Nemetic and Magnetic orders in Fe-based Superconductors

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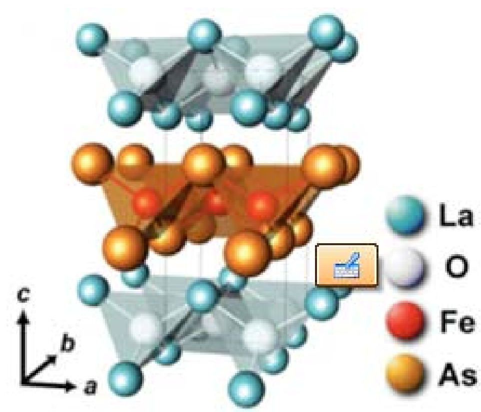

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Discussion with B. Halperin

Nematic and Magnetic orders in Fe-based Superconductors

Outline:

1, Ising nematic and magnetic transitions at finite temperature

2, Quantum nematic and magnetic transitions at finite doping and pressure

3, special system, FeTe, FeSe

4, Quantum nematic order with SC, experimental observables

Nematic and Magnetic orders in Fe-based Superconductors

Common phenomena:

1, SDW and structure distortion in almost all samples: neutron scattering...

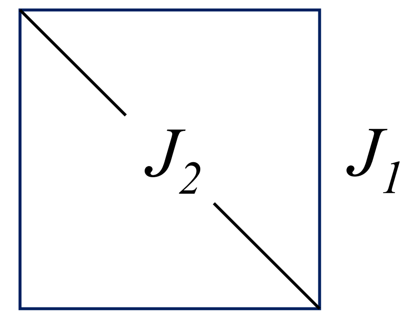
2, Lattice distortion and SDW do not always occur at the same temperature: $T_{c1,ld} \sim 150\text{K}$, $T_{c2,sdw} \sim 137\text{K}$, $T_{c1} \geq T_{c2}$

3, both lattice distortion and SDW suppressed by doping and pressure

First goal: unified picture of lattice distortion and SDW

Nematic and Magnetic orders in Fe-based Superconductors

Simplest toy model for SDW: Abrahams, Si, 2008



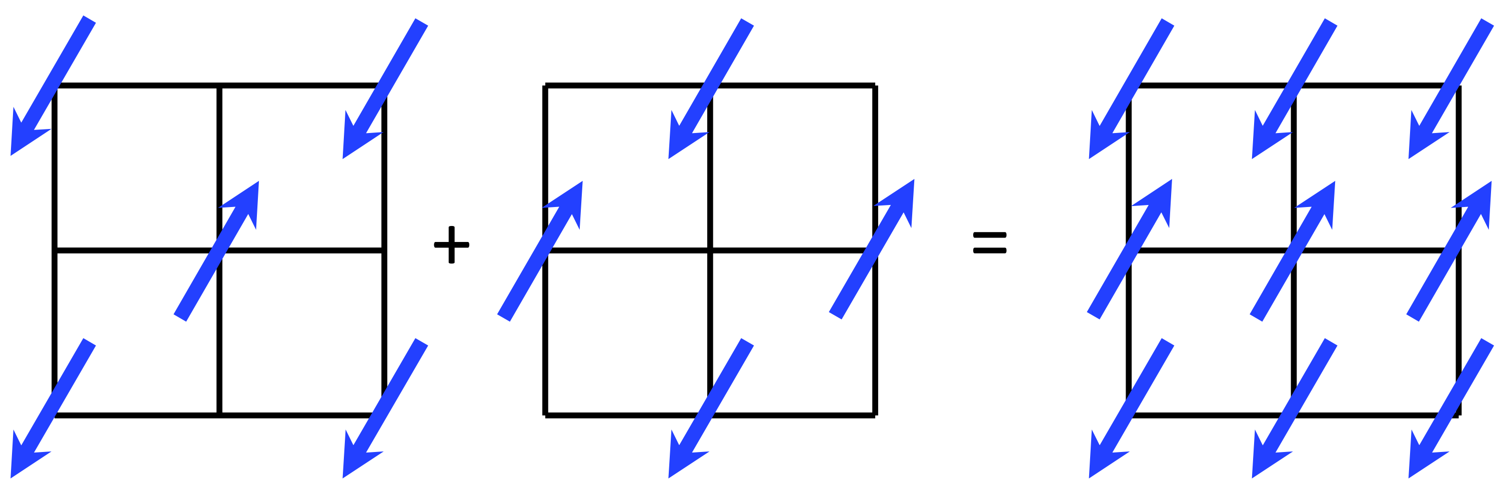
$$H = \sum_{<i,j>} J_1 \vec{S}_i \cdot \vec{S}_j + \sum_{\ll i,j \gg} J_2 \vec{S}_i \cdot \vec{S}_j.$$

Critical point: $J_1 = 2J_2$. If $J_1 < 2J_2$, Classical ground state is

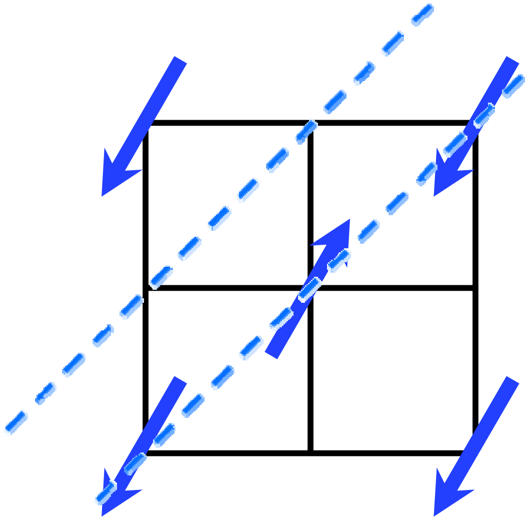
$$S^2 \otimes S^2$$

fluctuations will lead to GSM (moduli space)

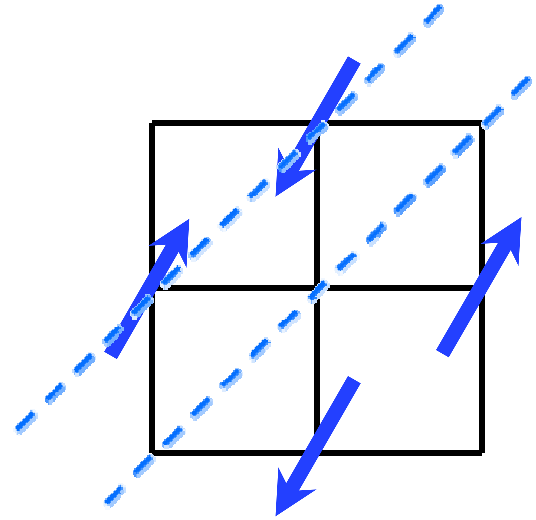
$$S^2 \otimes Z_2$$



Nematic and Magnetic orders in Fe-based Superconductors



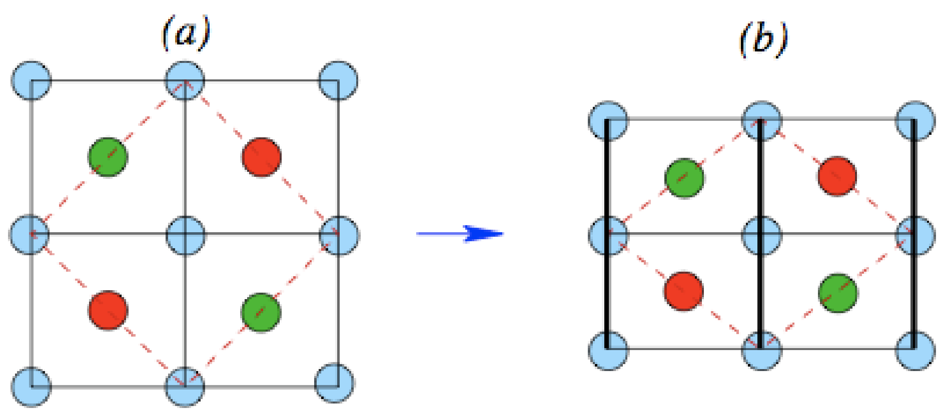
$-\vec{\phi}_1$



$-\vec{\phi}_2$

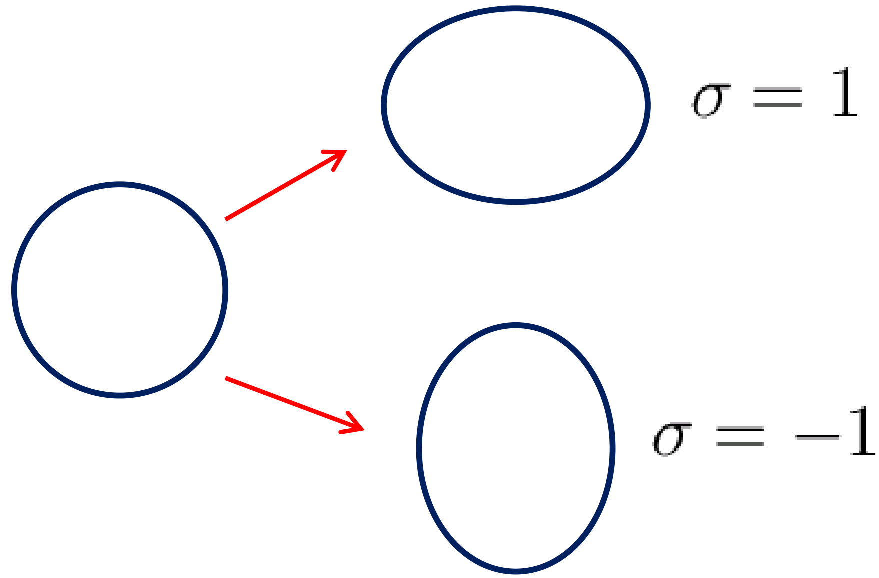
Natural Ising quantity: $\sigma = \vec{\phi}_1 \cdot \vec{\phi}_2$

Has the same symmetry as the lattice distortion!



Nematic and Magnetic orders in Fe-based Superconductors

$$\sigma = \vec{\phi}_1 \cdot \vec{\phi}_2$$



Can deform fermi surface
i.e. **nematic order**

Energy scales:

In pure 2d system, Ising order transition at $T_{Ising} \sim J_{in}$, and there is no SDW O(3) transition.

In weakly coupled 2d layers, $T_{sdw} \sim J_{in} / \ln(J_{in}/J_{\perp})$

Nematic and Magnetic orders in Fe-based Superconductors

The Ising order parameter breaks reflection symmetry along

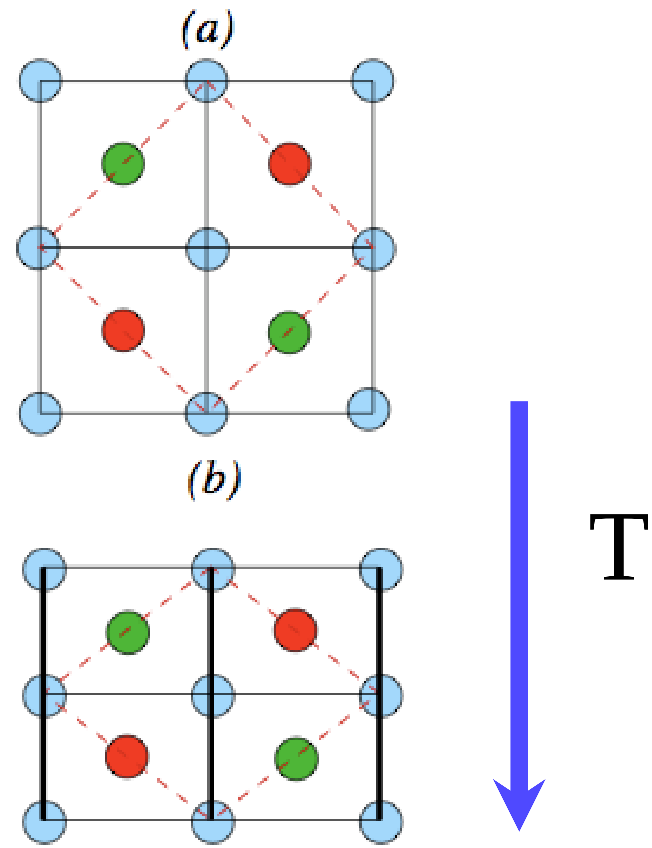
$$x = \pm y$$

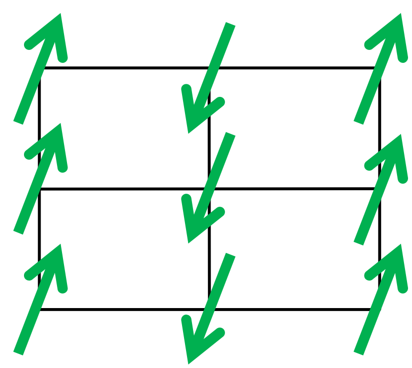
Lattice distortion may be driven by magnetism

Straightforward conclusion:

Nature of transitions: two separate transitions, one 3D Ising, one 3D O(3); if one single transition, first order.

PRB, 78, 020501, 2008, Cenke Xu et.al.
Similar story, Chen Fang et.al.



