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Magnetism in Parent Compound for Fe-Chalcogenides

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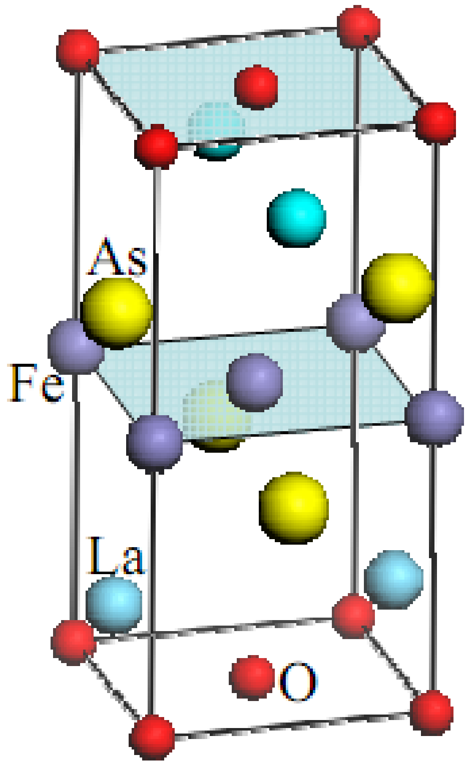
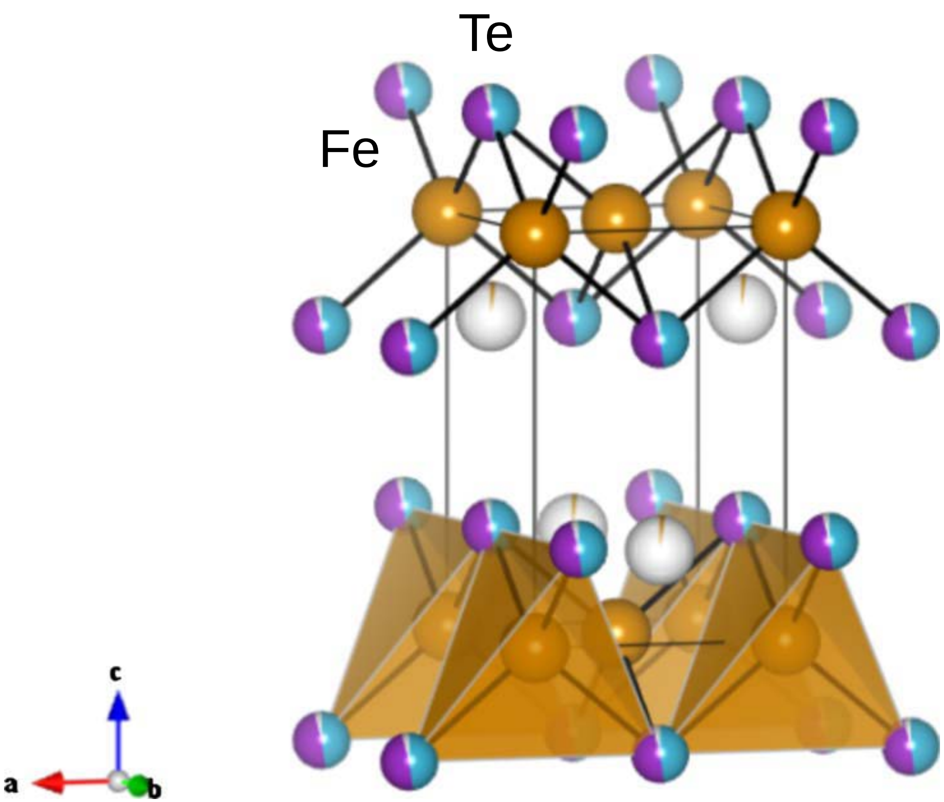
Fe-pnictides and chalcogenides



