Spin or Orbital-based Physics in the Fe-based Superconductors?

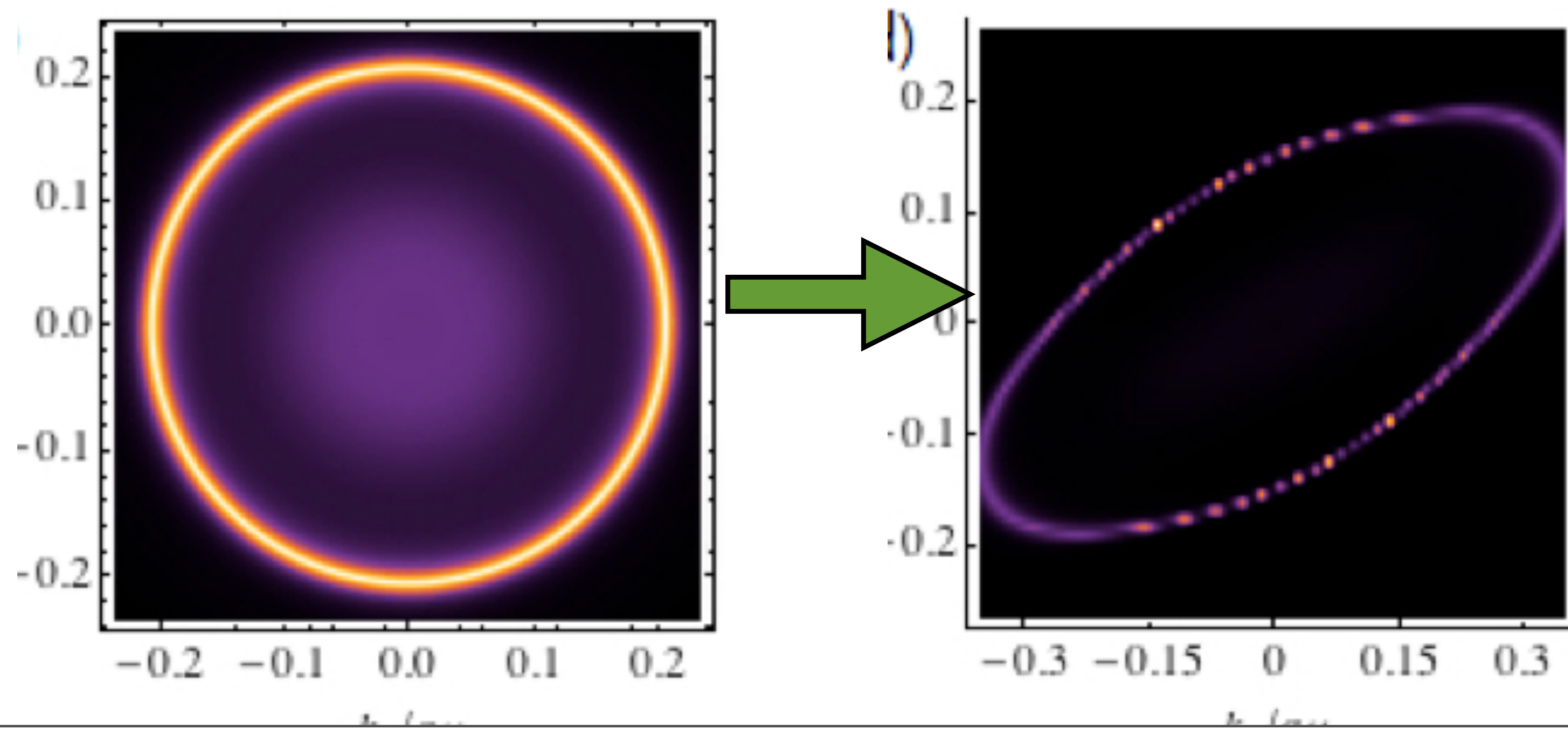
W. Lv, W. Lee, F. Kruger, Z. Leong, J. Tranquada

Thanks to: DOE (EFRC)+BNL

Spin or Orbital-based Physics in the Fe-based Superconductors?

W. Lv, W. Lee, F. Kruger, Z. Leong, J. Tranquada

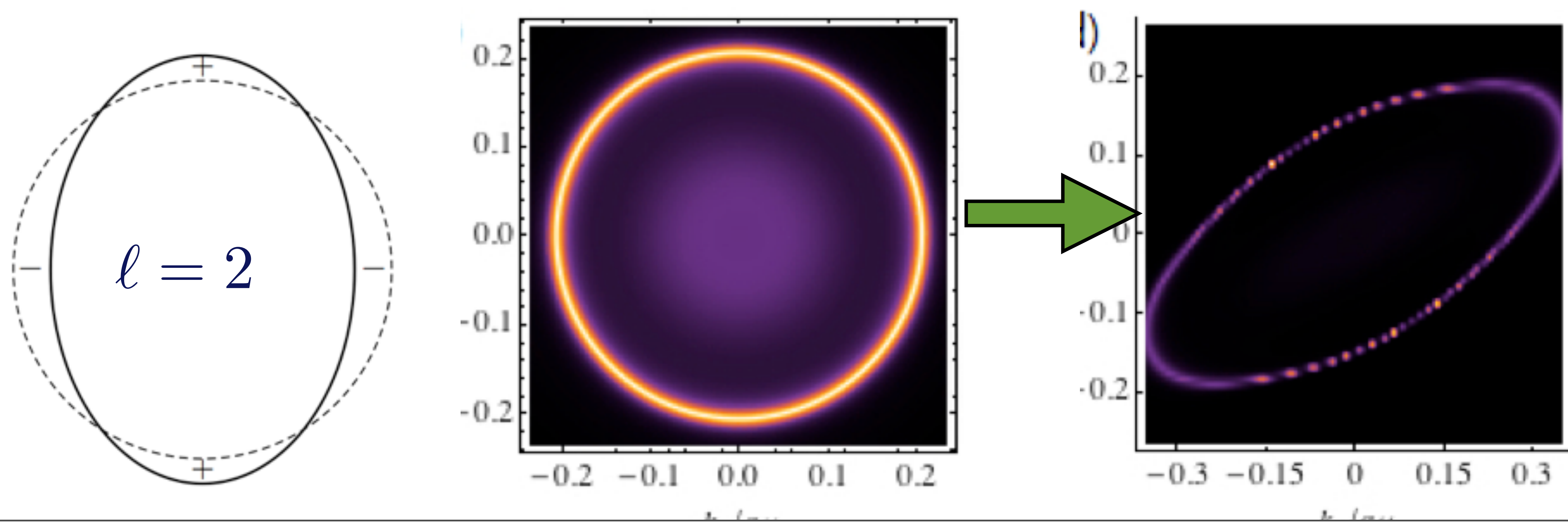
Thanks to: DOE (EFRC)+BNL

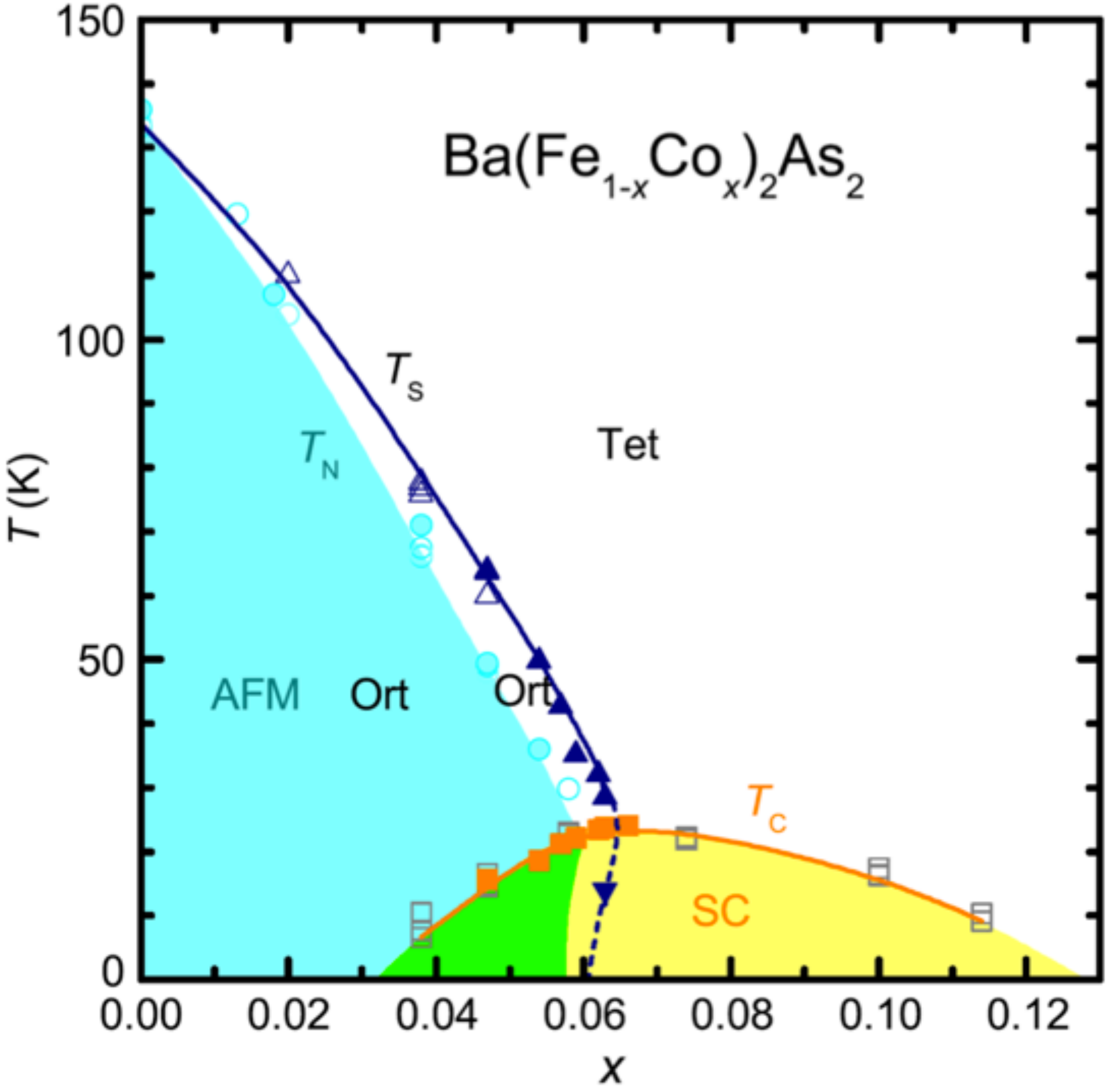


Spin or Orbital-based Physics in the Fe-based Superconductors?

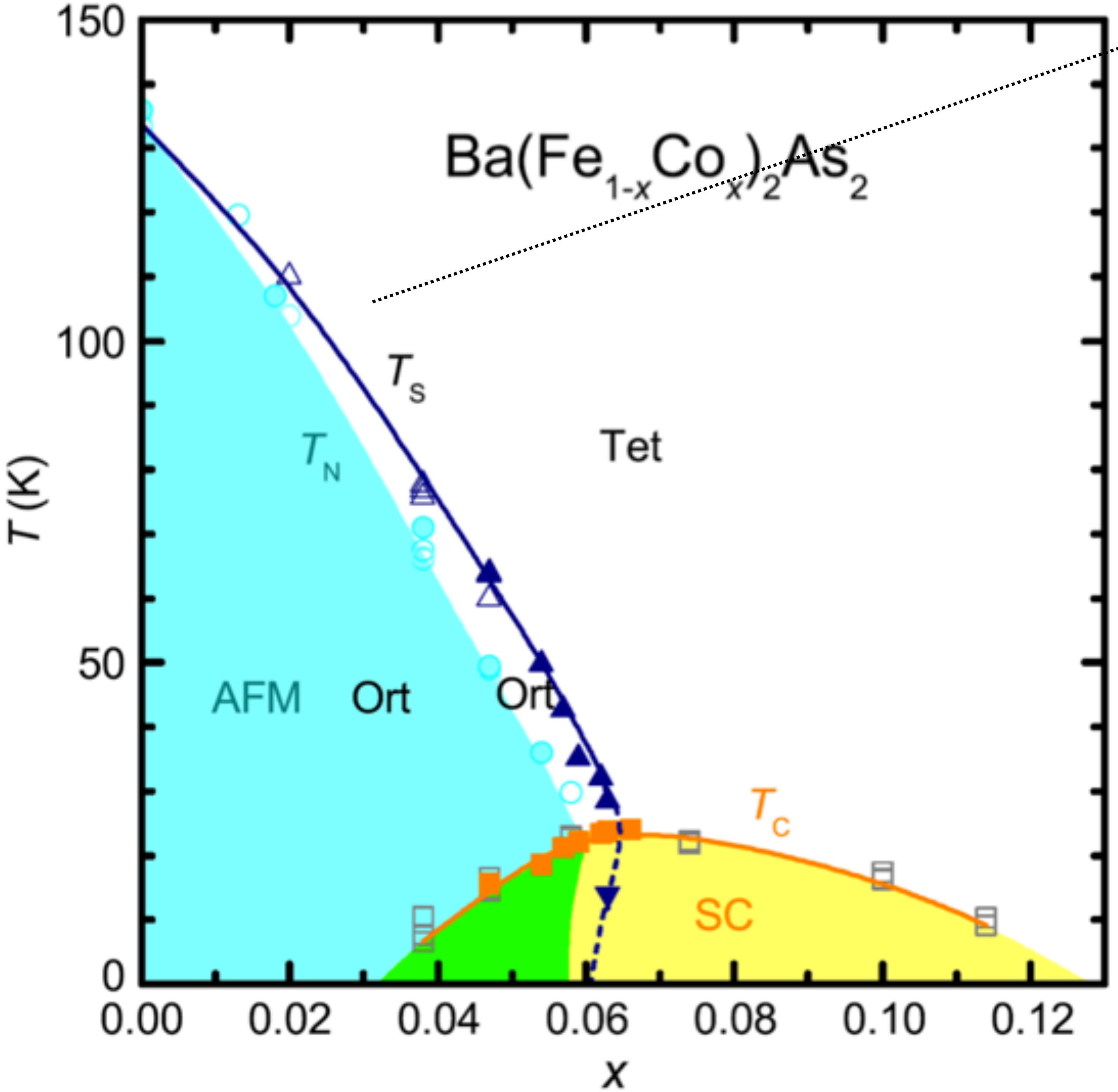
W. Lv, W. Lee, F. Kruger, Z. Leong, J. Tranquada