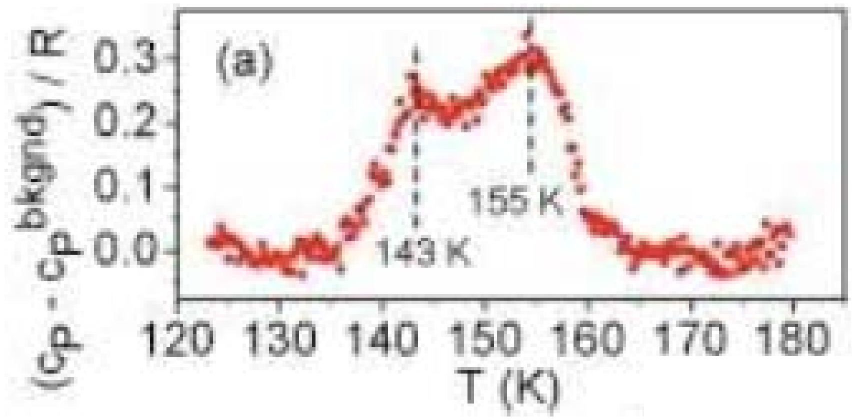


P. Dai *et.al.*

Mazin *et.al.*

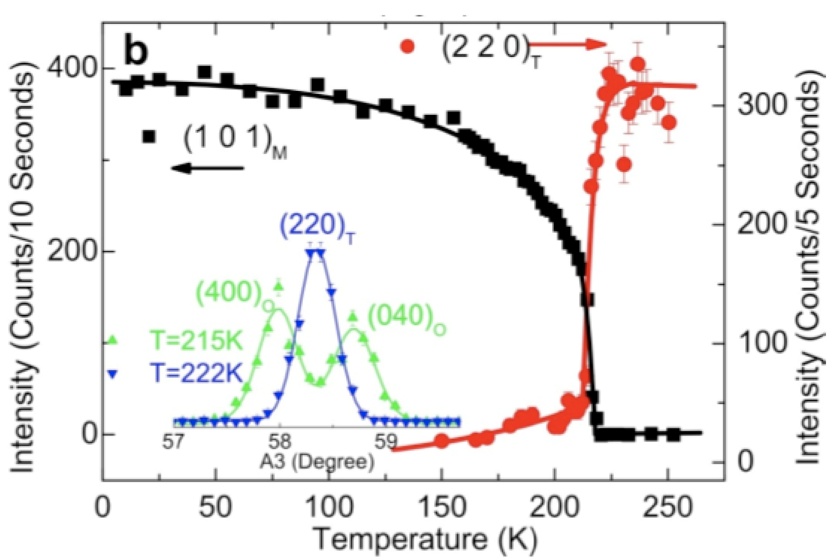
Nematic and Magnetic orders in Fe-based Superconductors

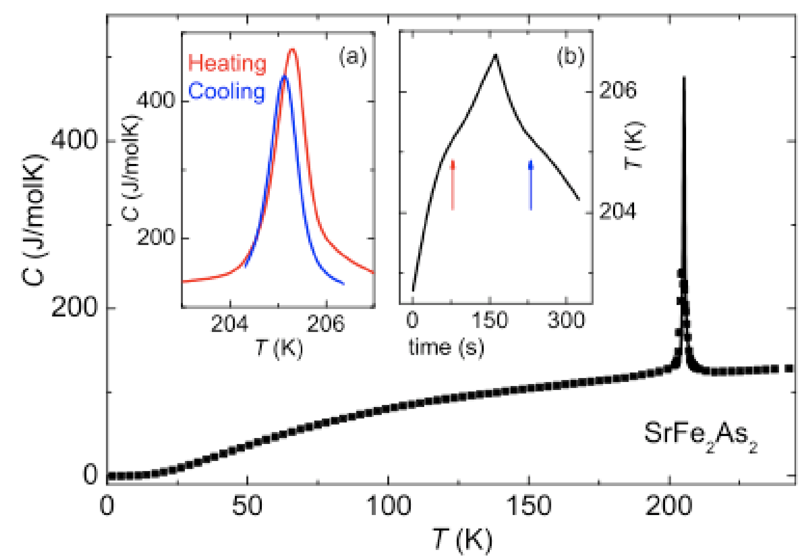
$LaFeAsO$



0806.3878
McGuire et.al.

MFe_2As_2





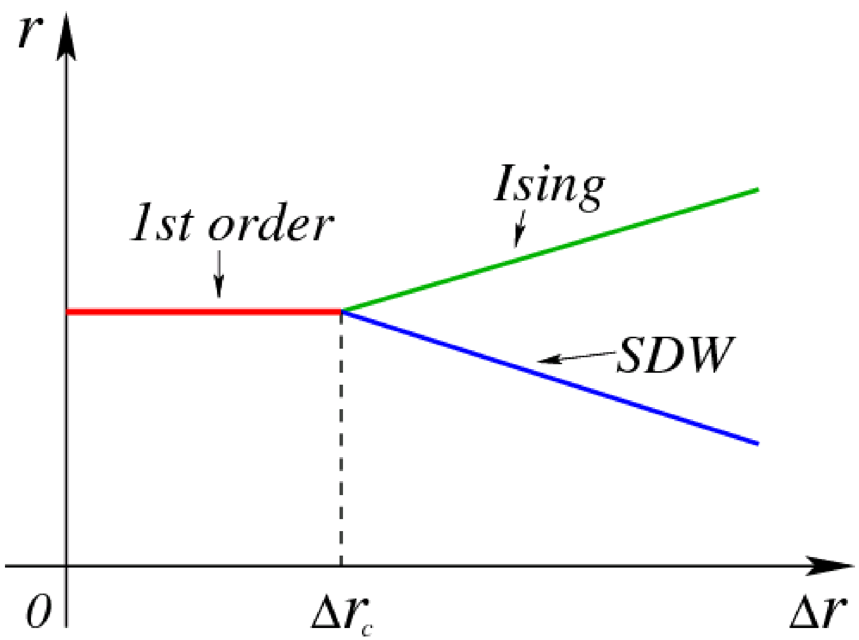
0807.1077 Zhao et.al.

0806.1043 Krellner et.al.

SDW and lattice distortion are intimately related.

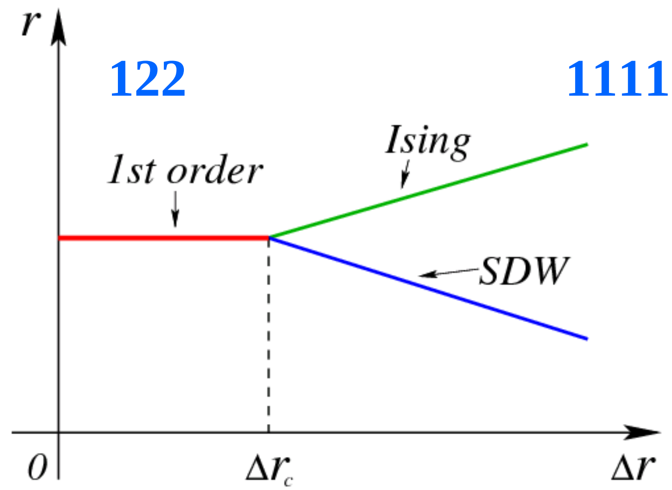
Question: Why are 1111 and 122 samples different?

$$F_{GL} = (\nabla_\mu \sigma)^2 + r_\sigma \sigma^2 + \sum_{a=1}^{2} (\nabla_\mu \vec{\phi}_a)^2 + r_\phi |\vec{\phi}_a|^2 + \tilde{u}\sigma \vec{\phi}_1 \cdot \vec{\phi}_2 + \cdots$$



$r = r_\sigma + r_\phi$ $\Delta r = r_\phi - r_\sigma$

r is tuned by temperature,
how about Δr ?



$$r = r_\sigma + r_\phi \qquad \Delta r = r_\phi - r_\sigma$$

Recall equations:

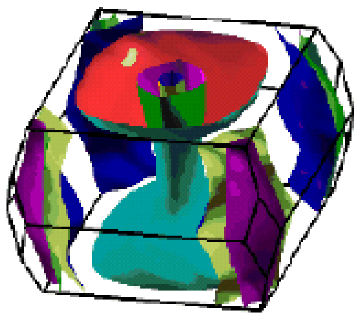
$$T_{ising} \sim J_{in}$$

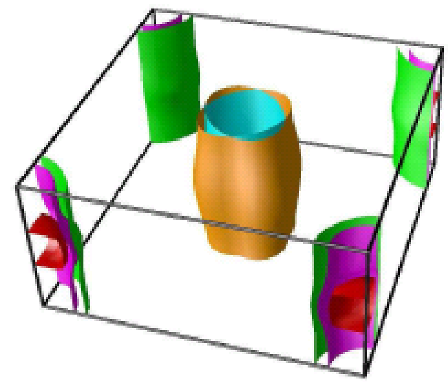
$$T_{sdw} \sim J_{in} / \ln(J_{in}/J_\perp)$$

Δr is tuned by the anisotropy of the system.

122 materials are much more isotropic than 1111 materials

Evidence 1: Strong *z* direction electron dispersion for 122 samples from LDA calculation, APRES;

122 

1111 

0806.3526 Ma et.al.

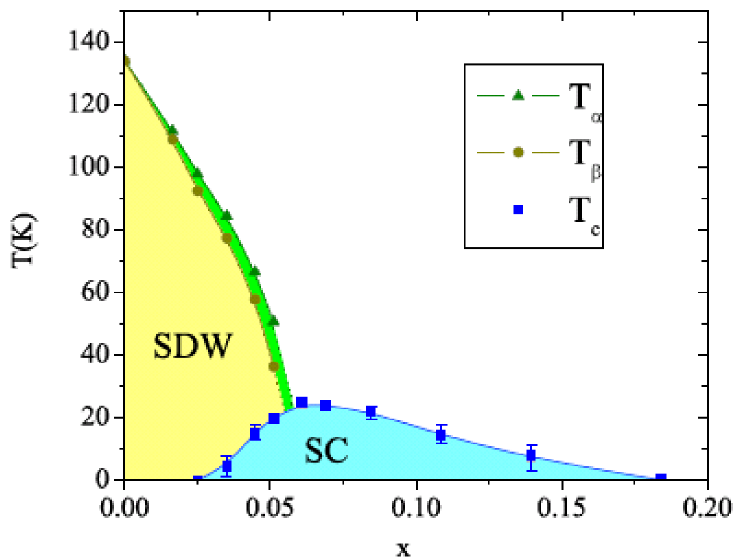
0806.1869 Mazin et.al.

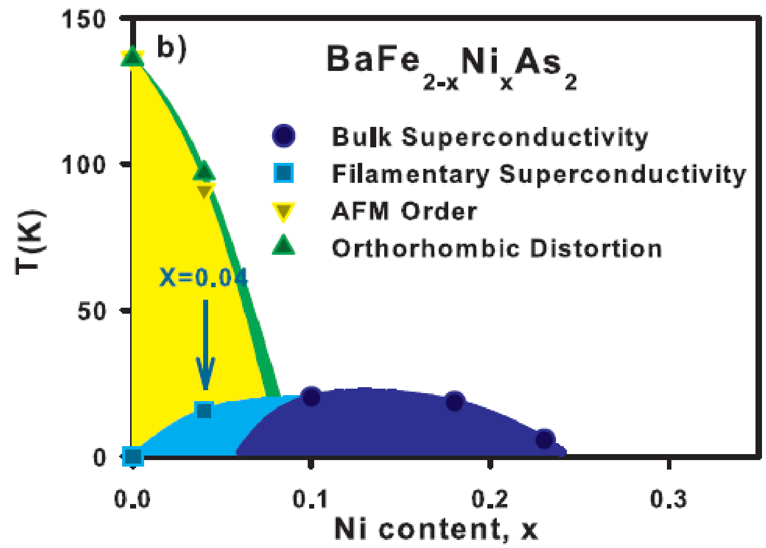
Evidence 2: almost isotropic H_{c2} for 122s. *0807.3137 Yuan et.al.*

$$H_{c2,z}/H_{c2,xy} \sim 1.5 - 2 \text{ for 122s}, \sim 7 - 8 \text{ for 1111s}.$$

Evidence 3: Strong *z* direction spin wave dispersion for 122s, from inelastic neutron, $J_z/J_{in} \sim 1/20 - 1/10$. *0808.2455 Zhao et.al.*

Electron doped 122s:





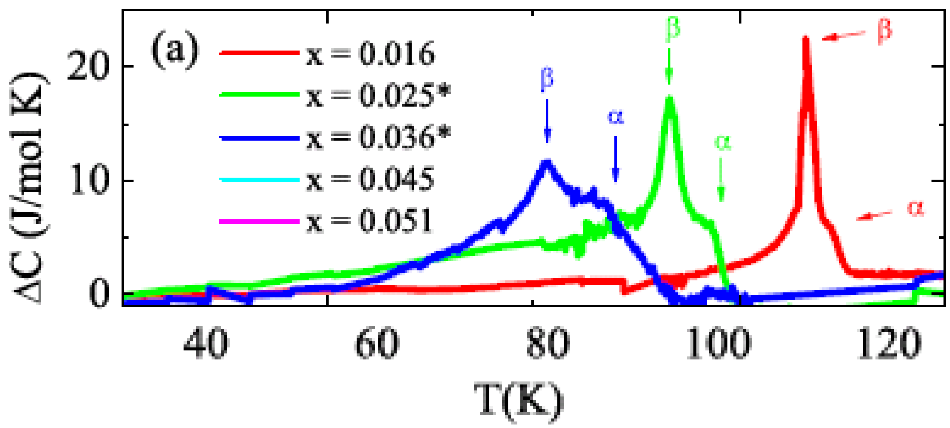
After electron doping, the transition splits into two second order transitions.