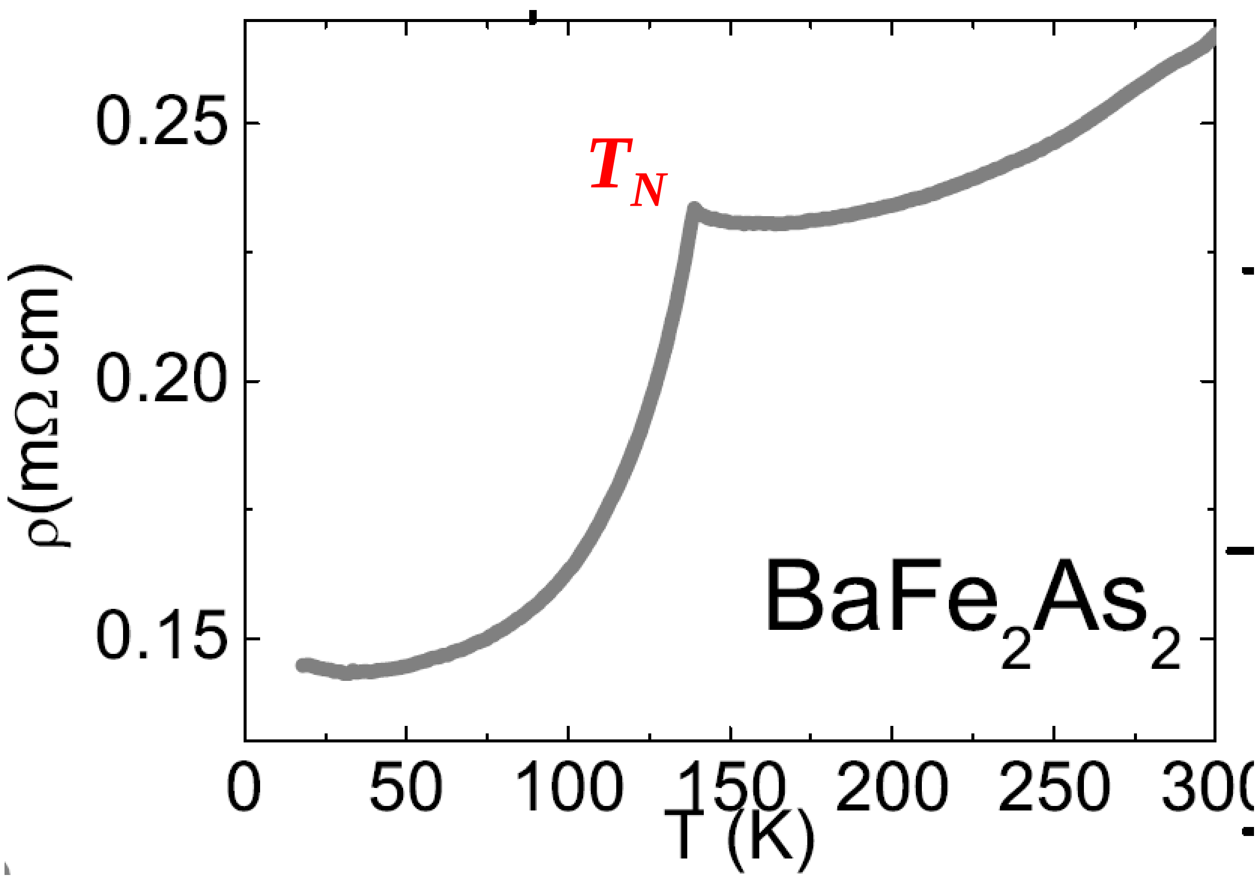
LaFeAsO



2D Fe-As layers with As above and below a square lattice formed by Fe

$Fe_{1+y}Te$: the simplest structure composed of only the FeTe layers

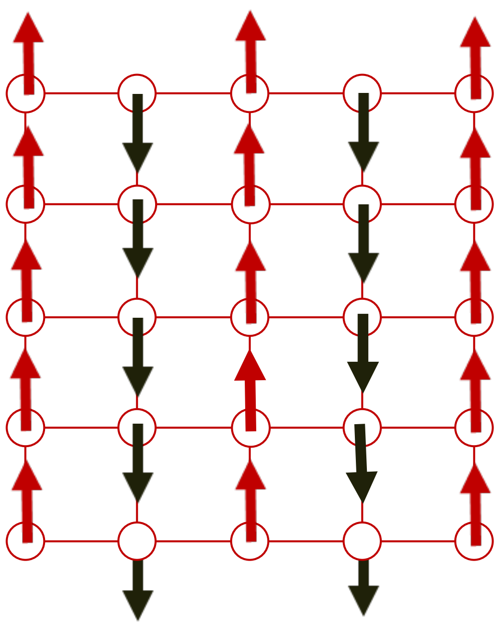
Metallic behavior of parent FeAs compounds



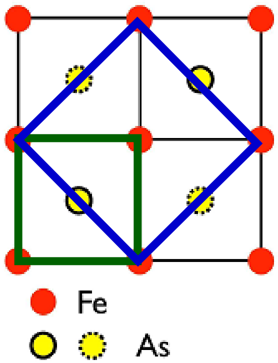
Fe-pnictides are doped metals

Two phase transitions
in parent compounds of Fe-pnictides
(1111 and 122)

Structural transition at high temperature:
tetragonal to orthorhombic

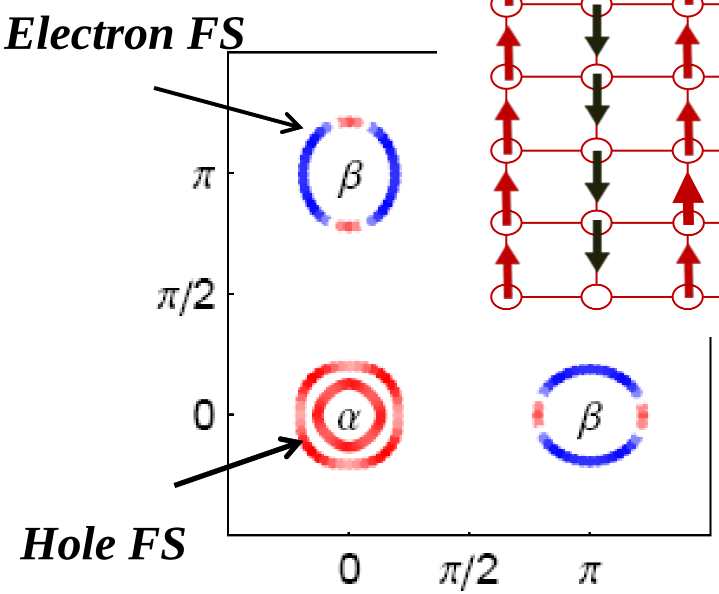


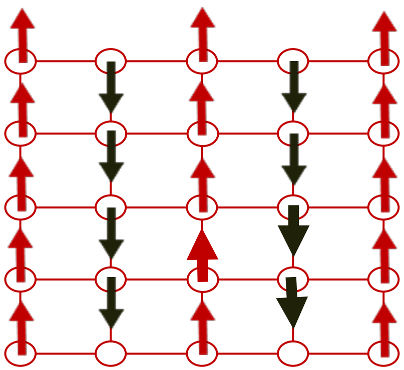
Magnetic transition to $(0,\pi)$ or $(\pi,0)$
state at lower temperature in the unfolded BZ



Magnetic order in pnictides can be reasonably well understood within itinerant scenario - the locations of the FSs and electron-electron interactions select two possible momenta for the order – $(0, \pi)$ and $(\pi, 0)$ – in the Fe-only BZ.