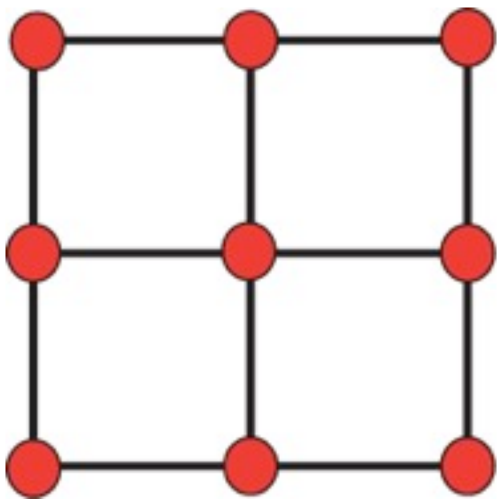
Thanks to: DOE (EFRC)+BNL



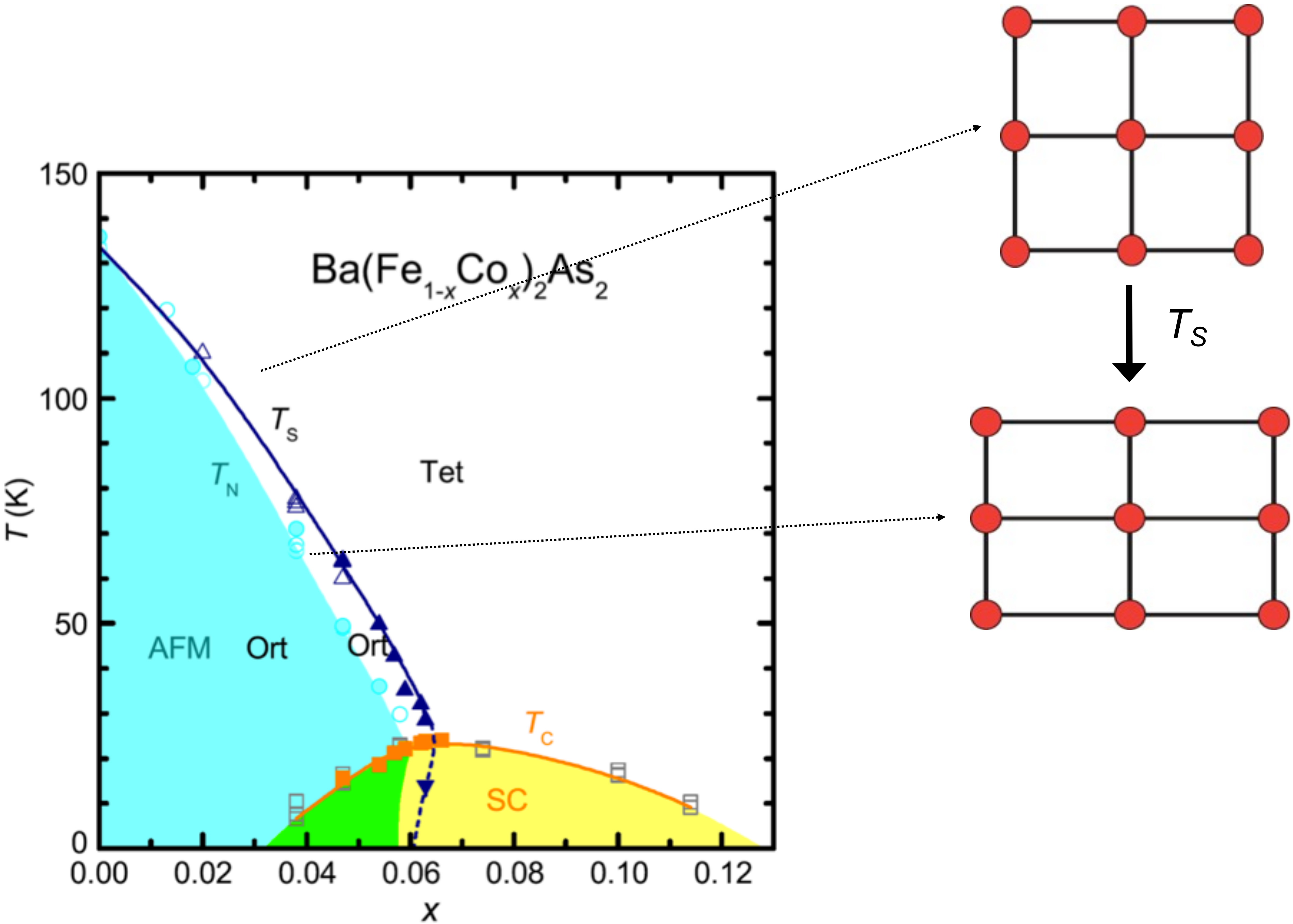


S. Nandi, et al. PRL (2010)

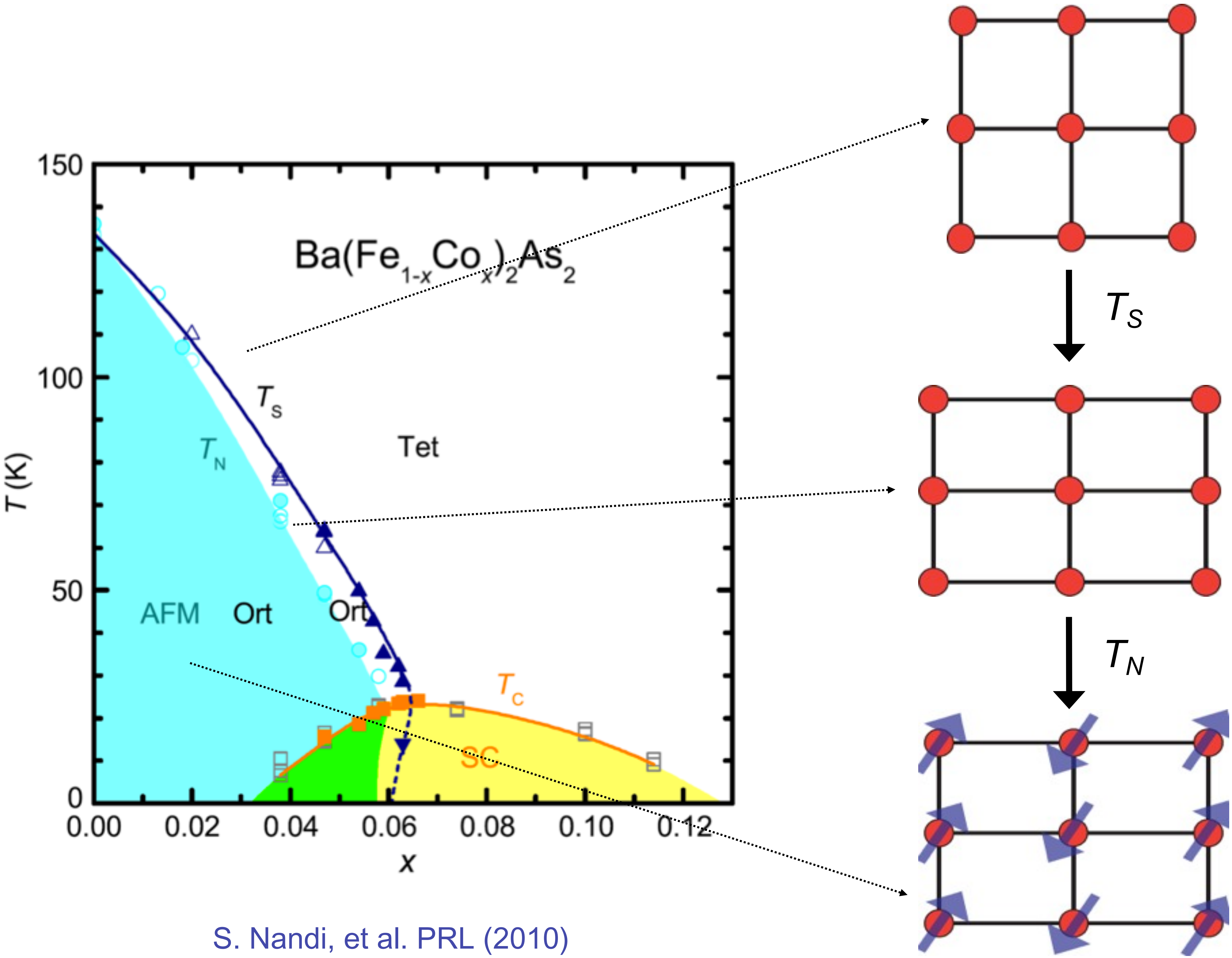




S. Nandi, et al. PRL (2010)



S. Nandi, et al. PRL (2010)



S. Nandi, et al. PRL (2010)

Who is in the Driver's Seat?

Who is in the Driver's Seat?

orbital order

F. Krüger, *et al.* PRB (2009)
R.R.P. Singh, arXiv:0903.4408
W. Lv, *et al.* PRB (2009)
A.M. Turner, *et al.* PRB (2009)
C.-C. Lee, *et al.* PRL (2009)
……

Who is in the Driver's Seat?

orbital order

F. Krüger, *et al.* PRB (2009)
R.R.P. Singh, arXiv:0903.4408
W. Lv, *et al.* PRB (2009)
A.M. Turner, *et al.* PRB (2009)
C.-C. Lee, *et al.* PRL (2009)
……

spin order

C. Fang, et al. PRB (2008)
C. Xu, et al. PRB (2008)
P. Chandra, et al. PRL (1990)

Nematic order in iron superconductors – who is in the driver's seat?

R. M. Fernandes, A. V. Chubukov, J. Schmalian

Who is in the Driver's Seat?

orbital order

F. Krüger, *et al.* PRB (2009)
R.R.P. Singh, arXiv:0903.4408
W. Lv, *et al.* PRB (2009)
A.M. Turner, *et al.* PRB (2009)
C.-C. Lee, *et al.* PRL (2009)
……

spin order

?

C. Fang, et al. PRB (2008)
C. Xu, et al. PRB (2008)
P. Chandra, et al. PRL (1990)

Nematic order in iron superconductors – who is in the driver's seat?

R. M. Fernandes, A. V. Chubukov, J. Schmalian

Who is in the Driver's Seat?

orbital order

F. Krüger, *et al.* PRB (2009)
R.R.P. Singh, arXiv:0903.4408
W. Lv, *et al.* PRB (2009)
A.M. Turner, *et al.* PRB (2009)
C.-C. Lee, *et al.* PRL (2009)
……

…n o…er

C. Fa… PRB (2008)
C. Xu, e… (2008)
P. Char…ra, … (1990)

Nematic order in iro… …rs – wh… …he driver's seat?