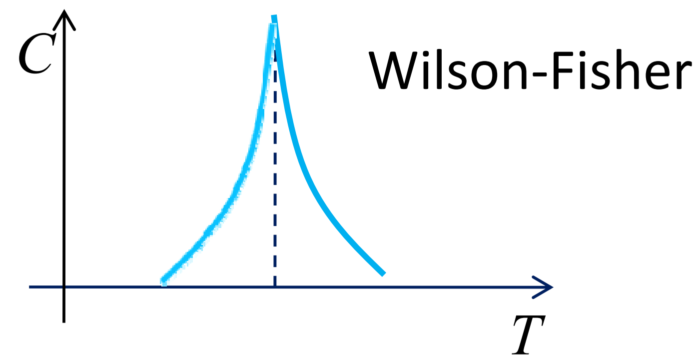
It turns out, electron doping rapidly suppresses z direction spin coupling. *0904.3775 Harriger, et.al.*

Can we measure anisotropic spin correlation in the window?

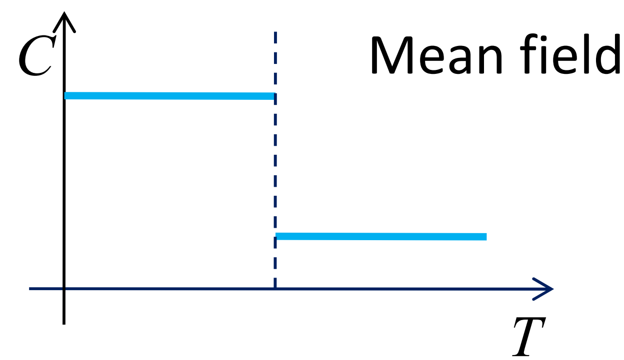
Nature of the transitions:

0811.2463 Chu et.al.





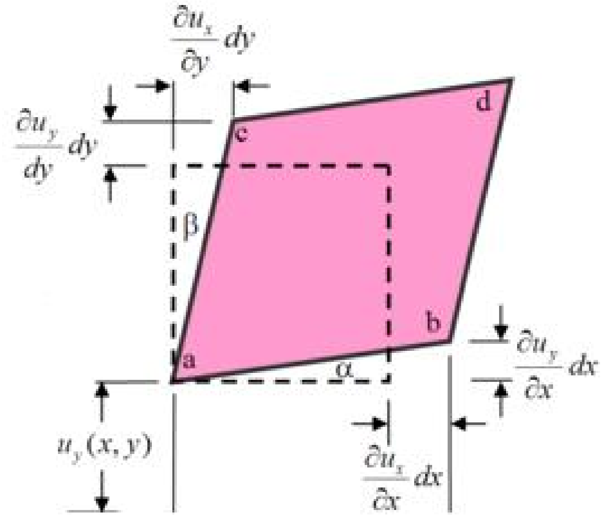
The lattice distortion transition is mean field like, while the SDW transition is a nontrivial WF universality class in 3D



Mean field is only applicable to dimensions higher than 4, where is the extra dimension? Why SDW unaffected?

Soft lattice coupled with 3D Ising transition:

$$g\sigma(\partial_x u_y + \partial_y u_x) + K(\vec{\nabla}\cdot\vec{u})^2 + \cdots$$

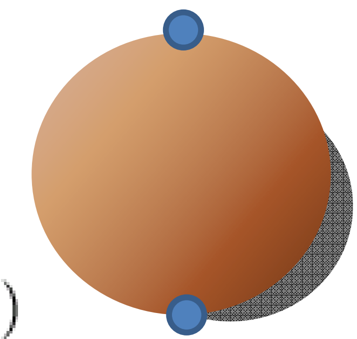


Integrating out displacement vector, obtaining angle dependent quadratic term:

$$F_{\theta,\phi} \sim f(\theta,\phi)|\sigma_{k,\theta,\phi}|^2 \sim 10K$$

Expanded at the minima:

$$F = \int q^2 dq \theta d\theta (q^2 + \lambda\theta^2 + r)|\sigma_{q,\theta}|^2 + O(\sigma^4)$$



$$F = \int dq_x dq_y dq_z (q_x^2 + q_y^2 + q_z^2 + \frac{q_x^2 + q_y^2}{q_z^2})|\sigma_q|^2 + O(\sigma^4)$$

Equivalent to 5 dimension! $\rightarrow$ **mean field transition!**

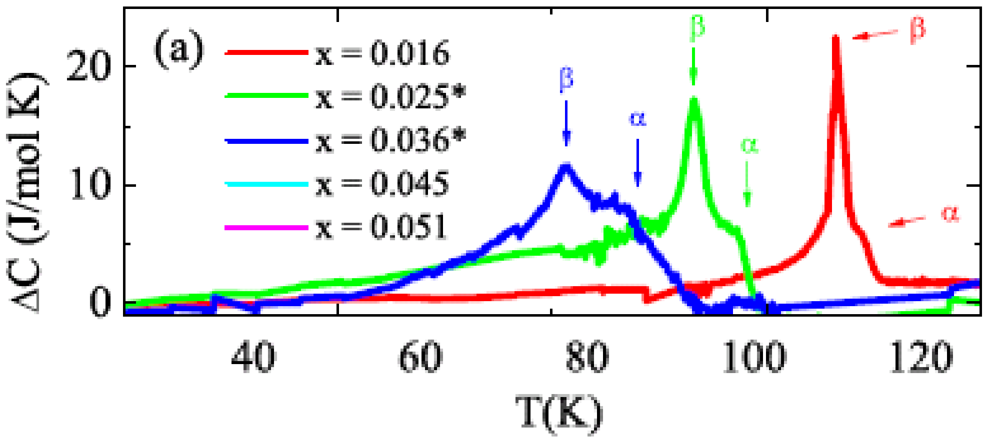
Soft lattice coupled with 3D O(3) transition (SDW):

$$|\vec{\phi}|^2(\partial_x u_x + \partial_y u_y + \lambda' \partial_z u_z)$$

Only generates irrelevant terms at the 3D O(3) transition, because $\alpha < 0$ for 3D O(3) or XY transition.

The lattice elasticity will leave the SDW transition unaffected, but drive the Ising transition more mean field like.

Yang Qi, Cenke Xu, arXiv:0812.0016



Outline:

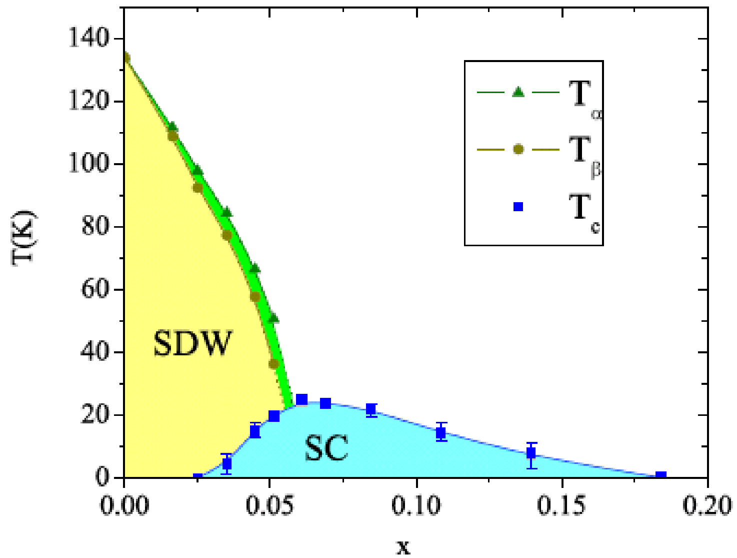
1, Ising nematic and magnetic transitions at finite temperature

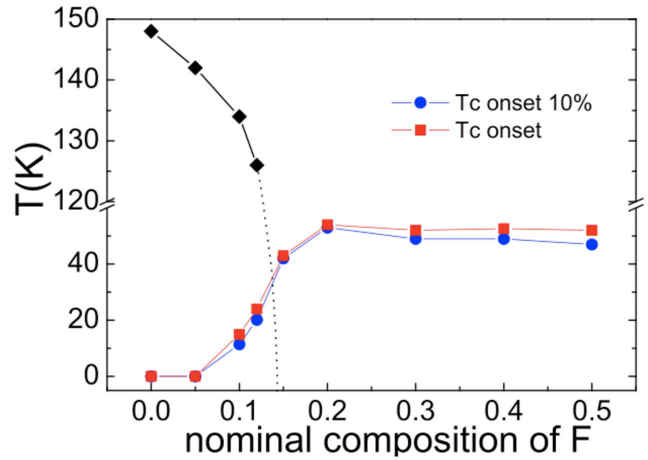
2, Quantum nematic and magnetic transitions at finite doping and pressure

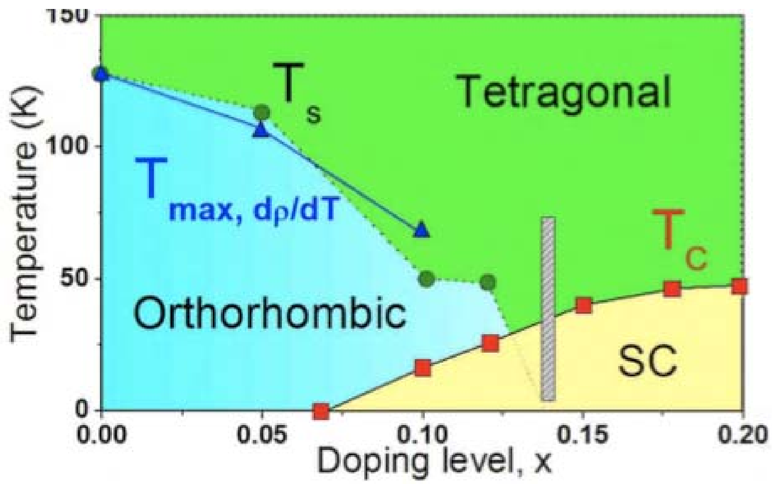
3, special system, FeTe, FeSe

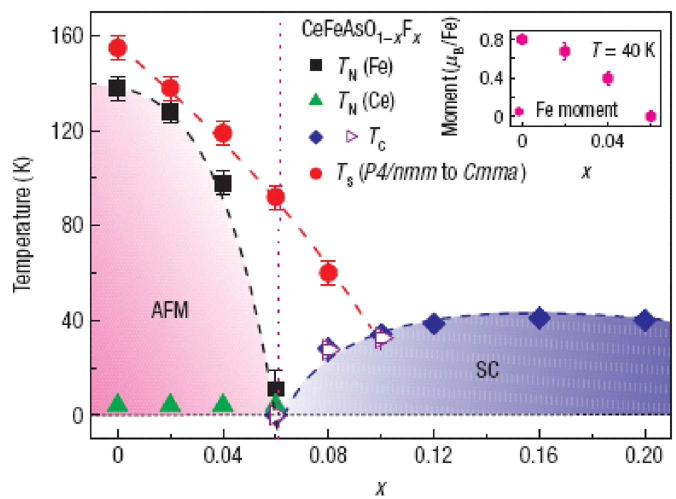
4, Quantum nematic order with SC, experimental observables

2, Quantum phase transitions at zero temperature:



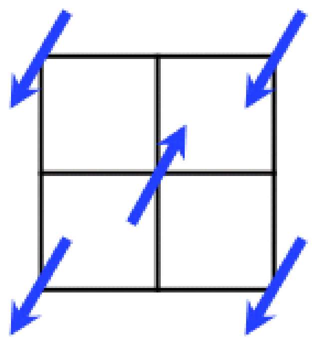




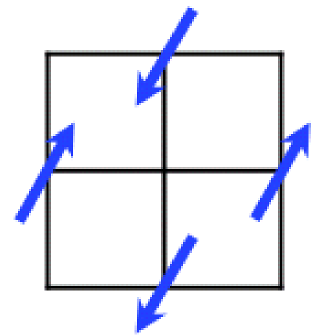


Nematic and Magnetic orders in Fe-based Superconductors

Recall:



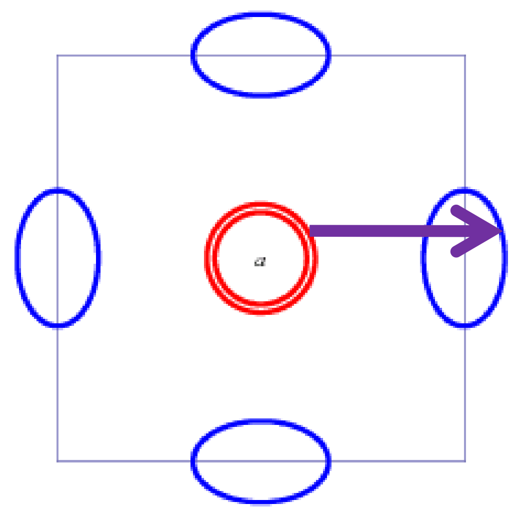
$\vec{\phi}_1$



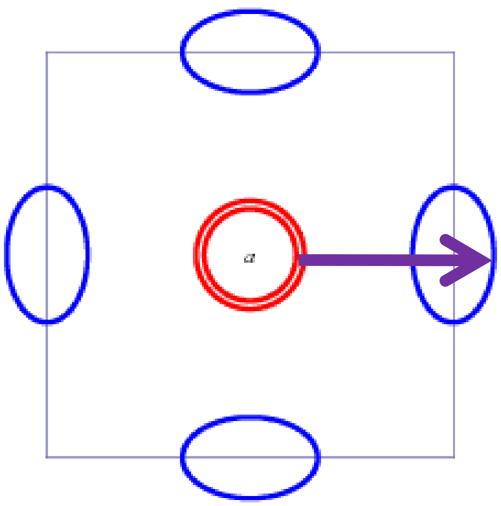
$\vec{\phi}_2$

Without the charge sectors, the transitions in the spin sector will have dynamical exponent $z=1$.

