacting electrons is non-polarized

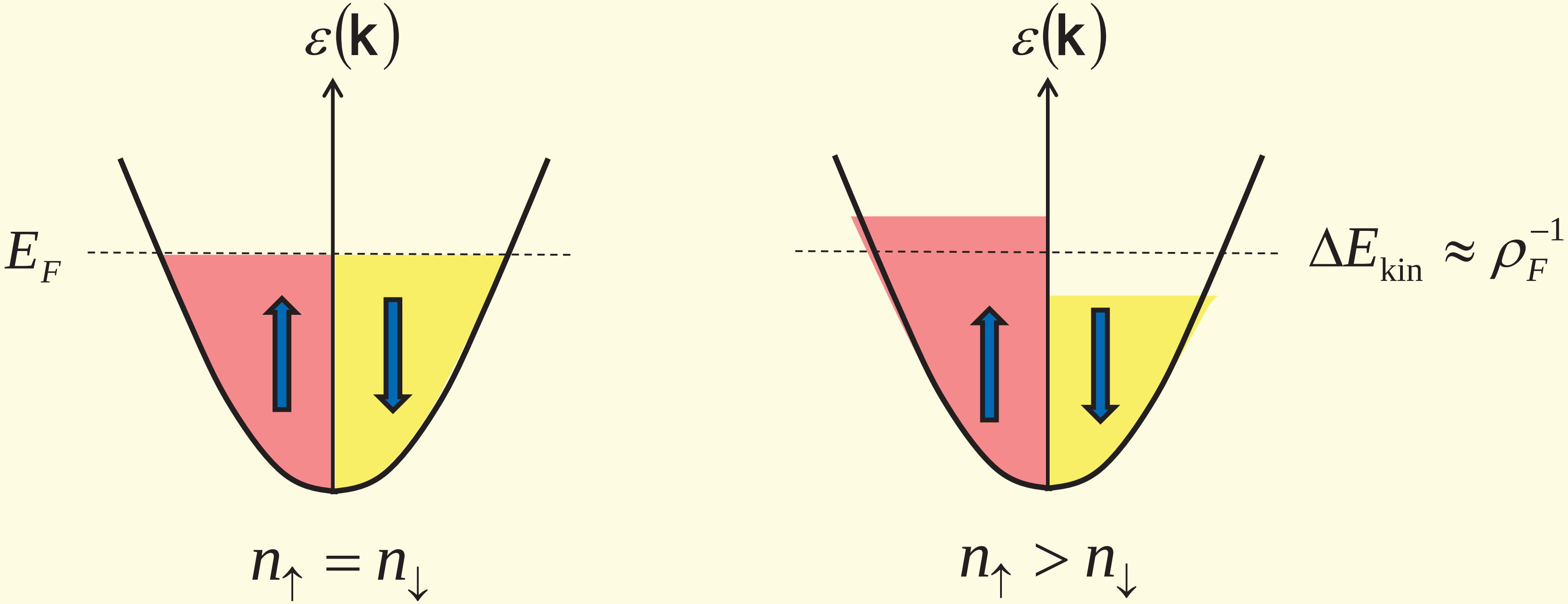


$$n_{\uparrow} = n_{\downarrow}$$

Digression: localized and itinerant magnetism

- *Itinerant limit*: to simplify, first consider the case of a ferromagnet (Stoner model)

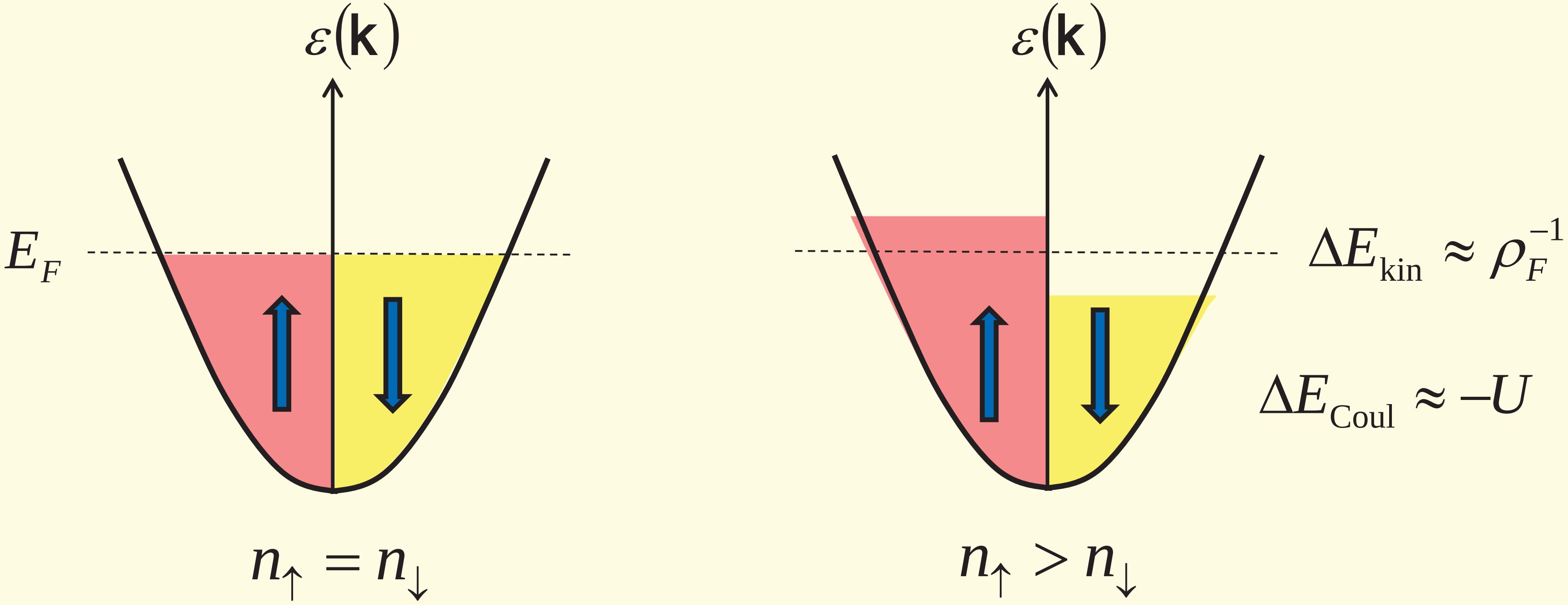
forcing a polarized state costs kinetic energy



Digression: localized and itinerant magnetism

- *Itinerant limit*: to simplify, first consider the case of a ferromagnet (Stoner model)

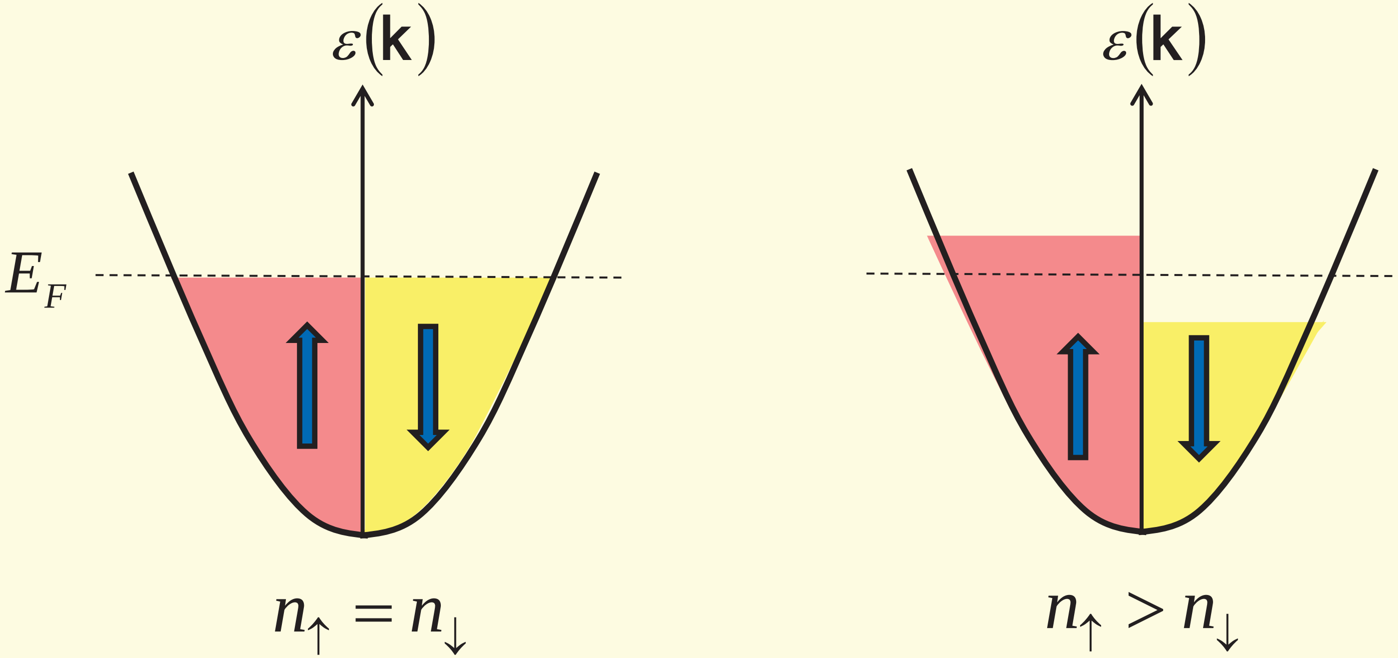
however, when the electrons are polarized, they pay less local Coulomb energy due to Pauli principle



Digression: localized and itinerant magnetism

- *Itinerant limit*: to simplify, first consider the case of a ferromagnet (Stoner model)

Stoner criterion for ferromagnetism: $\Delta E_{\text{kin}} + \Delta E_{\text{Coul}} = 0 \;\Rightarrow\; U\rho_F = 1$



energy gain comes from the Coulomb repulsion term

Digression: localized and itinerant magnetism

- *Itinerant limit*: to simplify, first consider the case of a ferromagnet (Stoner model)
  - Hubbard model in the limit of small $U << t$

$$H = -t \sum_{\langle ij \rangle, \sigma} \left(c_{i\sigma}^{+} c_{j\sigma} + c_{j\sigma}^{+} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

  - Coulomb repulsion enhances uniform susceptibility (RPA)

$$\chi = \frac{\chi_{\text{Pauli}}}{1 - \underbrace{U\rho_F}}$$

favored near van-Hove singularity

Digression: localized and itinerant magnetism

- *Itinerant limit*: Stoner condition can be generalized for the case of a magnetically ordered state with ordering vector **Q**

$$\chi(\mathbf{Q}) = \frac{\chi_0(\mathbf{Q})}{1 - U_{\mathbf{Q}}\chi_0(\mathbf{Q})}$$

- Instability usually assisted by nesting: $\varepsilon(\mathbf{k}+\mathbf{Q}) = -\varepsilon(\mathbf{k})$

$$\chi_0(\mathbf{Q}) = -T\sum_{\mathbf{k},\omega_n} G(\mathbf{k},\omega_n)G(\mathbf{k}+\mathbf{Q},\omega_n)$$

$$\chi_0(\mathbf{Q}) = \sum_{\mathbf{k}} \frac{\tanh(\varepsilon_{\mathbf{k}}/2T) - \tanh(\varepsilon_{\mathbf{k}+\mathbf{Q}}/2T)}{2(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{Q}})}$$

Digression: localized and itinerant magnetism

- *Itinerant limit*: Stoner condition can be generalized for the case of a magnetically ordered state with ordering vector **Q**

$$\chi(\mathbf{Q})=\frac{\chi_0(\mathbf{Q})}{1-U_{\mathbf{Q}}\chi_0(\mathbf{Q})}$$

- Instability usually assisted by nesting: $\varepsilon(\mathbf{k}+\mathbf{Q})=-\varepsilon(\mathbf{k})$

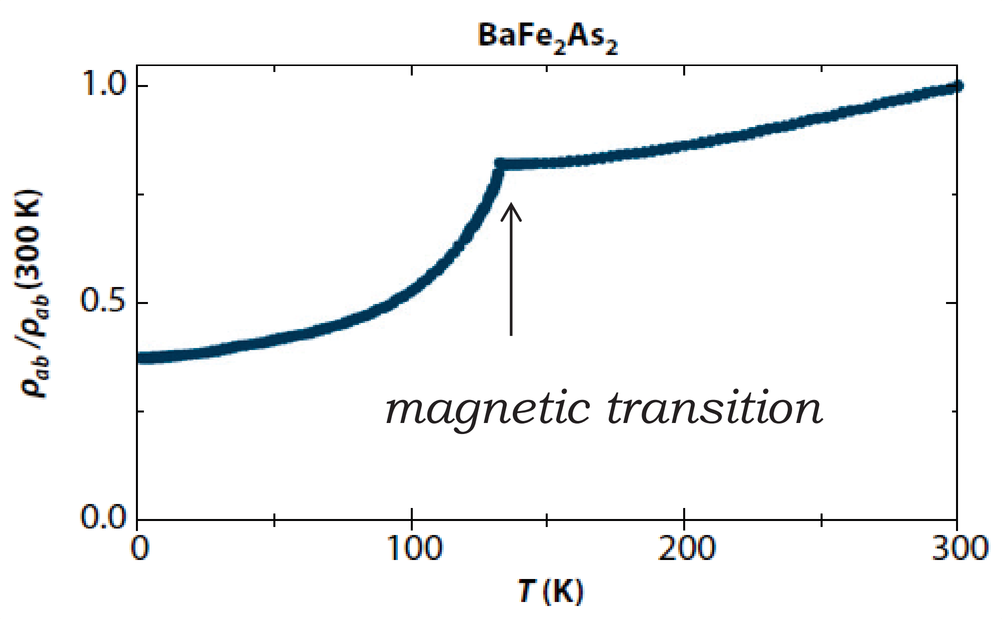
$$\chi_0(\mathbf{Q})=\rho_F\int_0^{\Lambda}\frac{d\varepsilon}{\varepsilon}\tanh\left(\frac{\varepsilon}{2T}\right)$$

same equation as BCS!

$$\chi_0(\mathbf{Q})\propto\rho_F\log\left(\frac{\Lambda}{T}\right)\qquad T_{\mathrm{mag}}\propto\Lambda\exp\left(-\frac{1}{U_{\mathbf{Q}}\rho_F}\right)$$

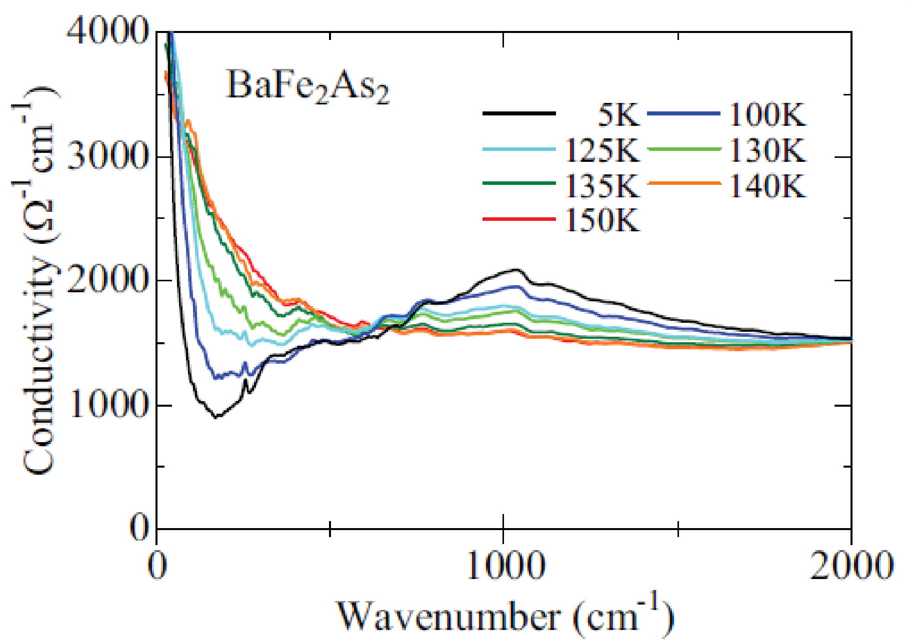
Iron pnictides: magnetic order

- from itinerant to localized magnetism
  - several known systems are in the intermediate coupling regime (such as elemental Ni and Fe)
  - *since the ground state of the iron pnictides is a metal, we choose here the itinerant limit as our starting point*



Iron pnictides: magnetic order

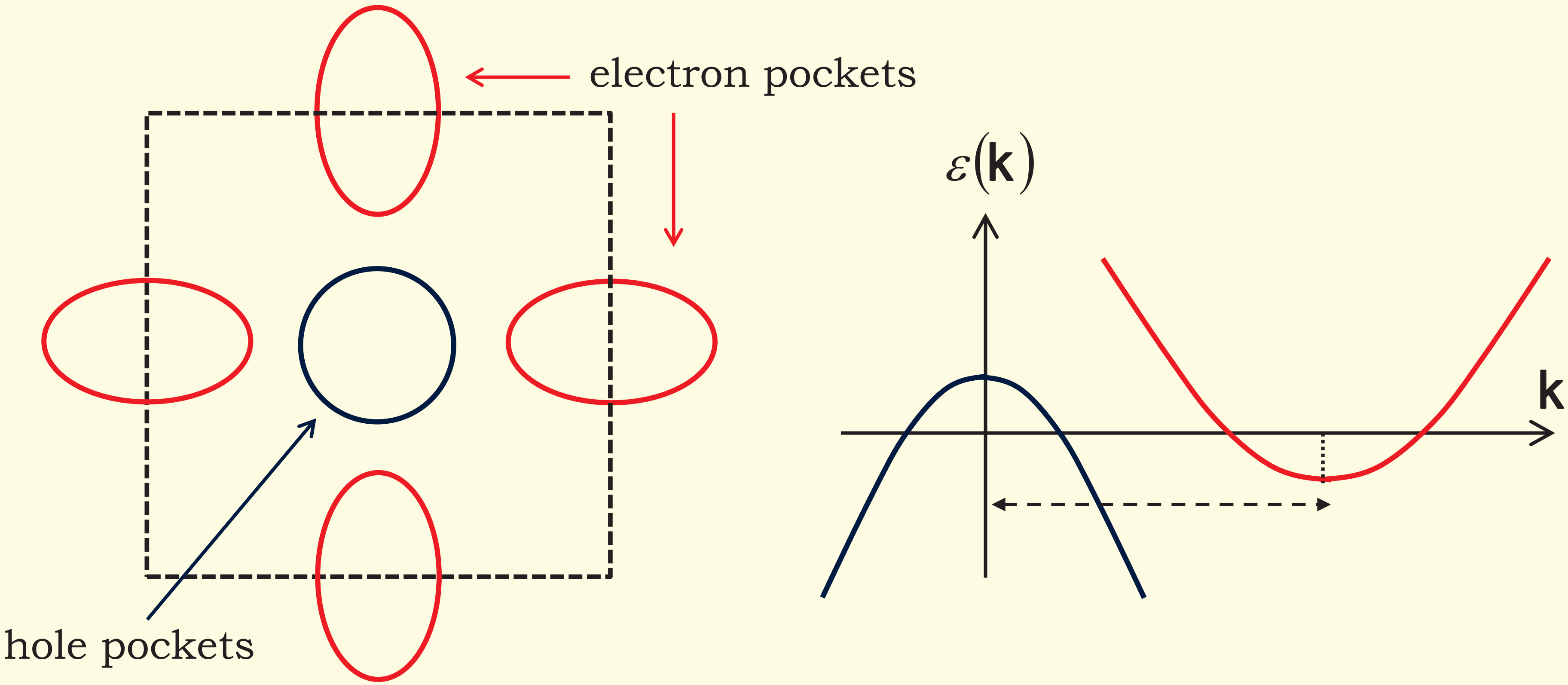
- from itinerant to localized magnetism
  - several known systems are in the intermediate coupling regime (such as elemental Ni and Fe)
  - *optical conductivity: transfer of spectral weight from the Drude peak to the mid-infrared region*



Nakajima et al, PRB (2010)

Iron pnictides:
itinerant approach to SDW

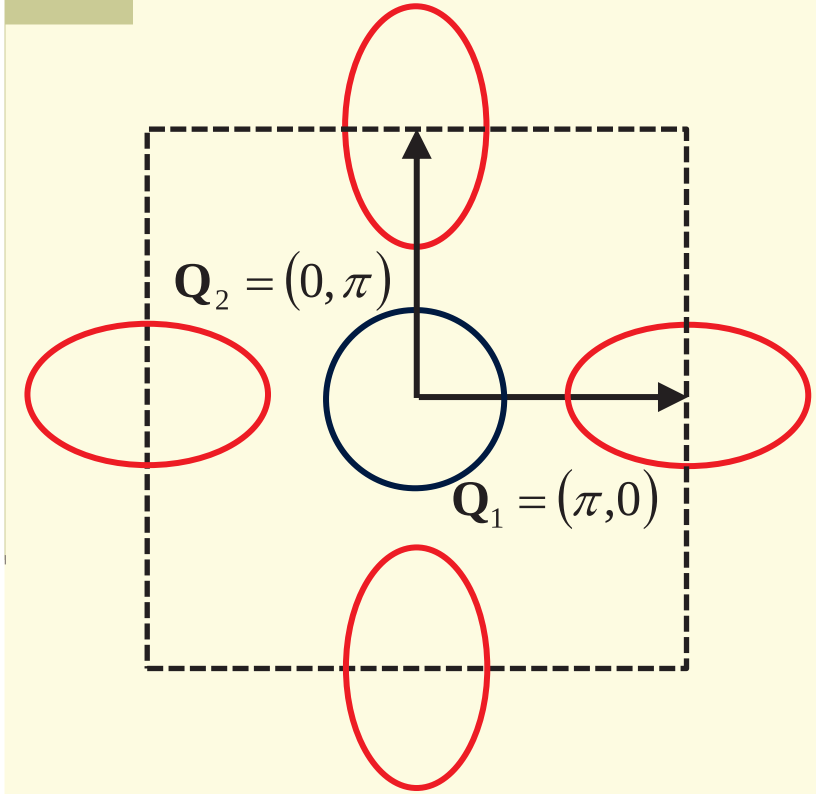
- Fermi surface of the iron pnictides:

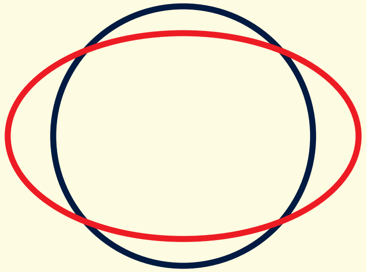


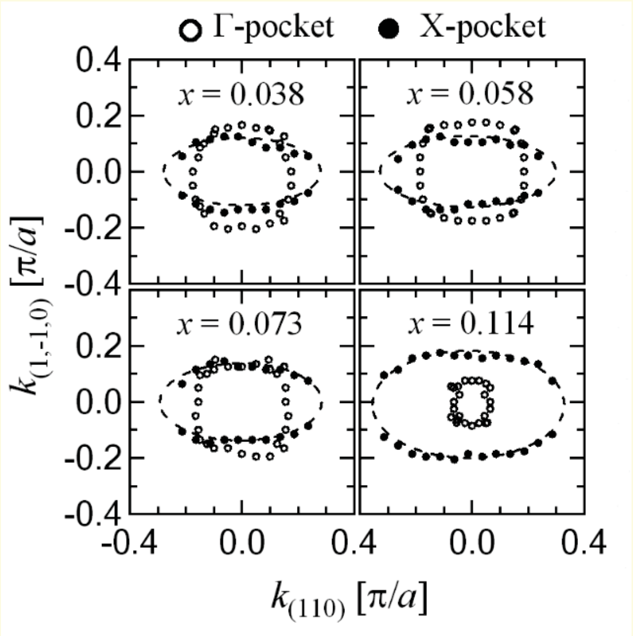
Iron pnictides: itinerant approach to SDW

- Bands have good nesting features (but not perfect)

$$\chi_0(\mathbf{Q}) \propto \log \frac{E_F}{\max\left(T,\delta_{\text{nesting}}\right)}$$





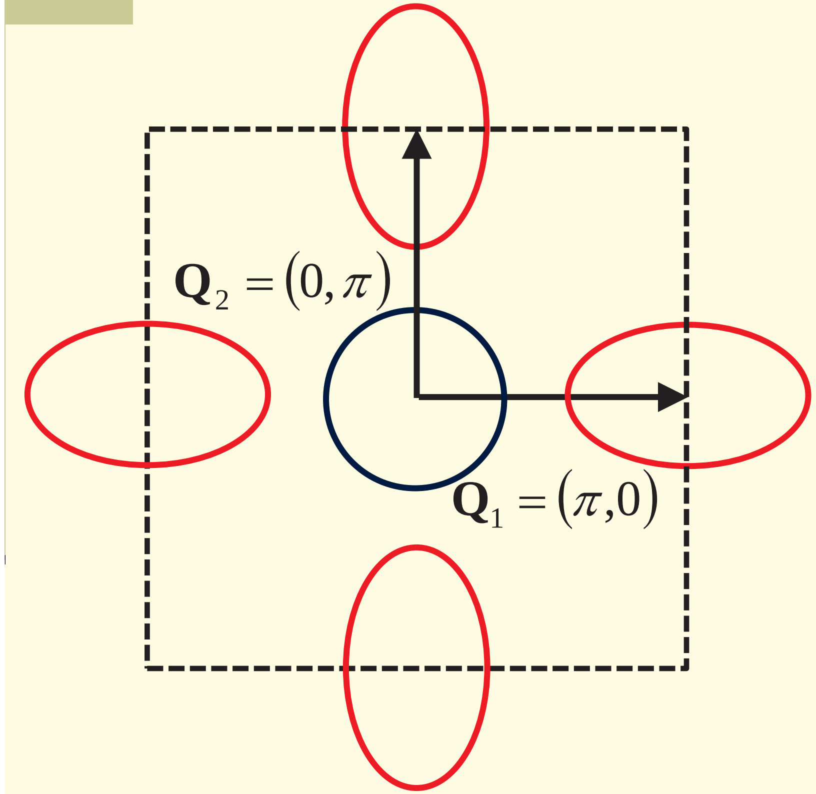


ARPES data

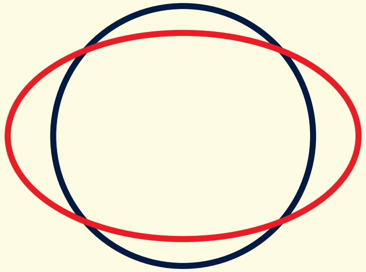
Liu *et al, Nature Phys. (2010)*

Iron pnictides: itinerant approach to SDW

- Bands have good nesting features (but not perfect)



$$\chi_0(\mathbf{Q}) \propto \log \frac{E_F}{\max(T, \delta_{\text{nesting}})}$$

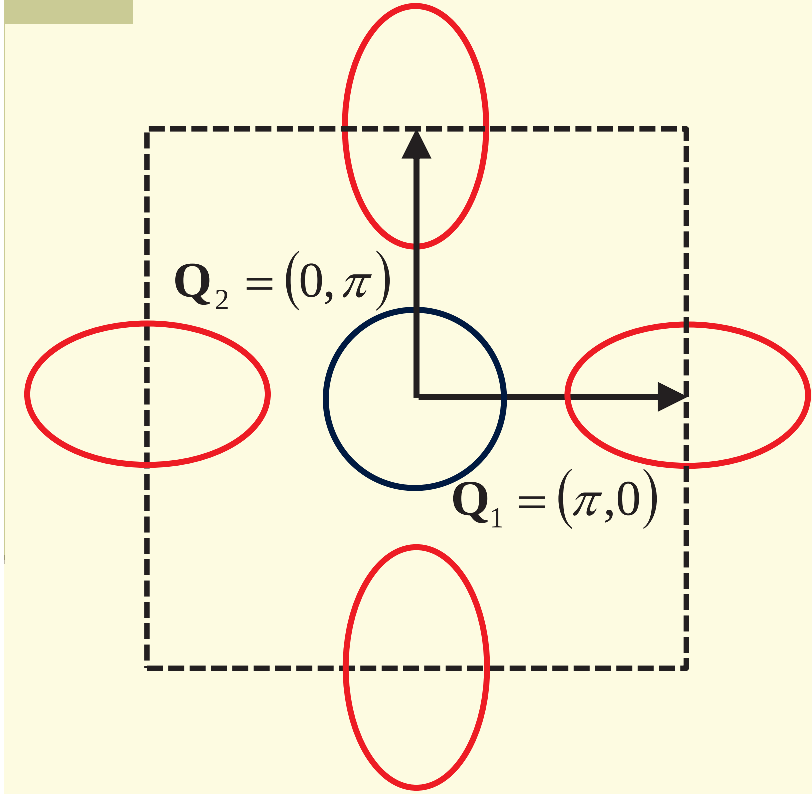


include interaction:

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

electronic interaction above threshold leads to a magnetically ordered state (SDW) with ordering vector Q_i

Theory of the itinerant magnetic state



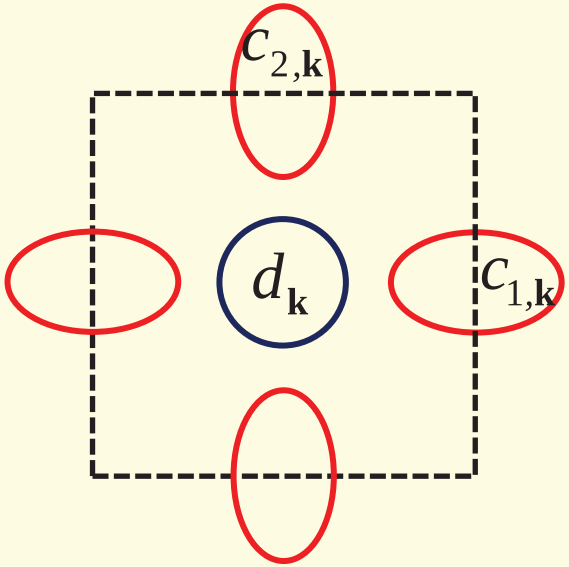
Two simultaneous spin-density wave instabilities:

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

microscopic calculation of the magnetic free energy by integrating out the electrons (Hertz-Millis approach)

derivation of the magnetic free energy

step 1: start with purely multi-band electronic interactions



$$H_0 = \sum_{\mathbf{k}} \varepsilon_{0,\mathbf{k}}\, d^{+}_{\mathbf{k}\alpha} d_{\mathbf{k}\alpha} + \sum_{\mathbf{k},i=1,2} \varepsilon_{i,\mathbf{k}}\, c^{+}_{i,\mathbf{k}\alpha} c_{i,\mathbf{k}\alpha}$$

electrons in
the hole pocket

electrons in
the electron pockets

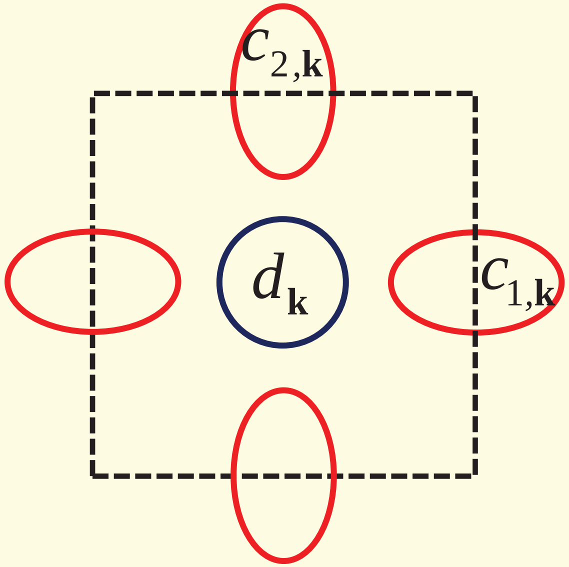
$$H_{\text{int}} = \sum_{i,\mathbf{k}_j} u_1\, d^{+}_{\mathbf{k}_1\alpha} d_{\mathbf{k}_3\alpha} c^{+}_{i,\mathbf{k}_2\beta} c_{i,\mathbf{k}_4\beta} + \sum_{i,\mathbf{k}_j} u_2\, d^{+}_{\mathbf{k}_1\alpha} c^{+}_{i,\mathbf{k}_2\beta} d_{\mathbf{k}_4\beta} c_{i,\mathbf{k}_3\alpha}$$

$$+ \sum_{i,\mathbf{k}_j} \frac{u_3}{2}\, d^{+}_{\mathbf{k}_1\alpha} d^{+}_{\mathbf{k}_2\beta} c_{i,\mathbf{k}_4\beta} c_{i,\mathbf{k}_3\alpha} + (\cdots)$$

equivalent to multi-orbital Hubbard model

derivation of the magnetic free energy

step 2: project the interactions in charge channel and spin channel



use the identity between
Kronecker deltas and Pauli matrices:

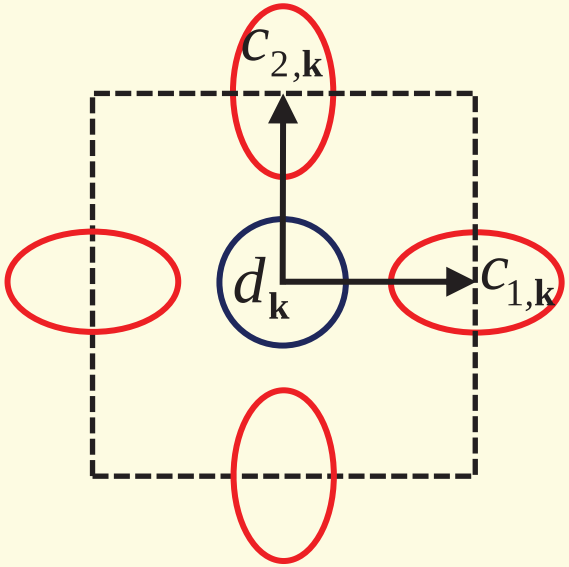
$$\delta_{\alpha\beta}\delta_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\gamma\beta} - \vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta}$$

$$H_{\text{int}} = -u_s \sum_{\mathbf{q},i} \left(d^{+}_{\mathbf{k}+\mathbf{q}\alpha}\vec{\sigma}_{\alpha\beta}c_{i,\mathbf{k}\beta}\right)\cdot\left(c^{+}_{i,\mathbf{p}-\mathbf{q}\gamma}\vec{\sigma}_{\gamma\delta}d_{i,\mathbf{p}\delta}\right)$$

$$u_s = u_1 + u_3$$

derivation of the magnetic free energy

step 3: introduce collective variables for the two SDW instabilities



$$Z \propto \int dc_{\mathbf{k}} df_{\mathbf{k}} \ \exp\left(-H/T\right)$$

$$\mathbf{M}_i \propto \sum_{\mathbf{k}} \left\langle d^{+}_{\mathbf{k}\alpha} \vec{\sigma}_{\alpha\beta} c_{i,\mathbf{k}\beta} \right\rangle$$

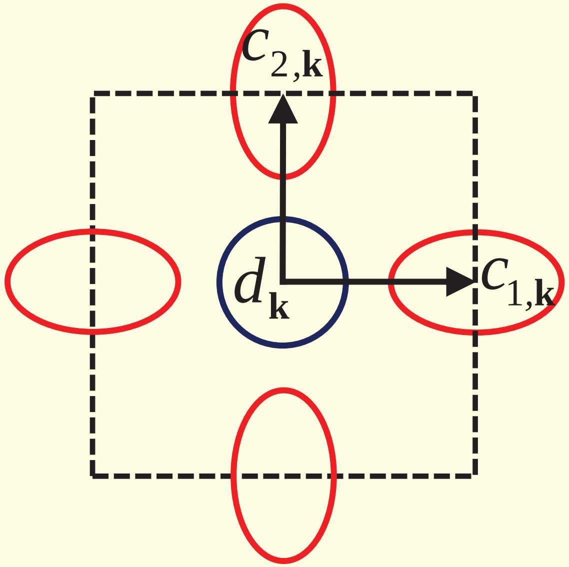
use the Hubbard-Stratonovich transformation:

$$\exp\left[u_s \left(d^{+}_{\mathbf{k}+\mathbf{q}\alpha} \vec{\sigma}_{\alpha\beta} c_{i,\mathbf{k}\beta}\right) \cdot \left(c^{+}_{i,\mathbf{p}-\mathbf{q}\gamma} \vec{\sigma}_{\gamma\delta} d_{\mathbf{p}\delta}\right)\right] =$$

$$\int d\mathbf{M}_i \exp\left[-\frac{u_s}{2} \mathbf{M}_{i,\mathbf{q}} \cdot \mathbf{M}_{i,-\mathbf{q}} + \mathbf{M}_{i,\mathbf{q}} \cdot \left(c^{+}_{i,\mathbf{k}-\mathbf{q}\alpha} \vec{\sigma}_{\alpha\beta} d_{\mathbf{k}\beta}\right) + \mathbf{M}_{i,-\mathbf{q}} \cdot \left(d^{+}_{\mathbf{k}+\mathbf{q}\alpha} \vec{\sigma}_{\alpha\beta} c_{i,\mathbf{k}\beta}\right)\right]$$

derivation of the magnetic free energy

step 4: introduce "Nambu operators" (simplify the notation)



$$\hat{\Psi}_{\mathbf{k}}^{+} = \begin{pmatrix} d_{\mathbf{k}\uparrow}^{+} & d_{\mathbf{k}\downarrow}^{+} & c_{1,\mathbf{k}\uparrow}^{+} & c_{1,\mathbf{k}\downarrow}^{+} & c_{2,\mathbf{k}\uparrow}^{+} & c_{2,\mathbf{k}\downarrow}^{+} \end{pmatrix}$$

$$Z \propto \int d\hat{\Psi}_{\mathbf{k}} d\mathbf{M}_i \exp\left(-F\left[\hat{\Psi}_{\mathbf{k}}, \mathbf{M}_i\right]\right)$$

$$F = -\int_k \hat{\Psi}_{\mathbf{k}}^{+} \hat{G}_k^{-1} \hat{\Psi}_{\mathbf{k}} + \frac{2}{u_s} \int_{x,i} M_i^2$$

$$\hat{G}_k^{-1} = \begin{pmatrix} G_{0,k}^{-1} & \mathbf{M}_1 \cdot \sigma & \mathbf{M}_2 \cdot \sigma \\ \mathbf{M}_1 \cdot \sigma & G_{1,k}^{-1} & 0 \\ \mathbf{M}_2 \cdot \sigma & 0 & G_{2,k}^{-1} \end{pmatrix}$$

with: $G_{j,k}^{-1} = i\omega_n - \varepsilon_{j,\mathbf{k}}$ $\qquad k = (\omega_n, \mathbf{k})$

derivation of the magnetic free energy

step 5: "integrate out" the electrons (Gaussian integration)

$$\hat{G}_k^{-1} = \left(\hat{G}_k^0\right)^{-1} - \hat{V}$$

$$\left(\hat{G}_k^0\right)^{-1} = \begin{pmatrix} G_{0,k}^{-1} & 0 & 0 \\ 0 & G_{1,k}^{-1} & 0 \\ 0 & 0 & G_{2,k}^{-1} \end{pmatrix} \qquad \hat{V} = -\begin{pmatrix} 0 & \mathbf{M}_1 \cdot \sigma & \mathbf{M}_2 \cdot \sigma \\ \mathbf{M}_1 \cdot \sigma & 0 & 0 \\ \mathbf{M}_2 \cdot \sigma & 0 & 0 \end{pmatrix}$$

$$Z \propto \int d\mathbf{M}_i \exp\left(-F_{\text{mag}}\left[\mathbf{M}_i\right]\right)$$

with the effective action:

$$F_{\text{mag}} = -\mathrm{Tr}\log\left(1 - \hat{G}_k^0 \hat{V}\right) + \frac{2}{u_s}\int_{x,i} M_i^2$$

derivation of the magnetic free energy

step 6: do perturbation theory

$$\left(\hat{G}_k^0\right)^{-1} = \begin{pmatrix} G_{0,k}^{-1} & 0 & 0 \\ 0 & G_{1,k}^{-1} & 0 \\ 0 & 0 & G_{2,k}^{-1} \end{pmatrix} \qquad \hat{V} = -\begin{pmatrix} 0 & \mathbf{M}_1 \cdot \sigma & \mathbf{M}_2 \cdot \sigma \\ \mathbf{M}_1 \cdot \sigma & 0 & 0 \\ \mathbf{M}_2 \cdot \sigma & 0 & 0 \end{pmatrix}$$

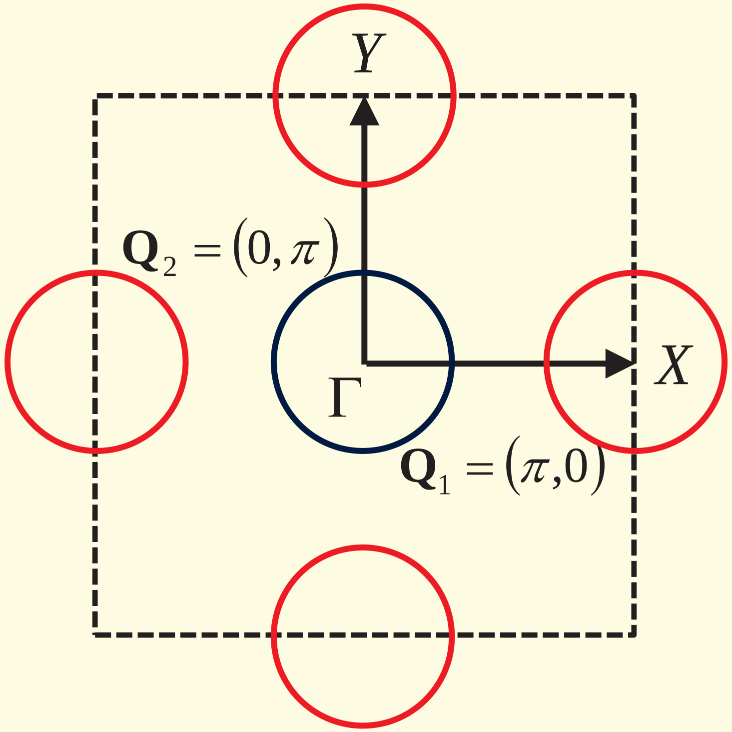
$$F_{\text{mag}} \approx \frac{1}{2} \mathrm{Tr}\left(\hat{G}_k^0 \hat{V}\right)^2 + \frac{1}{4} \mathrm{Tr}\left(\hat{G}_k^0 \hat{V}\right)^4 + \frac{2}{u_s} \int_{x,i} M_i^2 + O\left(M_i^6\right)$$

we obtain the Ginzburg-Landau derived from the microscopic model!

$$F_{\text{mag}} = \frac{a}{2}\left(M_1^2 + M_2^2\right) + \frac{u_{11}}{4} M_1^4 + \frac{u_{22}}{4} M_2^4 + \frac{u_{12}}{4} M_1^2 M_2^2 + \left(\cdots\right)$$