very schematically





stripe order:
$Q = (\pi,0)$ or $Q=(0,\pi)$

ground state manifold
$\boldsymbol{O(3) \times Z_2}$

Pre-emptive Ising (nematic) order: $C_4 \to C_2$

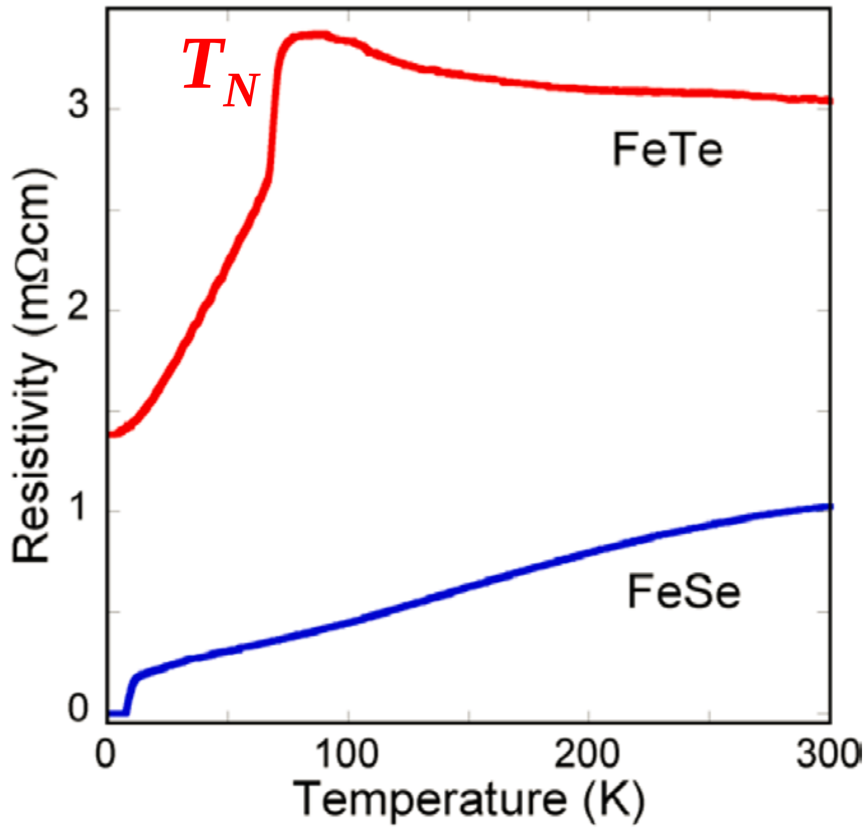
Details in lectures of Rafael Fernandes last week

nearly perfect nesting between electron and hole FSs

Upon doping, LRO is lost, but magnetic fluctuations evolve smoothly and remain peaked at or near $(0, \pi)$ and $(\pi, 0)$.

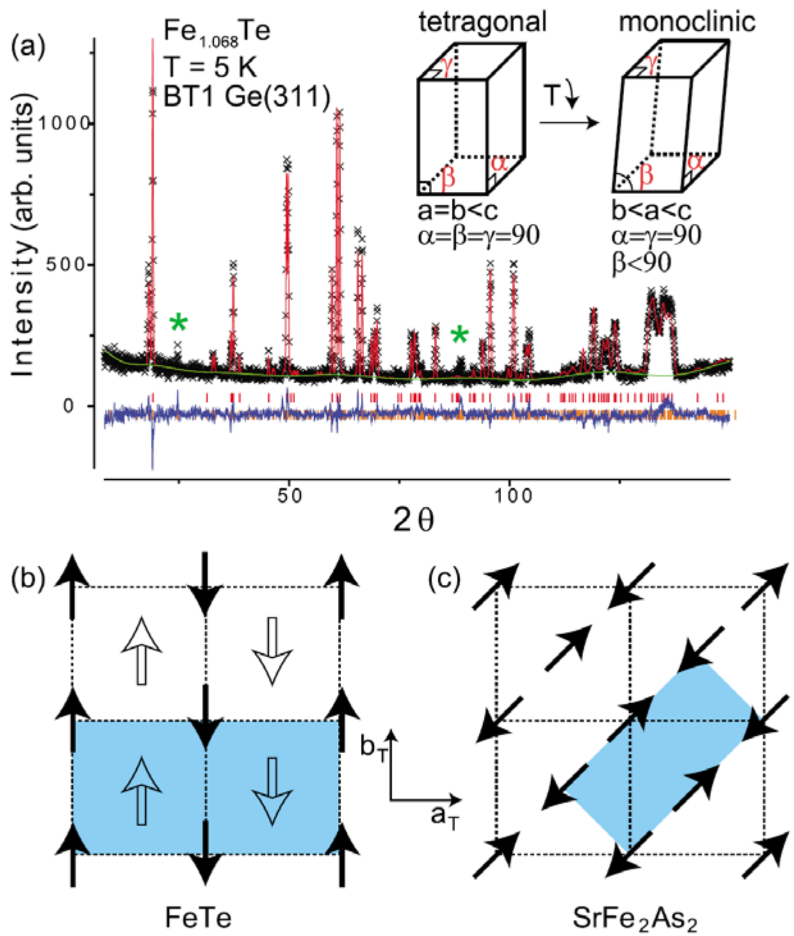
The same magnetic order is selected in the strong coupling approach, in which magnetic properties are reasonably well described by J1 − J2 model (Goes back to Larkin, Coleman,Chandra (1990)).

FeTe may be more strongly correlated



Y.Mizuguchi and Y. Takano (2010)

The single first-order magnetic and structural transition to the monoclinic P21/m space in FeTe at T=69 K

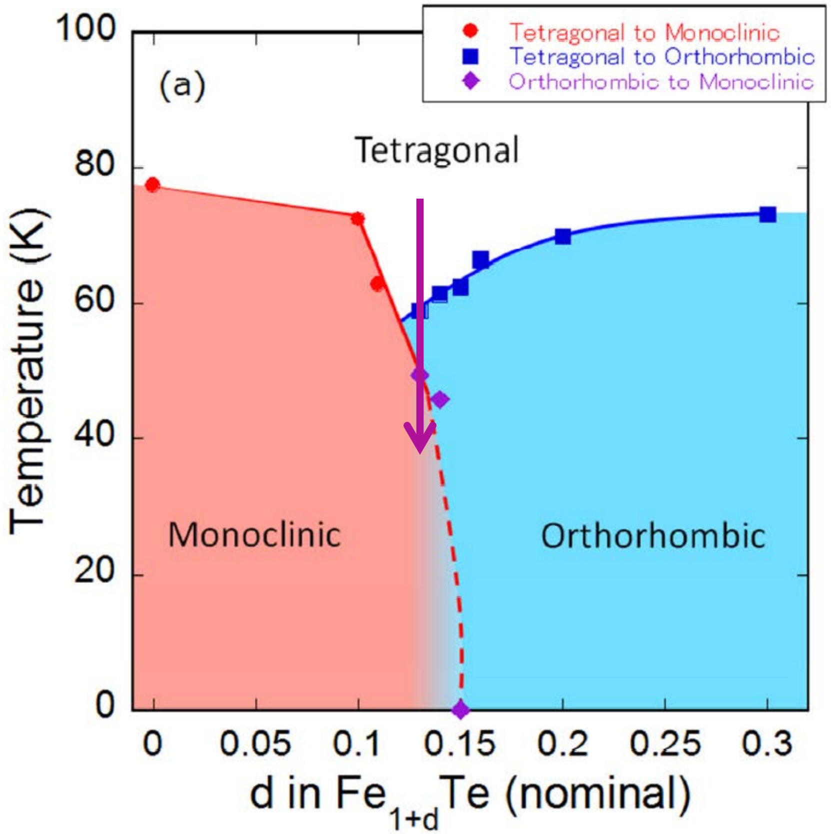


Li et. al., PRB (2009).