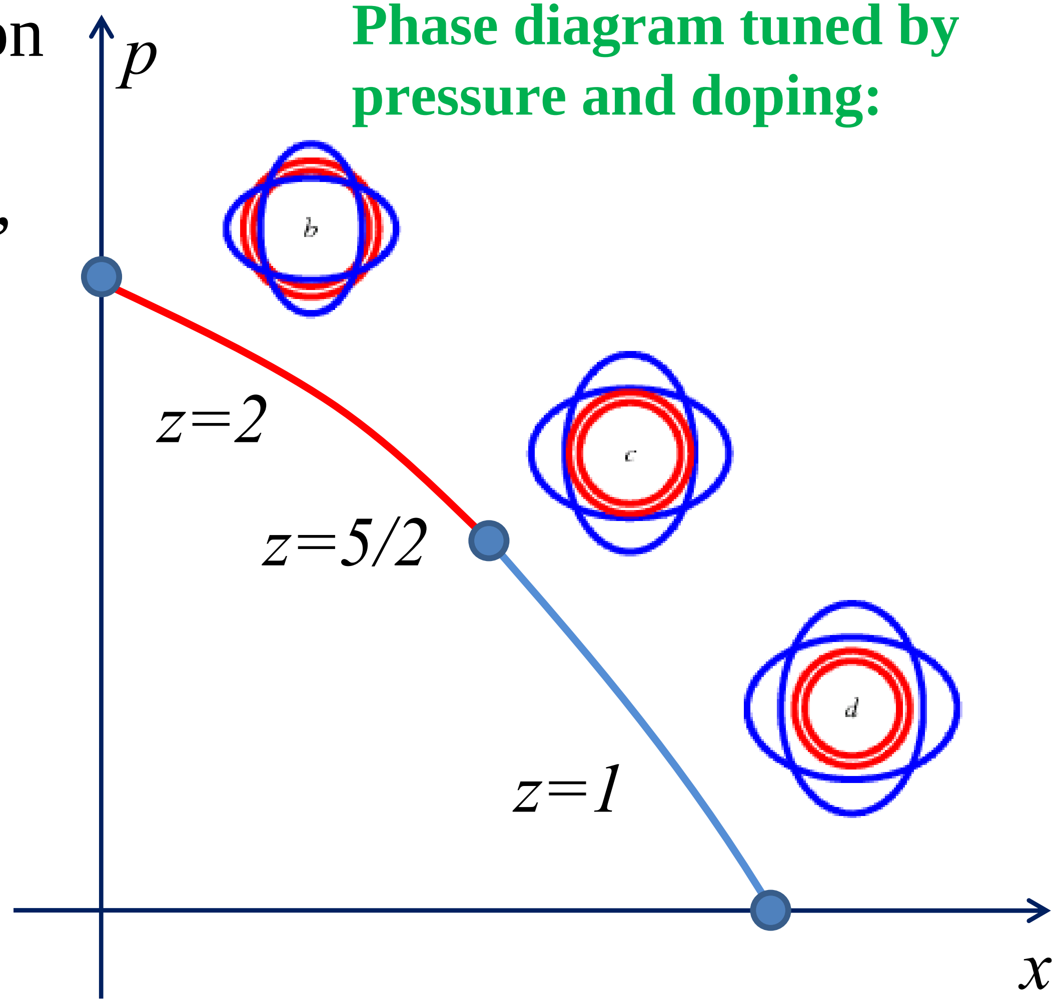
By coupling to the Fermi pockets, the exponent z may be modified.



The exponent *z* depends on the overlapping between hole and electron pockets, after translation by the SDW wave-vector:



Phase diagram tuned by pressure and doping:



Transitions at large doping, low pressure

$$L = \sum_{i=1}^{2} \sum_{\mu=\tau,x,y} \partial_\mu \vec{\phi}_i \cdot \partial_\mu \vec{\phi}_i - r\vec{\phi}_i^2 + u|\vec{\phi}_i|^4 + L',$$

$$L' = \gamma \vec{\phi}_1 \partial_x \partial_y \cdot \vec{\phi}_2 + \gamma_1 |\vec{\phi}_1|^2 |\vec{\phi}_2|^2 - \alpha(\vec{\phi}_1 \cdot \vec{\phi}_2)^2,$$

Estimate the scaling dimensions at the 3D O(3) transition

$$\Delta[\gamma] = D - (2 + D - 2 + \eta) = -\eta.$$

$$\Delta[\gamma_1] = D - 2\Delta[|\vec{\phi}|^2] = D - 2(D - \frac{1}{\nu}) = \frac{2}{\nu} - D,$$

$$\Delta[\alpha] \simeq 0.581$$

One obvious relevant perturbation, can split the transition to one SDW transition and one Ising nematic transition

Ising nematic transition without SC

Ordered at (0, 0), ferromagnetic type, decay with *ph*-pair

$$\mathrm{Im}[\chi(\omega,q)] \sim \int \frac{d^2k}{(2\pi)^2}[f(\epsilon_{k+q})-f(\epsilon_k)]\delta(\omega-\epsilon_{k+q}+\epsilon_k) \times |\langle k|\Phi_q|k+q\rangle|^2 \sim c_0\frac{\omega}{q}. \quad (7)$$

$$L = \Phi_{-q}\left(\frac{|\omega|}{c_0 q}+c_1 q^2+r\right)\Phi_q+\cdots$$

$$C_v \sim T^{d/z}=T^{2/3},$$

$$T_{c1} \sim \delta x^{z/(d-2+z)}=\delta x,$$

$$\rho \sim T^{(d+2)/z}=T^{4/3}.$$

PRB, 64, 195109, 2001, V. Oganesyan et.al.

PRB, 78, 020501, 2008, C. Xu et.al.

The exponent *z* depends on the overlapping between hole and electron pockets, after translation by the SDW wave-vector:

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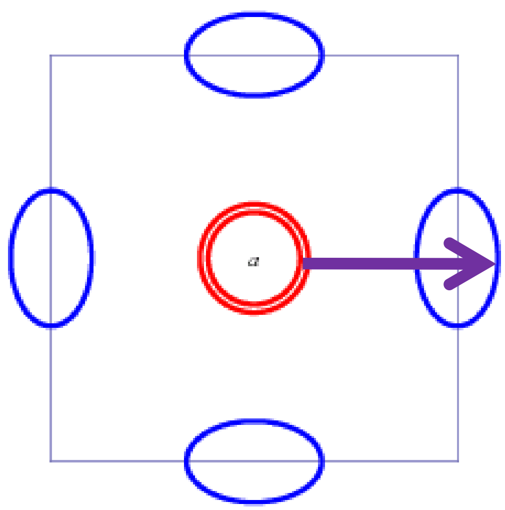

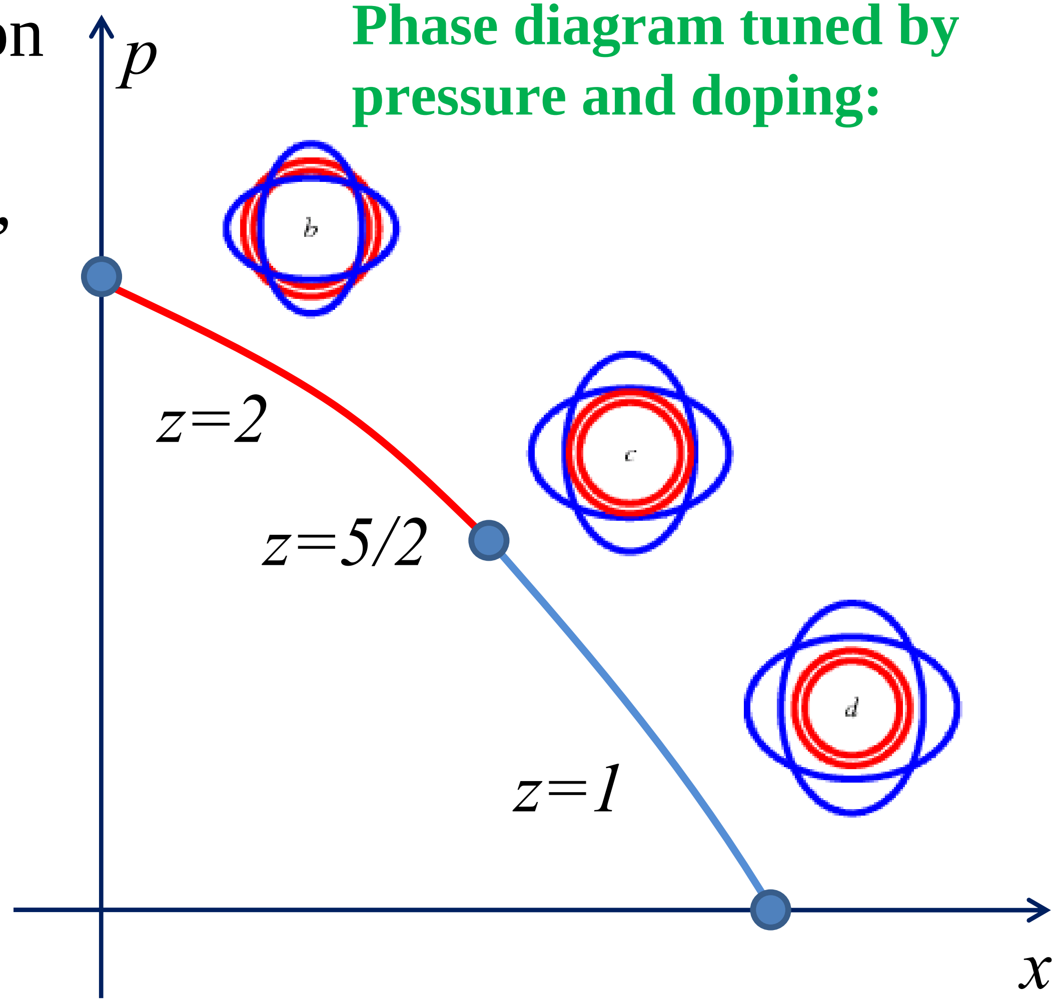

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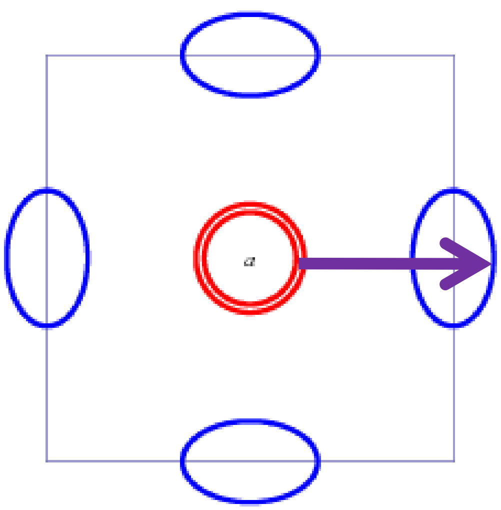

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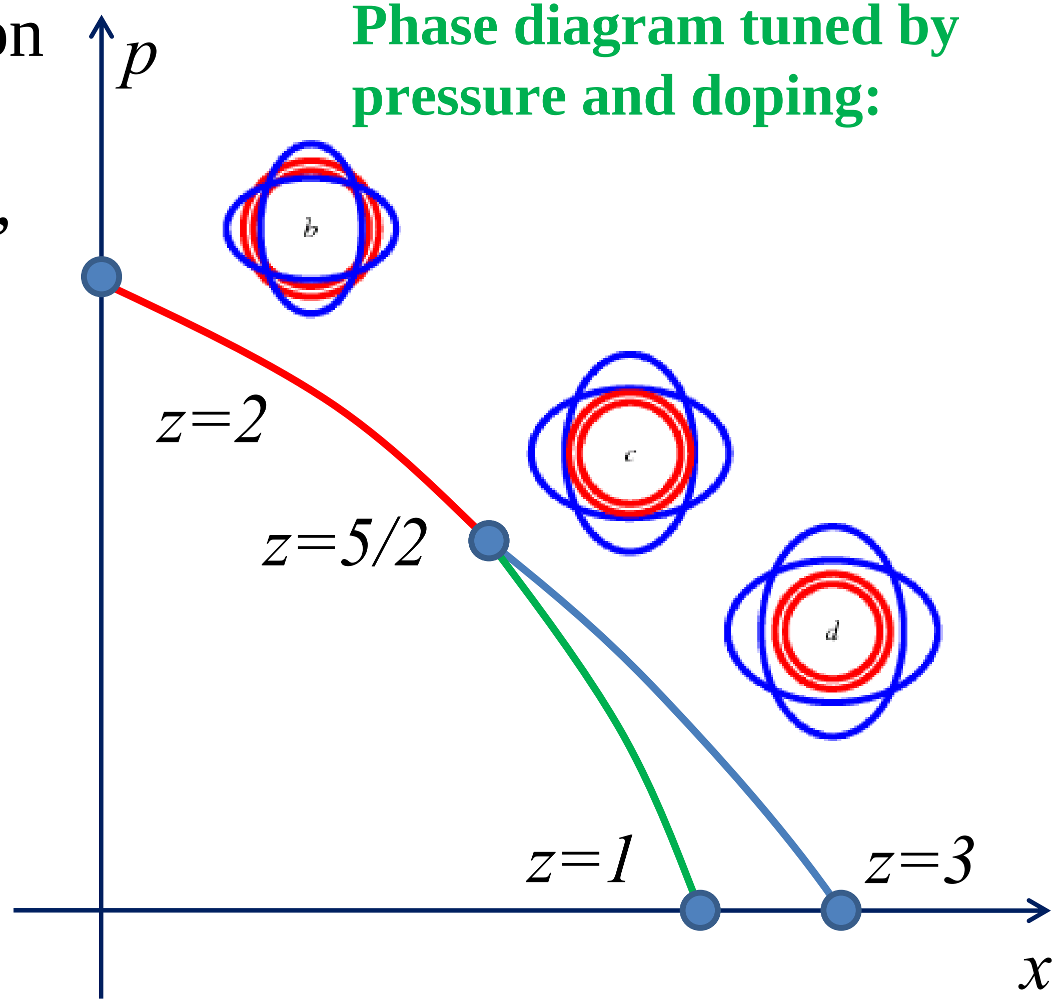
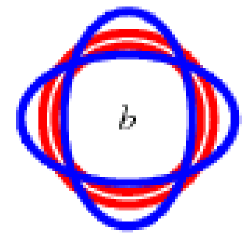