Theory of the itinerant magnetic state

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

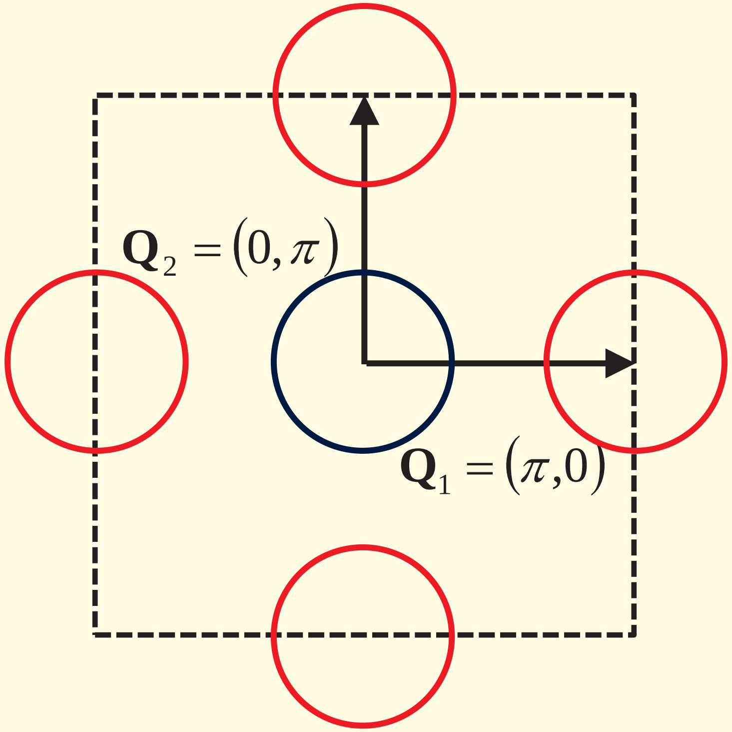


$$\begin{cases} a = \frac{2}{u_{\mathrm{s}}} + 2\int_k G_{\Gamma,k} G_{X,k} \\ u = \frac{1}{2}\int_k G_{\Gamma,k}^2 \left(G_{X,k} + G_{Y,k}\right)^2 \end{cases}$$

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

Theory of the itinerant magnetic state

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

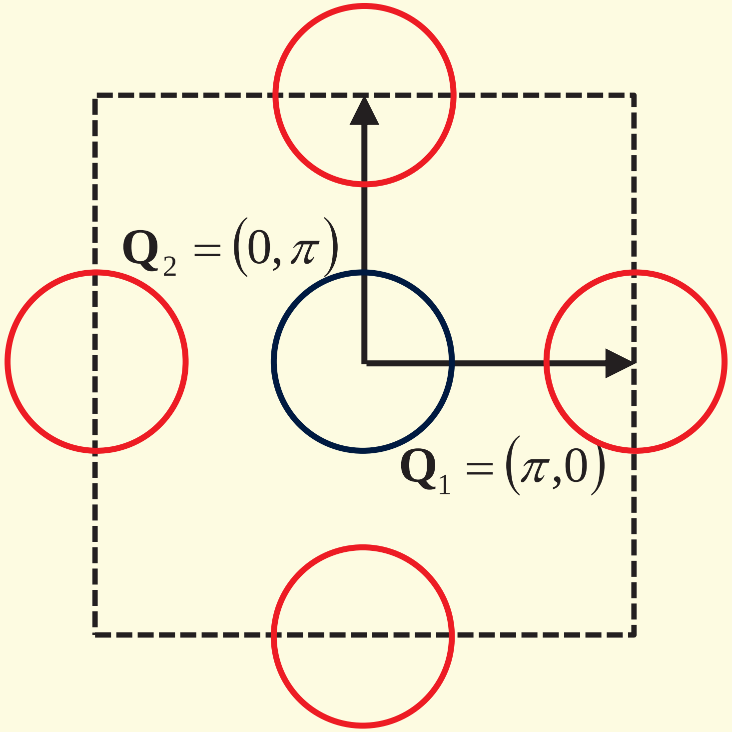


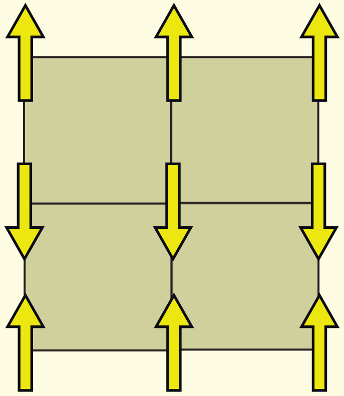
mean-field solution: $\frac{\partial F_{\mathrm{mag}}}{\partial M_i} = 0$

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

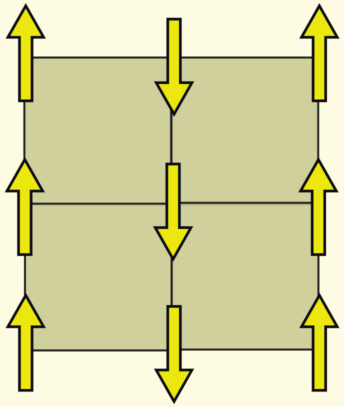
Theory of the itinerant magnetic state

For perfect nesting:

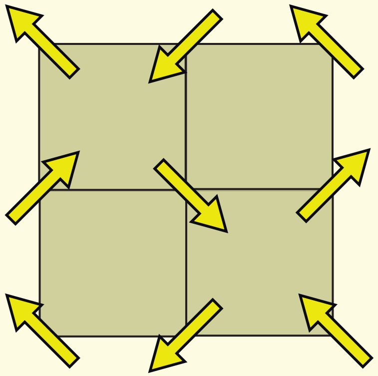




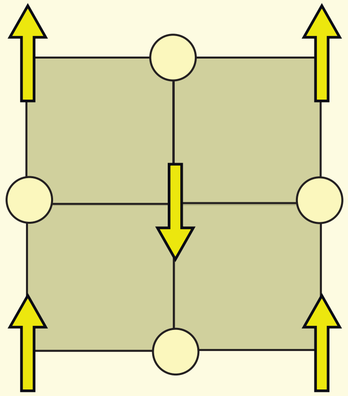
$\mathbf{M}_1 = 0 \; \& \; \mathbf{M}_2 \neq 0$



$\mathbf{M}_1 \neq 0 \; \& \; \mathbf{M}_2 = 0$



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

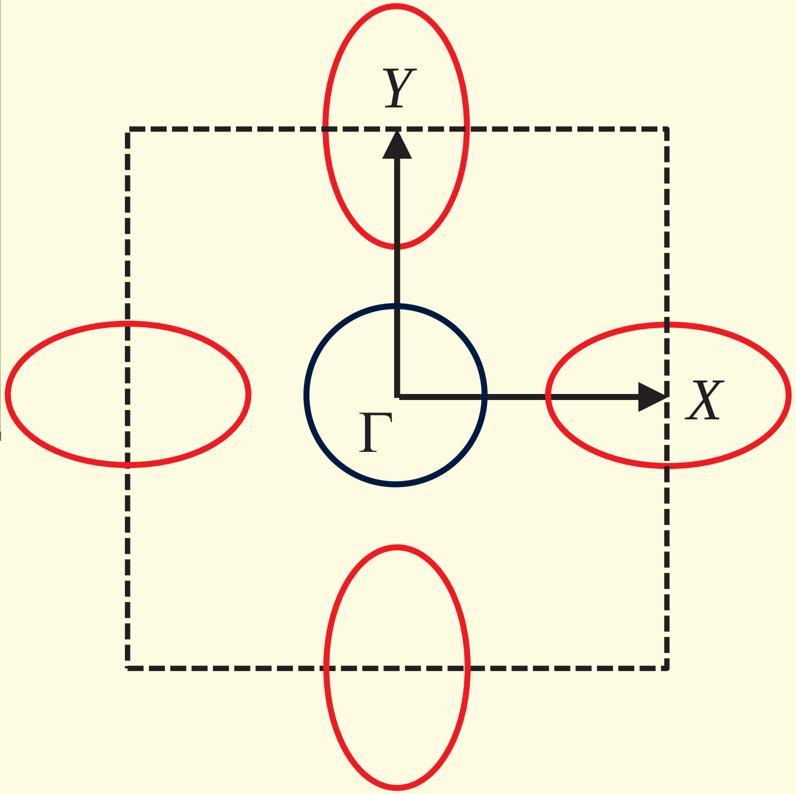


$\mathbf{M}_1 \parallel \mathbf{M}_2$

Theory of the itinerant magnetic state

Away from perfect nesting:

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

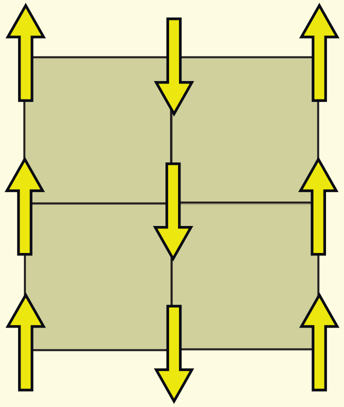


$$g = -\frac{1}{2}\int_k G_{\Gamma,k}^2 \left(G_{X,k} - G_{Y,k}\right)^2 > 0$$

Theory of the itinerant magnetic state

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

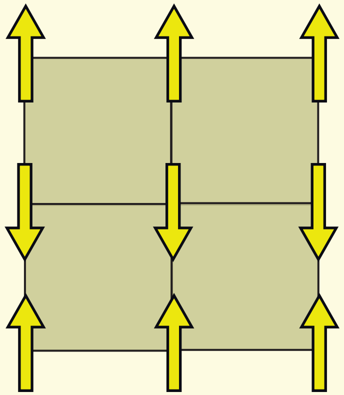
$$F_{\mathrm{mag}} = \frac{a}{2}\left(M_1^2 + M_2^2\right) + \frac{u}{4}\left(M_1^2 + M_2^2\right)^2 - \overbrace{\frac{g}{4}\left(M_1^2 - M_2^2\right)^2}^{+g\, M_1^2 M_2^2}$$



$M_1 \neq 0$

$M_2 = 0$

OR



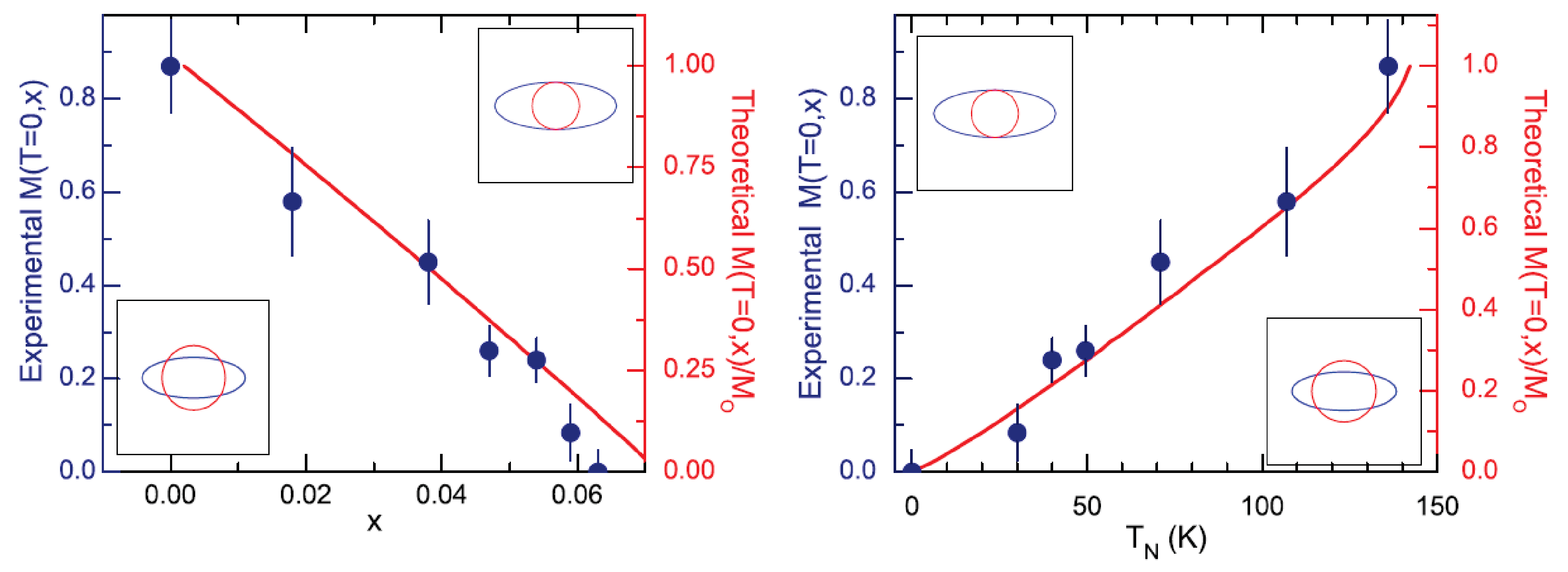
$M_1 = 0$

$M_2 \neq 0$

Iron pnictides: itinerant magnetism

- Solving the mean-field microscopic gap equations, we can also obtain the doping-dependence of the magnetization and transition temperature

good agreement with experimental measurements



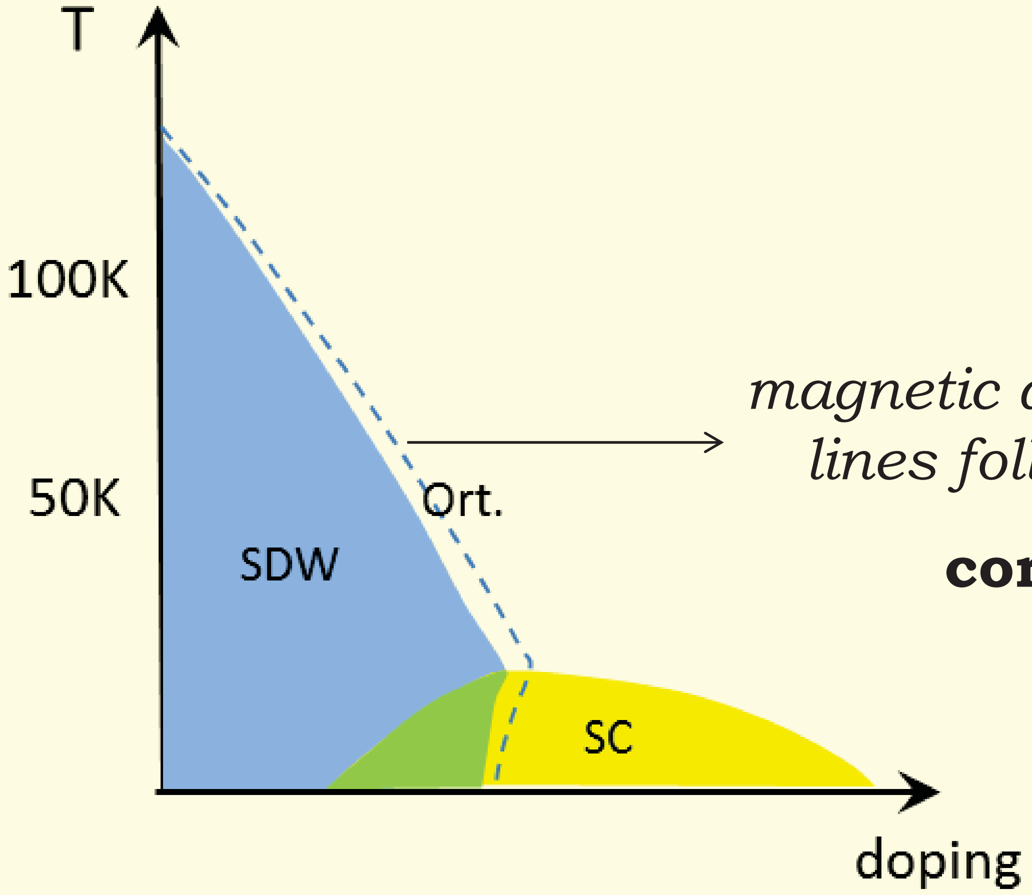
RMF *et al, PRB (2010)*

Outline

1. **The superconducting state (Lecture I)**
   - *unconventional superconductivity*
2. **The magnetic state (Lectures I & II)**
   - *itinerant or localized?*
3. **The nematic state (Lecture II)**
   - *a new electronic phase that emerges from magnetism and triggers structural and orbital order*
4. **Competing orders (Lecture II)**
   - *competition between SC, magnetism, and nematics*

Why nematics???

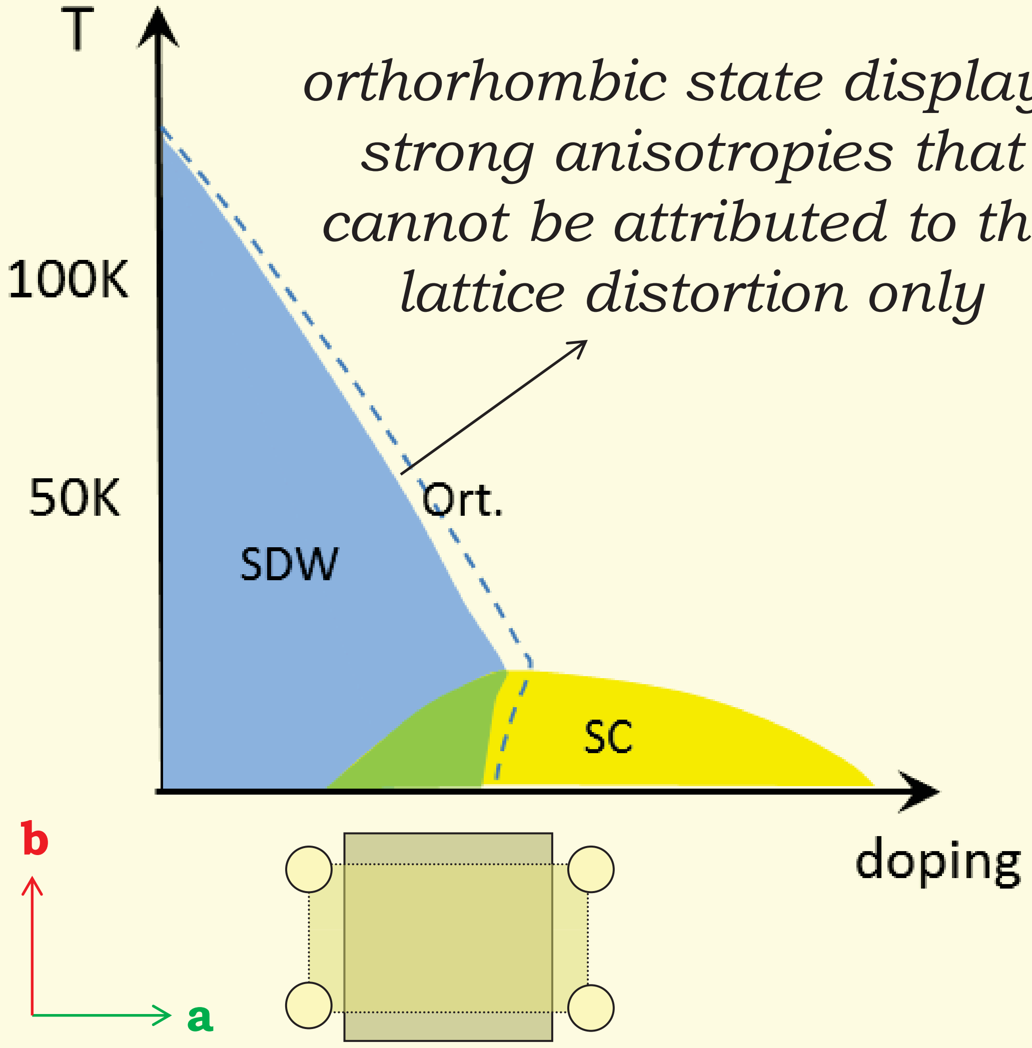
Iron pnictides: normal state properties



magnetic and structural transition lines follow closely each other

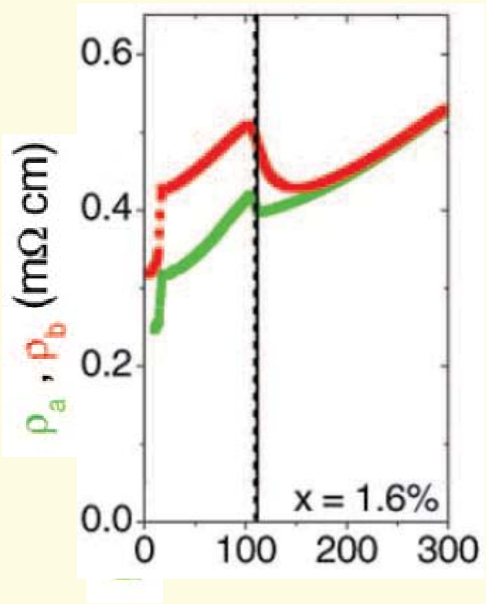
correlated phases!