Magnetic order in FeTe has momenta $\pm(\pi/2, \pm\pi/2)$. However, this does not uniquely determine spin configuration as a generic $\pm(\pi/2, \pm\pi/2)$ order is a superposition of two different Q−vectors: $(\pi/2, -\pi/2)$ and $(\pi/2, \pi/2)$.

Liu et al., (2010);
Mizuguchi and Takano(2010);
Lipsocombe et al.(2011);
I. Zaliznyak, *et al*,(2012)…

Doped Fe(1+d)Te



For 0.12<d<0.15 - two distinct transitions. Magnetic transition is at a higher T than the structural one.

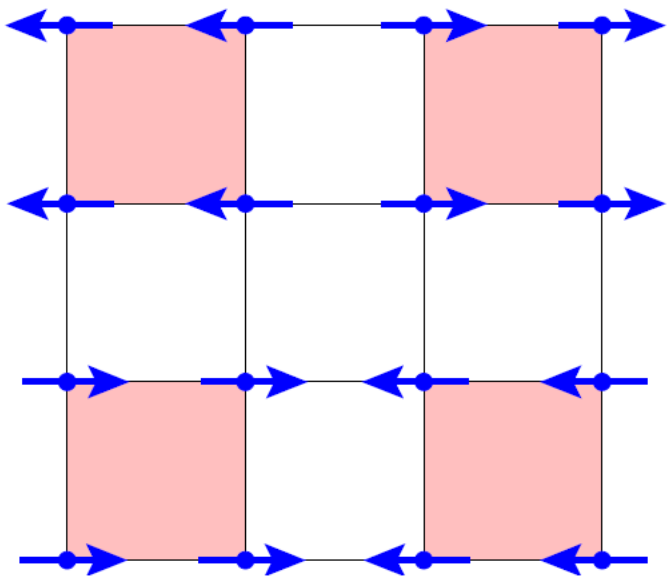
Roessler et. al., PRB (2011).

Two-step structural phase transition tetragonal-orthorhombic-monoclinic

Two-step magnetic transition?

Y.Mizuguchi et all 2012

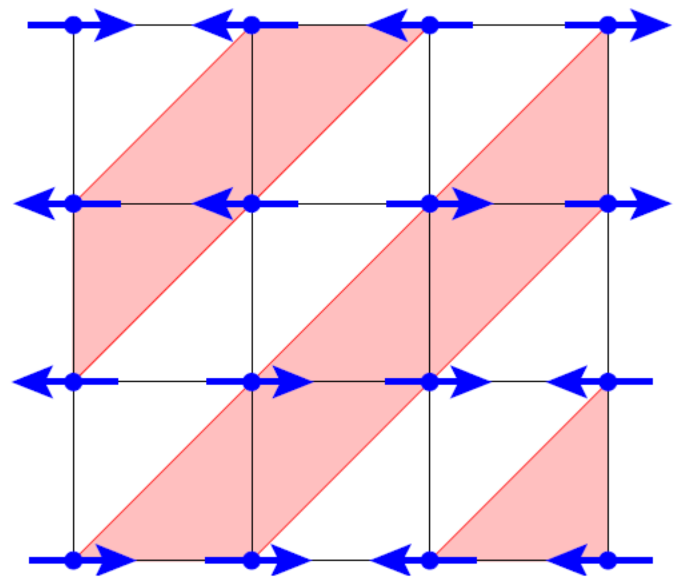
Two possible collinear configurations for parent compound FeTe



double Q plaquette
spin order

Orthogonal Double Stripe (ODS)

Preserves C4 rotational symmetry,
But breaks Z4 translational symmetry



single Q bi-collinear
spin order

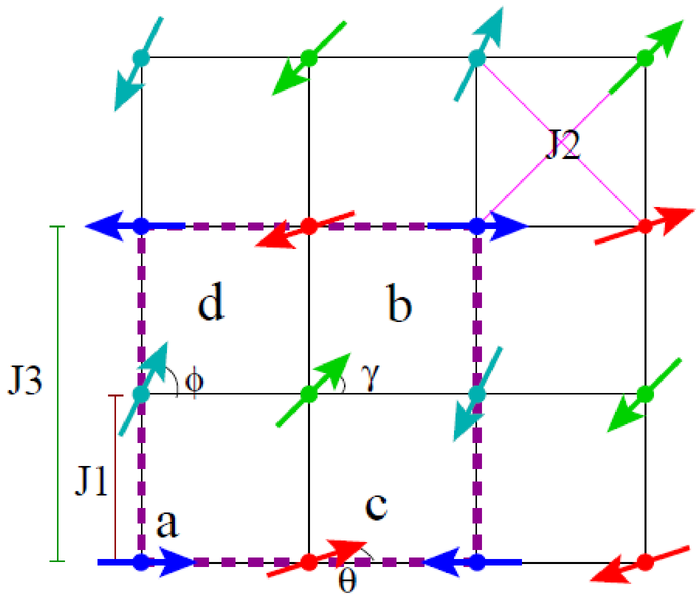
Diagonal Double Stripe (DDS)

Breaks C4 rotational symmetry

Minimal model and classical ground state

Heisenberg J_1- J_2- J_3 Model

$$H = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j + J_3 \sum_{\langle\langle\langle ij \rangle\rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$



F. Ma, *et.al* (2009)
R. Yu, *et. al* (2011)
P. Sindzingre,*et. al* (2010)
J. Reuther, *et al*.(2011)

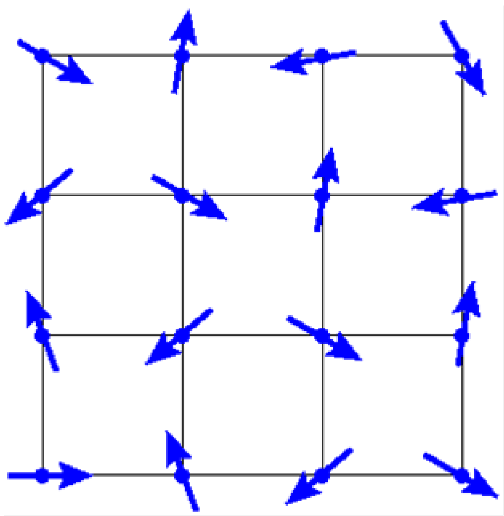
Minimal model and classical ground state

Heisenberg J_1- J_2- J_3 Model

$$H = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j + J_3 \sum_{\langle\langle\langle ij \rangle\rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$

$J_3 > J_2/2 >> J_1$

F. Ma et al, PRL (2009)



In this limit, the classical ground state is a spiral with the pitch vector $\mathbf{Q} = (\pm q, \pm q)$, where $q = \arccos\left(\frac{-J_1}{2J_2+4J_3}\right)$.