Transitions at low doping, large pressure

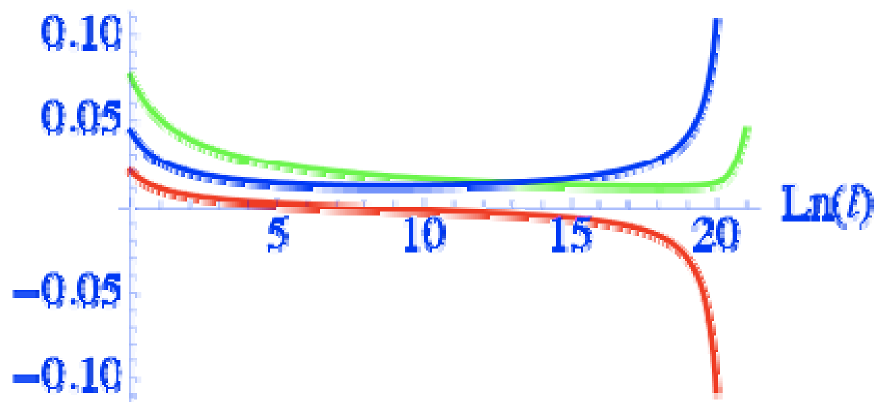
$$L = \sum_{i=a,b} |\omega||\vec{\phi}_i|^2 + c^2(k_x^2 + rk_y^2)|\vec{\phi}_a|^2 + c^2(k_y^2 + rk_x^2)|\vec{\phi}_b|^2$$
$$+ \; A|\vec{\phi}_i|^4 + B(\vec{\phi}_a \cdot \vec{\phi}_b) + C|\vec{\phi}_a|^2|\vec{\phi}_b|^2$$



$$\vec{\phi}_{a,b} = \vec{\phi}_1 \pm \vec{\phi}_2$$

Perturbative RG equation around a *z = d = 2* fixed point:

$$\frac{dA}{d\ln l} = -22A^2 - \frac{1}{2}B^2 - \frac{3}{2}C^2 - BC,$$
$$\frac{dB}{d\ln l} = -5\alpha B^2 - 8AB - 8\alpha BC,$$
$$\frac{dC}{d\ln l} = -\alpha B^2 - 4AB - 20AC - 4\alpha C^2.$$



Extremely weak run-away flow, relevant only very close to critical point Cut-off: ~50K

Special multicritical point

$Q = 2k_f$ decay rate

$$\frac{|\omega|}{\sqrt{|q_x|}} + \frac{|\omega|}{\sqrt{|q_y|}}$$

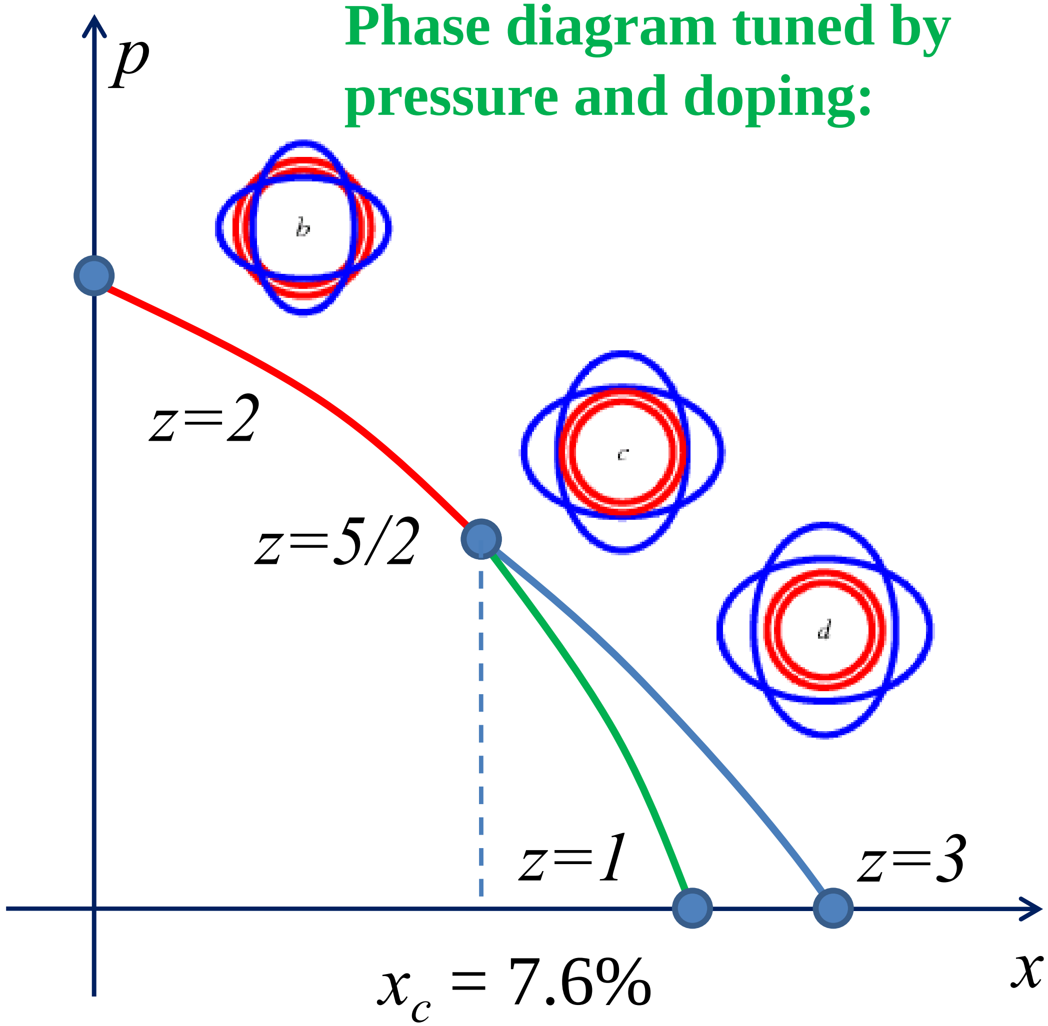
Naively, $z = 5/2$, but singular term generated:

$$|\vec{\phi}|^{5/2}$$

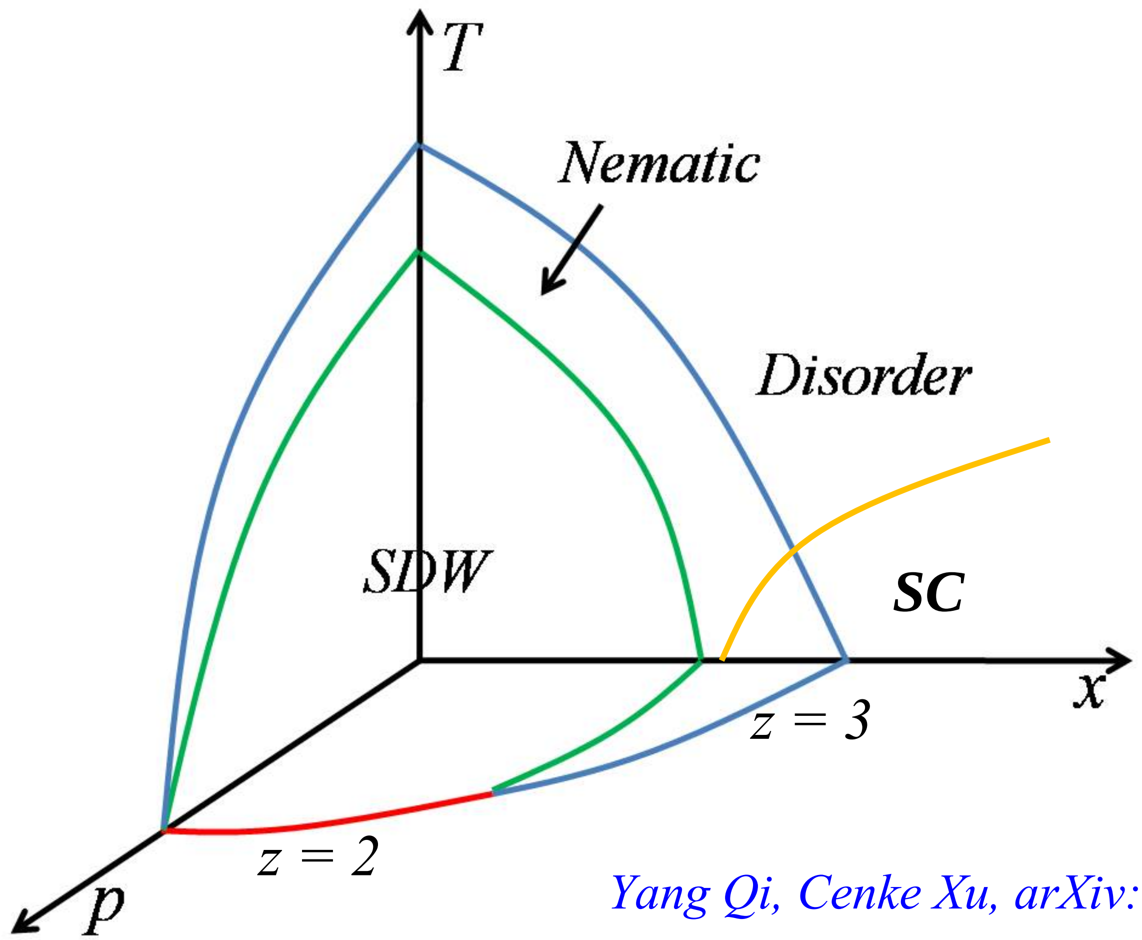
No longer a mean field solution

Similar: nematic-smectic transition, K. Sun *et.al.* 2008

Phase diagram tuned by pressure and doping:



Global Phase diagram of 1111



Yang Qi, Cenke Xu, arXiv:0812.0016

For 122, more 3d, more mean field like, less splitting

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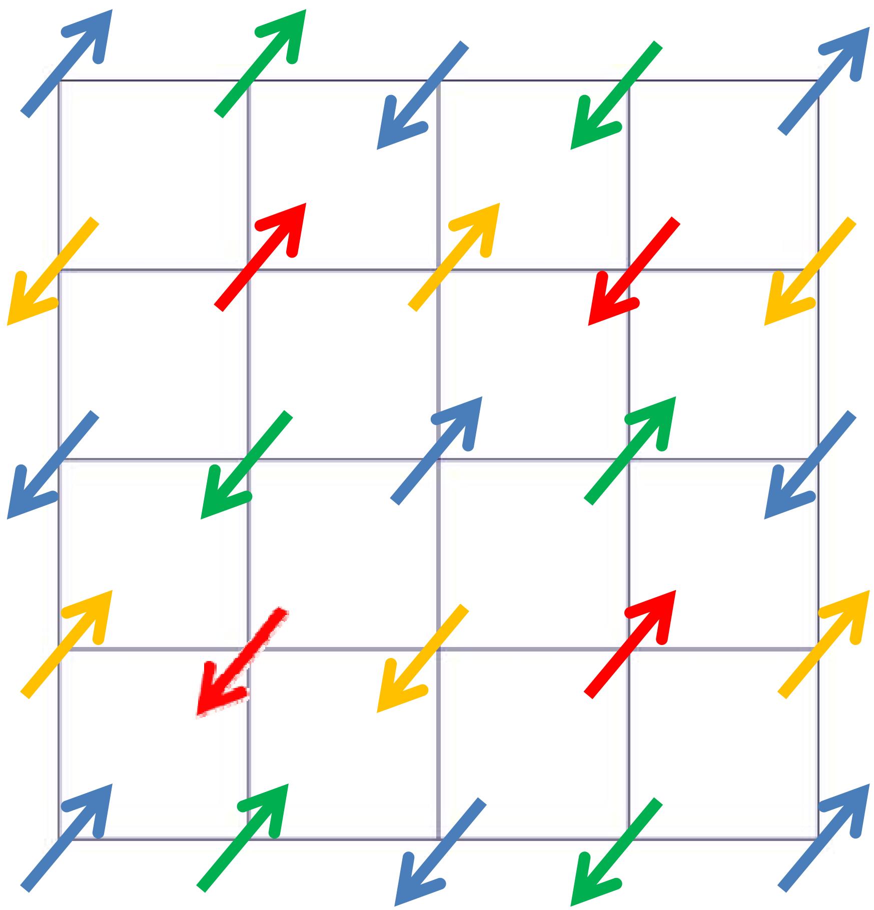
Nematic and Magnetic orders in Fe-based Superconductors