R. M. Fernandes, A. V. Chubukov, J. Schma…

orbitals vs spins

Why do I care?

orbitals vs spins

Why do I care?

what are the pnictides?

orbitals vs spins

Why do I care?

what are the pnictides?

cuprates

$$d^9$$

no orbital
degree of freedom

orbitals vs spins

Why do I care?

what are the pnictides?

manganites

cuprates

$$d^9$$

no orbital
degree of freedom

orbitals vs spins

Why do I care?

what are the pnictides?

manganites

cuprates

d^9

no orbital
degree of freedom

pnictides

d^6

orbital degeneracy
d_xz, d_yz

orbitals vs spins

Why do I care?

what are the pnictides?

manganites

cuprates

pnictides

d^9

d^6

no orbital
degree of freedom

orbital degeneracy
d_xz, d_yz

orbital degree of freedom: Hund physics

subtle problem

$$O(3) \times Z_2$$

subtle problem

$$O(3) \times Z_2$$

$$\rightarrow (\pi, 0), (0, \pi)$$

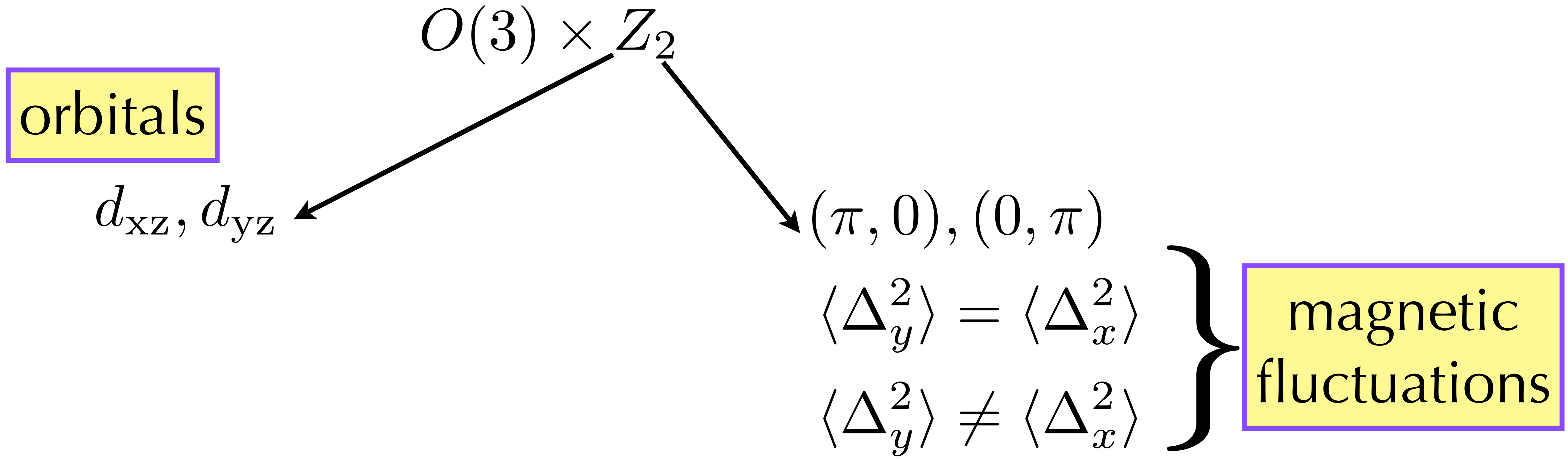
subtle problem

$$O(3) \times Z_2$$

orbitals

$d_{\rm xz}, d_{\rm yz}$ ← $O(3) \times Z_2$ → $(\pi, 0), (0, \pi)$

subtle problem



subtle problem

$O(3) \times Z_2$

orbitals

$d_{\rm xz}, d_{\rm yz}$

$(\pi, 0), (0, \pi)$

$\langle \Delta_y^2 \rangle = \langle \Delta_x^2 \rangle$

$\langle \Delta_y^2 \rangle \neq \langle \Delta_x^2 \rangle$

magnetic fluctuations

$\langle \Delta_y \rangle = \langle \Delta_x \rangle$

structural transition

$\langle n_{\rm xz} \rangle \neq \langle n_{\rm yz} \rangle$

nematic

magnetism $\langle \Delta_y \rangle \neq \langle \Delta_x \rangle$

subtle problem

$$O(3) \times Z_2$$

orbitals

$$d_{\rm xz}, d_{\rm yz}$$

$$\langle n_{\rm xz}^2 \rangle = \langle n_{\rm yz}^2 \rangle$$

$$\langle n_{\rm xz}^2 \rangle \neq \langle n_{\rm yz}^2 \rangle$$

$$\langle n_{\rm xz} \rangle \neq \langle n_{\rm yz} \rangle$$

structural transition

magnetism

$$(\pi, 0), (0, \pi)$$

$$\langle \Delta_y^2 \rangle = \langle \Delta_x^2 \rangle$$

$$\langle \Delta_y^2 \rangle \neq \langle \Delta_x^2 \rangle$$

magnetic fluctuations

$$\langle \Delta_y \rangle = \langle \Delta_x \rangle$$

structural transition

$$\langle n_{\rm xz} \rangle \neq \langle n_{\rm yz} \rangle$$

nematic

magnetism $\langle \Delta_y \rangle \neq \langle \Delta_x \rangle$

can this debate be settled?

orbitals

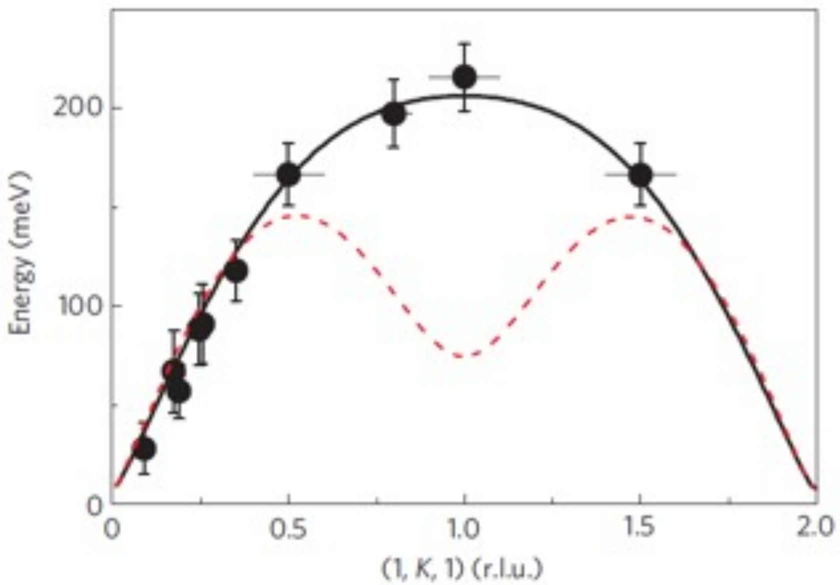
$d_{\mathrm{xz}}, d_{\mathrm{yz}}$

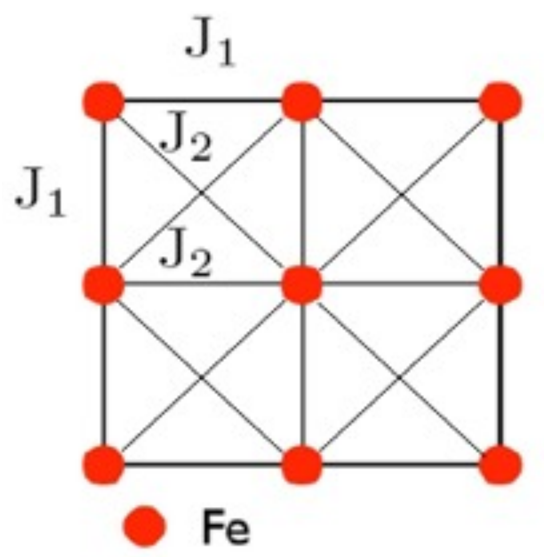
spins

$(\pi, 0), (0, \pi)$

• *Inelastic neutron scattering*

Experimental Puzzle 1?





J. Zhao, *et al.* Nature Physics (2009)

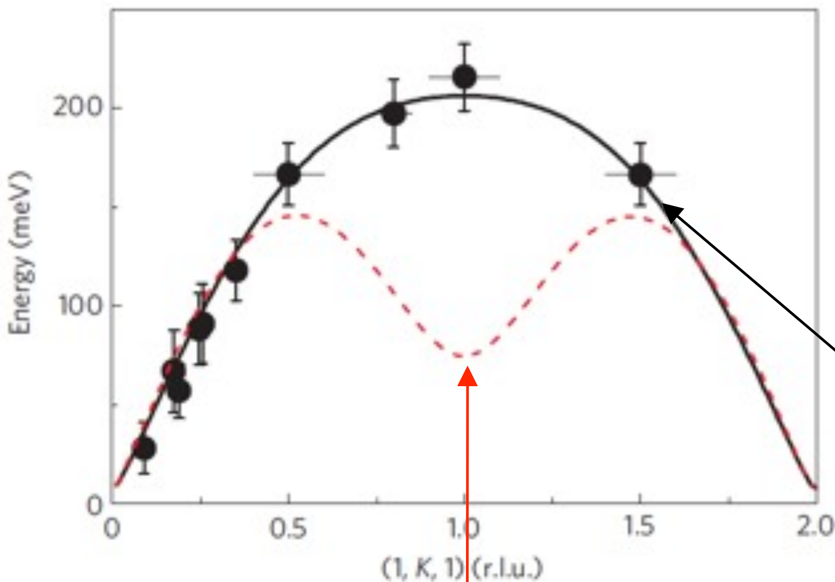
$$SJ_1^a = 27\,\mathrm{meV}$$
$$SJ_1^b = 25\,\mathrm{meV}$$
$$SJ_2 = 36\,\mathrm{meV}$$

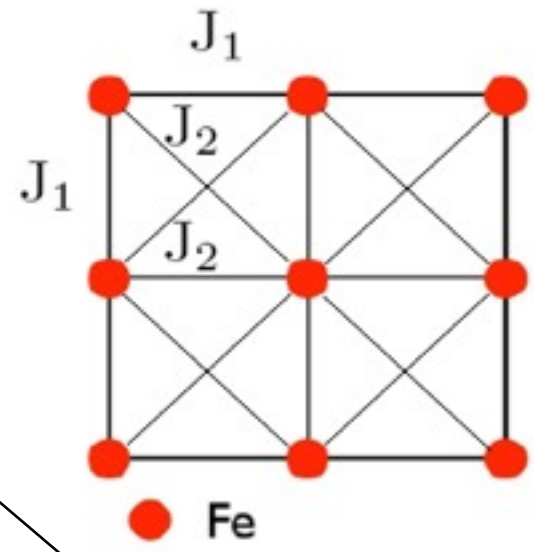
$$SJ_1^a = 49.9 \pm 9.9\,\mathrm{meV}$$
$$SJ_1^b = -5.7 \pm 4.5\,\mathrm{meV}$$
$$SJ_2 = 18.9 \pm 3.4\,\mathrm{meV}$$

Why is the magnetism frustrated?

Experimental Puzzle 1?

- *Inelastic neutron scattering*





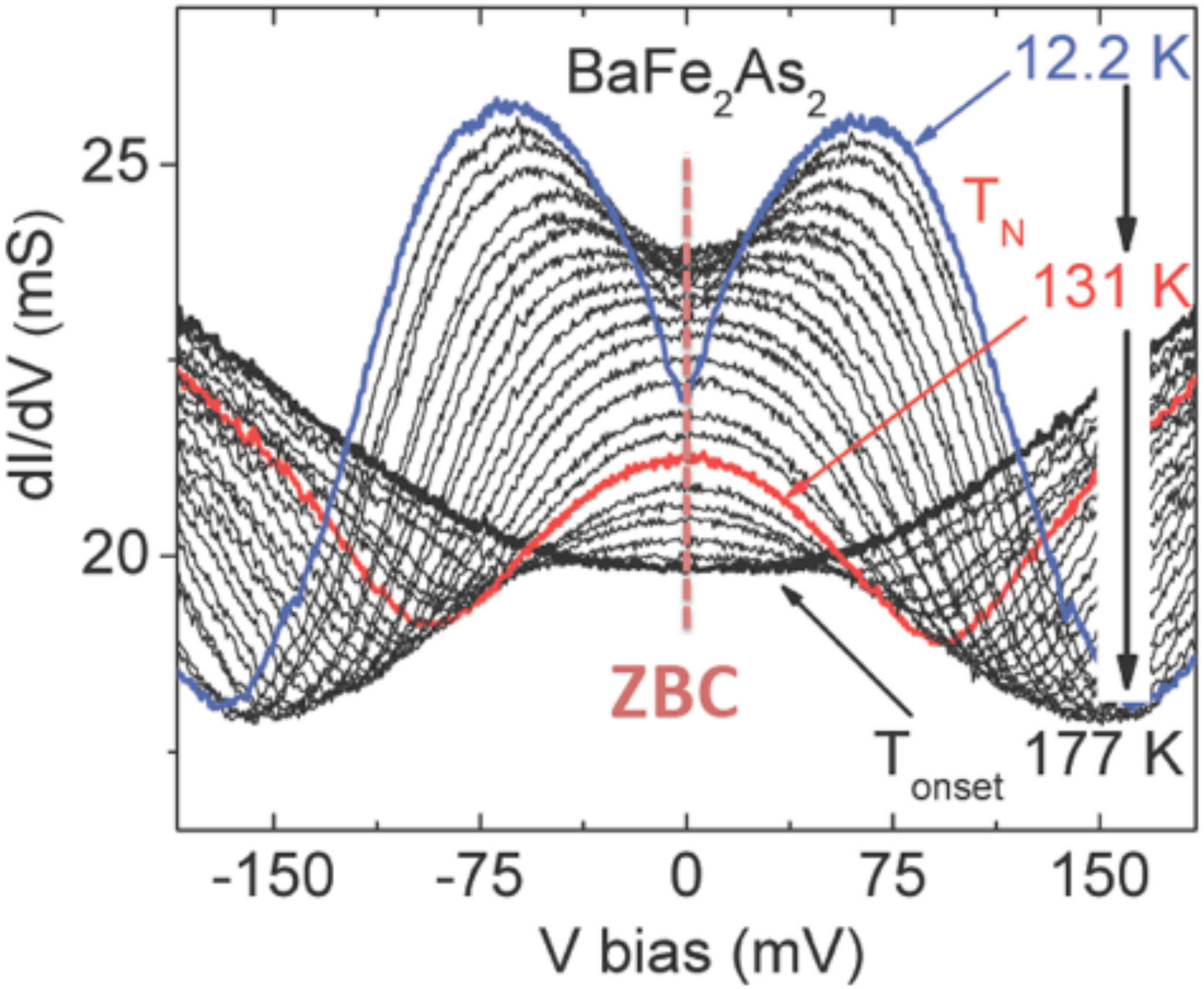
J. Zhao, *et al.* Nature Physics (2009)