Classical energy of the spiral is

$$\boxed{E_{cl} = -\left(2J_3 + \frac{J_1^2}{2J_2 + 4J_3}\right) NS^2}$$

Classical energy of the double stripes is $\boxed{E_{cl}=-2J_3NS^2}$

Quantum fluctuations

- Classically both DDS and ODS are unstable with respect to the spiral state at any $J_1 \neq 0$.
- We study if quantum fluctuations within $1/S$ expansion can stabilize either ODS or DDS.
- We argue that quantum fluctuations lift accidental degeneracies and gap out some of the spinwave modes which in the classical limit become unstable at $J_1 \neq 0$.

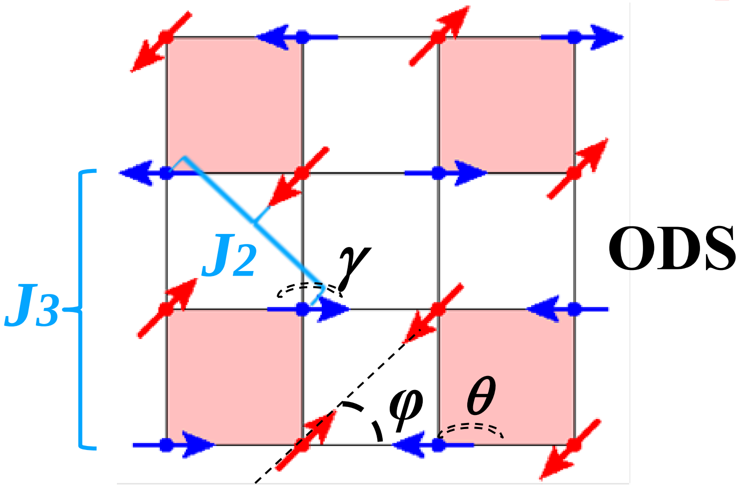
Order by disorder

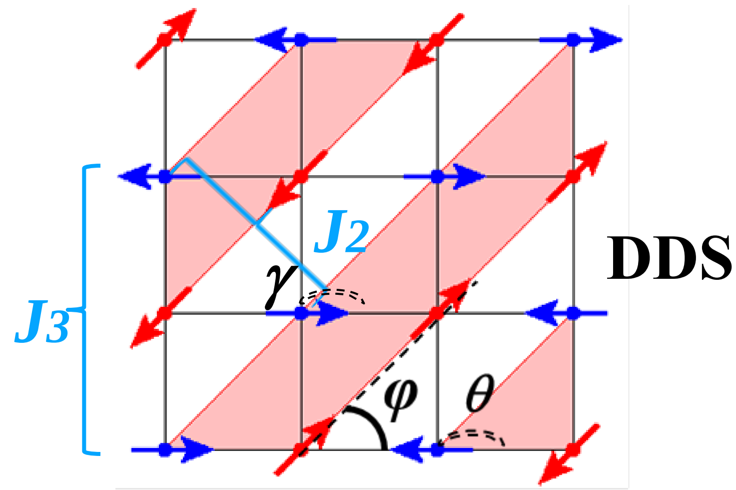
$J_1 = 0 \longrightarrow J_2 - J_3$ model

effective "$J_1 - J_2$"

J_2 plays the role of "J_1"

J_3 plays the role of "J_2"





For $J_3 > J_2/2$ quantum fluctuations select stripe configuration for each sublattice:
the angle γ is locked at $\gamma = 0$ or $\gamma = \pi$,
and the angle θ is locked at $\theta = \phi$ or $\theta = \pi + \phi$.
The collinear DDS and ODS states have different locking of ϕ between the nearest-neighbor spins. DDS: $\phi = 0, \theta = \pi$ or $\phi = \pi, \theta = 0$
ODS: $\phi = \theta = 0$ or $\phi = \theta = \pi$.

$J_1 = 0$: Spin-wave excitations

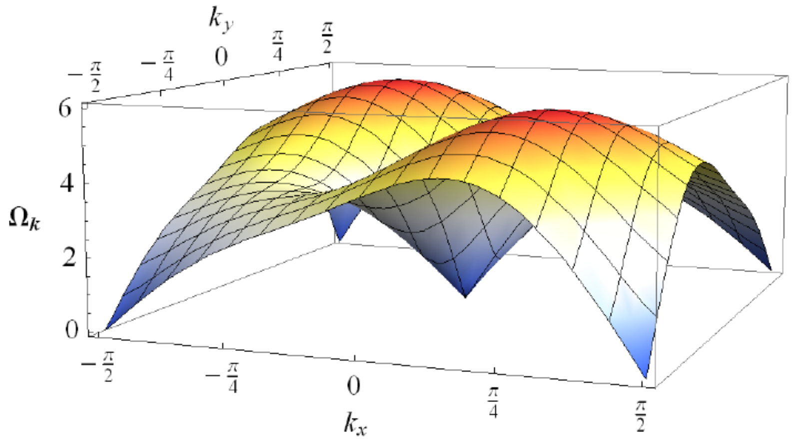
The linear spin-wave spectrum is the same for all selected states.

$$H_{sw} = S(\Omega_{\alpha\mathbf{k}}\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}} + \Omega_{\beta\mathbf{k}}\beta^\dagger_{\mathbf{k}}\beta_{\mathbf{k}})$$