The 11 family: FeTe **4-sublattice Neel order**

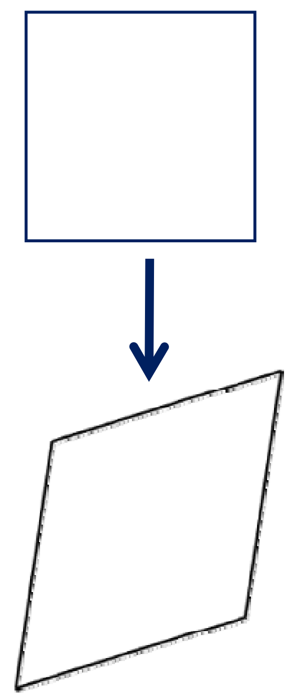
Shiliang Li, *et.al.* 2008



Lattice distortion:

Tetragonal to monoclinic

(in contrast to orthorhombic)

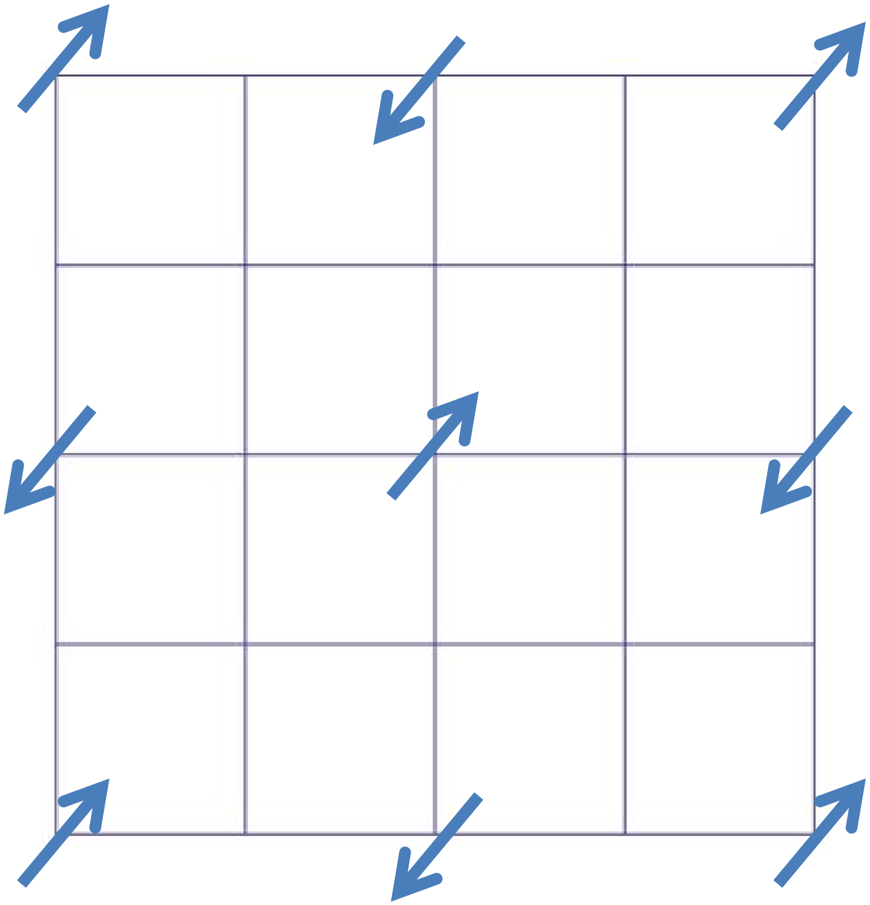


Nematic and Magnetic orders in Fe-based Superconductors

The 11 family: FeTe

4-sublattice Neel order

Shiliang Li, *et.al.* 2008



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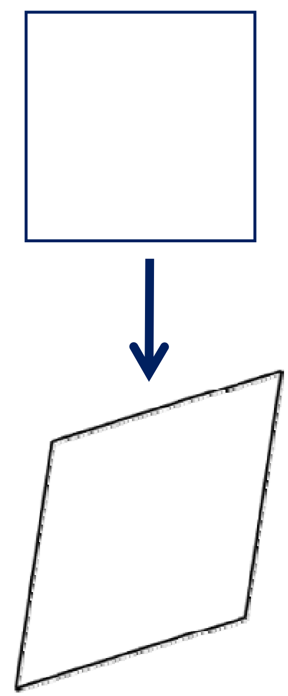

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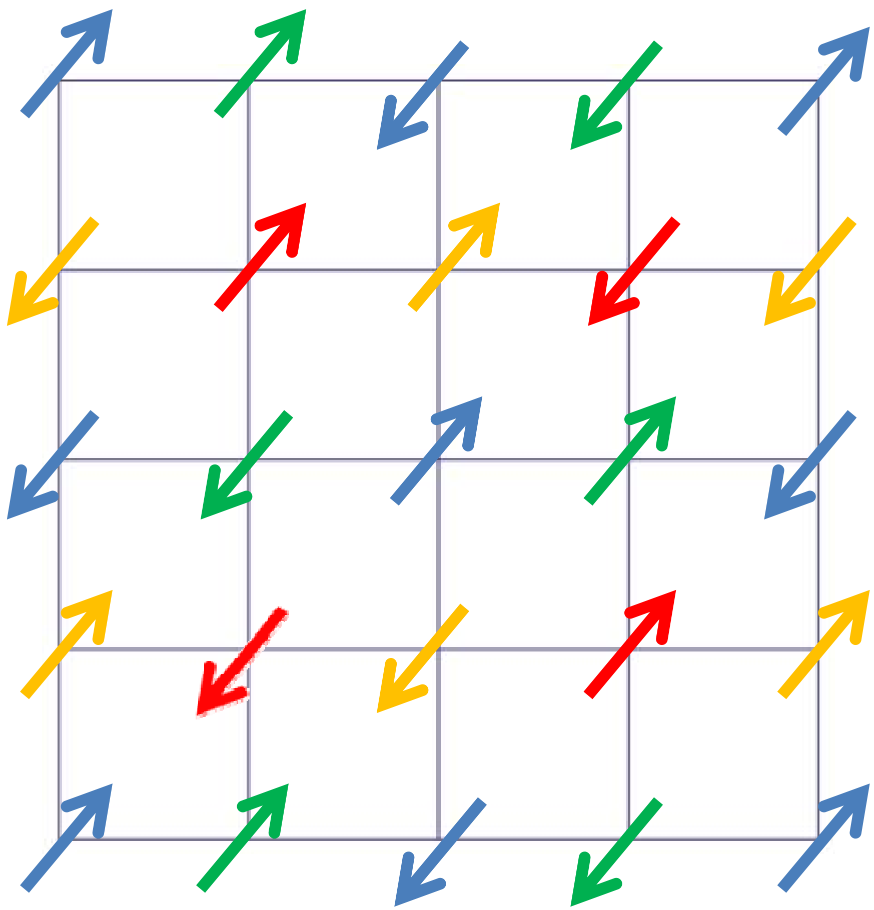
The 11 family: FeTe **4-sublattice Neel order**

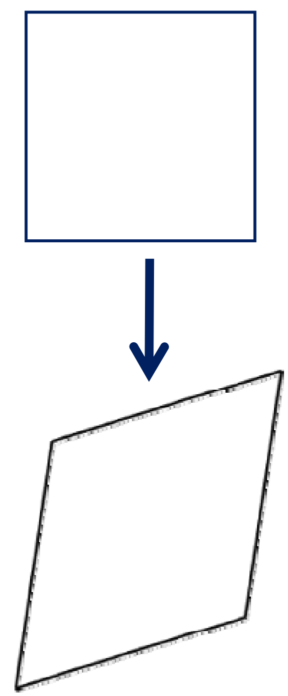
Shiliang Li, *et.al.* 2008



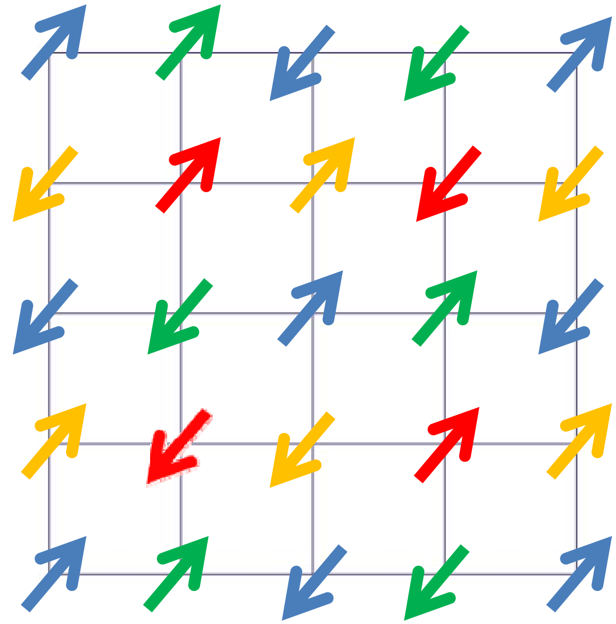
Lattice distortion:

Tetragonal to monoclinic

(in contrast to orthorhombic)



Lattice symmetry guarantees that reversing the direction of the spins on any two sublattices simultaneously will not change the energy



There are in total two independent Ising quantities defined.

$S^2 \times Z_2 \times Z_2$

In contrast to $S^2 \times Z_2$

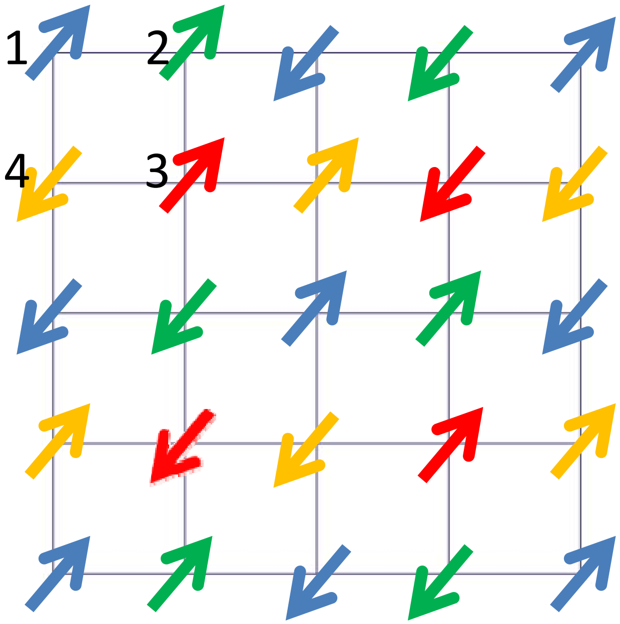
Richer phase diagrams!

Cenke Xu, Jiangping Hu, arXiv:0903.4477

Commensurate v.s. incommensurate order, both orbserved.

Wei Bao, *et.al.* 2008

Nematic and Magnetic orders in Fe-based Superconductors



$$F_{\vec{\phi}} = \sum_{a=1}^{4} J_3(\nabla_\mu \vec{\phi}_a)^2 + \beta\vec{\phi}_1 \cdot \nabla_x \vec{\phi}_2 + \beta\vec{\phi}_4 \cdot \nabla_x \vec{\phi}_3 - \beta\vec{\phi}_2 \cdot \nabla_y \vec{\phi}_3 - \beta\vec{\phi}_1 \cdot \nabla_y \vec{\phi}_4$$

$$F_{\sigma,\vec{\phi}} = \gamma\sigma_1(\vec{\phi}_1 \cdot \vec{\phi}_2 + \vec{\phi}_2 \cdot \vec{\phi}_3 - \vec{\phi}_3 \cdot \vec{\phi}_4 - \vec{\phi}_1 \cdot \vec{\phi}_4) + \gamma\sigma_2(\vec{\phi}_1 \cdot \vec{\phi}_2 - \vec{\phi}_2 \cdot \vec{\phi}_3 - \vec{\phi}_3 \cdot \vec{\phi}_4 + \vec{\phi}_1 \cdot \vec{\phi}_4)$$

Commensurate v.s. incommensurate order, both orbserved.