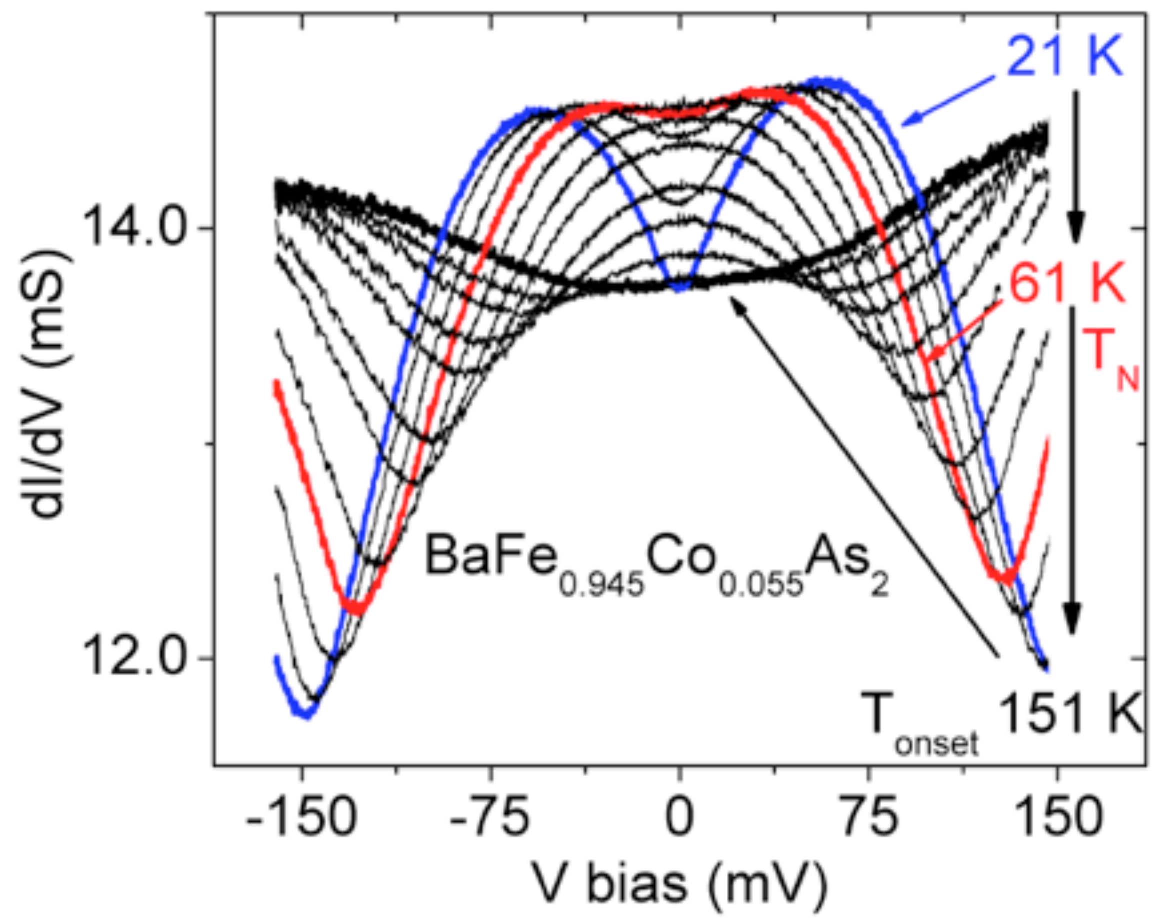
$$
\begin{aligned}
SJ_1^a &= 27\,\mathrm{meV} \\
SJ_1^b &= 25\,\mathrm{meV} \\
SJ_2 &= 36\,\mathrm{meV}
\end{aligned}
$$

$$
\begin{aligned}
SJ_1^a &= 49.9 \pm 9.9\,\mathrm{meV} \\
SJ_1^b &= -5.7 \pm 4.5\,\mathrm{meV} \\
SJ_2 &= 18.9 \pm 3.4\,\mathrm{meV}
\end{aligned}
$$

Why is the magnetism frustrated?

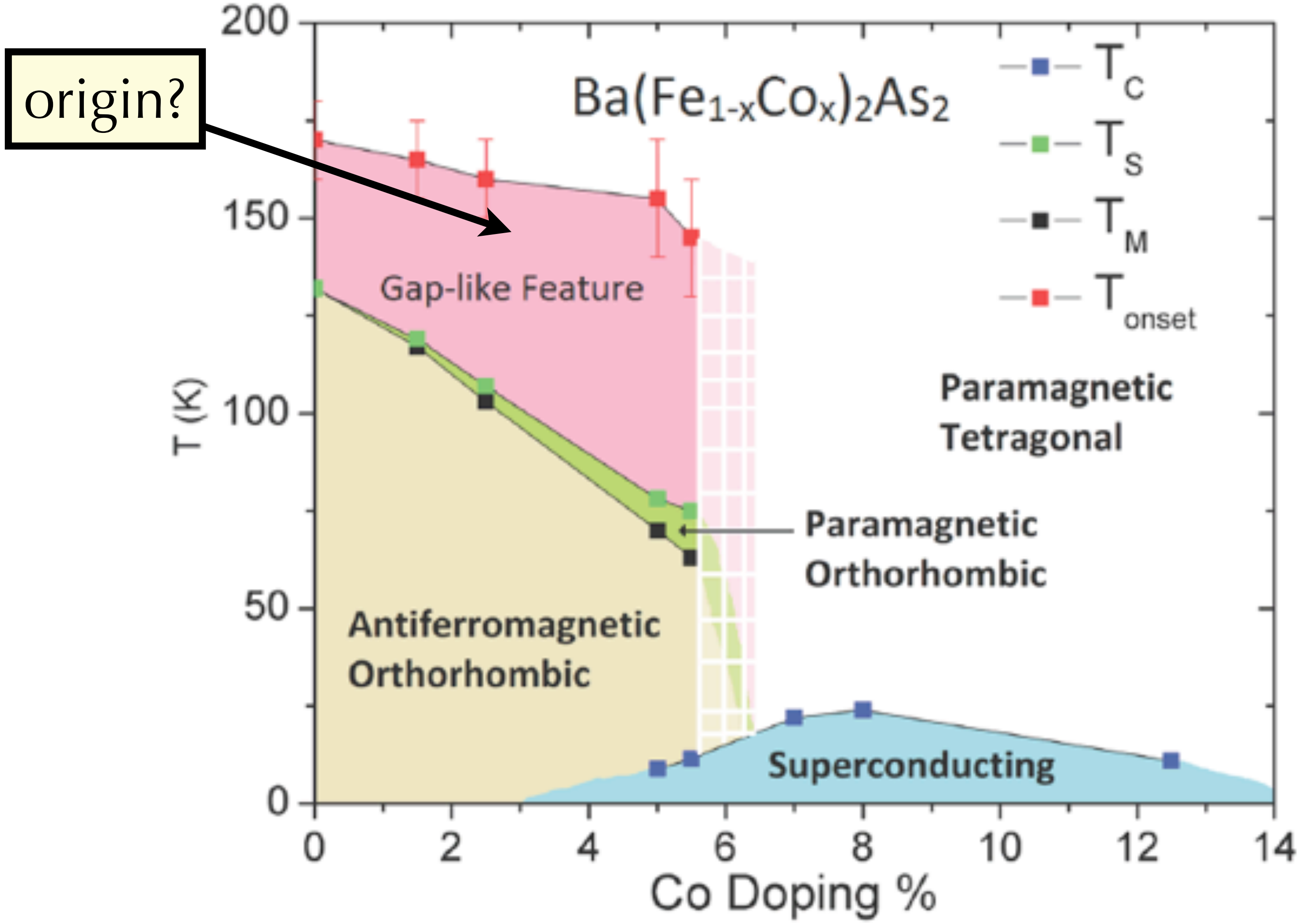
Experimental puzzle 2: What is the origin of the gap-like feature above the structural transition?





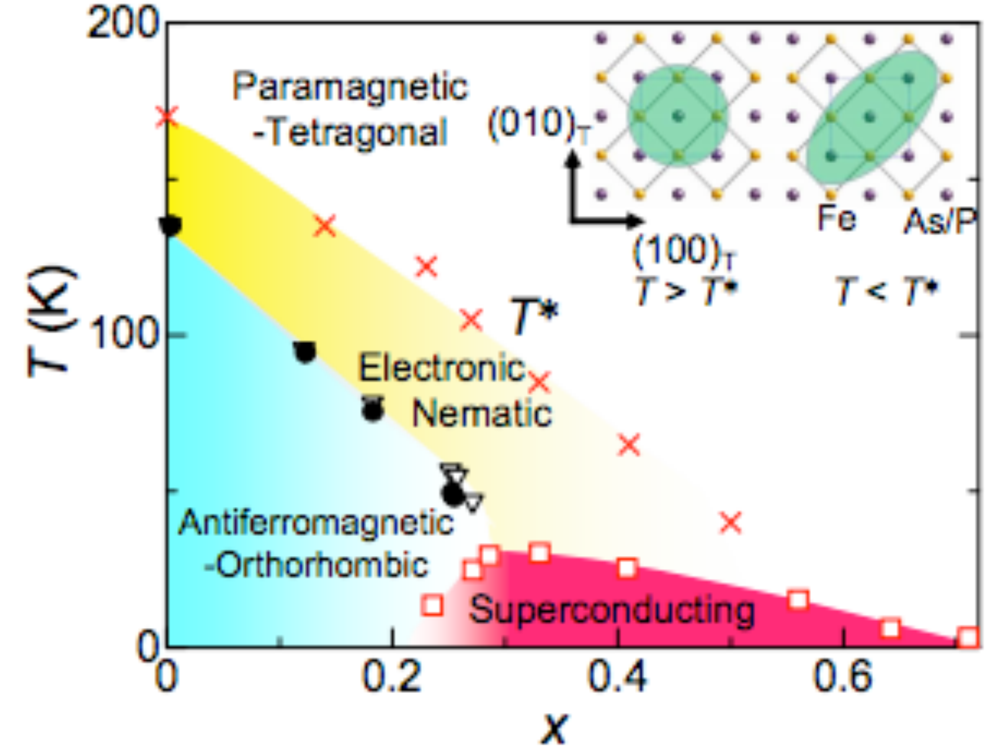
H. Ahram, L. Greene, ... (UIUC)

Crossover into a strongly correlated state on the underdoped side of the phase diagram



Greene, et al.

Nature 486, 382-385 (2012)