Iron pnictides: normal state properties

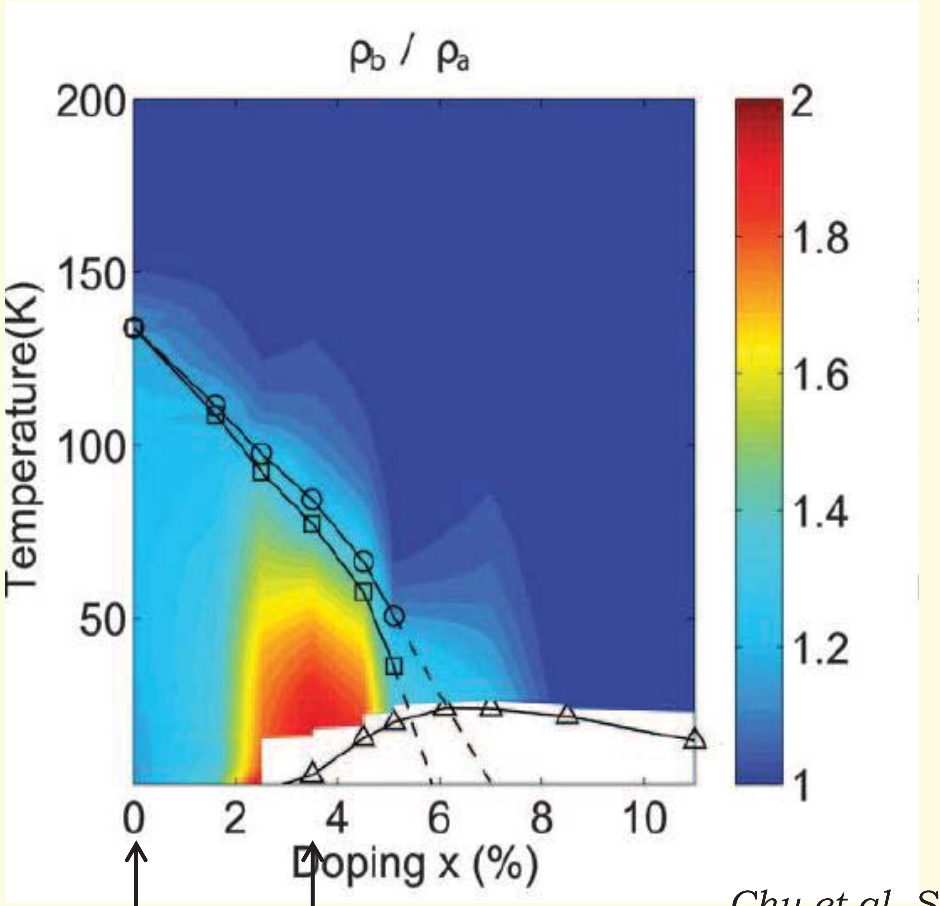


orthorhombic state displays strong anisotropies that cannot be attributed to the lattice distortion only

- **resistivity**



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



Chu et al, Science (2010)

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

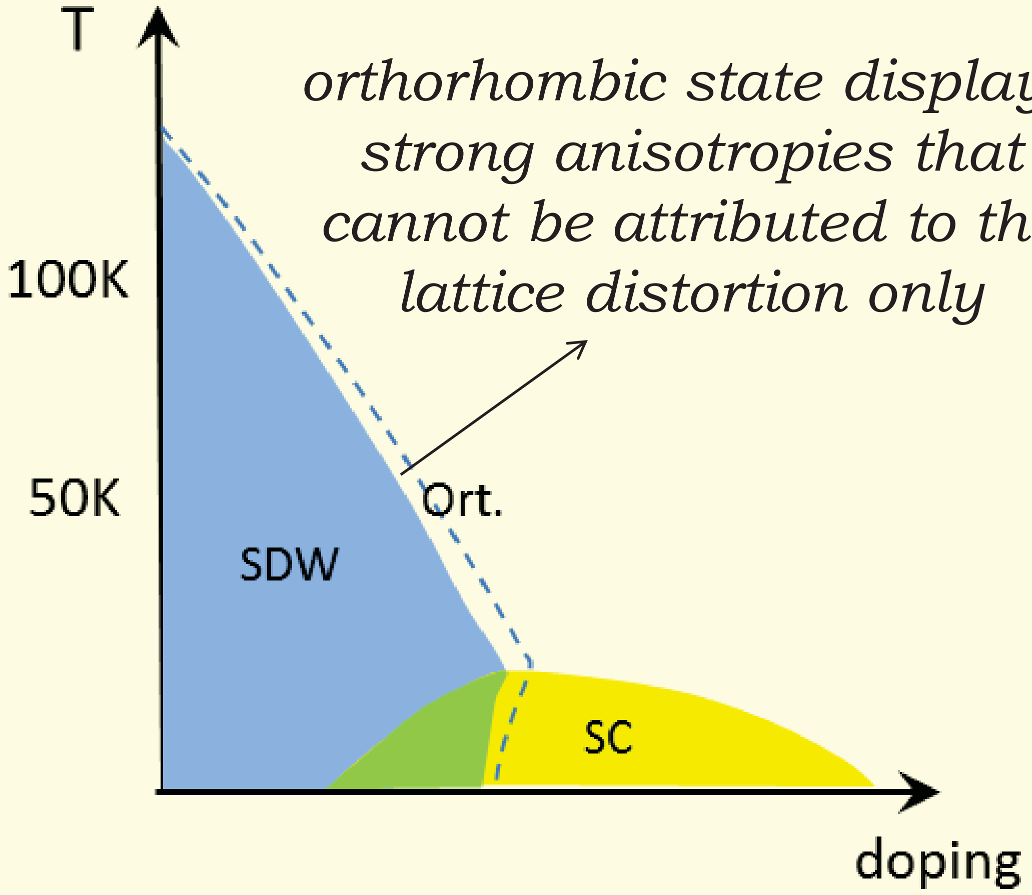
maximum orthorhombic distortion

maximum resistivity anisotropy

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

resistivity anisotropy cannot be attributed only to the orthorhombic distortion

Iron pnictides: normal state properties



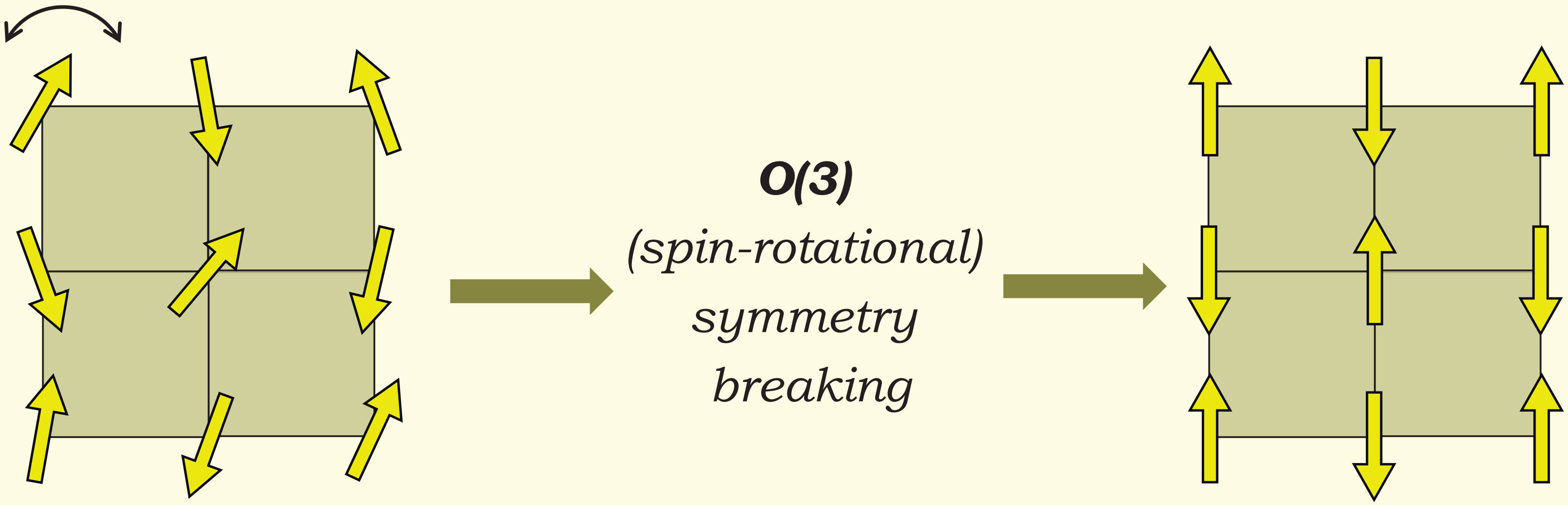
orthorhombic state displays strong anisotropies that cannot be attributed to the lattice distortion only

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

underlying electronic order that spontaneously breaks tetragonal symmetry: nematic phase

Nematic order: qualitative argument

- Symmetry breaking in a regular antiferromagnet:



O(3)

(spin-rotational)

symmetry

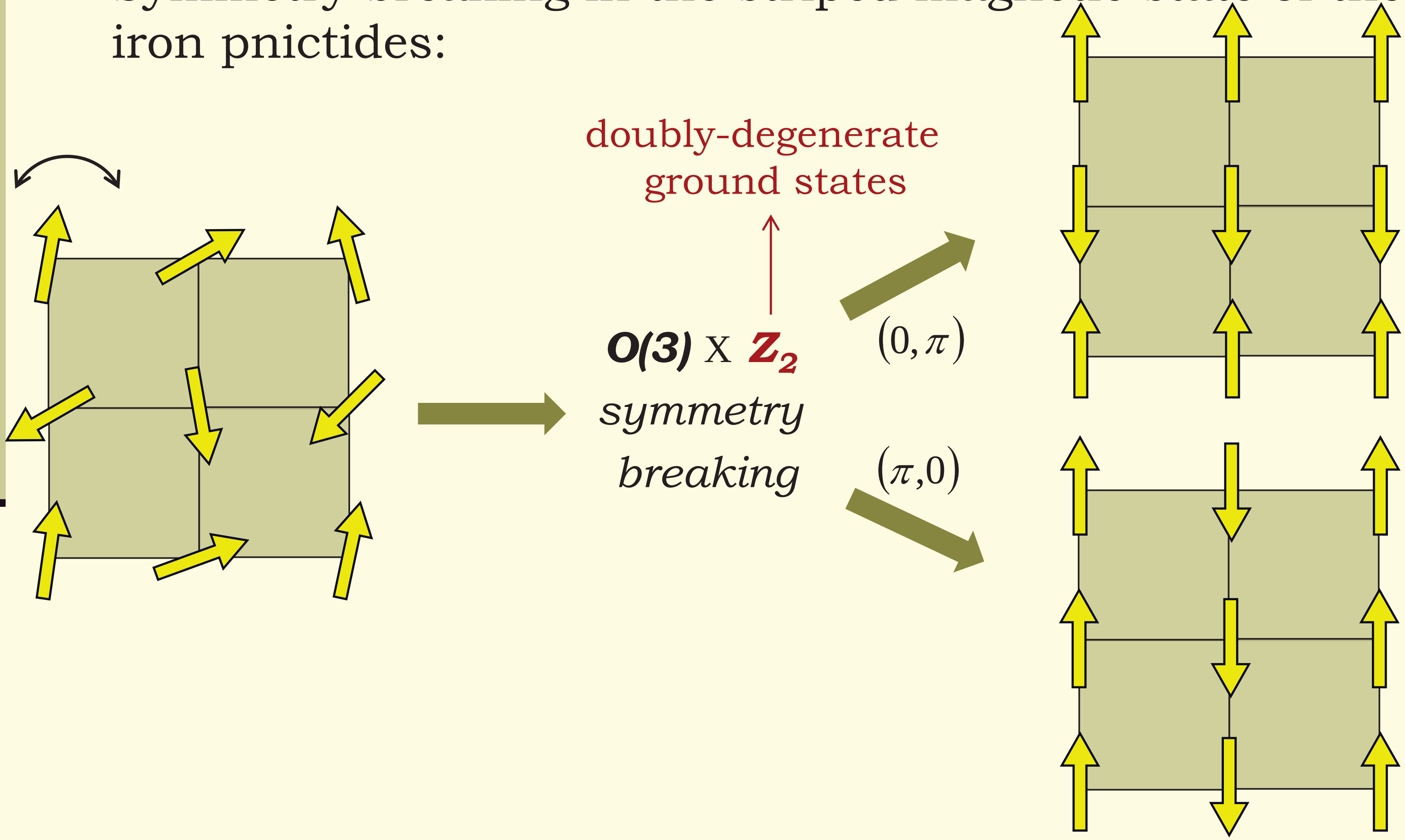
breaking

disordered
state

magnetic
state

Nematic order: qualitative argument

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



doubly-degenerate ground states

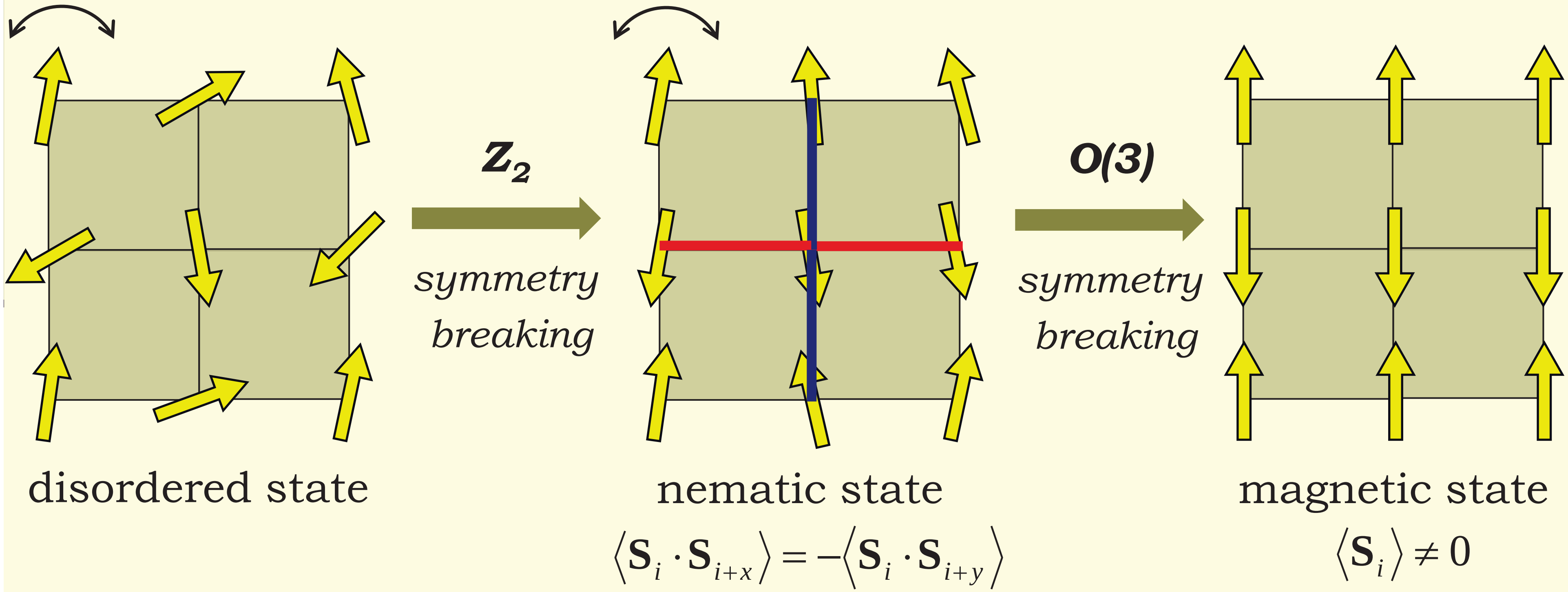
O(3) x $\mathbf{Z_2}$ *symmetry breaking*

$(0,\pi)$

$(\pi,0)$

Nematic order: qualitative argument

- A state that breaks Z_2 symmetry but remains paramagnetic
  - 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

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

Itinerant approach to the nematic state

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

$$F_{\mathrm{mag}} = \chi^{-1}_{\mathrm{mag}}(\mathbf{q})\left(M_1^2 + M_2^2\right) + \frac{u}{2}\left(M_1^2 + M_2^2\right)^2 - \frac{g}{2}\left(M_1^2 - M_2^2\right)^2$$

$$Z = \int dM_i \exp\left(-F_{\mathrm{mag}}\left[M_i\right]\right)$$

Hubbard-Stratonovich transformation: auxiliary fields

$$\exp\left[-\frac{u}{2}\left(M_1^2 + M_2^2\right)^2\right] = \int d\psi \exp\left[-\psi\left(M_1^2 + M_2^2\right) + \frac{\psi^2}{2u}\right]$$

$$\psi \propto M_1^2 + M_2^2$$

Gaussian fluctuations

Itinerant approach to the nematic state

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

$$F_{\text{mag}} = \chi^{-1}_{\text{mag}}(\mathbf{q})\left(M_1^2 + M_2^2\right) + \frac{u}{2}\left(M_1^2 + M_2^2\right)^2 - \frac{g}{2}\left(M_1^2 - M_2^2\right)^2$$

$$Z = \int dM_i \exp\left(-F_{\text{mag}}\left[M_i\right]\right)$$

Hubbard-Stratonovich transformation: auxiliary fields

$$\exp\left[\frac{g}{2}\left(M_1^2 - M_2^2\right)^2\right] = \int d\varphi \exp\left[\varphi\left(M_1^2 - M_2^2\right) - \frac{\varphi^2}{2g}\right]$$

$\varphi \propto M_1^2 - M_2^2$ *nematic order parameter*

Itinerant approach to the nematic state

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

$$Z = \int dM_i \, d\psi \, d\varphi \exp\left(-F_{\mathrm{mag}}\left[M_i, \psi, \varphi\right]\right)$$

Now the partition function is quadratic in the magnetic degrees of freedom, which can be integrated out analytically

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

Itinerant approach to the nematic state

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

$$Z = \int d\psi \, d\varphi \exp\left(-F_{\text{eff}}[\psi, \varphi]\right)$$

Now the partition function is quadratic in the magnetic degrees of freedom, which can be integrated out analytically

$$F_{\text{eff}}[\psi, \varphi] = \int_q \left(\frac{\varphi^2}{2g} - \frac{\psi^2}{2u}\right) + \frac{3}{2} \operatorname{tr} \log\left[\left(\chi_{\text{mag}}^{-1} + \psi\right)^2 - \varphi^2\right]$$

Itinerant approach to the nematic state

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

$$F_{\mathrm{eff}}[\psi,\varphi]=\int_q\left(\frac{\varphi^2}{2g}-\frac{\psi^2}{2u}\right)+\frac{3}{2}\operatorname{tr}\log\left[\left(\chi^{-1}_{\mathrm{mag}}+\psi\right)^2-\varphi^2\right]$$

Saddle-point approximation gives two non-linear coupled equations:

$$\begin{cases}\dfrac{\partial F_{\mathrm{eff}}}{\partial\psi}=0\\[2ex]\dfrac{\partial F_{\mathrm{eff}}}{\partial\varphi}=0\end{cases}\Rightarrow\begin{cases}\psi=\dfrac{u}{2}\displaystyle\int_q\left[\dfrac{1}{\chi^{-1}_{\mathrm{mag}}(q)+\psi-\varphi}+\dfrac{1}{\chi^{-1}_{\mathrm{mag}}(q)+\psi+\varphi}\right]\\[2ex]\varphi=\dfrac{g}{2}\displaystyle\int_q\left[\dfrac{1}{\chi^{-1}_{\mathrm{mag}}(q)+\psi-\varphi}-\dfrac{1}{\chi^{-1}_{\mathrm{mag}}(q)+\psi+\varphi}\right]\end{cases}$$

Itinerant approach to the nematic state

Equation of state for the nematic order parameter:

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

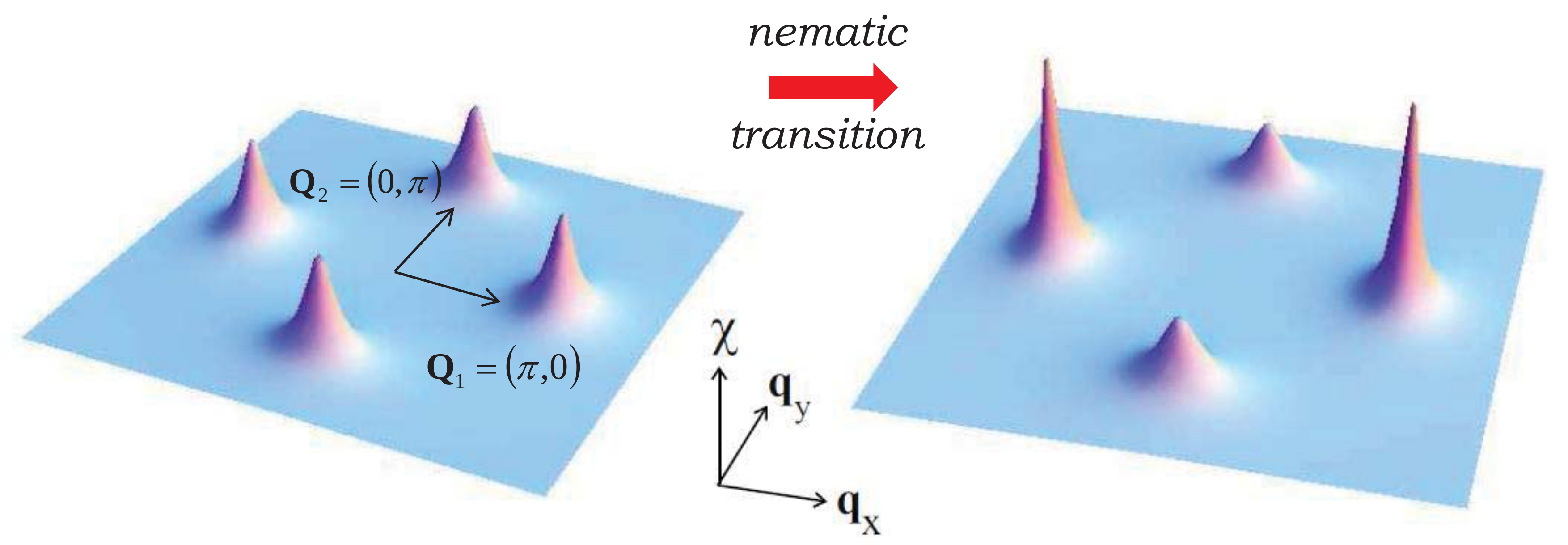
$\varphi \neq 0$ **solution already in the paramagnetic phase, when the magnetic susceptibility is large enough**

$$\left\langle M_{1}^{2}\right\rangle \neq \left\langle M_{2}^{2}\right\rangle$$

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:

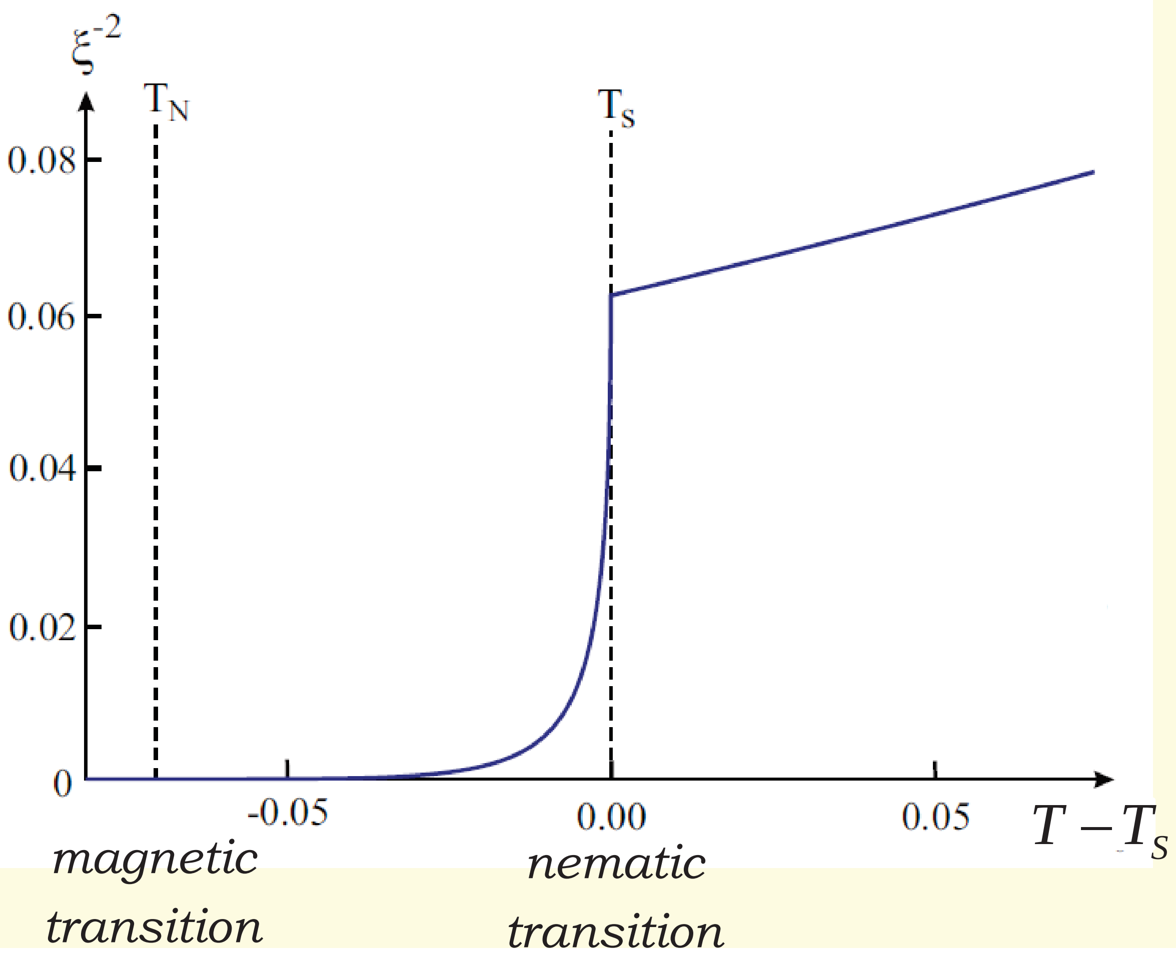
tetragonal symmetry breaking

(structural transition driven by magnetic fluctuations)

Enhanced magnetic fluctuations due to nematic order

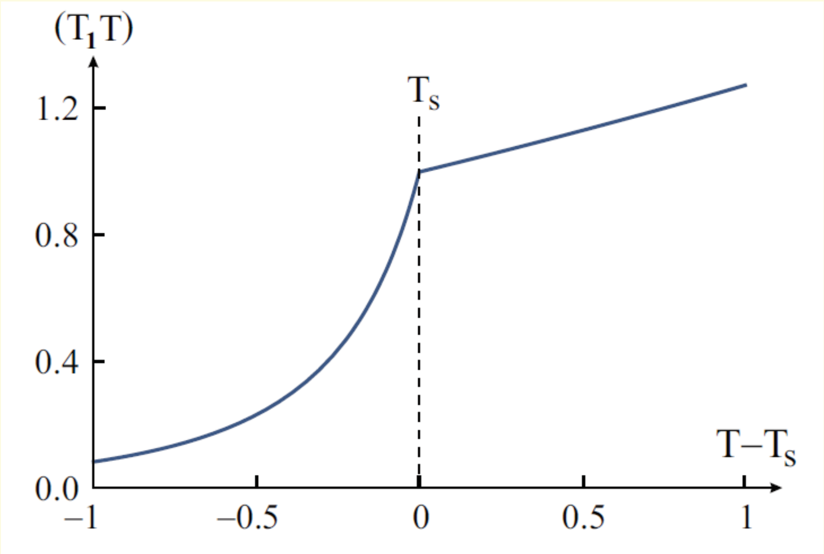
- Strong increase of the magnetic correlation length at the nematic transition

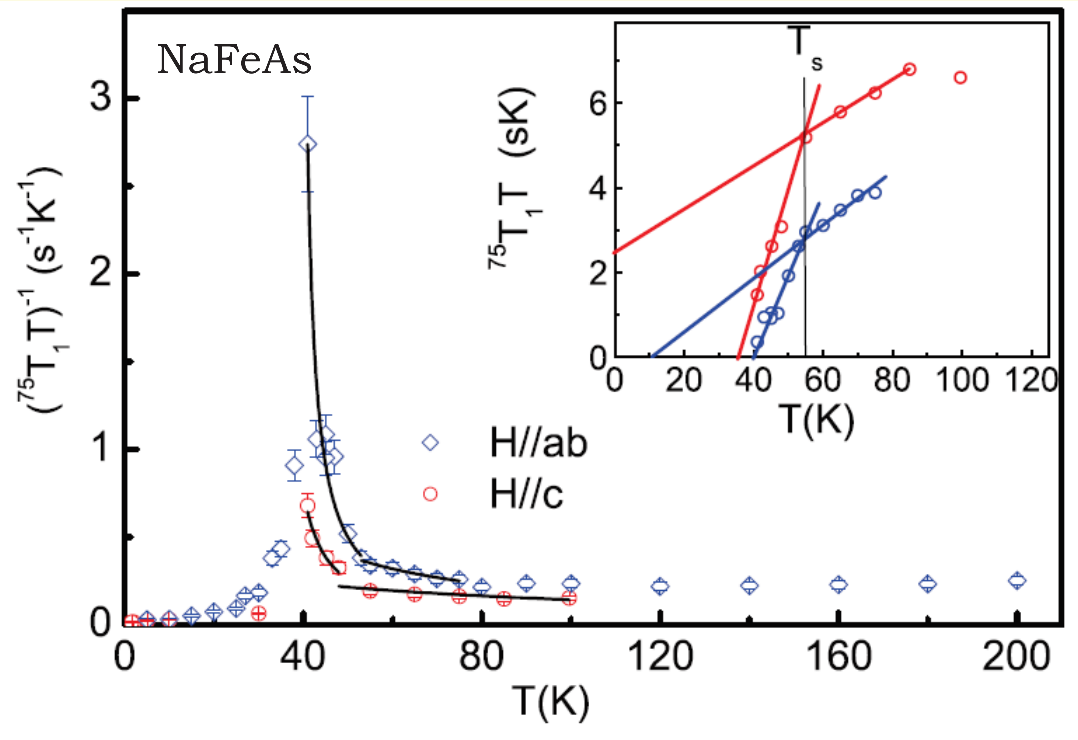
$$\xi^{-2} \rightarrow \xi^{-2} - \varphi$$



Enhanced magnetic fluctuations due to nematic order

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





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

RMF & Schmalian, SUST (2012)

Ma et al, PRB (2011)

Phase diagrams for the magnetic and structural transitions

magnetic fluctuations

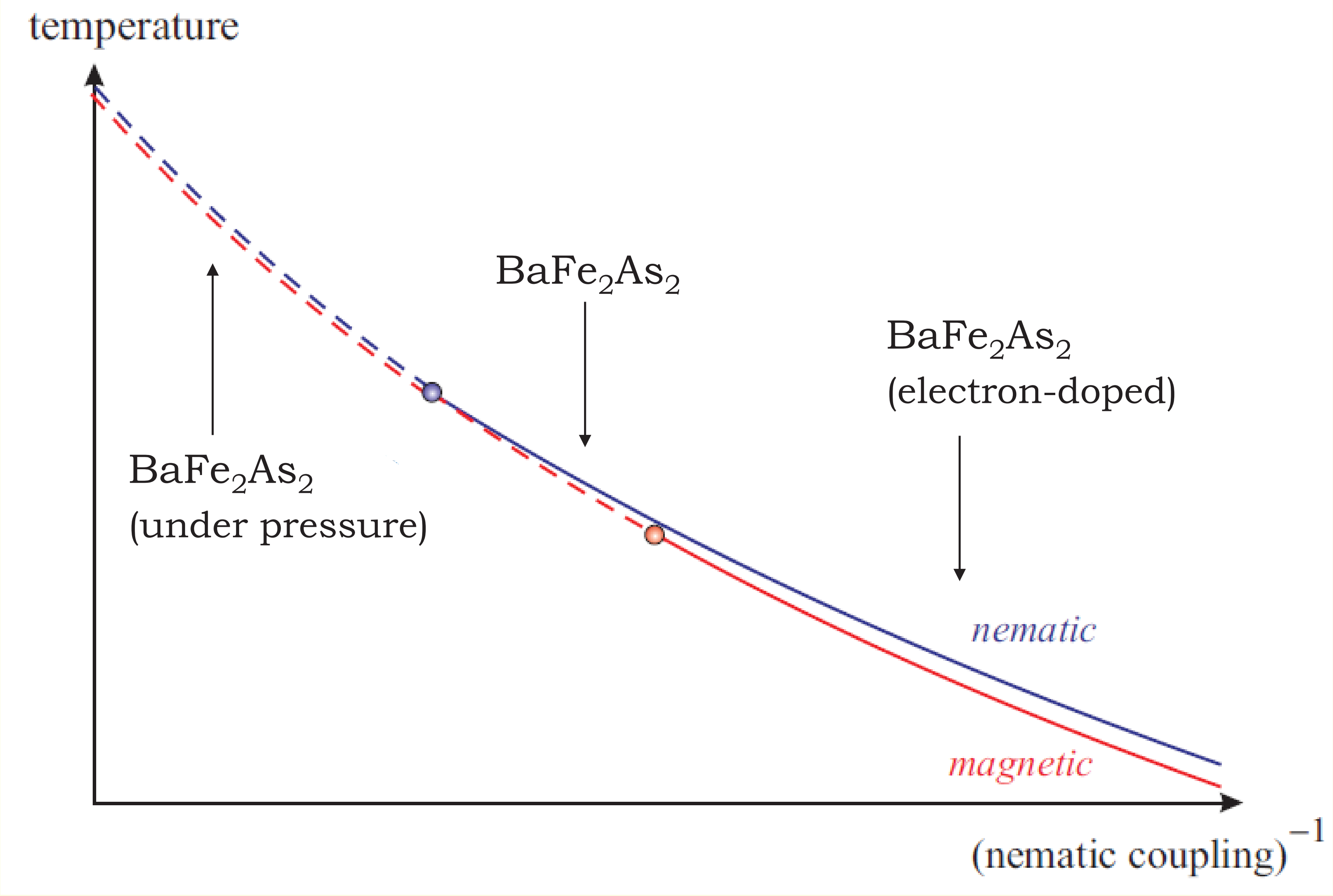
give rise to

enhances

nematic order

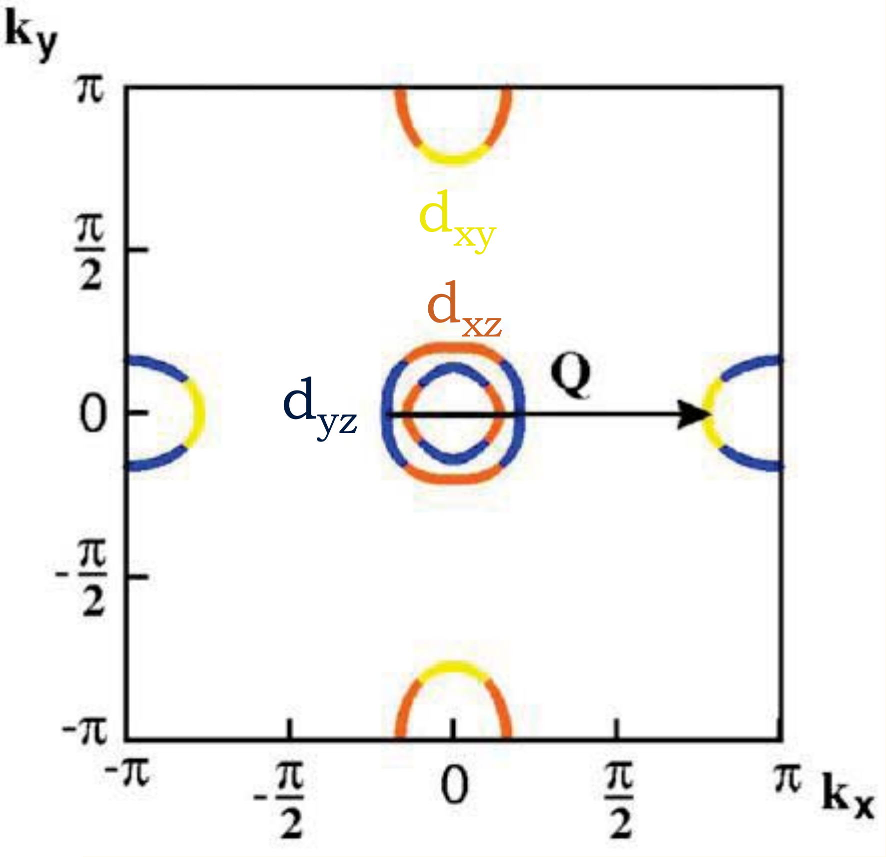
transitions naturally follow each other

magneto-structural phase diagram: itinerant approach

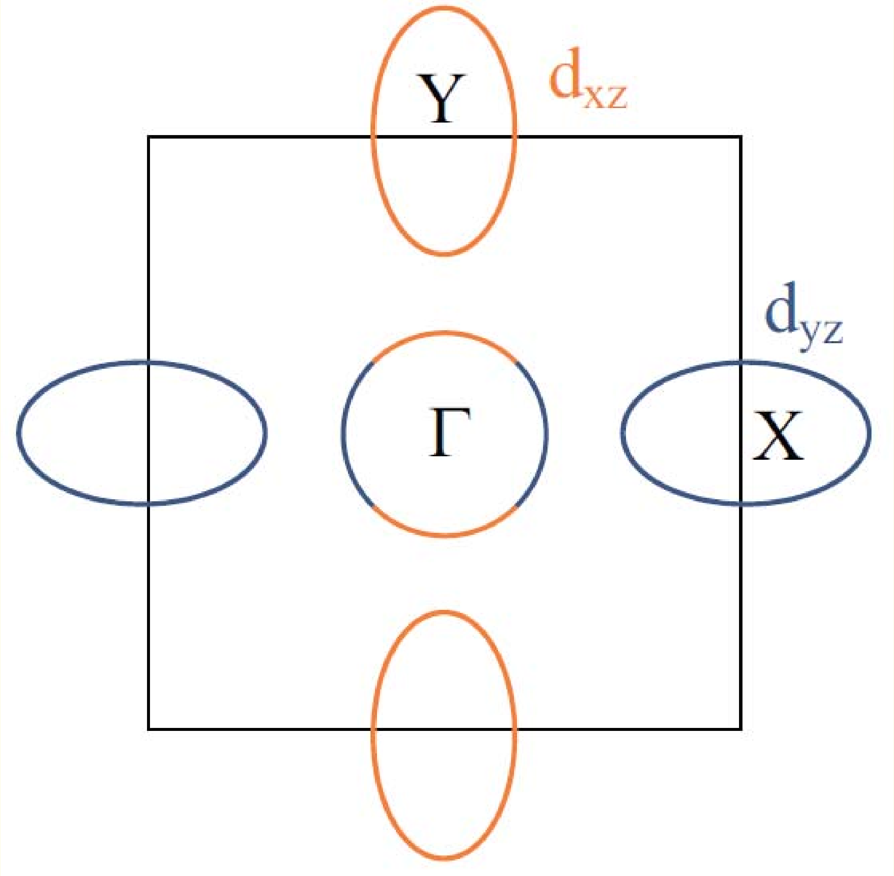


Nematic transition triggers orbital order

- Distinct Fermi pockets have different orbital content



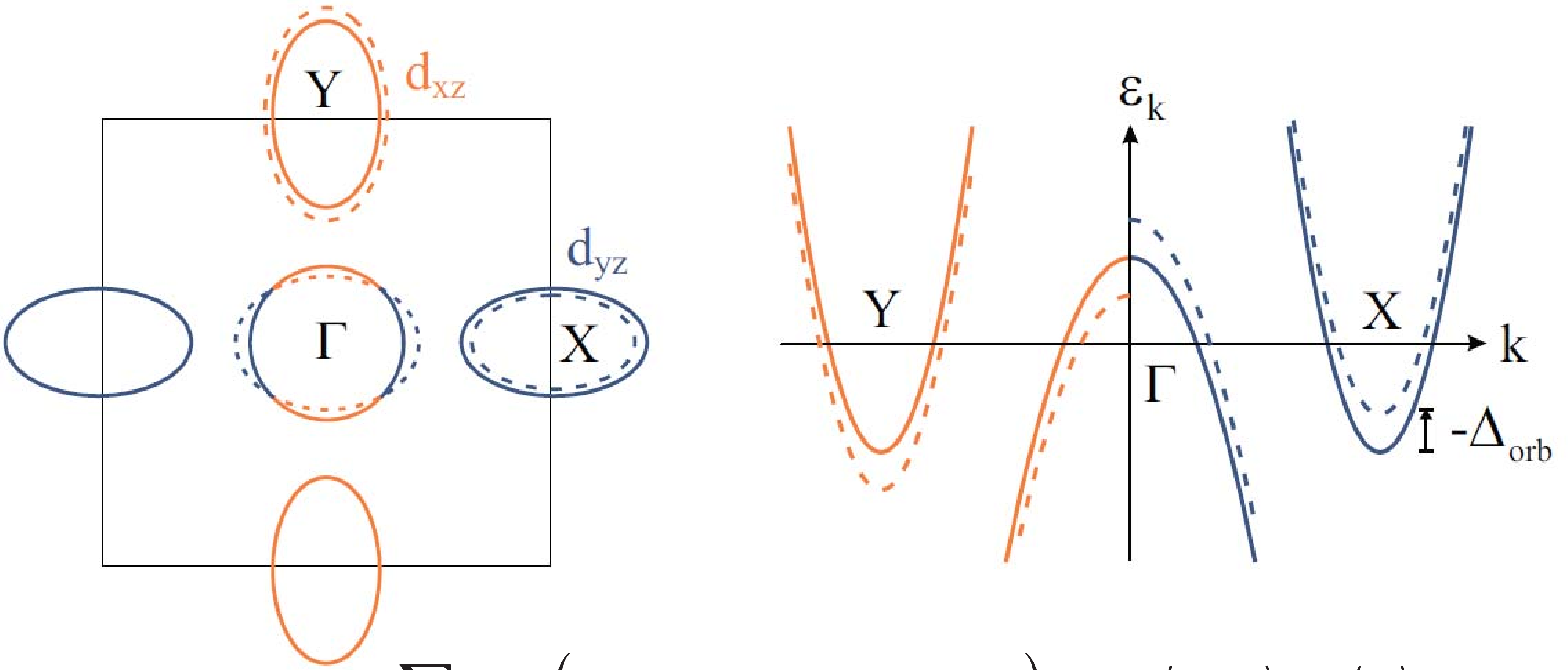
DFT calculation



simplified 2-orbital model

Nemratic transition triggers orbital order

- Nematic order leads to different onsite energies for the d_{xz} and d_{yz} orbitals: *ferro-orbital order*