Wei Bao, *et.al.* 2008

Nematic and Magnetic orders in Fe-based Superconductors

Outline:

1, Ising nematic and magnetic transitions at finite temperature

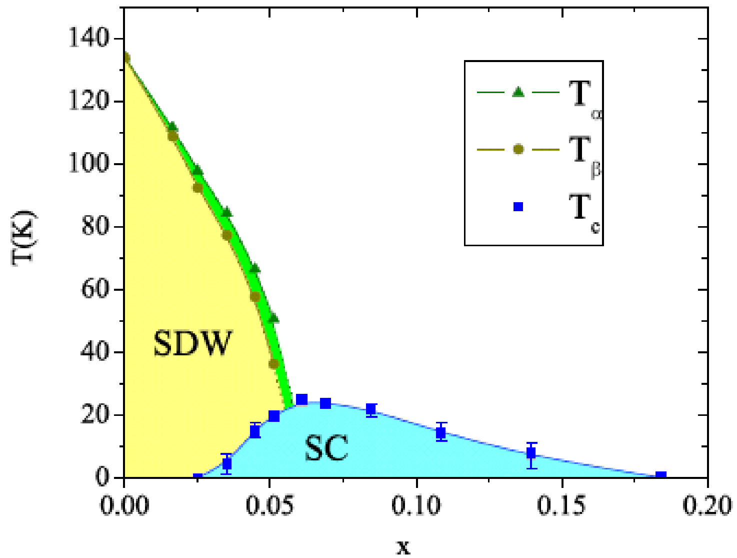
2, Quantum nematic and magnetic transitions at finite doping and pressure

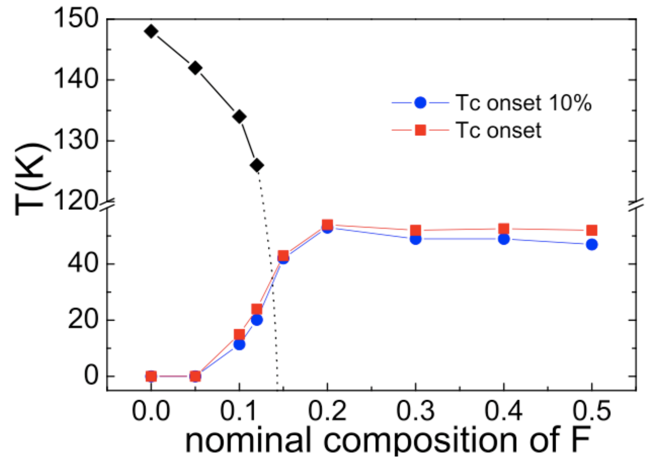
3, special system, FeTe, FeSe

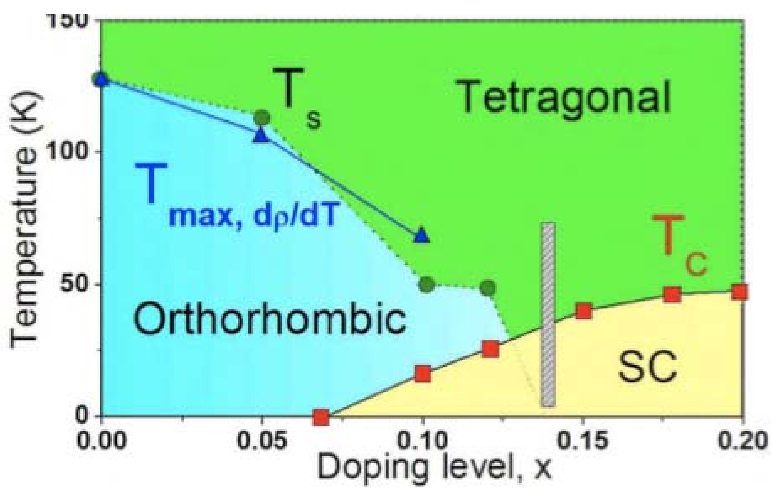
4, Quantum nematic order with SC, experimental observables

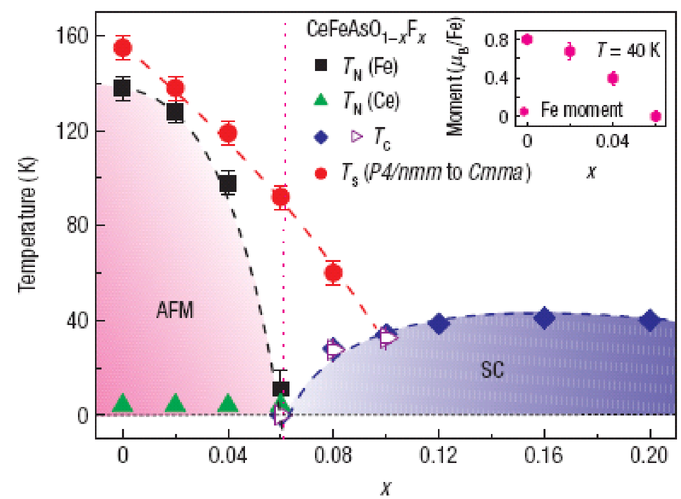
Nematic and Magnetic orders in Fe-based Superconductors

Quantum transition inside the superconductor:



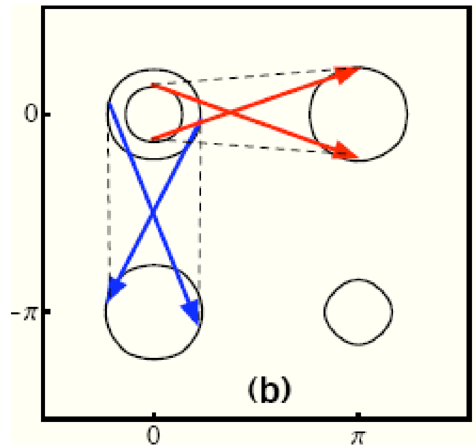




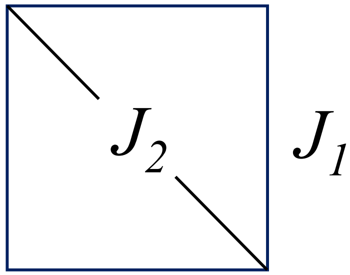


Why s±-wave ??

1, Approach 1: starting with Hubbard model, numerical RG, *Fa Wang et.al.*



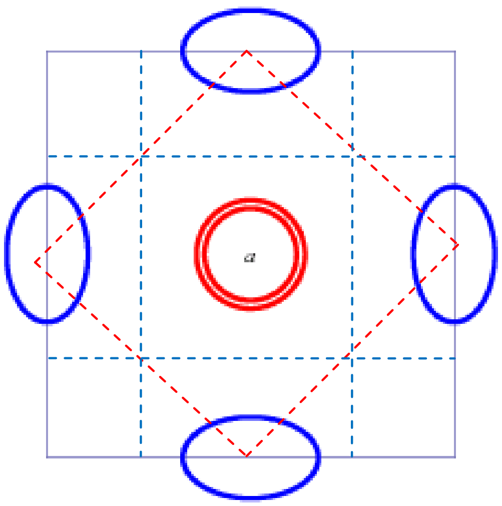
1, Approach 2: starting with *t-J1-J2* model, *K. Seo et.al.*



$$J_1\vec{S}\cdot\vec{S}+J_2\vec{S}\cdot\vec{S}\sim\sum_{k,k'}V_{k,k'}c^\dagger_{\alpha,k,\uparrow}c^\dagger_{\alpha,-k,\downarrow}c_{\alpha,-k',\downarrow}c_{\alpha,k',\uparrow}$$

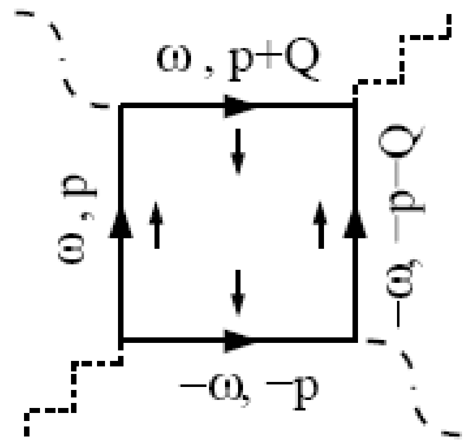
$$V_{k,k'}=-\frac{2J_1}{N}\sum_\pm(\cos k_x\pm\cos k_y)(\cos k'_x\pm\cos k'_y)$$

$$-\frac{8J_2}{N}(\cos k_x\cos k_y\cos k'_x\cos k'_y+\sin k_x\sin k_y\sin k'_x\sin k'_y)$$

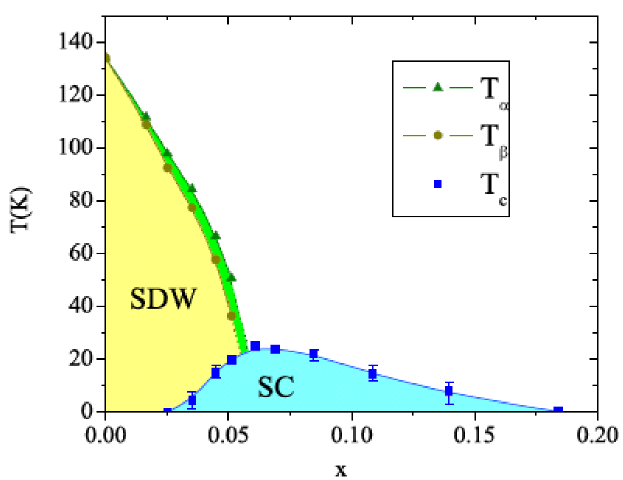


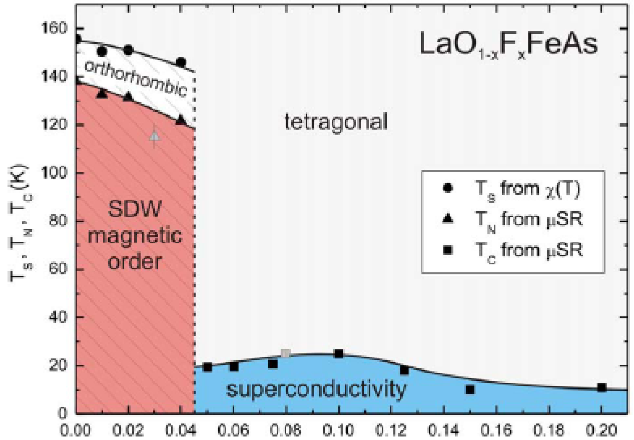
Do SDW and SC compete with each other?

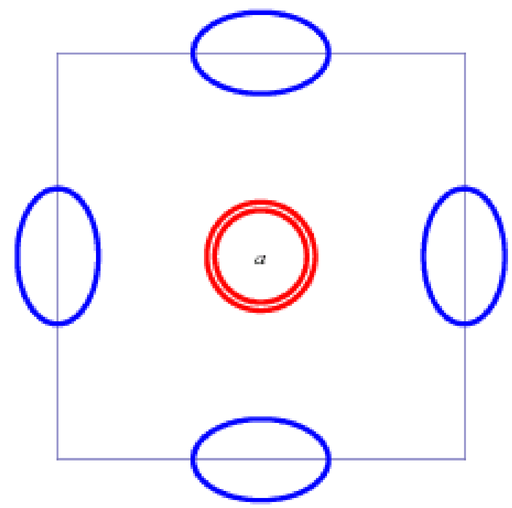
Direct calculations: $\kappa|\Delta|^2|\vec{\phi}|^2$



SDW competes with d-wave pairing, but not s±-wave; nematic order always competes with SC.

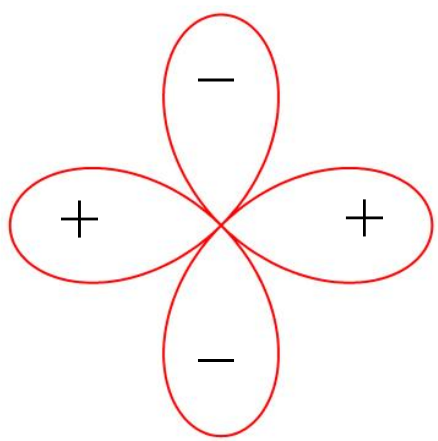


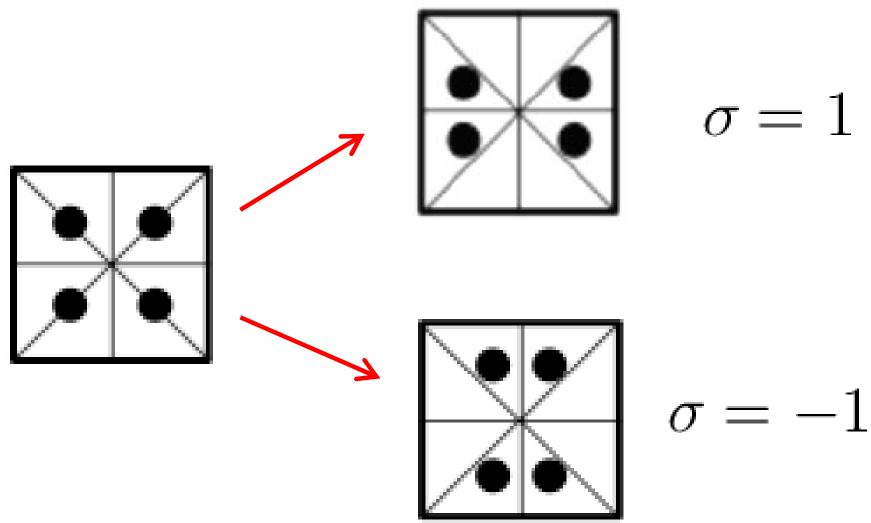




Superconductor (partially) gaps out the fermi surface, if the SC is *s*-wave, the low energy, long wavelength nature of the spin sector transition is unaffected, $z = 1$.

d-wave SC, the nematic order parameter couple with the nodal particle, and deform the location of the nodes





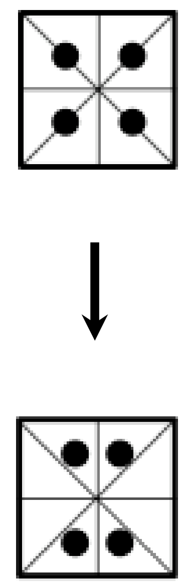
Effective low energy theory for nodal particles: Dirac fermions E. Kim *et.al.*

$$L = L_\Psi + L_\phi + L_{\Psi\phi},$$

$$L_\Psi = \sum_{a=1}^{N_f} \Psi_{1a}^\dagger(\partial_\tau - iv_f\partial_x\tau^z - iv_\Delta\partial_y\tau^x)\Psi_{1a}$$
$$+ \Psi_{2a}^\dagger(\partial_\tau - iv_f\partial_y\tau^z - iv_\Delta\partial_x\tau^x)\Psi_{2a},$$

$$L_\phi = \frac{1}{2}(\partial_\tau\phi)^2 + \frac{c^2}{2}(\nabla\phi)^2 + \frac{r}{2}\phi^2 + \frac{u_0}{4!}\phi^4,$$

$$L_{\Psi\phi} = \lambda_0\phi\sum_{a=1}^{N_f}(\Psi_{1a}^\dagger\tau^x\Psi_{1a} + \Psi_{2a}^\dagger\tau^x\Psi_{2a}).$$



Quantum fluctuation makes the velocity energy dependent, fixed point: $v_\Delta = 0$, Y. Huh *et.al.*

$1/N_f$ RG equations:

$$\frac{d\Sigma_1}{d\ln\Lambda} = C_1(-i\omega) + C_2 v_f k_x \tau^z + C_3 v_\Delta k_y \tau^x,$$

$$\frac{dv_f}{d\ln\Lambda} = (C_1 - C_2)v_f,$$

$$\frac{dv_\Delta}{d\ln\Lambda} = (C_1 - C_3)v_\Delta,$$

$$\frac{d(v_\Delta/v_f)}{d\ln\Lambda} = (C_2 - C_3)(v_\Delta/v_f).$$

C_i are functions of $1/N_f$ and v_Δ/v_f

$$C_1 = -0.4627\frac{(v_\Delta/v_F)}{N_f} + \mathcal{O}\left((v_\Delta/v_F)^3\right)$$

$$C_2 = -0.3479\frac{(v_\Delta/v_F)}{N_f} + \mathcal{O}\left((v_\Delta/v_F)^3\right)$$

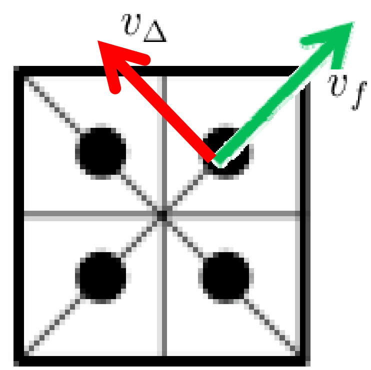
$$C_3 = \left(\frac{8}{\pi^2}\ln(v_F/v_\Delta) - 0.9601\right)\frac{(v_\Delta/v_F)}{N_f} + \mathcal{O}\left((v_\Delta/v_F)^3\right).$$

Fixed Point: $v_\Delta = 0.$ Y. Huh *et.al.* 2008

How does the nematic quantum critical point change the physical quantities?