Even sites

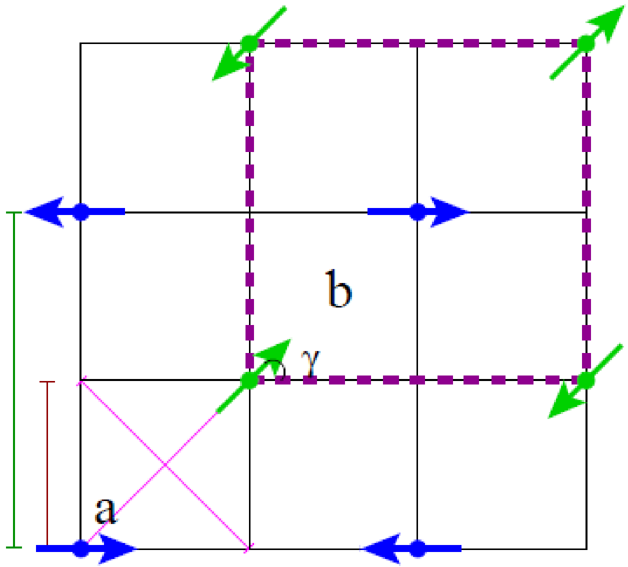
Odd sites

$$\Omega_{\mathbf{k}} = S(A^2_{\mathbf{k}} - B^2_{\mathbf{k}})^{1/2}, \; A_{\mathbf{k}} = 4J_3 + 2J_2\cos(k_x + k_y),$$
$$B_{\mathbf{k}} = 2J_2(\cos 2k_x + \cos 2k_y) + 2J_2\cos(k_x - k_y).$$

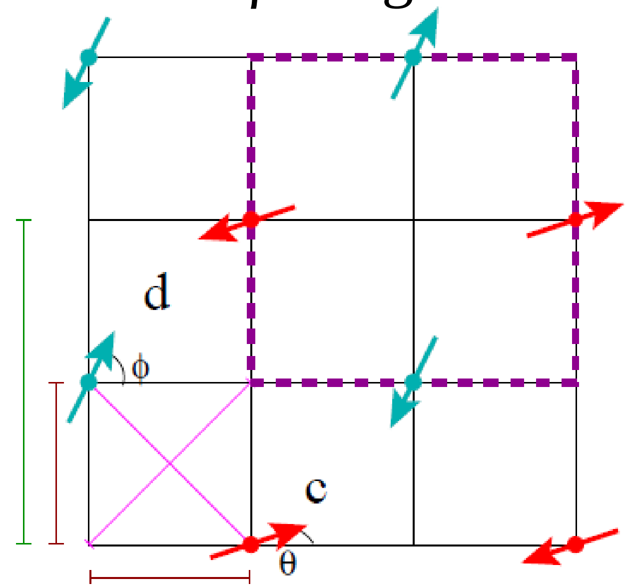


Nodes at $\pm(\pi/2,\pm\pi/2)$,but some of them are not symmetry-related and are lifted by quantum fluctuations.

Even sites:
α-magnons



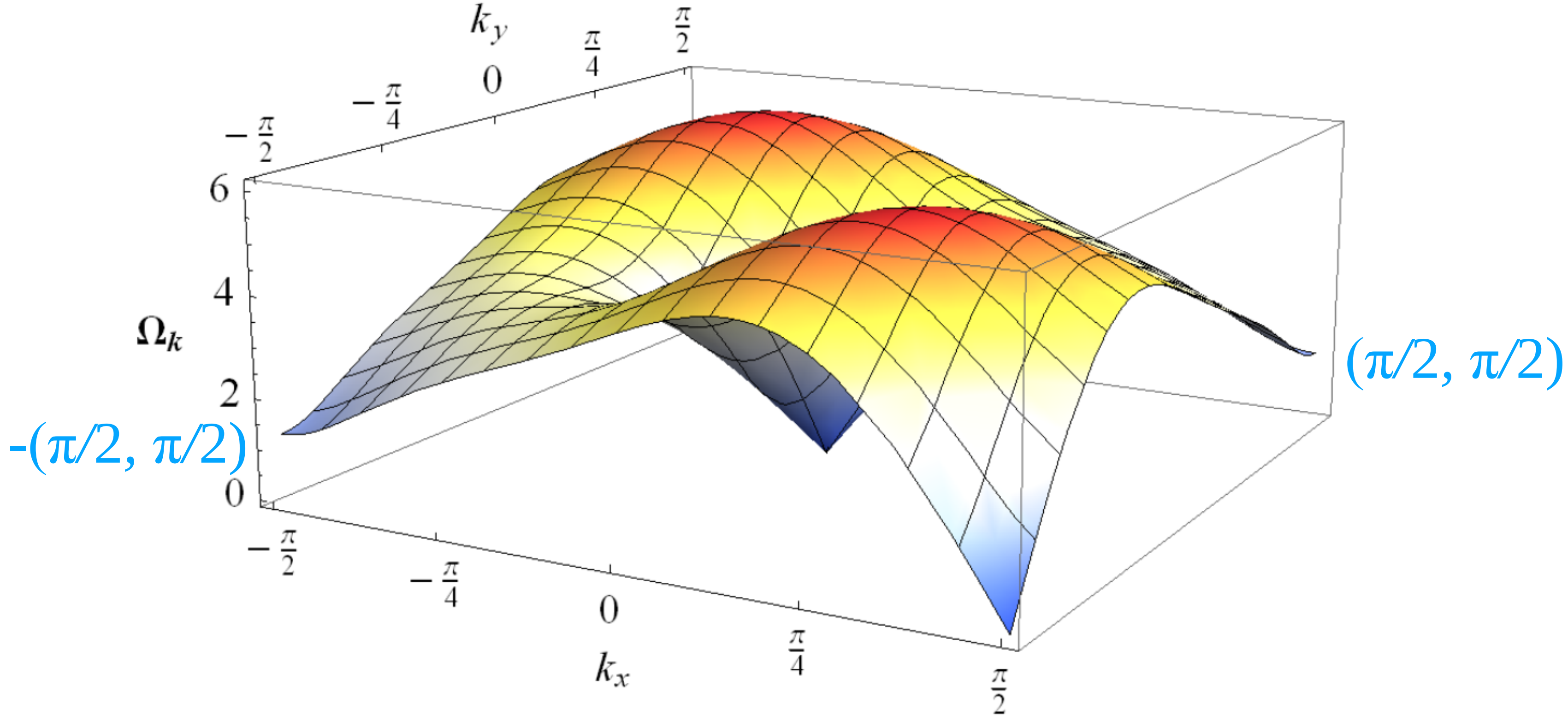
Odd sites:
β-magnons.



The order has momentum $\pm(\pi/2,-\pi/2)$ for both the ODS and the DDS states ($\gamma=0$ or $\gamma=\pi$). Thus, the nodes at $\pm(\pi/2, \pi/2)$ must be lifted by quantum fluctuations.