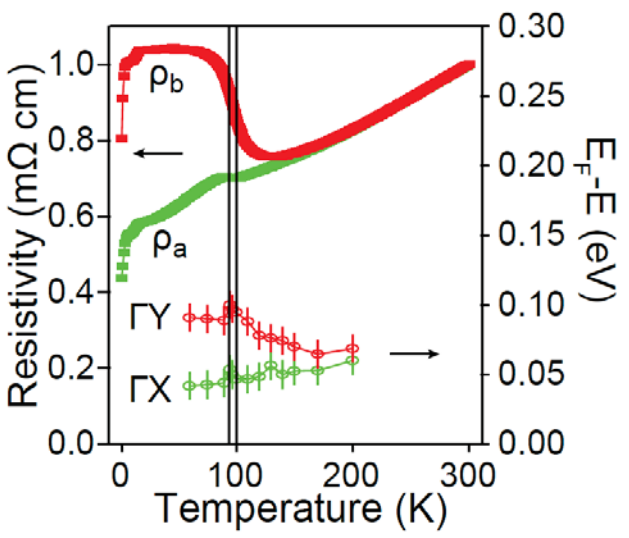


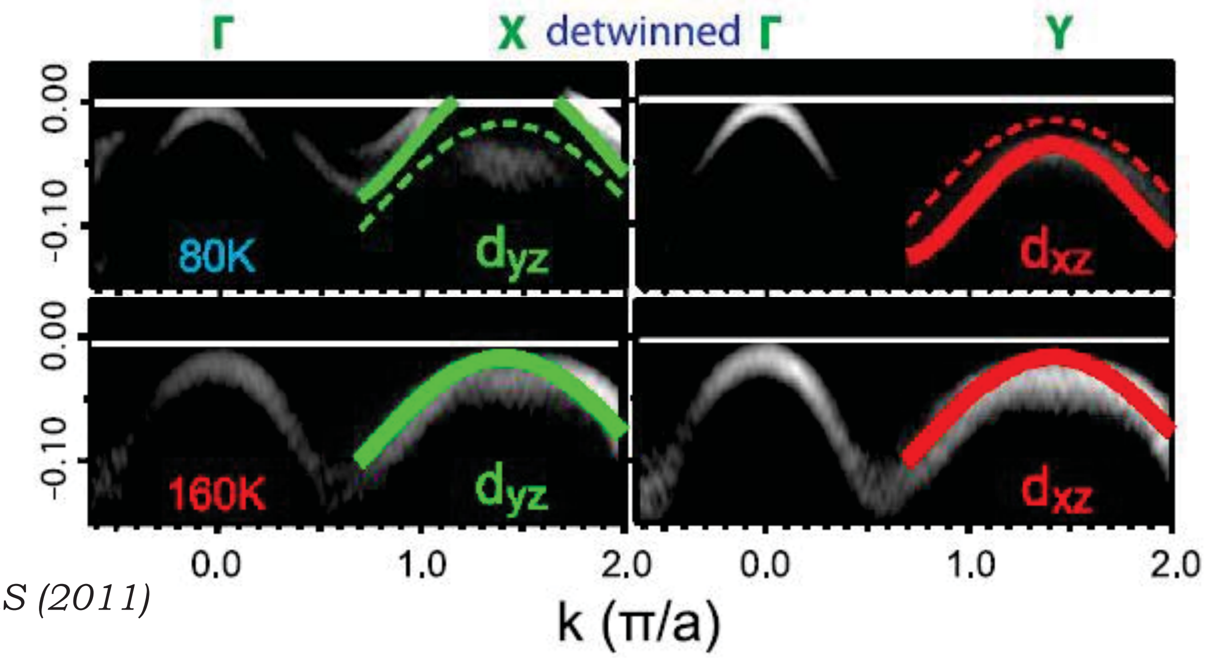
$$H_{\text{orb}} = -\sum_{\mathbf{k}} \Delta_{\text{orb}} \left(c^{+}_{X,\mathbf{k}\alpha} c_{X,\mathbf{k}\alpha} - c^{+}_{Y,\mathbf{k}\alpha} c_{Y,\mathbf{k}\alpha} \right) \Rightarrow \left\langle \Delta_{\text{orb}} \right\rangle \propto \left\langle \varphi \right\rangle$$

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

Nematic transition triggers orbital order

- polarized ARPES observes orbital splitting in $BaFe_2As_2$





Yi et al, PNAS (2011)

- so far, this is the only mechanism that, starting from an itinerant microscopic model, gives orbital order in the absence of long-range magnetic order

Outline

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   - *a new electronic phase that emerges from magnetism and triggers structural and orbital order*
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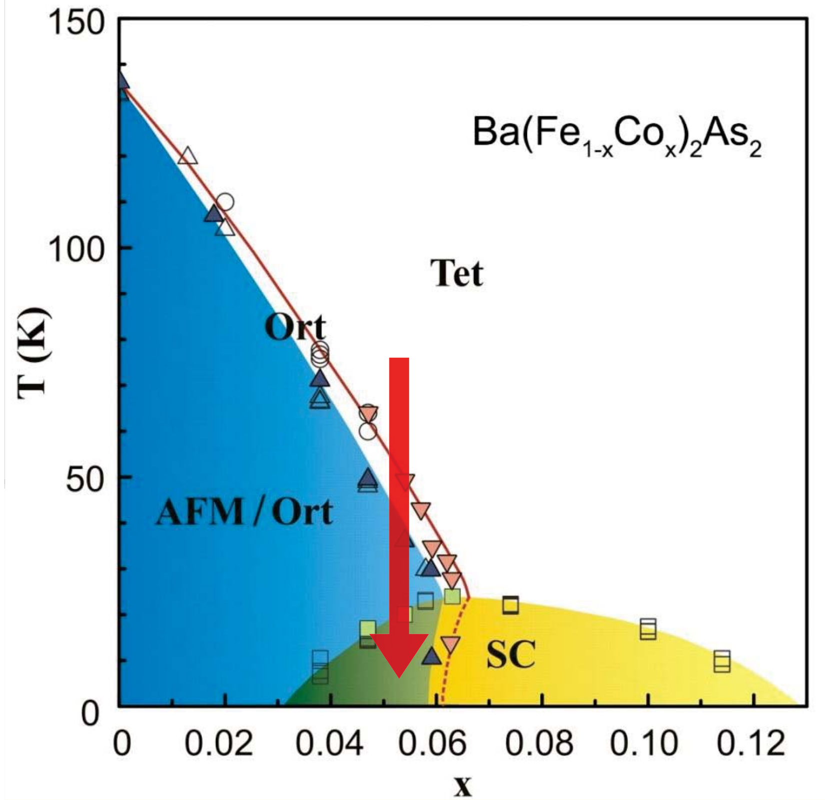
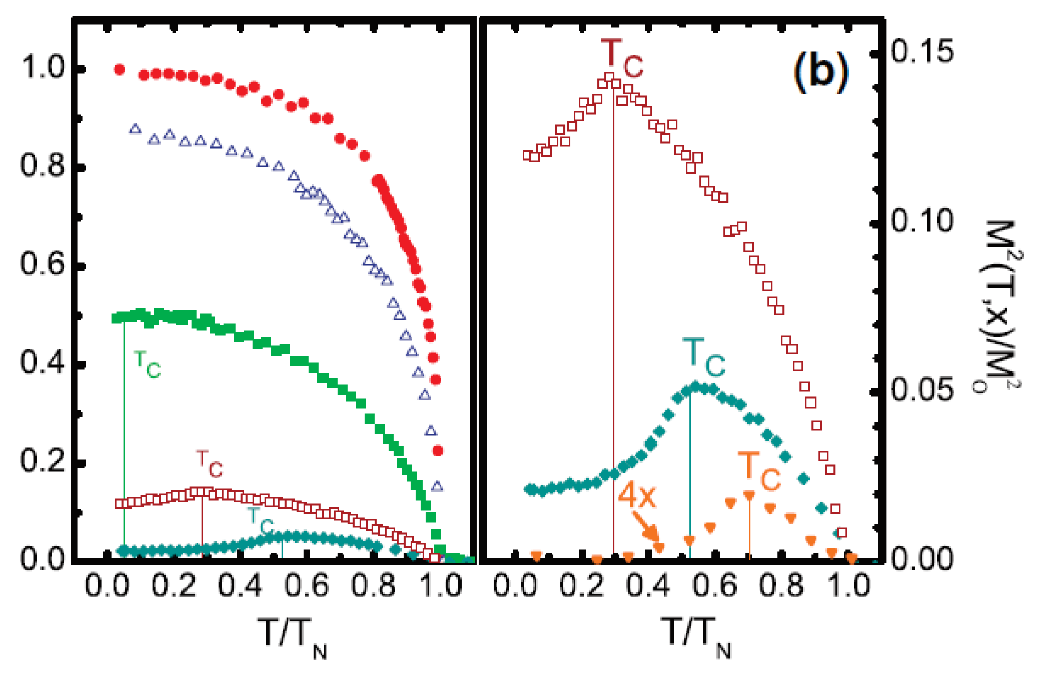
   - *competition between SC, magnetism, and nematics*

Competing phases: experimental observations

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



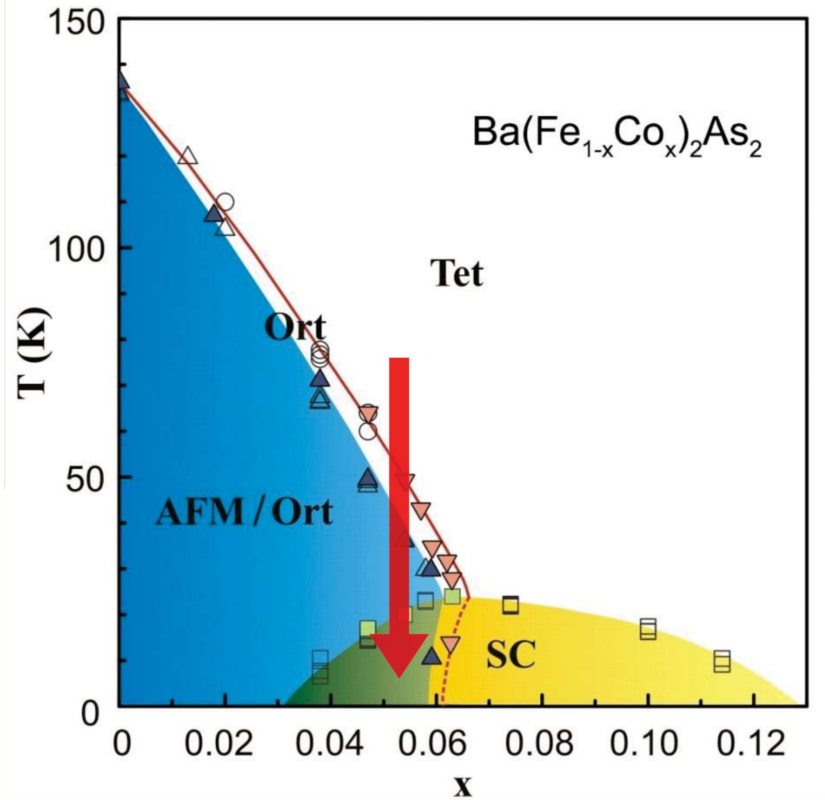


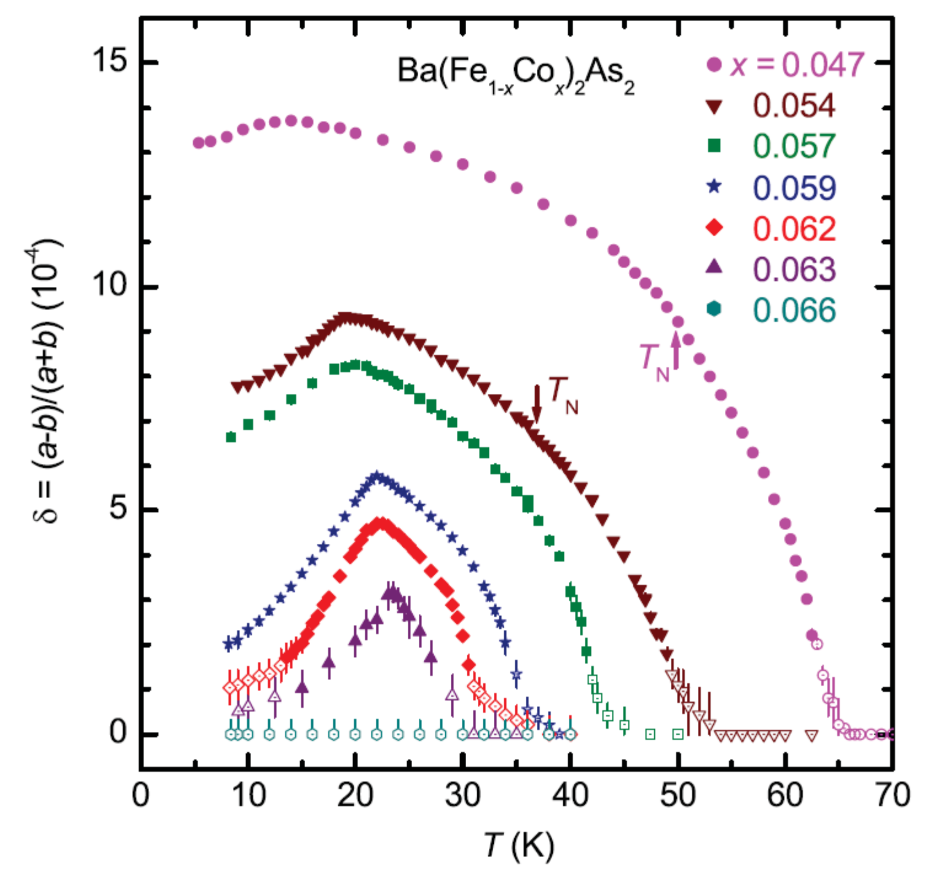
RMF et al, PRB (2010)

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

Competing phases: experimental observations

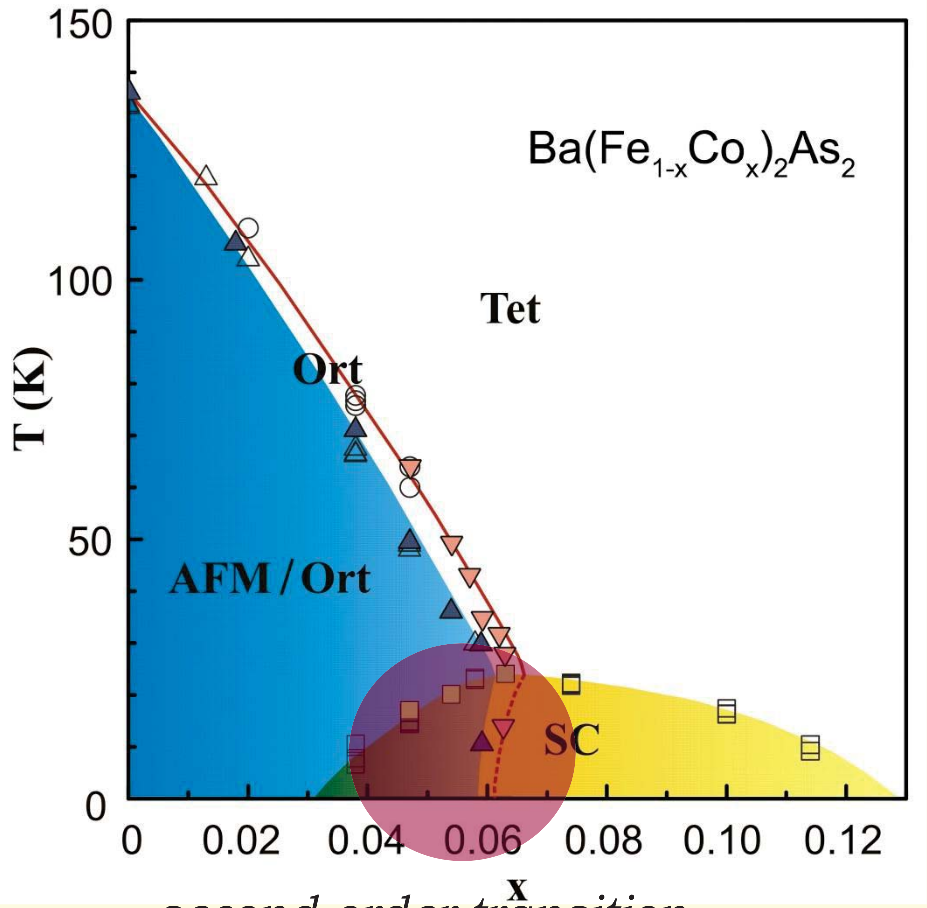
- X-ray diffraction: suppression of the **orthorhombic order parameter** below T_c





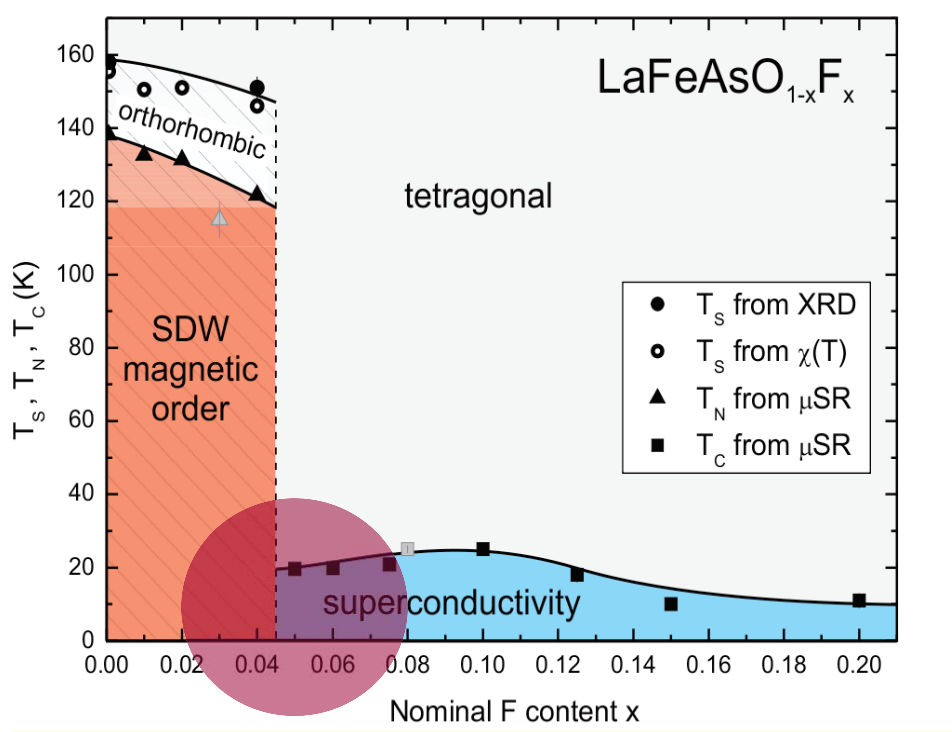
Nandi,…, RMF et al, PRL (2010)

Competition between SDW and SC: coexistence or phase separation?



second-order transition

(microscopic coexistence)

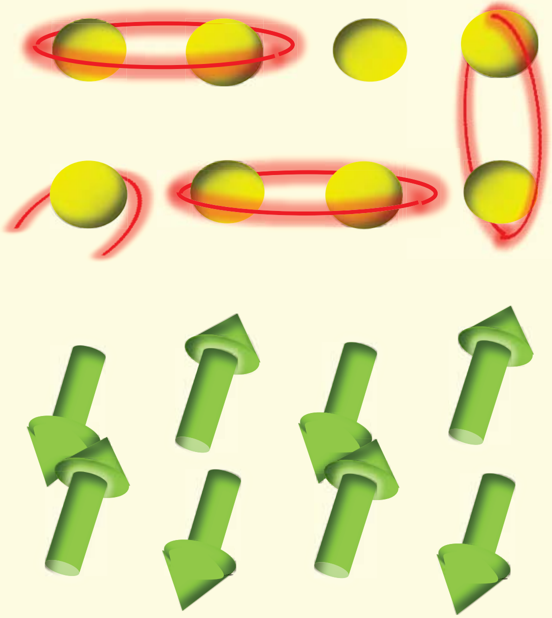


first-order transition

(phase separation)

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

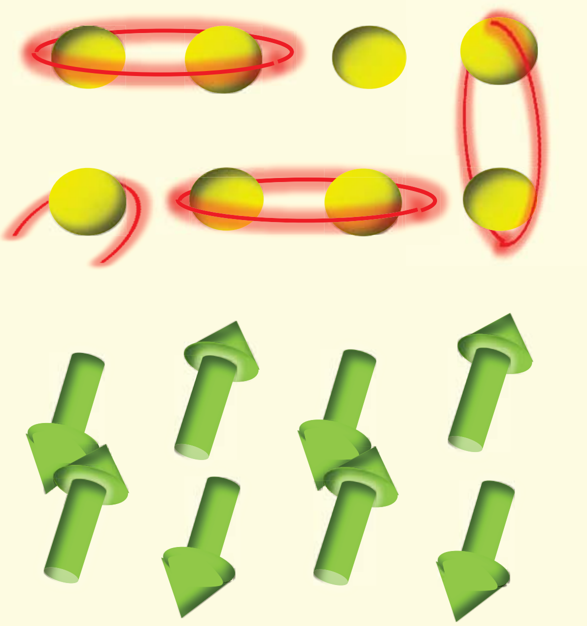


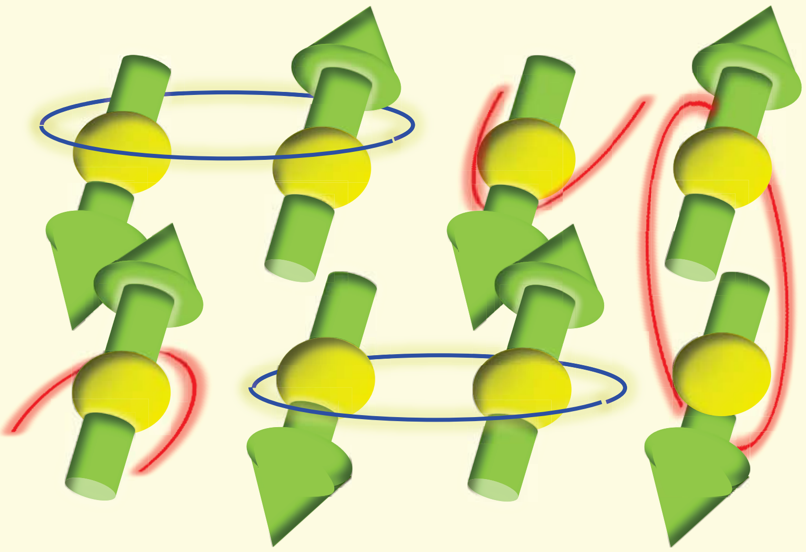
conduction electrons
(3d band)

localized spins
(4f band)