Due to coupling with nematic order, velocities are functions of frequency:

Physical Quantity 1: LDOS, measured by STM



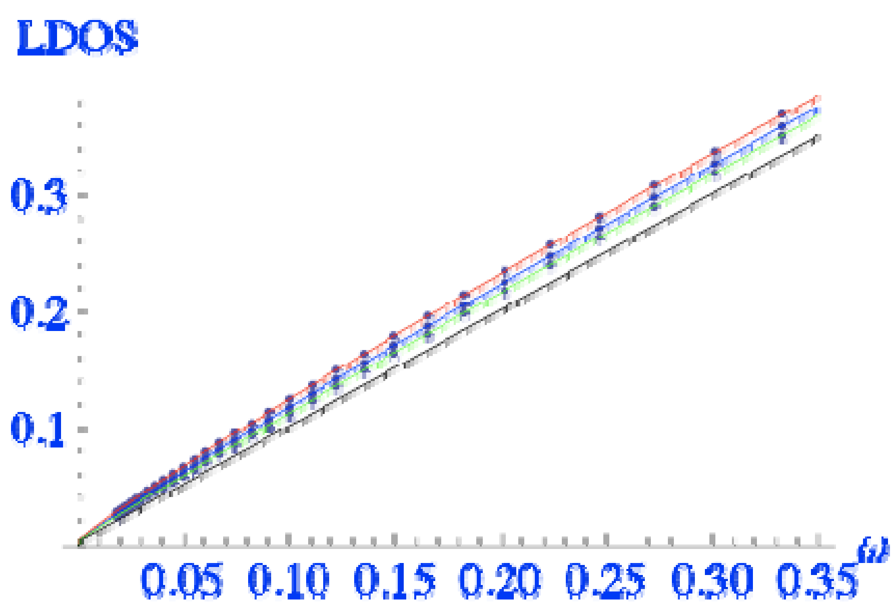
Naive equation:

$$\rho(\omega/\Lambda) \sim \frac{\omega}{v_\Delta v_f}$$

$$v_{\Delta 0}/v_{f0} = 1/5, \quad \rho \sim \omega^{0.91},$$

$$v_{\Delta 0}/v_{f0} = 1/10, \quad \rho \sim \omega^{0.935},$$

$$v_{\Delta 0}/v_{f0} = 1/20, \quad \rho \sim \omega^{0.955}.$$



Physical Quantity 2: Specific heat

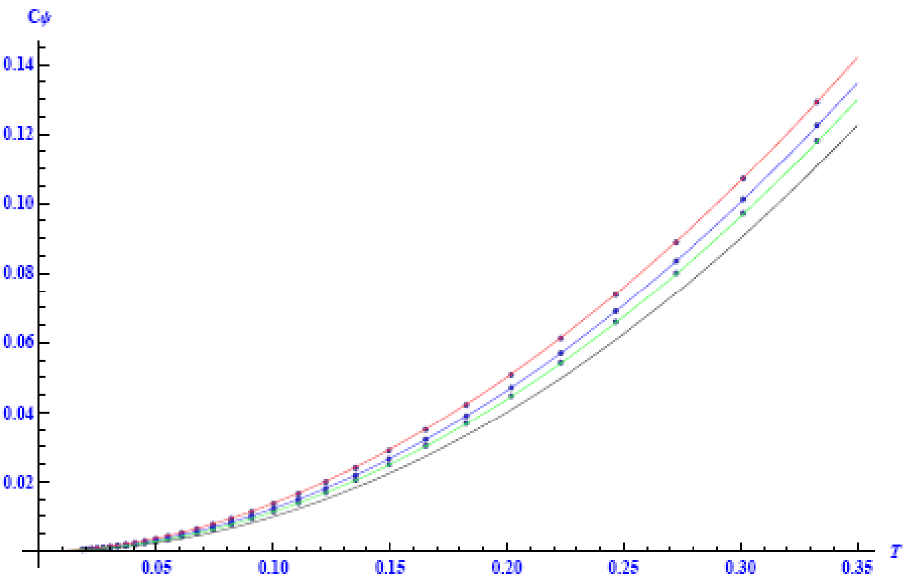
Naive equation:

$$C \sim \frac{1}{v_\Delta v_f} T^2$$

$$v_{\Delta 0}/v_{f0} = 1/5, \quad C \sim T^{1.86},$$

$$v_{\Delta 0}/v_{f0} = 1/10, \quad C \sim T^{1.91},$$

$$v_{\Delta 0}/v_{f0} = 1/20, \quad C \sim T^{1.95}.$$

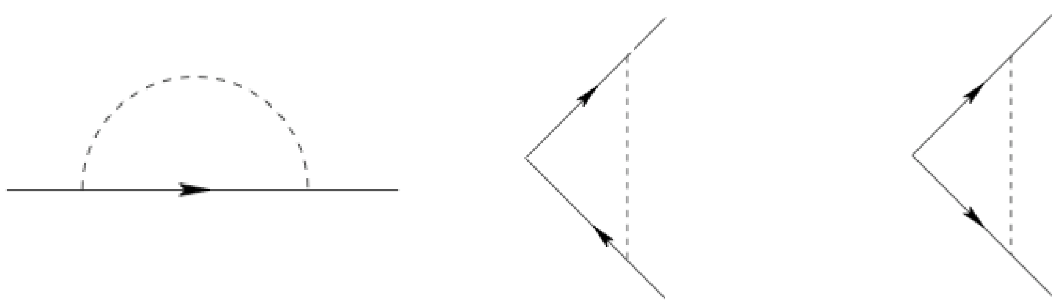


Physical Quantity 3: NMR spin lattice relaxation rate

$$F(\omega) \sim \int dq_x dq_y \frac{1}{\omega} \chi''(q_x, q_y, \omega),$$

Local probe, momentum integrated susceptibility, contribution from all the "slow" spin density wave should be considered.

Wave-function + vertex corrections



$$\begin{aligned}
\vec{q} &= (0,0), \quad \Psi_1^\dagger \sigma^a \Psi_1 + \Psi_2^\dagger \sigma^a \Psi_2; \\
\vec{q}_{12A} &= (2Q,0), \quad \Psi_2^\dagger \sigma^a \Psi_1; \\
-\vec{q}_{12A} &= (-2Q,0), \quad \Psi_1^\dagger \sigma^a \Psi_2; \\
\vec{q}_{12B} &= (0,2Q), \quad \Psi_1^t \tau^y \sigma^y \sigma^a \Psi_2; \\
-\vec{q}_{12B} &= (0,-2Q), \quad \Psi_2^\dagger \tau^y \sigma^a \sigma^y \Psi_1^*, \\
\vec{q}_{11} &= (2Q,2Q), \quad \Psi_1^t \tau^y \sigma^y \sigma^a \Psi_1; \\
-\vec{q}_{11} &= (-2Q,-2Q), \quad \Psi_1^\dagger \tau^y \sigma^a \sigma^y \Psi_1^*, \\
\vec{q}_{22} &= (-2Q,2Q), \quad \Psi_2^t \tau^y \sigma^y \sigma^a \Psi_2; \\
-\vec{q}_{22} &= (2Q,-2Q), \quad \Psi_2^\dagger \tau^y \sigma^a \sigma^y \Psi_2^*
\end{aligned}$$

Physical Quantity 3: NMR spin lattice relaxation rate

$$F(\omega) \sim \int dq_x dq_y \frac{1}{\omega} \chi''(q_x, q_y, \omega),$$

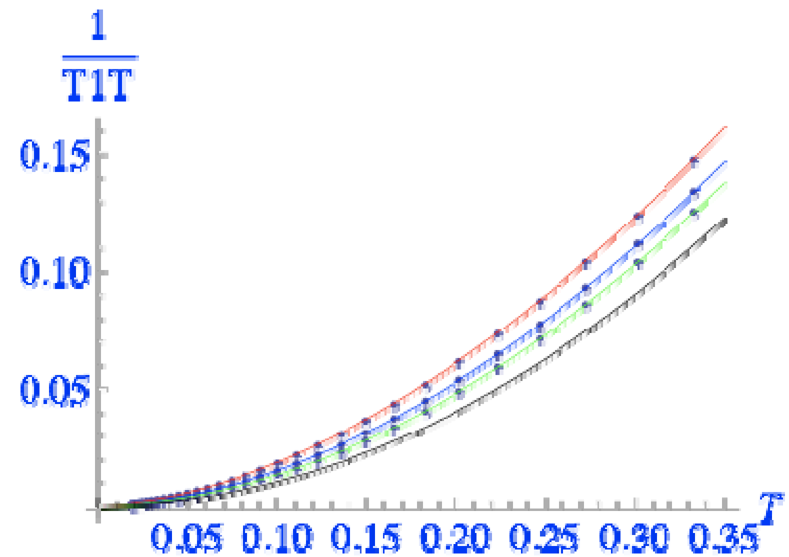
Naive equation:

$$1/T_1 T \sim T^2$$

$$v_{\Delta 0}/v_{f0} = 1/5, \quad 1/T_1 T \sim T^{1.74},$$

$$v_{\Delta 0}/v_{f0} = 1/10, \quad 1/T_1 T \sim T^{1.83},$$

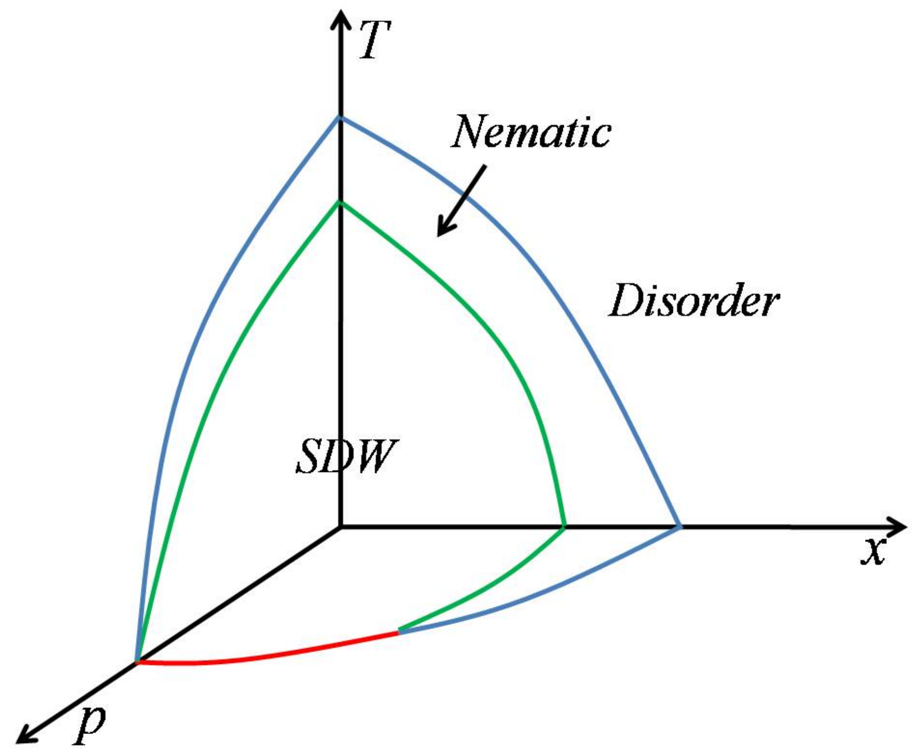
$$v_{\Delta 0}/v_{f0} = 1/20, \quad 1/T_1 T \sim T^{1.89}.$$



PRB, **78**, 134508 (2008), C. Xu, Y. Qi, S, Sachdev

Summary of Fe-SC:

1, Global phase diagram:



2, Unified theory of lattice distortion and SDW.

3, nature of the transitions when coupled to a soft lattice.

4, physical observables at the nematic transition in SC.