The order has momentum $\pm(\pi/2, \pi/2)$ for the ODS-state ($\phi = \theta = 0$ or $\phi = \theta = \pi$), and $\pm(\pi/2,-\pi/2)$ for the DDS-state ($\phi = 0$, $\theta = \pi$ or $\phi = \pi$, $\theta = 0$). Quantum fluctuations then must lift the nodes at $\pm(\pi/2,-\pi/2)$ for the ODS and at $\pm(\pi/2, \pi/2)$ for the ODS.

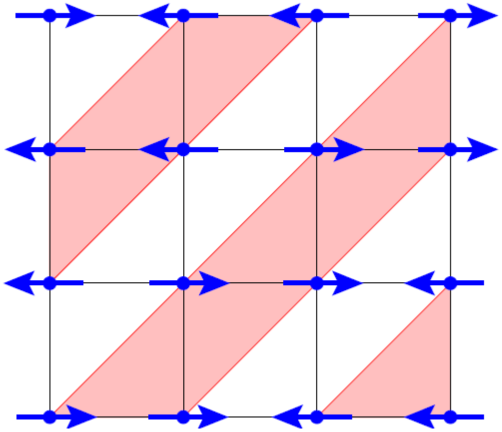
The spectrum renormalized by quantum fluctuations **for DDS state.**



The same is true for the ODS state: accidental nodes are lifted by quantum fluctuations and only true Goldstone modes remain.

$J_1 \neq 0$. DDS states.

- A non-zero J_1 couples the two sublattices
- For DDS states the stripes on even and odd sites are directed parallel to each other, and the dispersions of α_k and β_k magnons are identical, including $1/S$ corrections. The two dispersions are then gapless at the same momenta $\pm(\pi/2, -\pi/2)$. Expanding these true Goldstone points at gives $\boxed{\Omega^{\alpha}_{\tilde{\mathbf{k}}} = \Omega^{\beta}_{\tilde{\mathbf{k}}} \approx 4S\sqrt{J_3(2J_3+J_2)}(\tilde{k}_x^2 + \tilde{k}_y^2 - 2a\tilde{k}_x\tilde{k}_y)^{1/2}}$

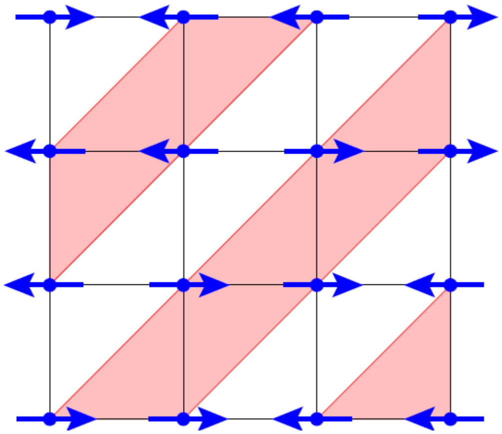


Coupling between sublattices:

$$\delta H_{DDS} = \Delta^{DDS}_{\tilde{\mathbf{k}}}(\alpha^{\dagger}_{\tilde{\mathbf{k}}}\beta_{\tilde{\mathbf{k}}} + \alpha_{\tilde{\mathbf{k}}}\beta_{-\tilde{\mathbf{k}}} + h.c)$$

$$\Delta^{DDS}_{\tilde{\mathbf{k}}} = \frac{J_1 S}{2}\left(\frac{2J_3+J_2}{J_3}\right)^{1/2} \frac{\tilde{k}_y - \tilde{k}_x}{(\tilde{k}_x^2 + \tilde{k}_y^2 - 2a\tilde{k}_x\tilde{k}_y)^{1/2}}$$

DDS state.



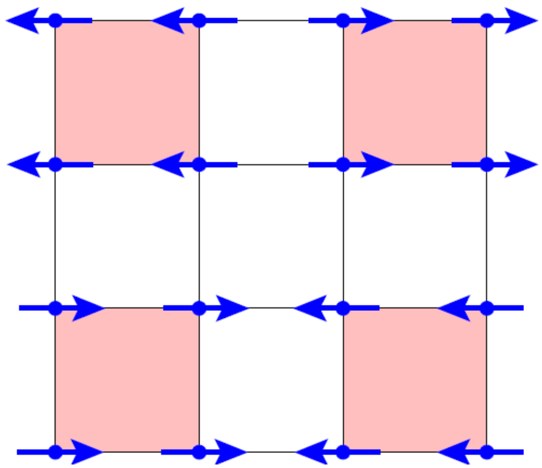
The coupling term δH_{DDS} remains finite when we approach to the Goldstone point. After diagonalizing one of the two solutions become negative:

$$E_{\tilde{k}}^2 \approx -2\Omega_{\tilde{\mathbf{k}}}^{\alpha(\beta)} \Delta_{\tilde{\mathbf{k}}}^{DDS}$$

The excitations become purely imaginary near Goldston modes. Fluctuations around a DDS state grow exponentially with time and make this state unstable.

$J_1 \neq 0$. ODS states.

- For ODS states the stripes on even and odd sites are directed perpendicular to each other, and the dispersions of $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ magnons are different. Near any of the points $\pm(\pi/2,-\pi/2)$ or $\pm(\pi/2, \pi/2)$, the zero in one branches ($\alpha_{\mathbf{k}}$ or $\beta_{\mathbf{k}}$) is lifted by quantum fluctuations. Again we expand near Goldstone points



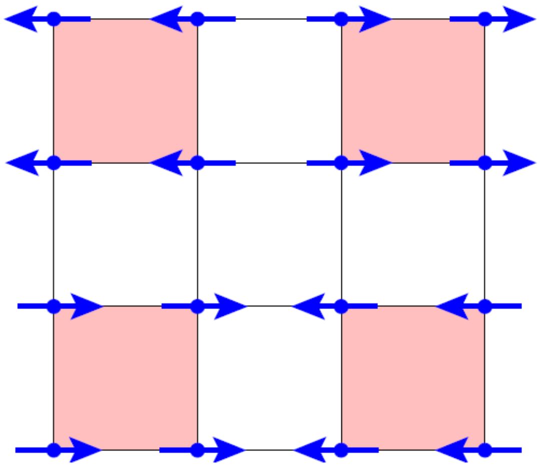
The interactions term has the same form

$$\delta H_{ODS} = \Delta^{ODS'}\tilde{\mathbf{k}}(\alpha^{\dagger}_{\tilde{\mathbf{k}}}\beta_{\tilde{\mathbf{k}}} + \alpha_{\tilde{\mathbf{k}}}\beta_{-\tilde{\mathbf{k}}} + h.c)$$

but

$$\Delta^{ODS}_{\tilde{\mathbf{k}}} = 2J_1S^2(2J_3+J_2)\frac{\tilde{k}_y - \tilde{k}_x}{(\Omega^{\alpha}_{\tilde{k}}\Omega^{\beta}_{\tilde{k}})^{1/2}} = O\left(J_1S^{3/2}|\tilde{k}|^{1/2}\right)$$

ODS state.