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

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

- Minimization with respect to M leads to

$$a_m + u_m M^2 = -\gamma |\Delta|^2$$

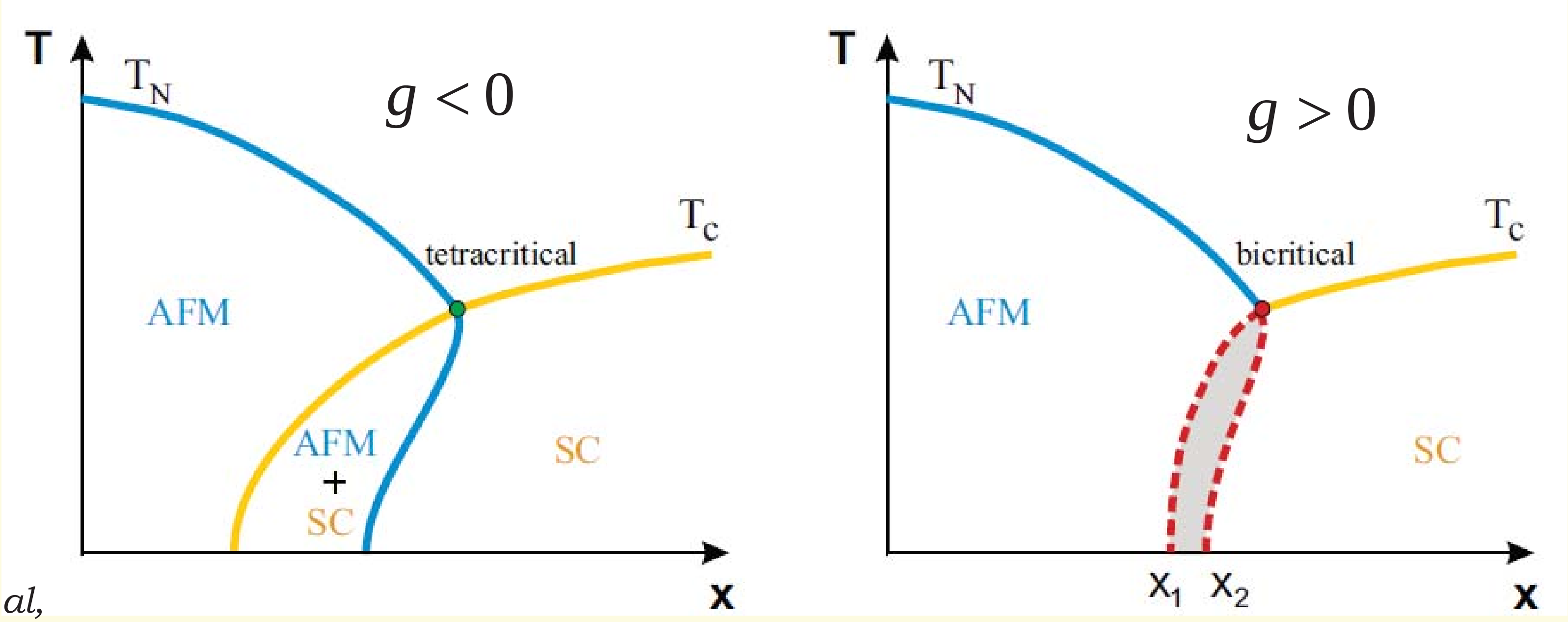
and we obtain the effective free energy

$$F[\Delta] = -\frac{a_m^2}{4u_m} + \frac{a_s}{2}\left(1 - \frac{a_m \gamma}{a_s u_m}\right)|\Delta|^2 + \frac{u_s}{4}\left(1 - \overbrace{\underbrace{\frac{\gamma^2}{u_s u_m}}_{>0\ :\ \text{second-order}}}^{<0\ :\ \text{first-order}}\right)|\Delta|^4$$

Competition between SDW and SC: phenomenological model

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

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



Kosterlitz et al, PRB (1976)

coexistence

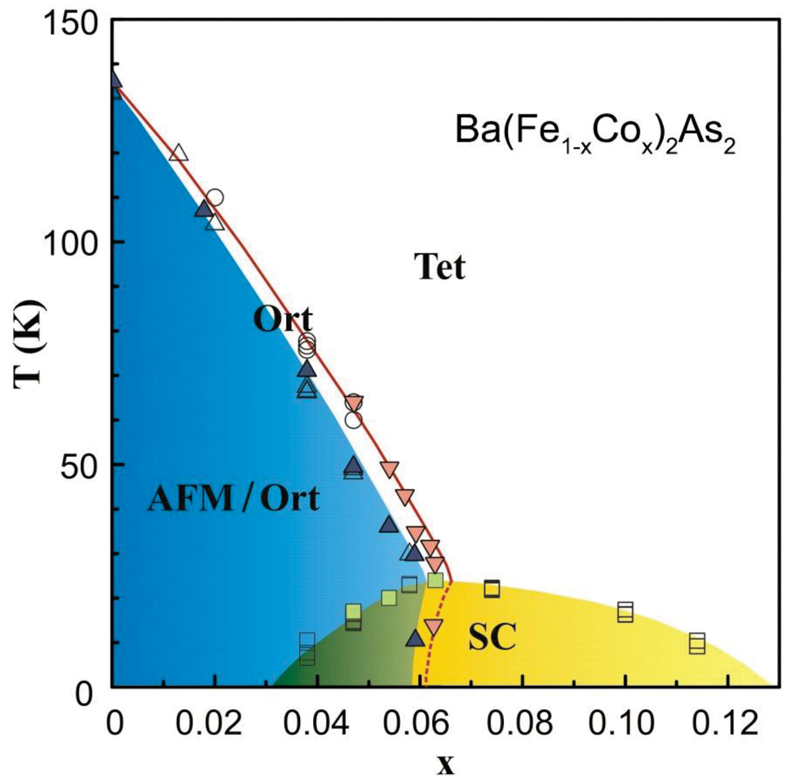
phase separation

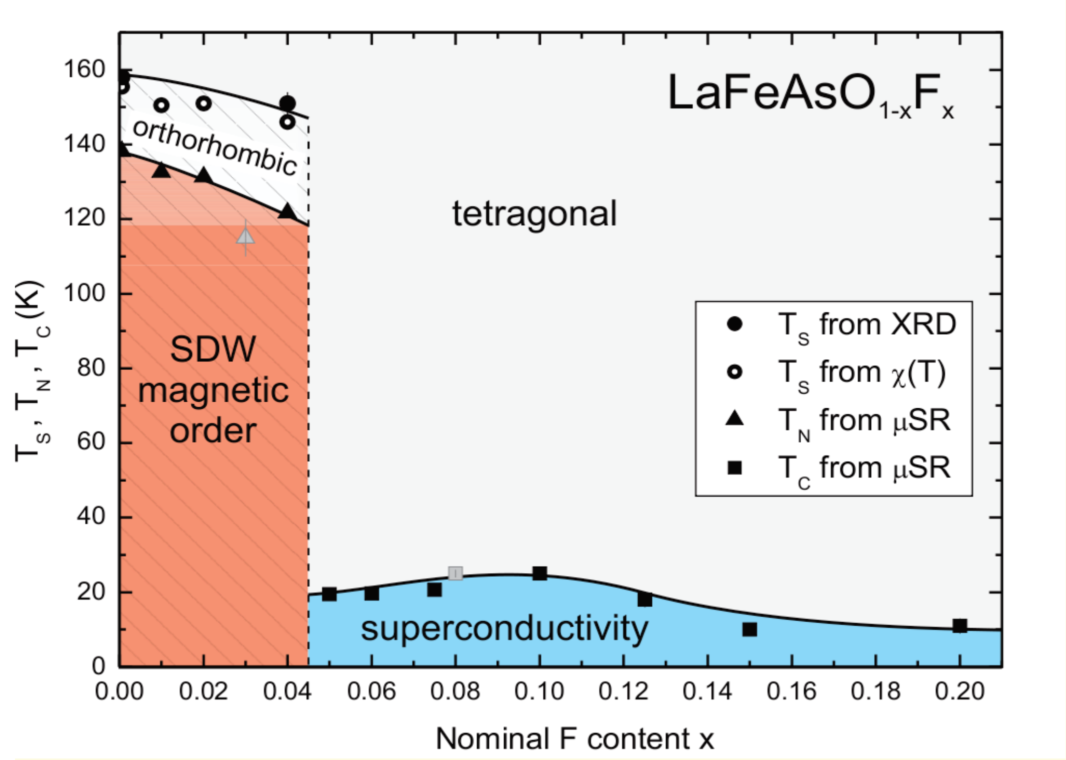
Competition between SDW and SC: phenomenological model

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

$g<0$

$g>0$

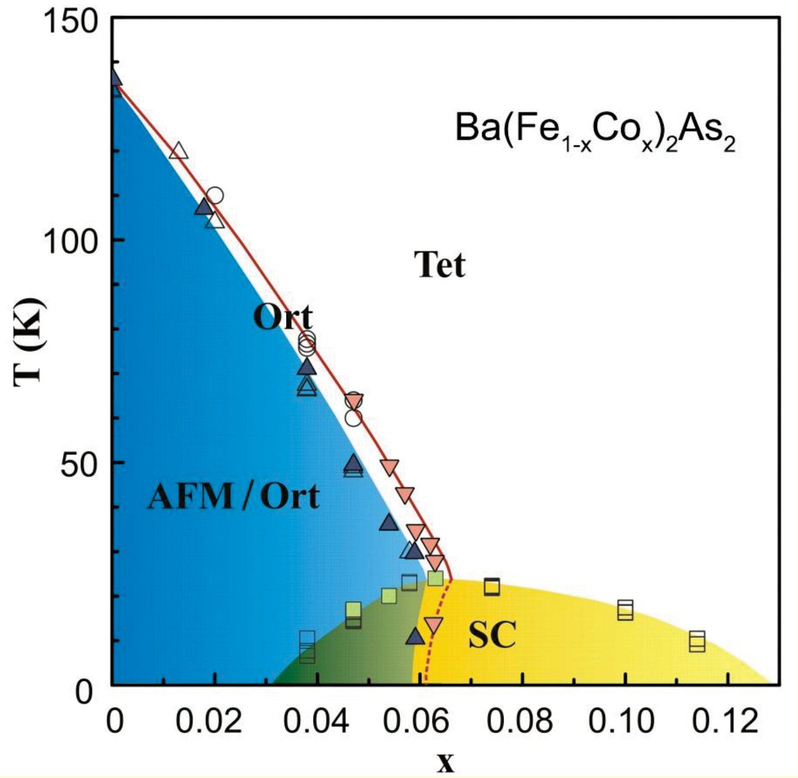




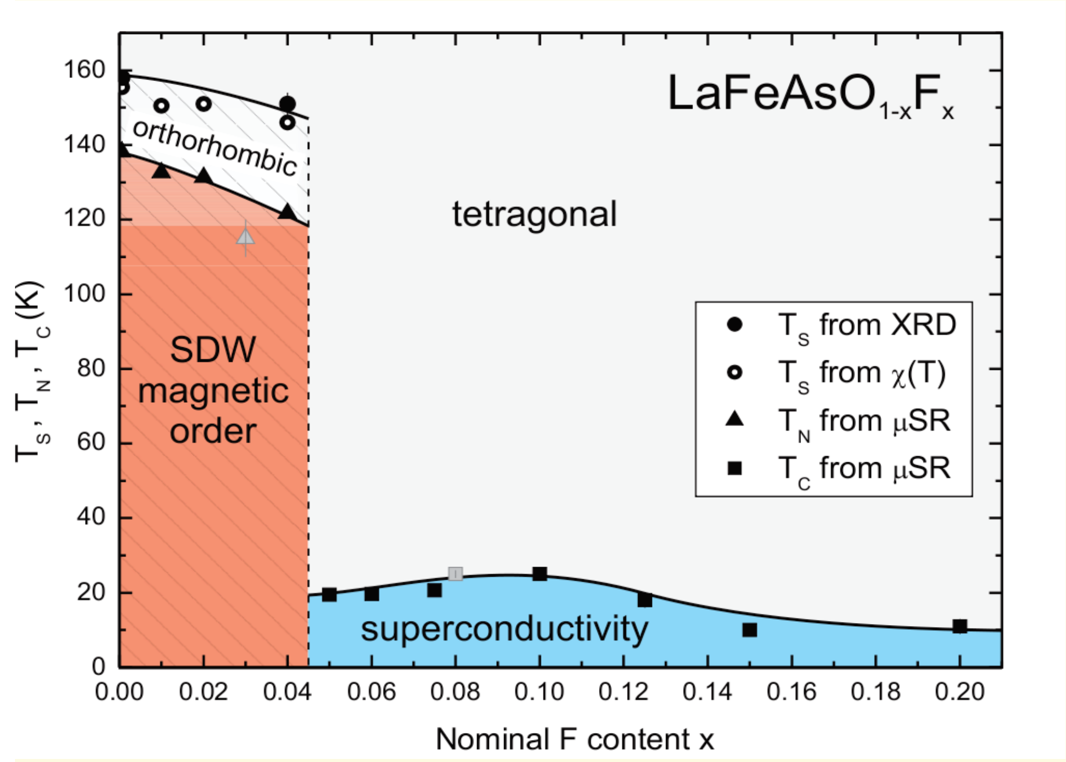
Competition between SDW and SC: phenomenological model

How to describe this competition from a microscopic model?

$g < 0$



$g > 0$



Competition between SDW and SC: microscopic model

- Hertz-Millis approach to the two-band model

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

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

Competition between SDW and SC: microscopic model

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

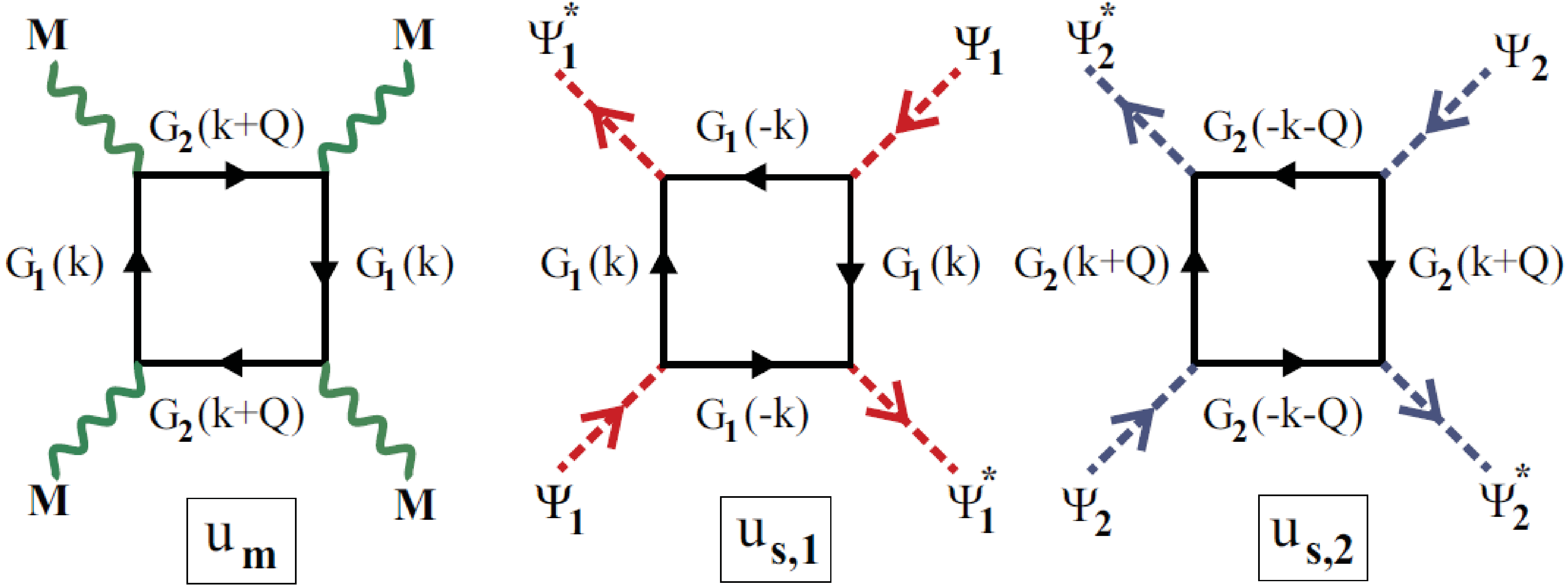
$$F[M,\Delta]=\frac{a_m}{2}M^2+\frac{u_m}{4}M^4+\frac{a_s}{2}|\Delta|^2+\frac{u_s}{4}|\Delta|^4+\frac{\gamma}{2}|\Delta|^2M^2$$

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

Competition between SDW and SC: microscopic model

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

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



Competition between SDW and SC: microscopic model

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

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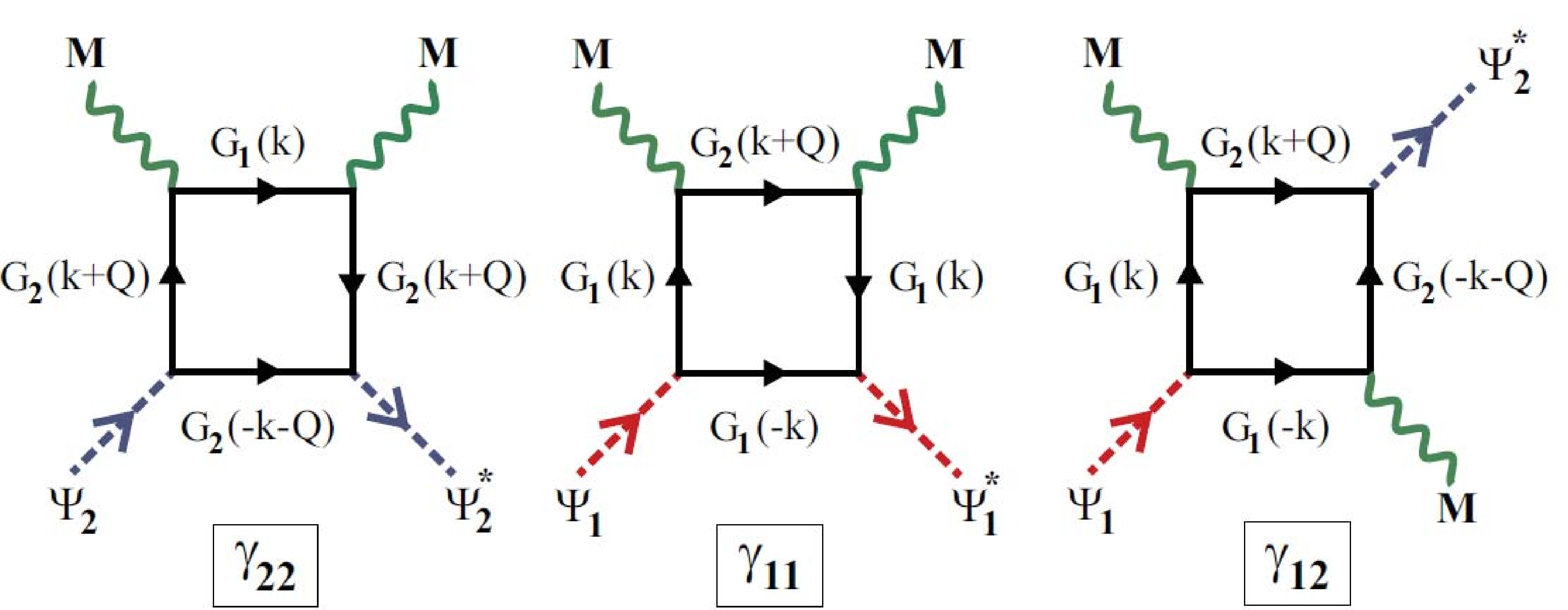
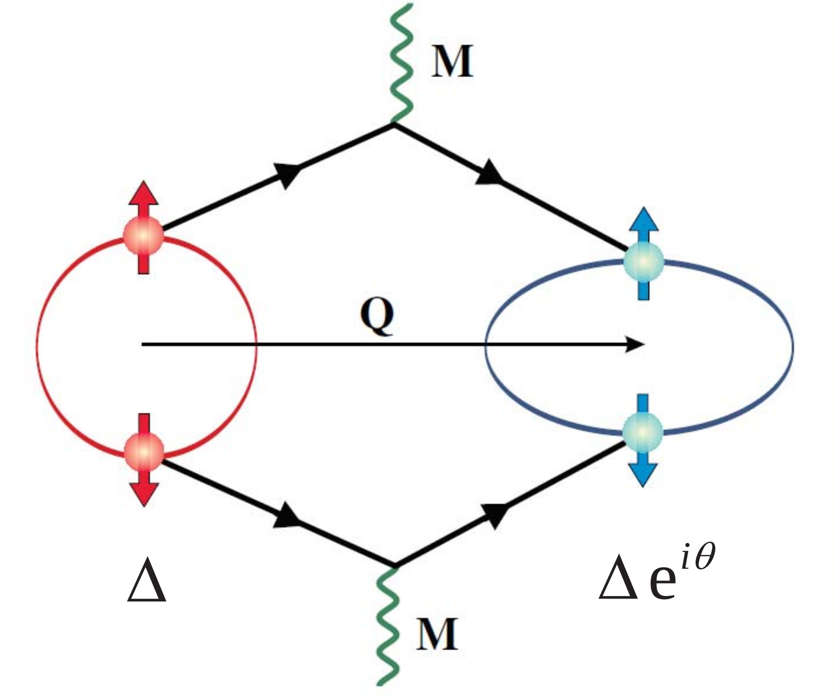