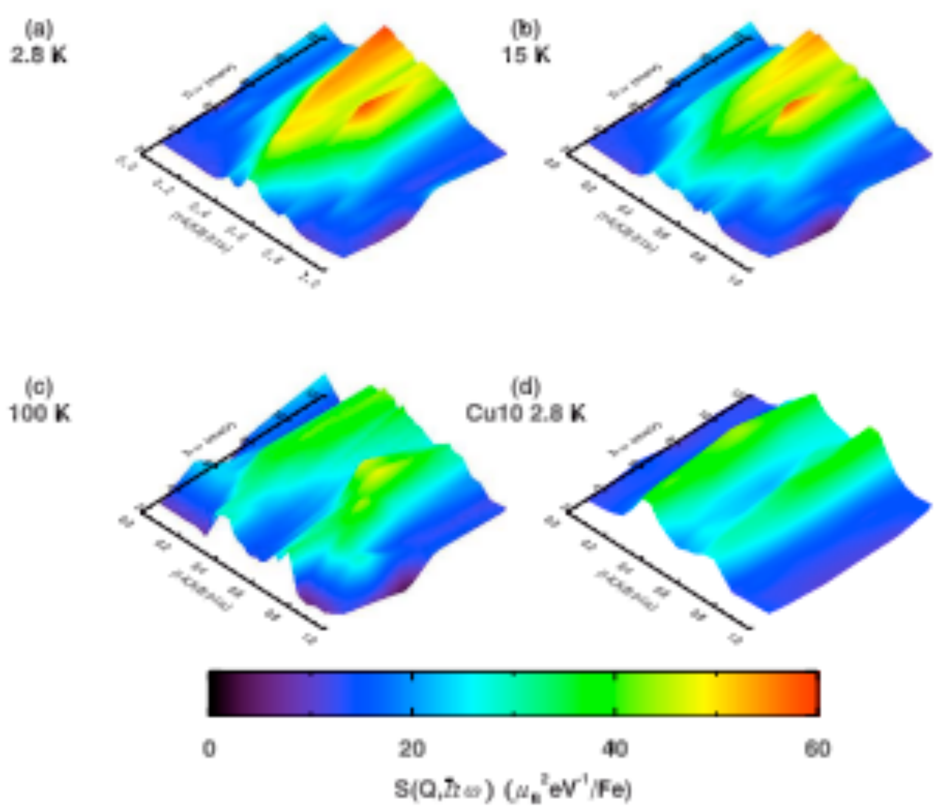


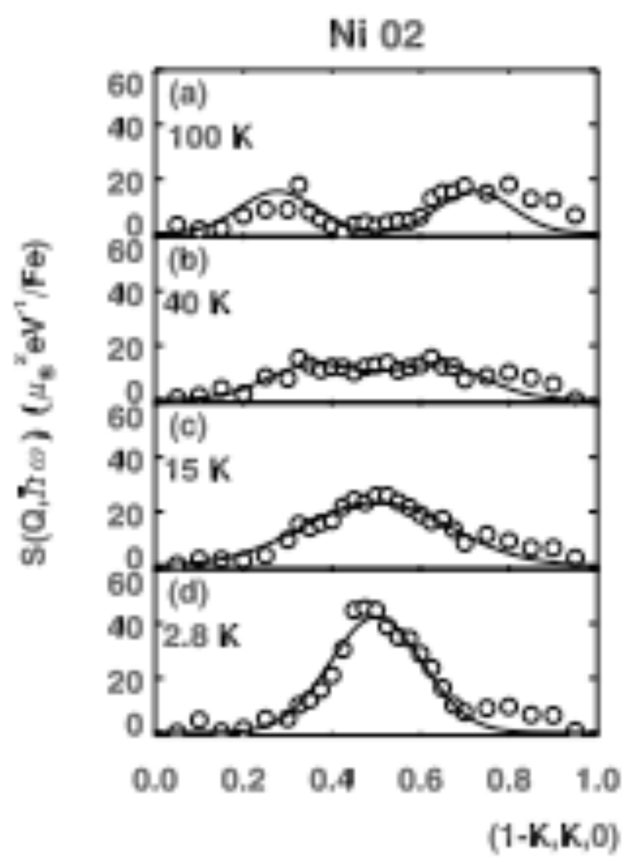
Matsuda, et al.

Experimental puzzle 3: What is the origin of the incommensurate-commensurate transition

Temperature-dependent transformation of the magnetic excitation spectrum on approaching superconductivity in $Fe_{1-x}(Ni/Cu)_xTe_{0.5}Se_{0.5}$

Zhijun Xu,[1,*] Jinsheng Wen,[1,2,3,*] Yang Zhao,[4,5] Masaaki Matsuda,[6] Wei Ku,[1] Xuerong Liu,[1] Genda Gu,[1] D.-H. Lee,[2,3] R. J. Birgeneau,[2,3] J. M. Tranquada,[1] and Guangyong Xu[1]
[1]*Condensed Matter Physics and Materials Science Department,*



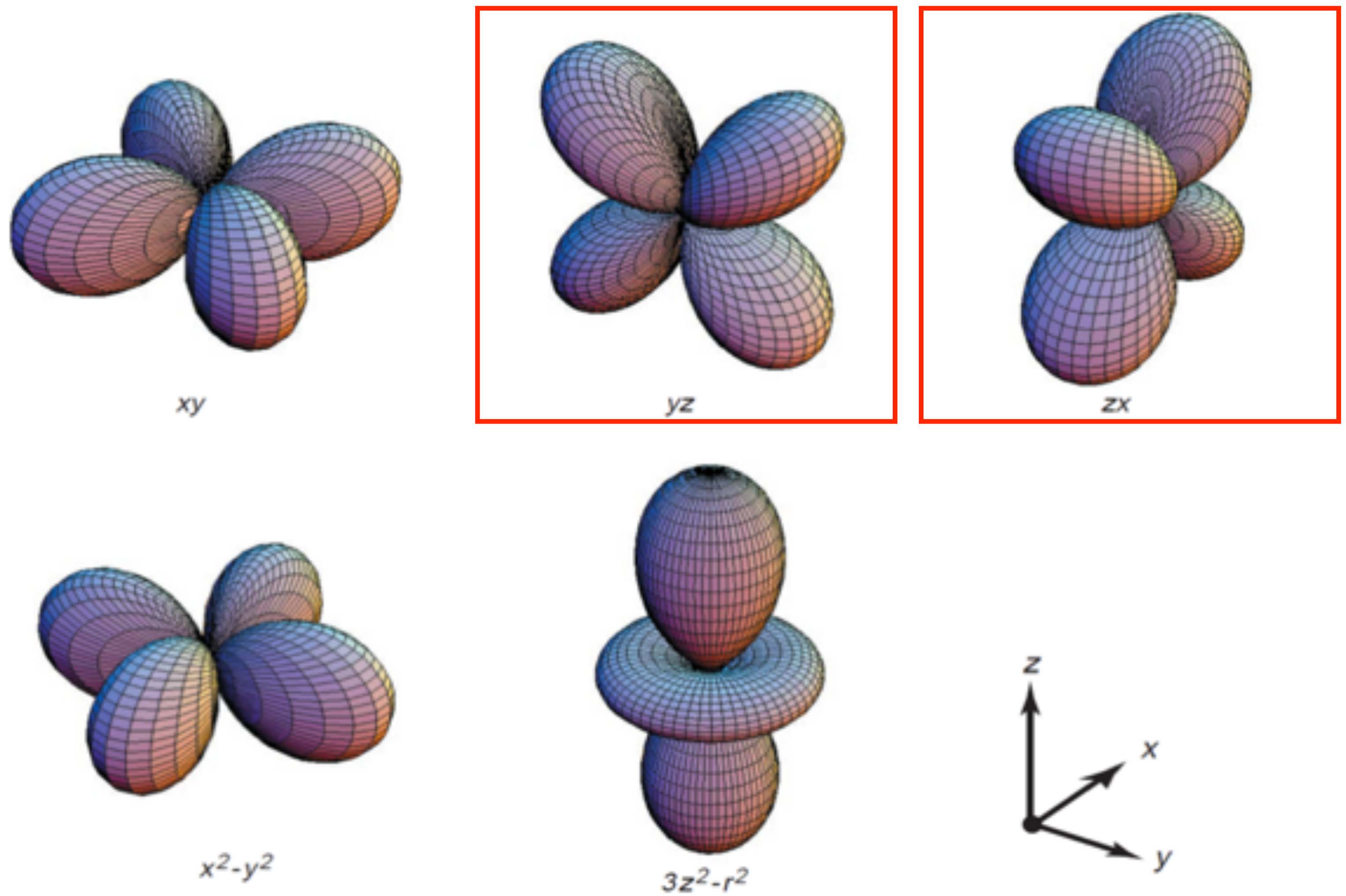


something besides spin degree of freedom

Orbital Ordering

t_{2g}

e_g

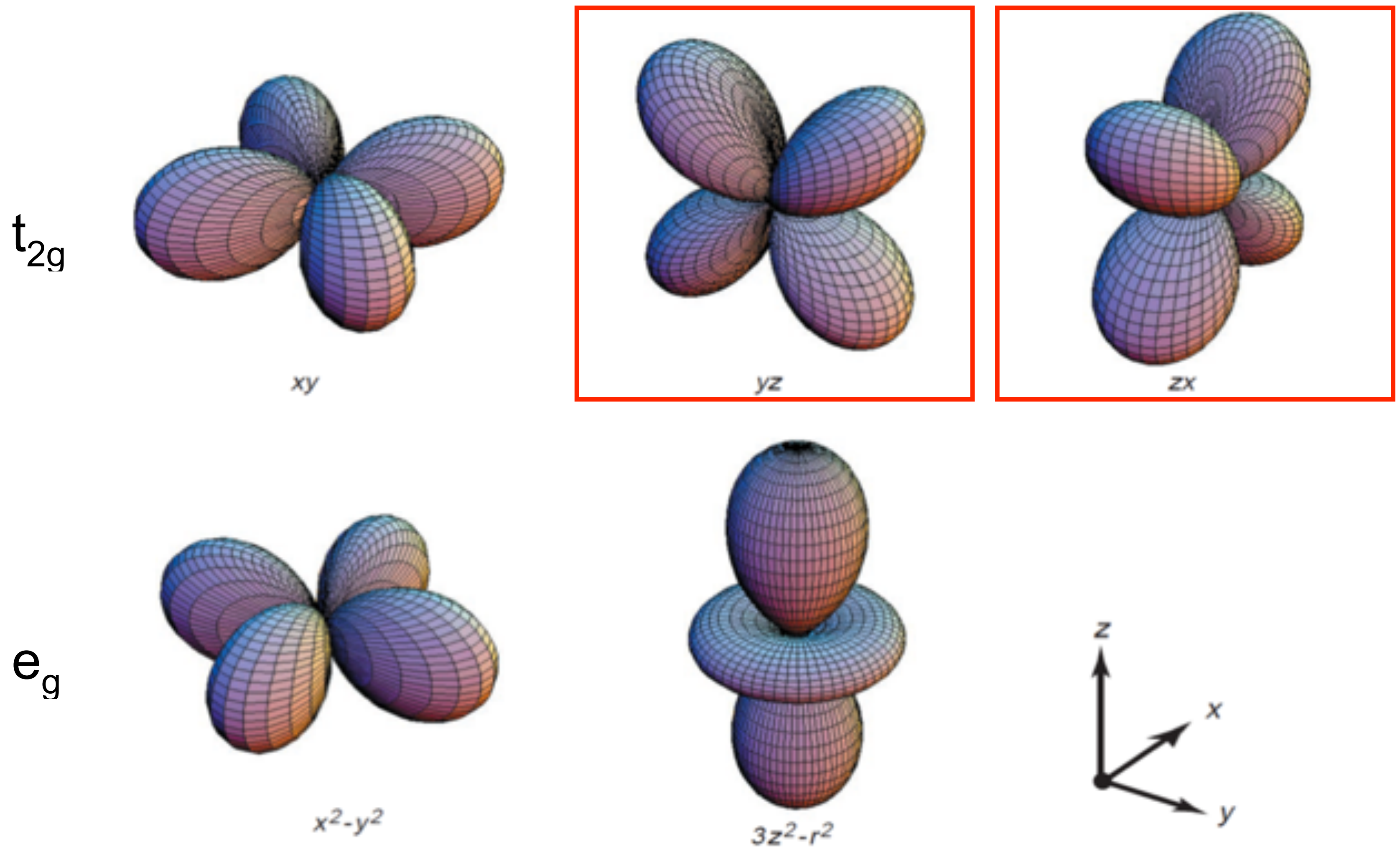


only d_yz and d_xz break rotational symmetry in xy plane.

Orbital Ordering

unequal occupancy of d_{xz} and d_{yz}

drive the structural transition, magnetism, ...

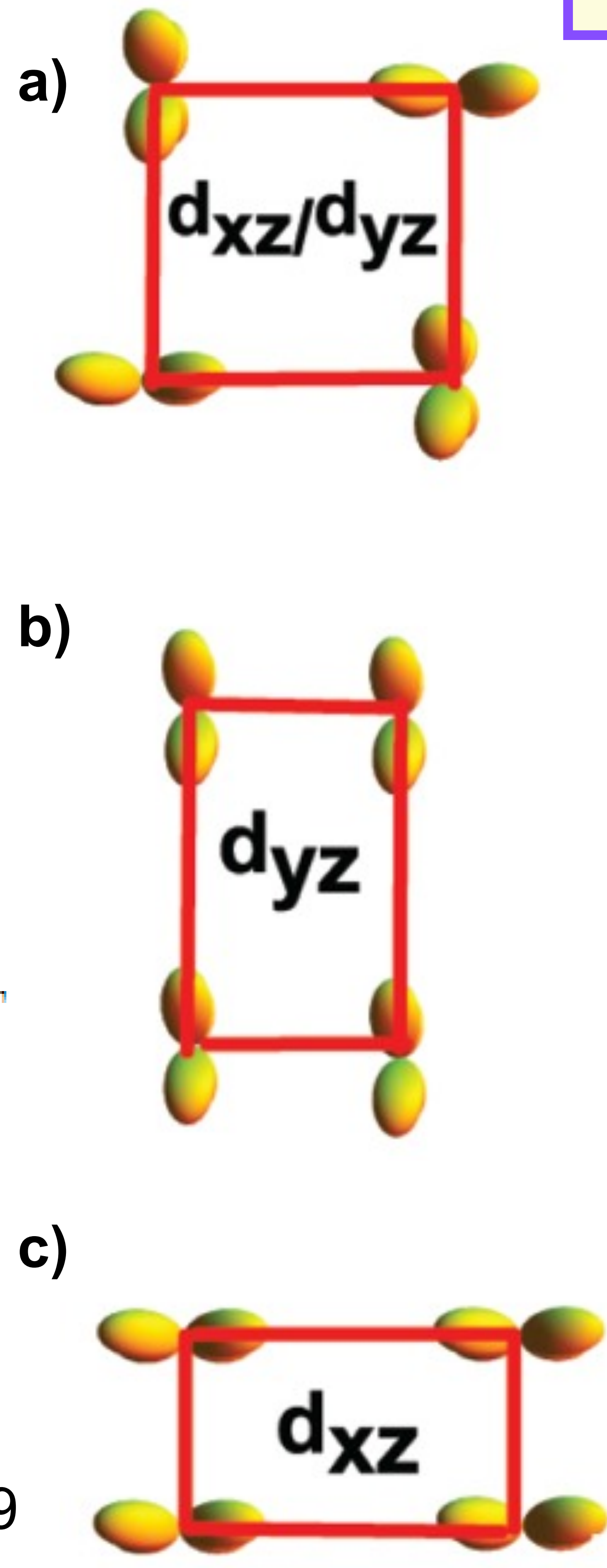


only d_yz and d_xz break rotational symmetry in xy plane.