The coupling term δH_{ODS} is linear in $\tilde{k}$ when we approach to the Goldstone point. After diagonalizing, we get

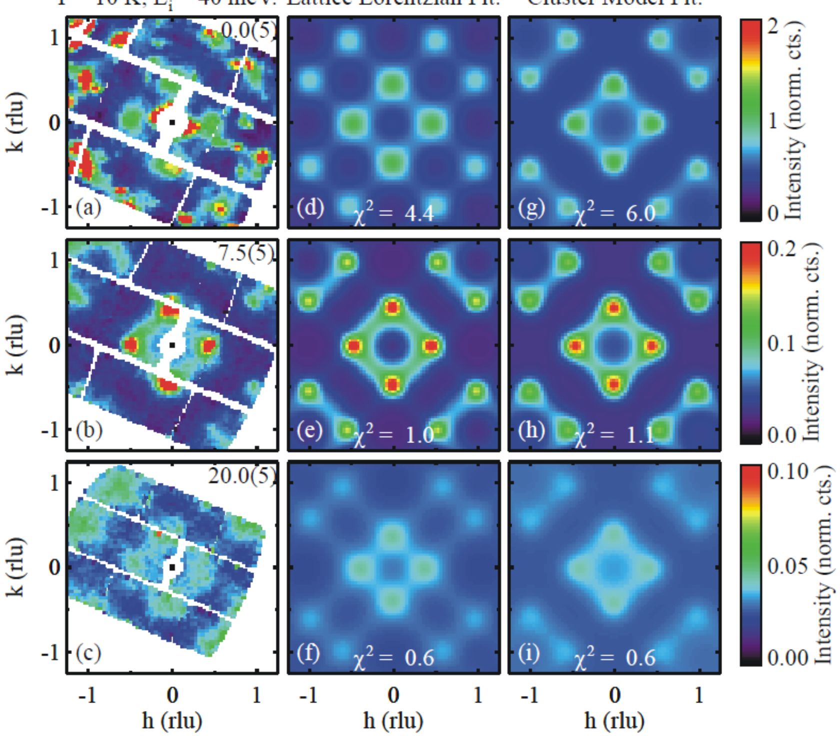
$$E^2_{1,2} = \frac{1}{2}\Big((\Omega^\alpha_{\tilde{k}})^2 + (\Omega^\beta_{\tilde{k}})^2 \pm\sqrt{((\Omega^\alpha_{\tilde{k}})^2 - (\Omega^\beta_{\tilde{k}})^2)^2 + 16(\Delta^{ODS}_{\tilde{\mathbf{k}}})^2\Omega^\alpha_{\tilde{k}}.\Omega^\beta_{\tilde{k}}}\Big)$$

One of the solutions is gapped to order 1/*S*, the other is linear in $\tilde{k}$ with the stiffness which differs from its value at $J_1 = 0$ by $O(J_1S/J_3)$.

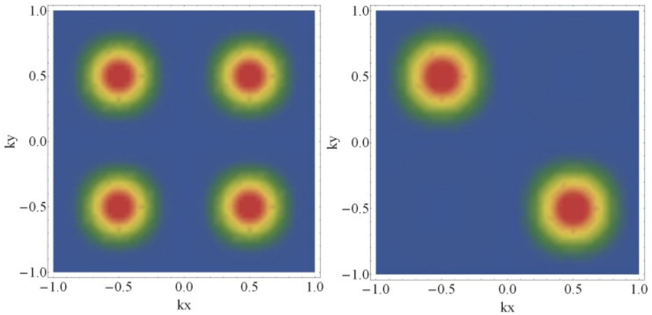
The ODS states are stable as long as J_1S/J_3 is small.

Final remarks (I)

- Experimental signatures of ODS state.



Neutron scattering experiments suggested the plaquette order.
I. Zaliznyak, et al (2011)



ODS DDS

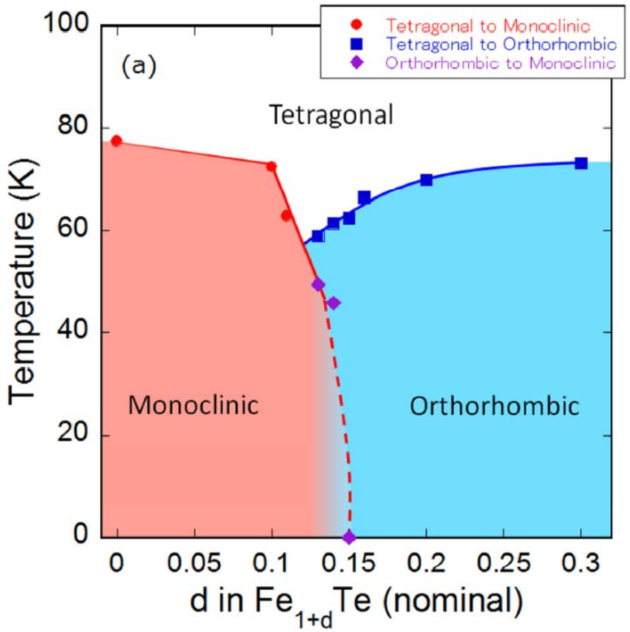
Final remarks(II)

- Absence of a pre-emptive spin-nematic transition plus monoclinic distortion below T_N point to more symmetric ODS state. On contrary, the DDS state has O(3)·Z(2) symmetry like in the simple stripe phase of other Fe-pnictides. Thus, one would expect pre-emptive nematic transition.

Final remarks(III)

- The succession of different pressure and temperature-induced structural and magnetic phases indicates the presence of strong magneto-elastic coupling effects in Fe-chalcogenides.

To be studied in the future!



Y.Mizuguchi et all 2012

Thank you