Competition between SDW and SC: microscopic model

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



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

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

Coexistence between AFM and SC: perfect nesting

- For perfect nesting:

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

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

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

borderline

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

phase separation

Coexistence between AFM and SC: perfect nesting

- For perfect nesting:

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

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

borderline

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

phase separation

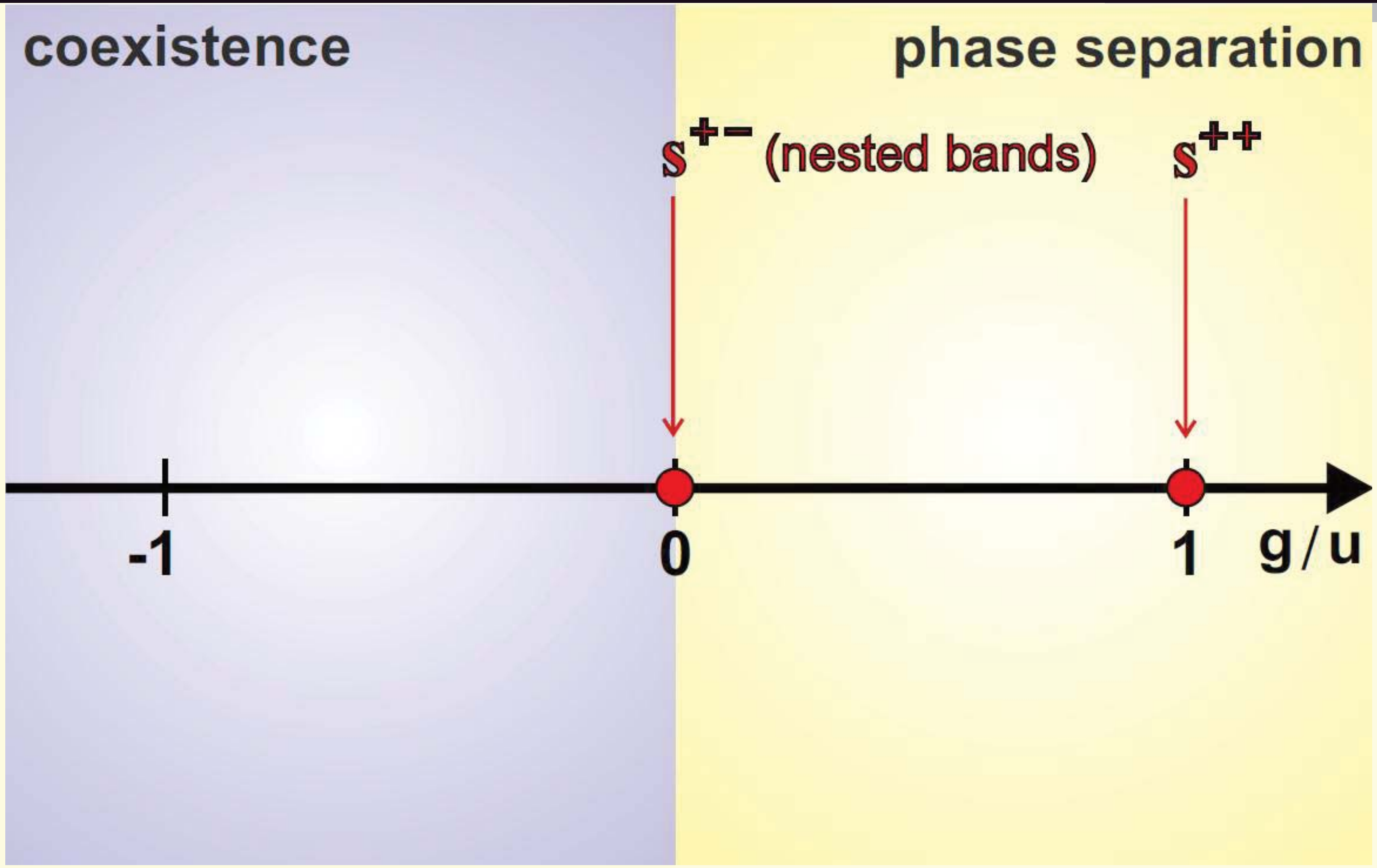
Note that $g=0 \Rightarrow$ emergent SO(5) symmetry

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

Podolsky et al, EPL (2009)

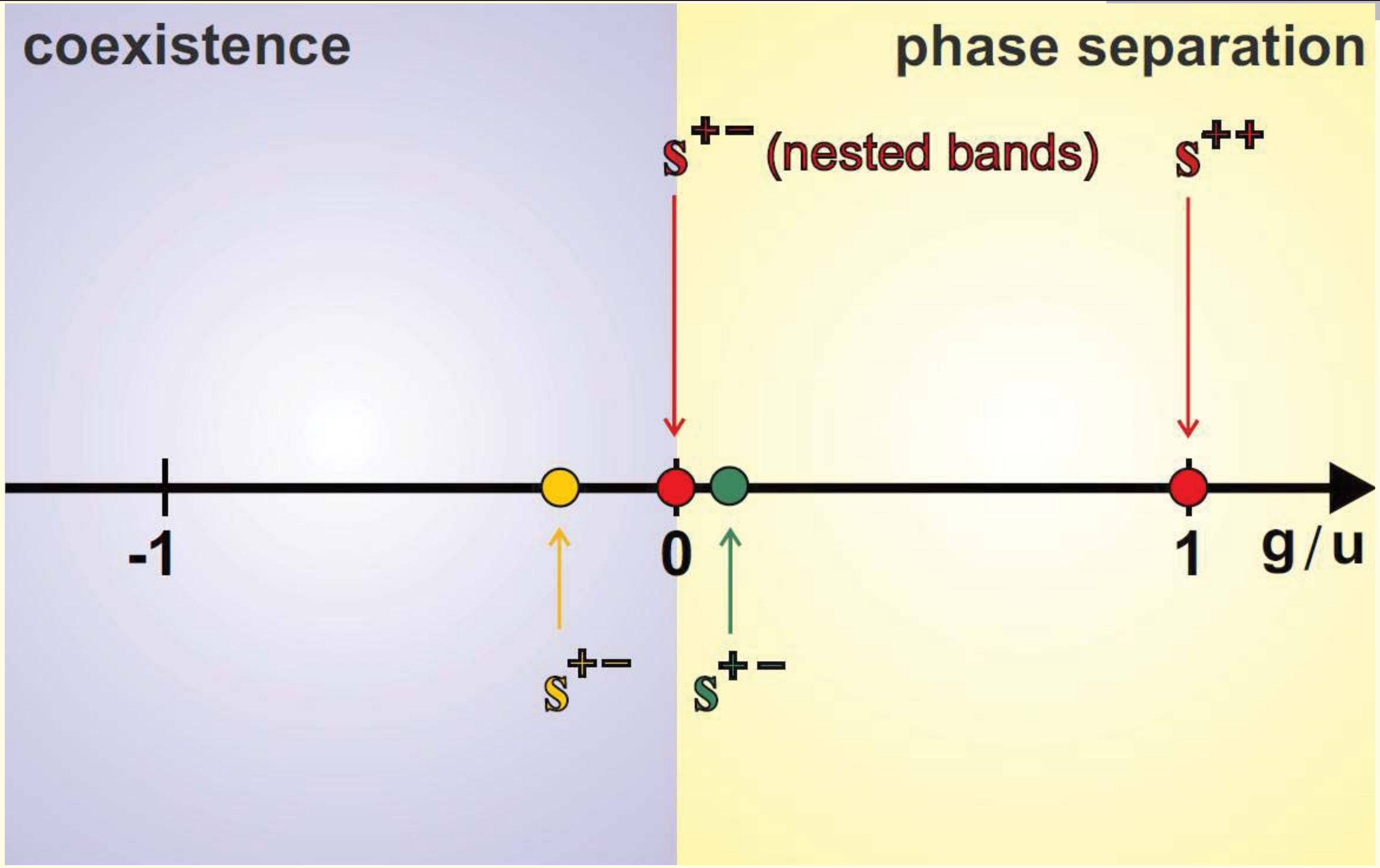
Chubukov, Physica C (2008)

Competition between SDW and SC: coexistence

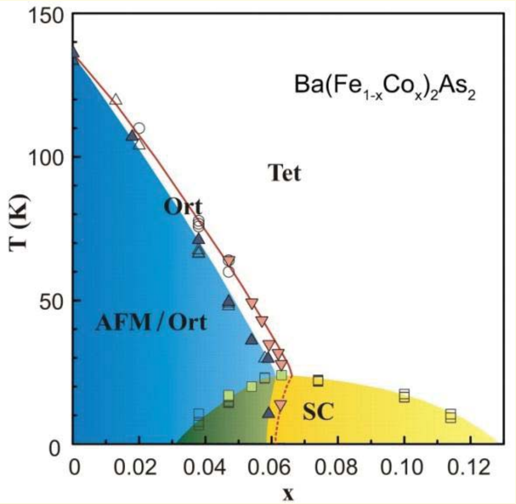


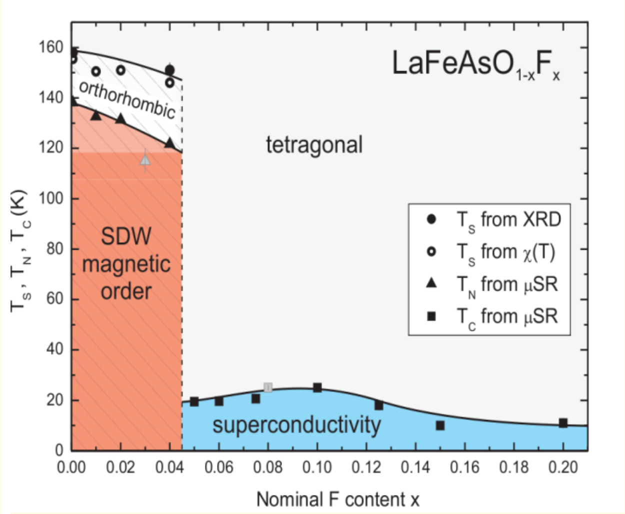
perfect nesting: $g = \dfrac{1+\cos\theta}{2}$

Competition between SDW and SC: coexistence



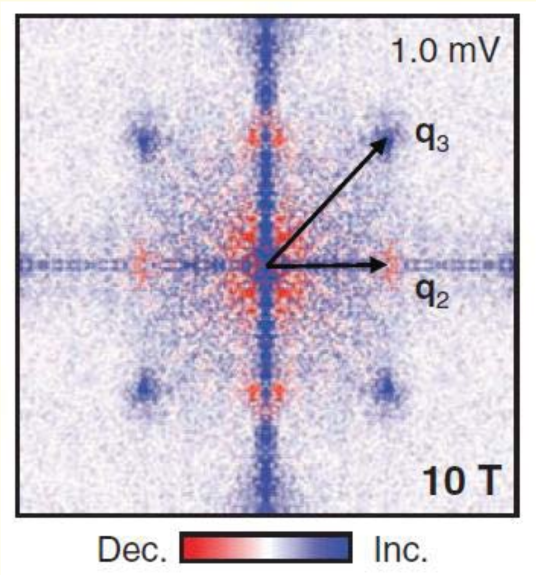
- s^{++} cannot coexist with magnetism
- s^{+-} may or may not coexist





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)

Competition between superconductivity and nematicity

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

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

  - magnetic fluctuations suppressed by superconductivity

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

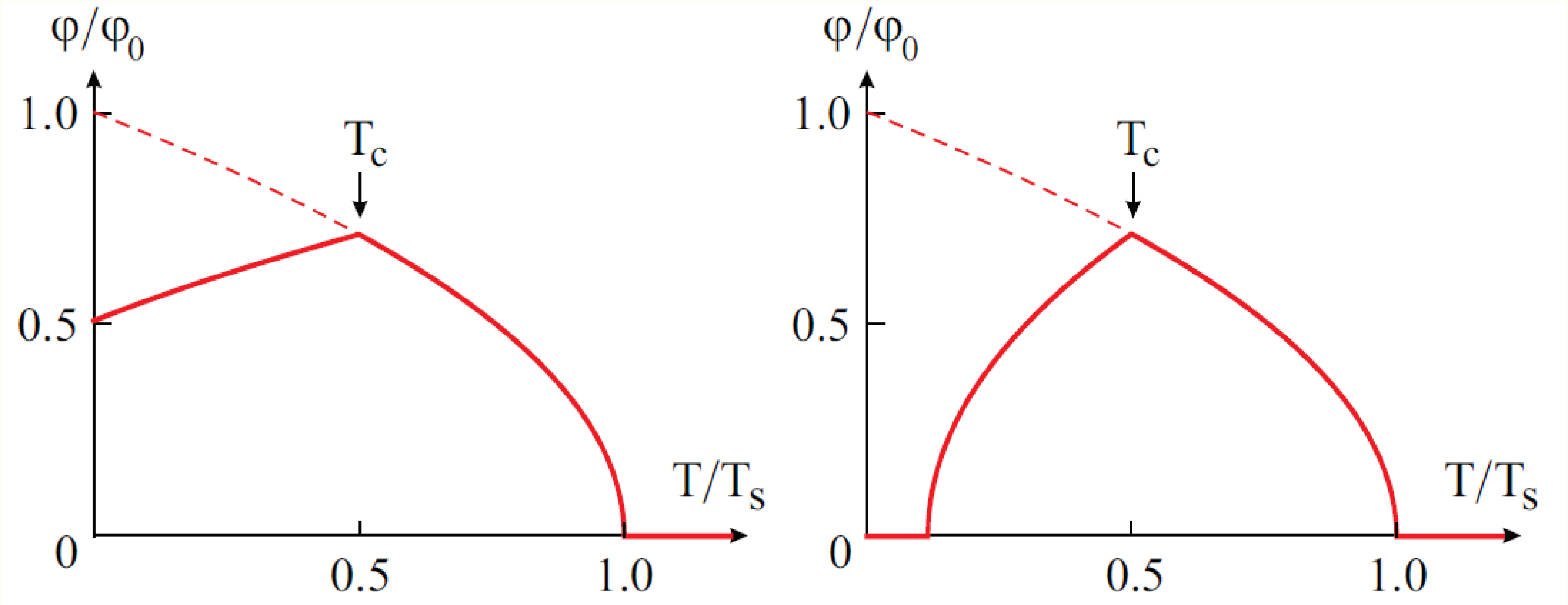
$$\tilde{\chi}_{\text{mag}}^{-1} = \chi_{\text{mag}}^{-1} + \gamma\,\Delta^2$$

Competition between superconductivity and nematicity

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

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

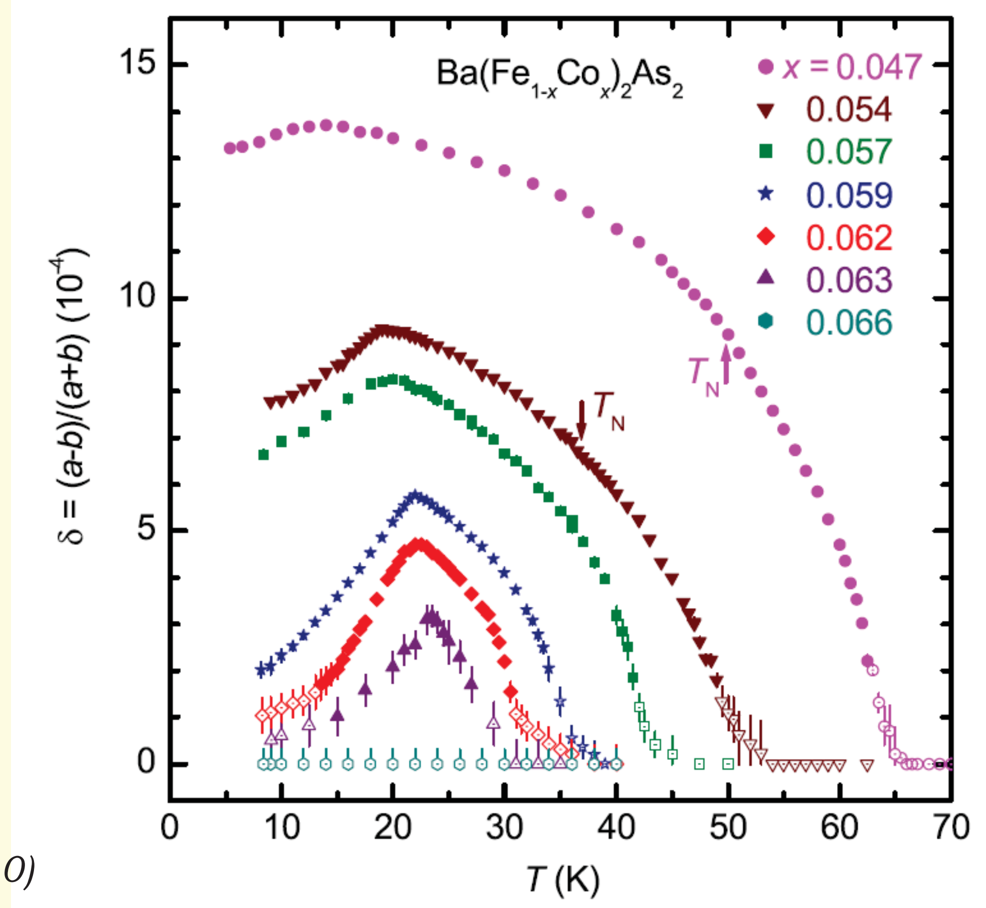
  - *even in the absence of long-range magnetic order*



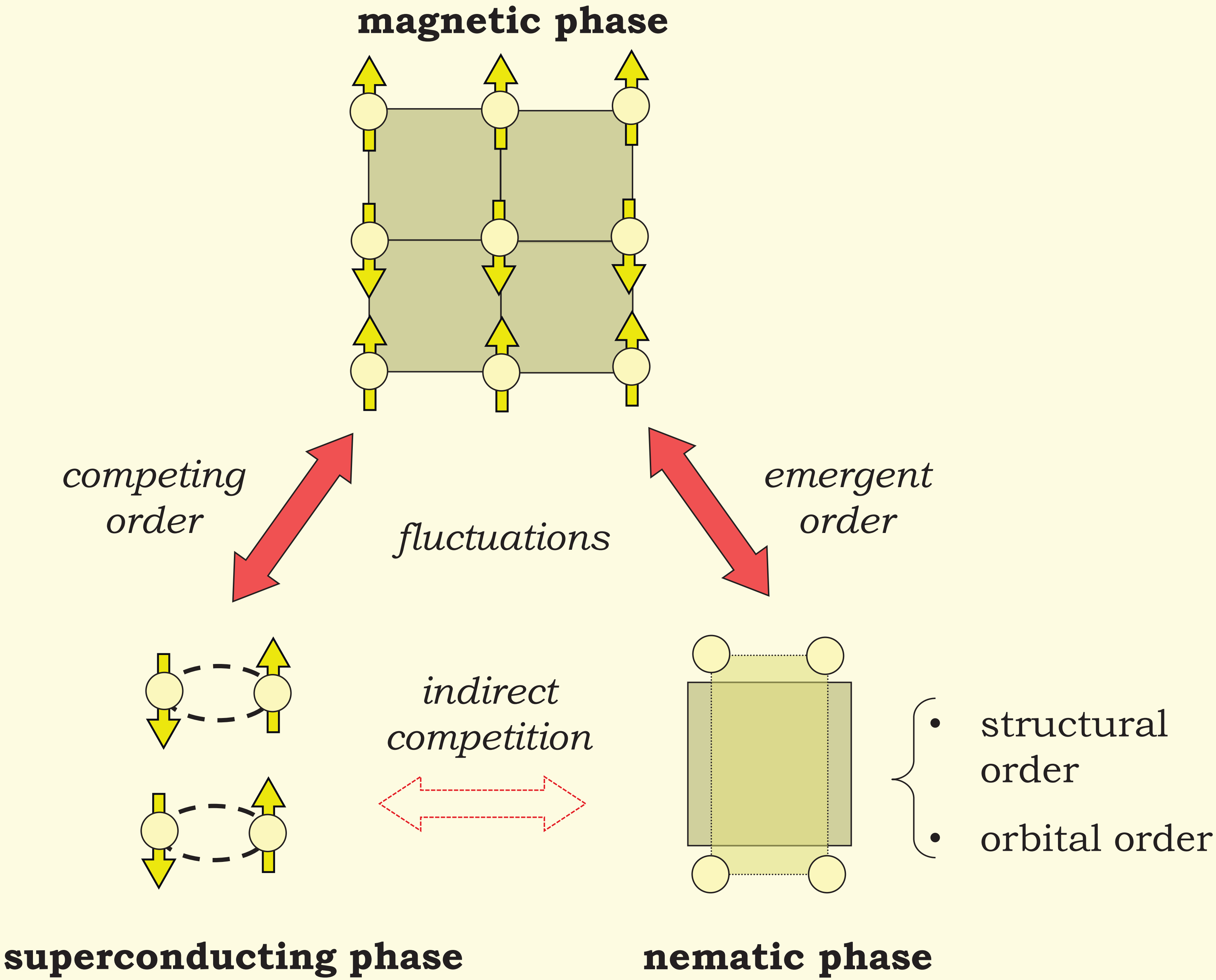
RMF & Schmalian, SUST (2012)

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)



magnetic phase

competing order

fluctuations

emergent order

indirect competition

- structural order
- orbital order

superconducting phase

nematic phase