structural transition

$T > T_{SPT}$

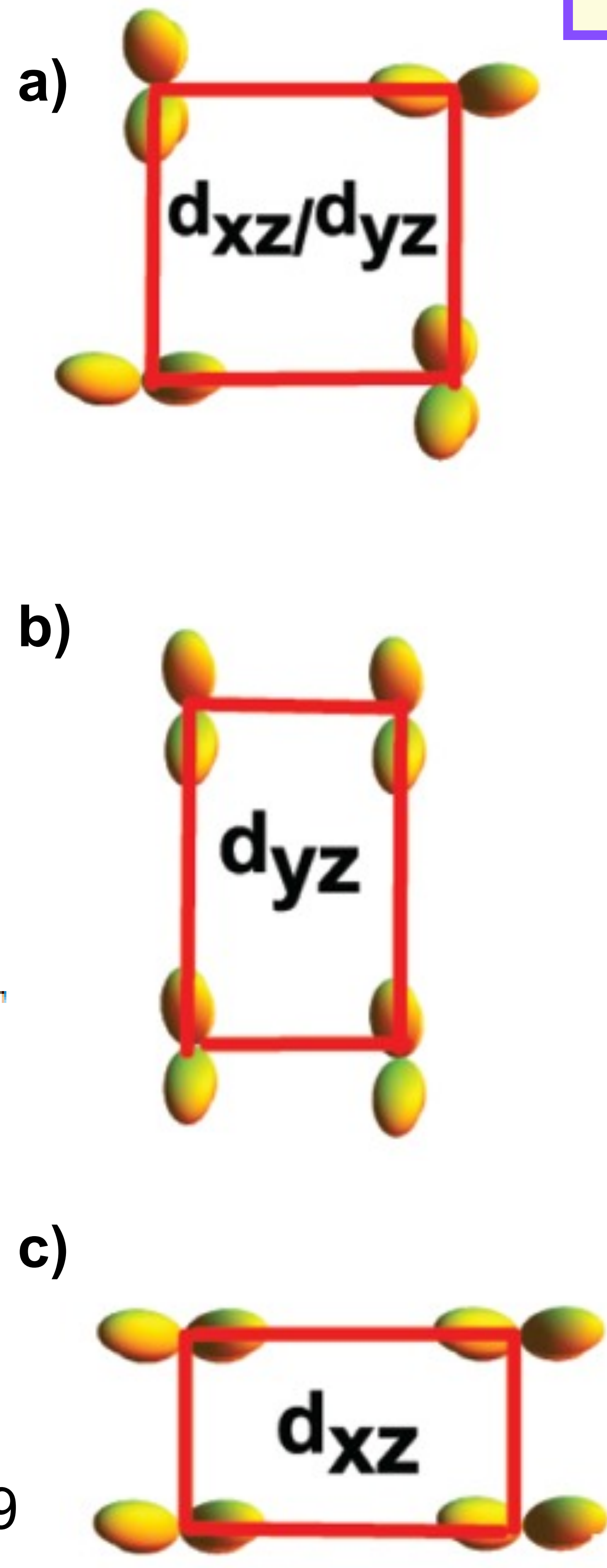
$T < T_{SPT}$



Lv, Wu, PP, 2009

structural transition

$T > T_{SPT}$



$T < T_{SPT}$

Coulomb Repulsion:

$$U = e^2 \int |\psi_{i_1 m_1}(\mathbf{r})|^2 \frac{e^{-|\mathbf{r}-\mathbf{r}'|/r_0}}{|\mathbf{r}-\mathbf{r}'|} |\psi_{i_2 m_2}(\mathbf{r}')|^2$$

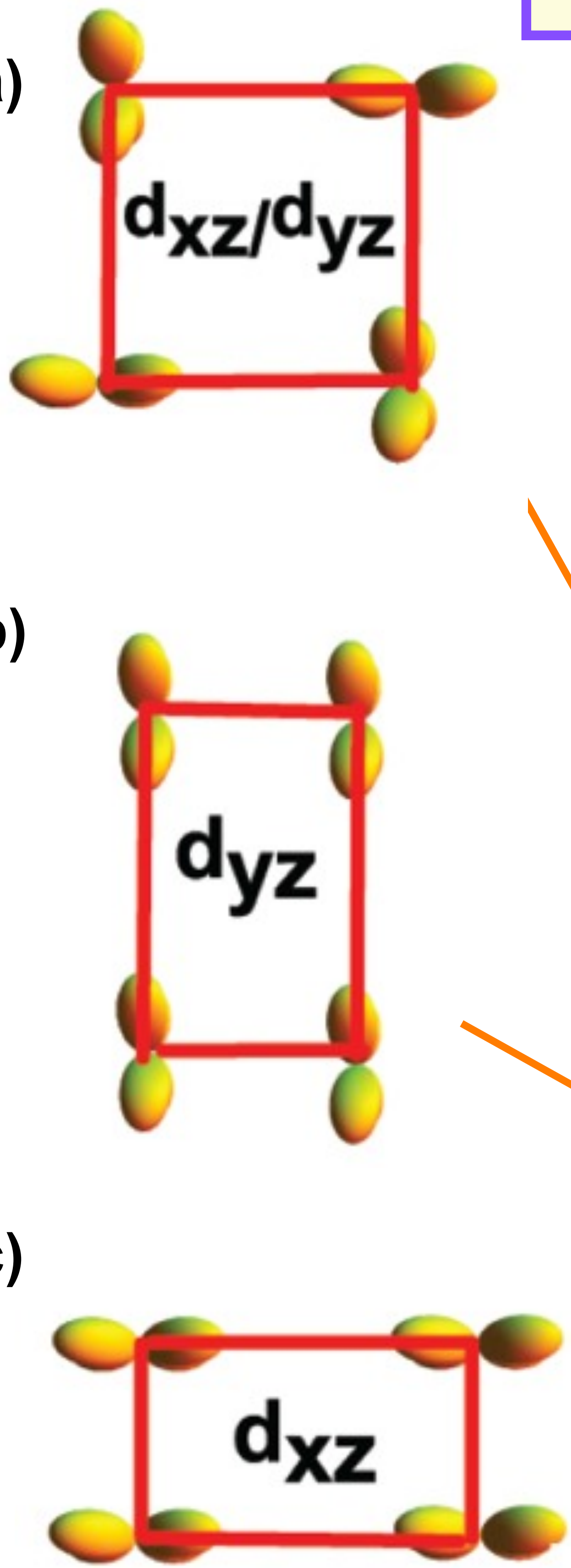
Energy Difference:

$$\Delta(\delta) = \frac{U_b(\delta) - U_a}{U_a}$$

Lv, Wu, PP, 2009

structural transition

$T > T_{SPT}$



$T < T_{SPT}$

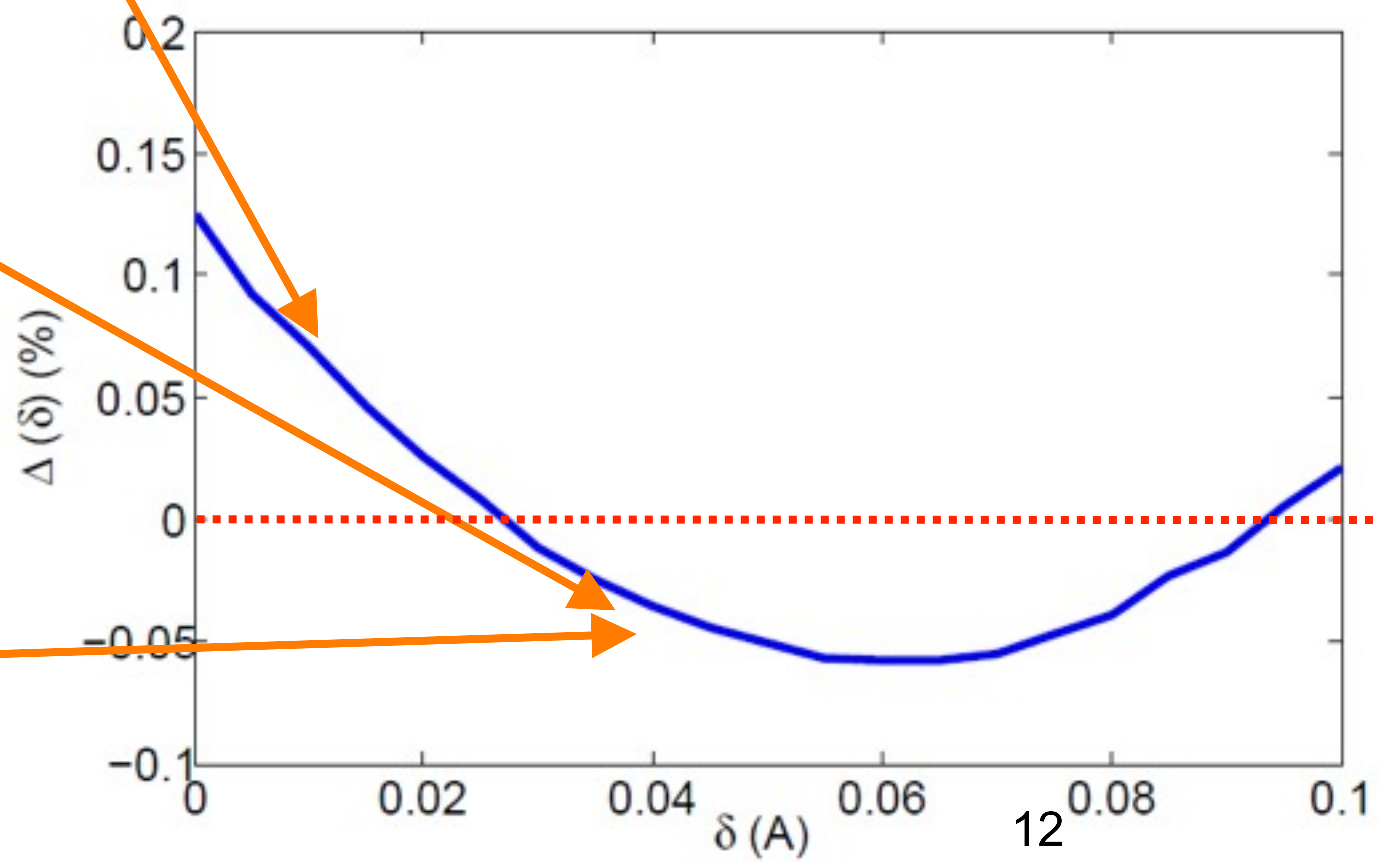
Lv, Wu, PP, 2009

Coulomb Repulsion:

$$U = e^2 \int |\psi_{i_1 m_1}(\mathbf{r})|^2 \frac{e^{-|\mathbf{r}-\mathbf{r}'|/r_0}}{|\mathbf{r}-\mathbf{r}'|} |\psi_{i_2 m_2}(\mathbf{r}')|^2$$

Energy Difference:

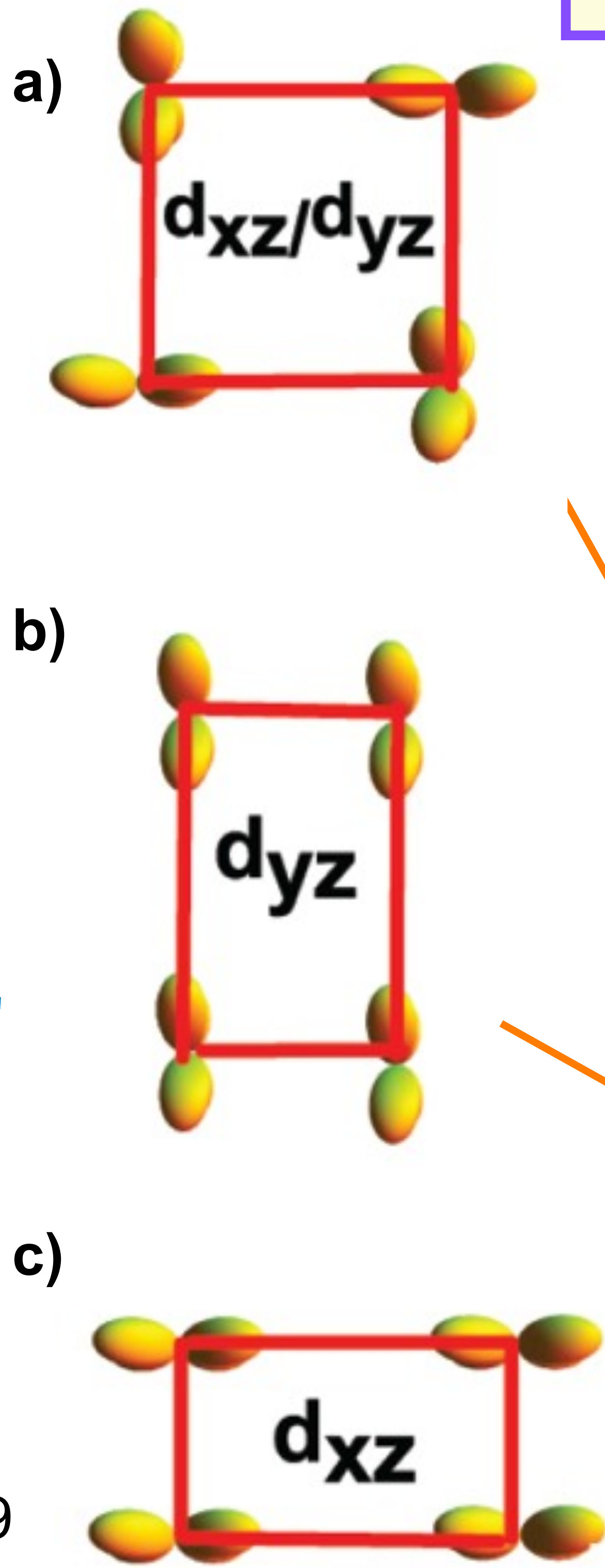
$$\Delta(\delta) = \frac{U_b(\delta) - U_a}{U_a}$$



structural transition

$T > T_{SPT}$

a)



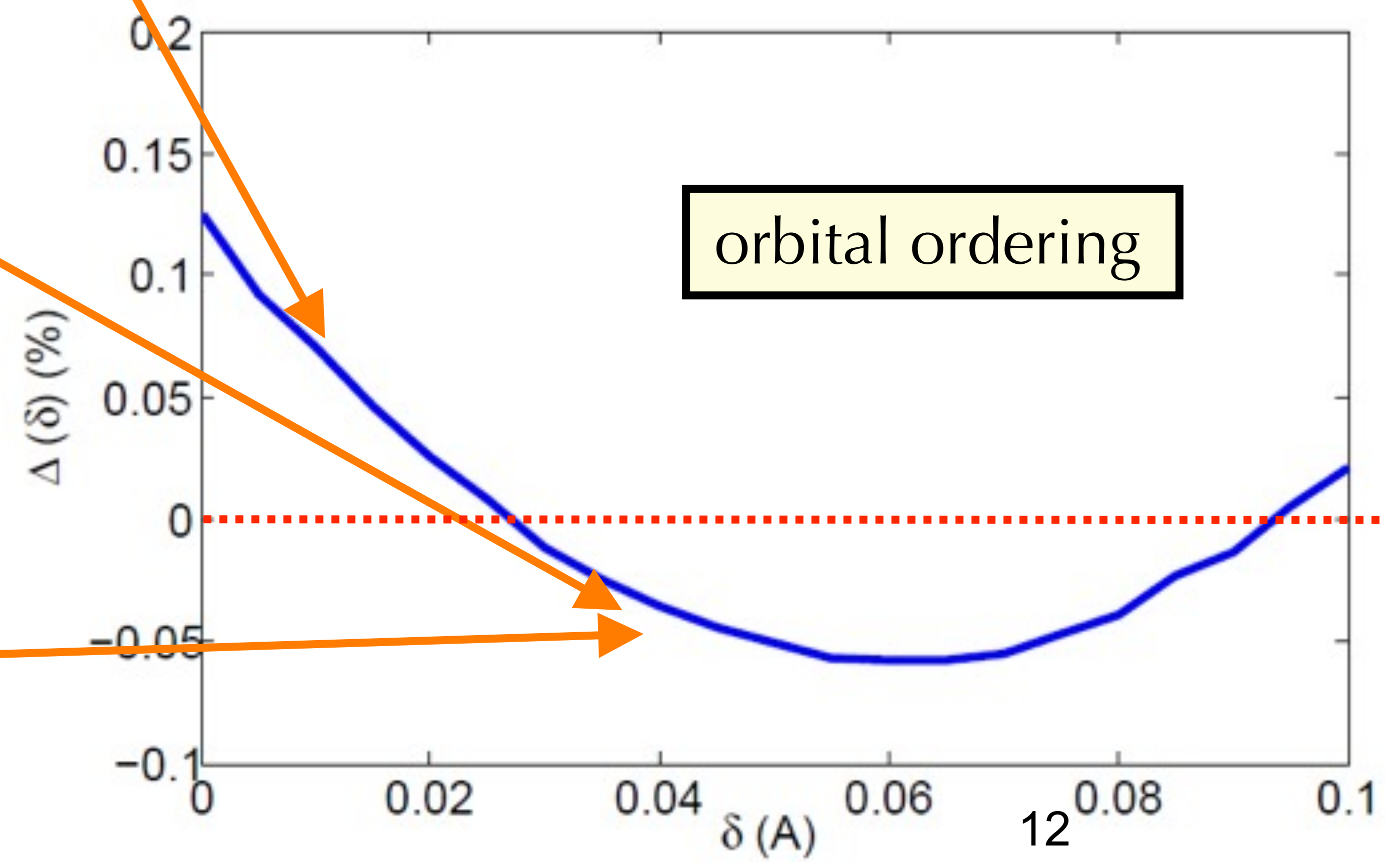
$T < T_{SPT}$

Coulomb Repulsion:

$$U = e^2 \int |\psi_{i_1 m_1}(\mathbf{r})|^2 \frac{e^{-|\mathbf{r}-\mathbf{r}'|/r_0}}{|\mathbf{r}-\mathbf{r}'|} |\psi_{i_2 m_2}(\mathbf{r}')|^2$$

Energy Difference:

$$\Delta(\delta) = \frac{U_b(\delta) - U_a}{U_a}$$



Lv, Wu, PP, 2009

SPT in Ising Universality Class

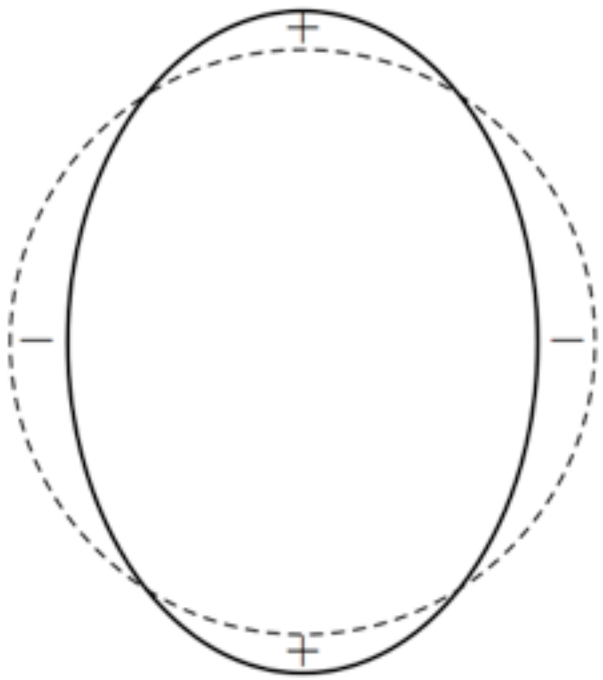
$$H_{\mathrm{SPT}} = -J_{\mathrm{SPT}} \sum_{\langle i,j \rangle} M_i M_j$$

$$M_i = \pm 1, i = d_{yz}, d_{xz}$$

structural transition=nematic?

structural transition=nematic?

electron nematic

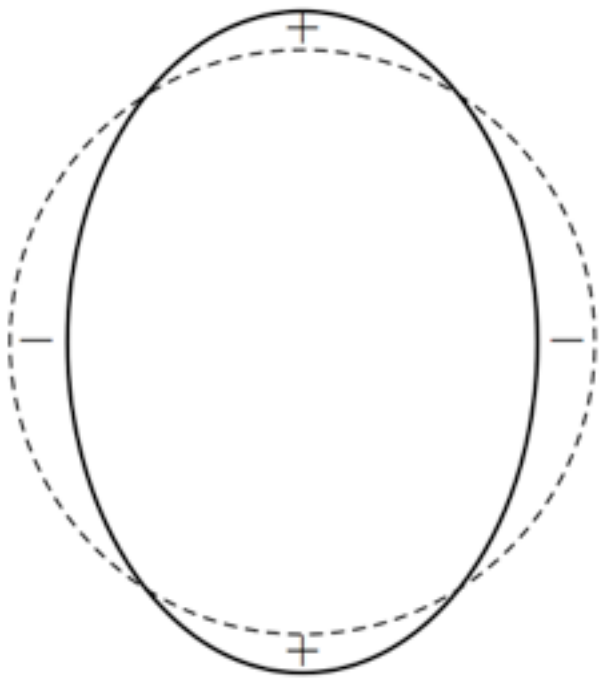


continuous symmetry breaking

goldstone boson

structural transition=nematic?

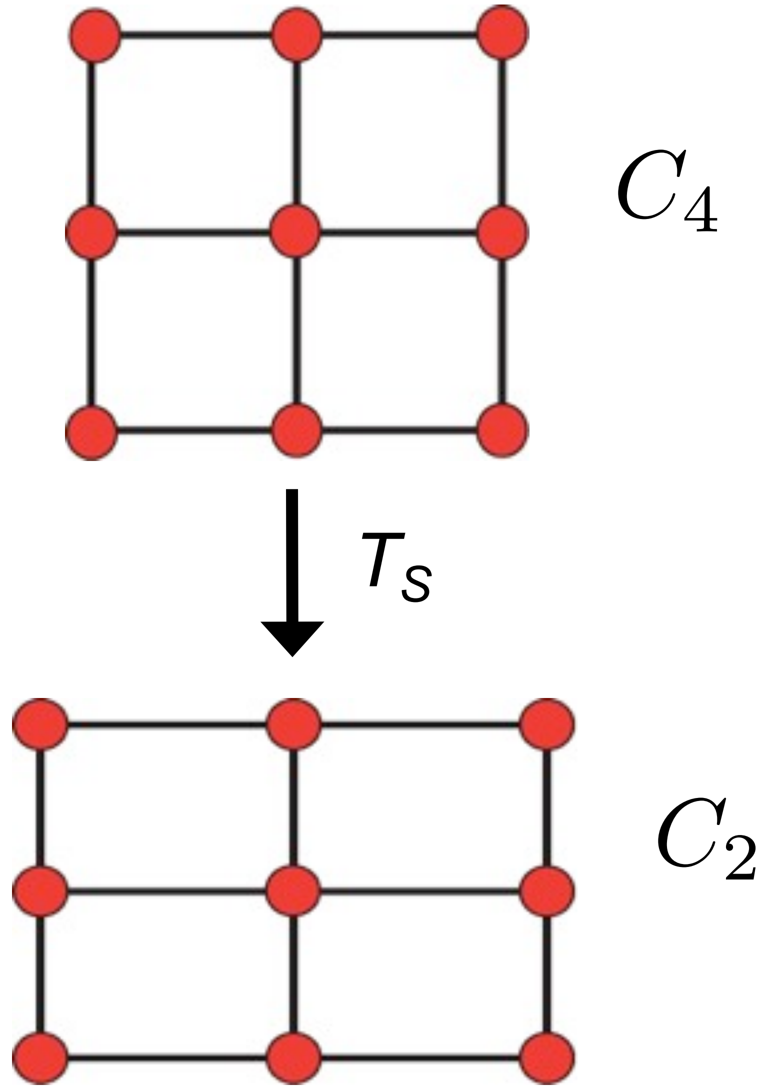
electron nematic



continuous symmetry breaking

goldstone boson

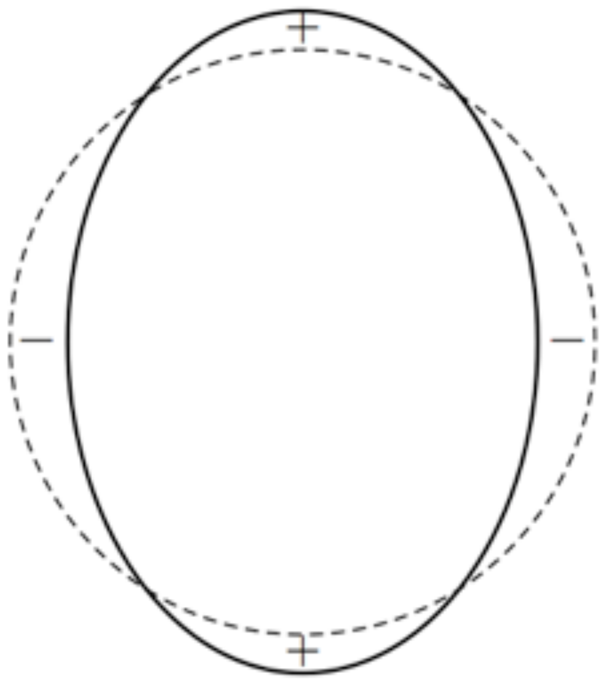
pnictides



no goldstone boson

structural transition=nematic?

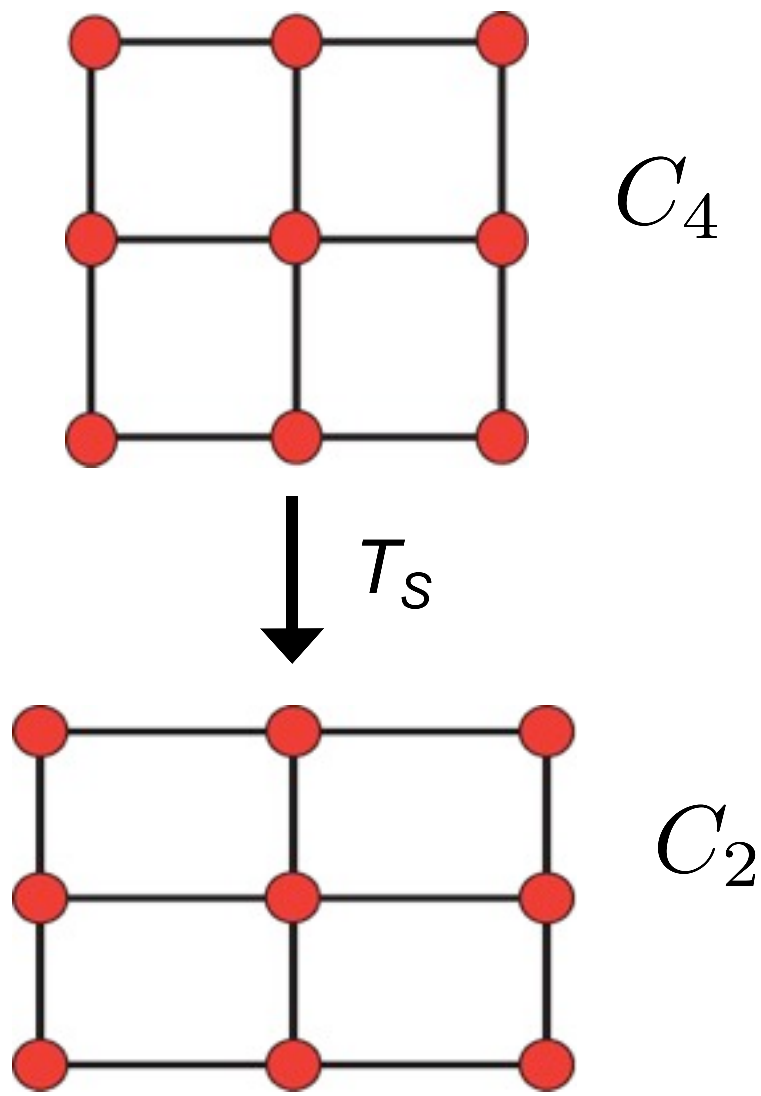
electron nematic



continuous symmetry breaking

goldstone boson

pnictides



no goldstone boson

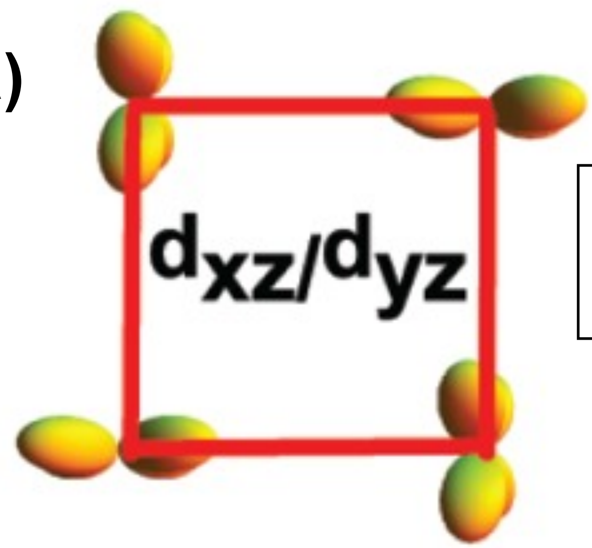
not really but this is not stopping anyone

SPT-induced Collinear AF

SPT-induced Collinear AF

$T > T_{SPT}$

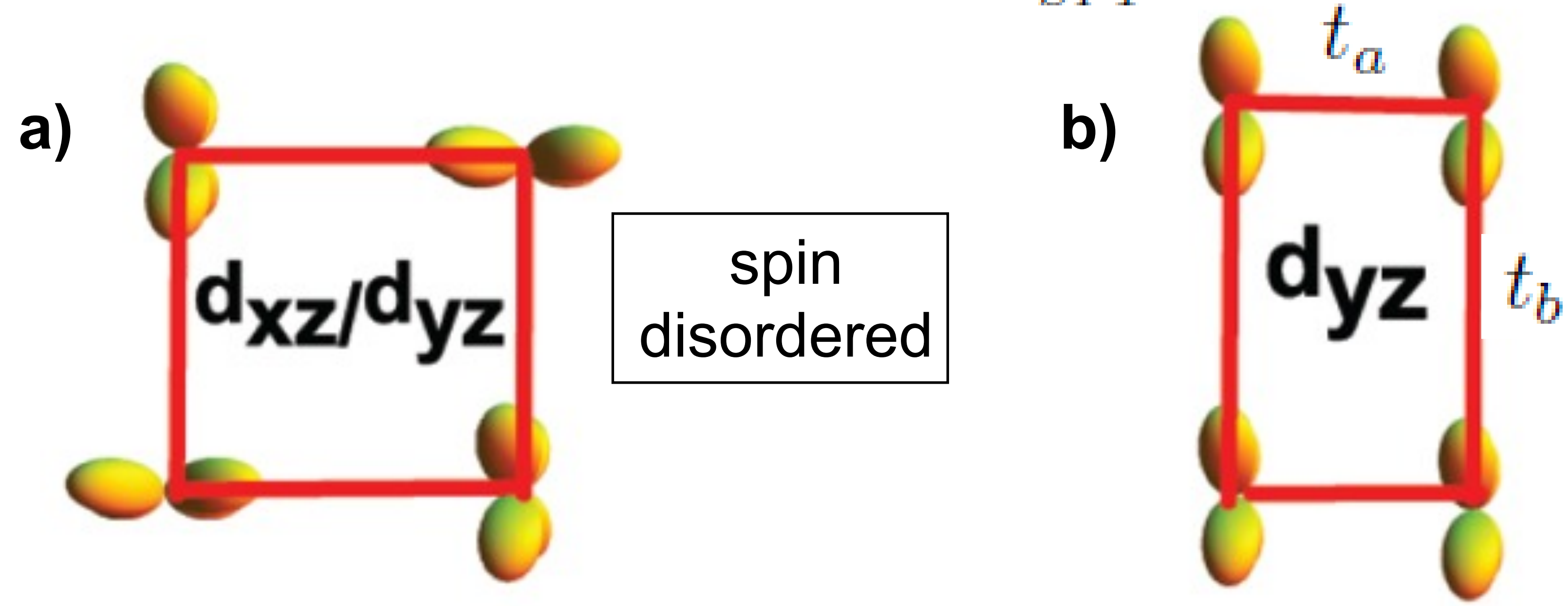
a)



spin disordered

SPT-induced Collinear AF

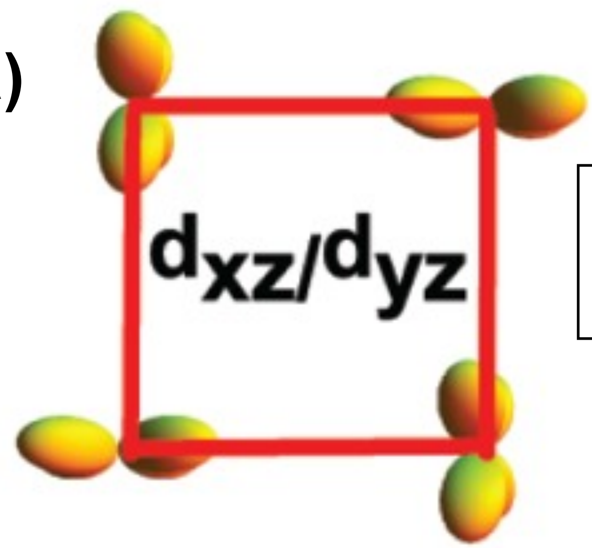
$T > T_{SPT}$ $T < T_{SPT}$



SPT-induced Collinear AF

$T > T_{SPT}$

a)



spin
disordered

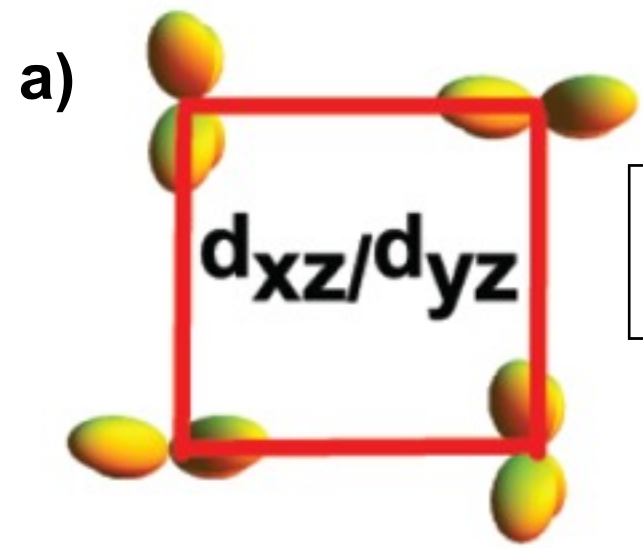
$T < T_{SPT}$

b)

$$t_b > t_a$$
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$

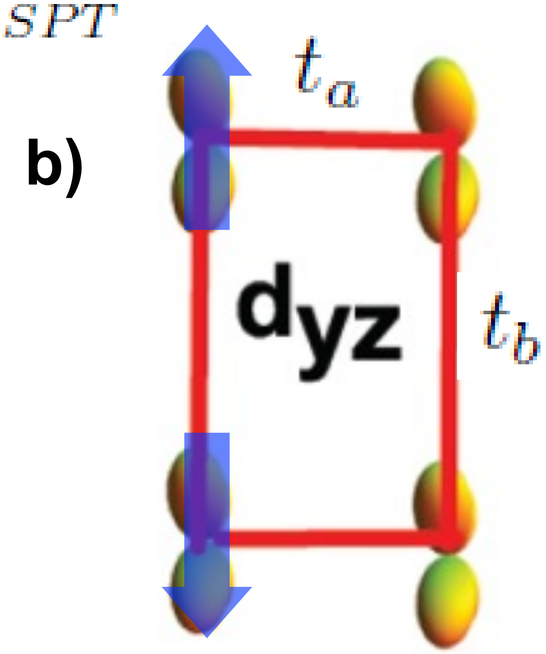
SPT-induced Collinear AF

$T > T_{SPT}$



spin disordered

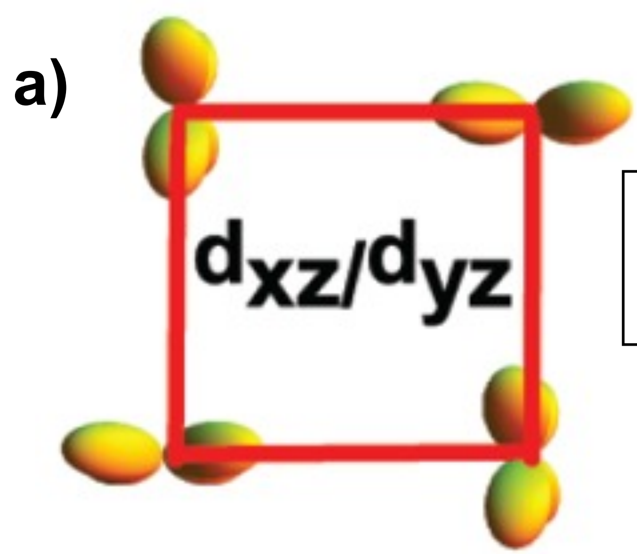
$T < T_{SPT}$



$$t_b > t_a$$
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$

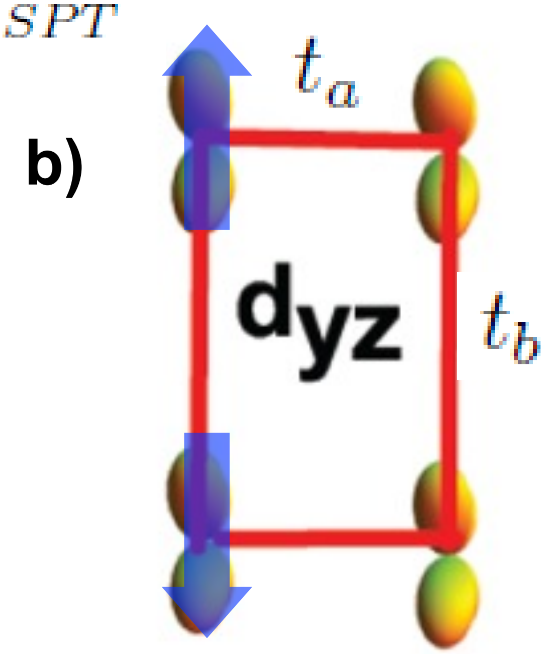
SPT-induced Collinear AF

$T > T_{SPT}$



spin disordered

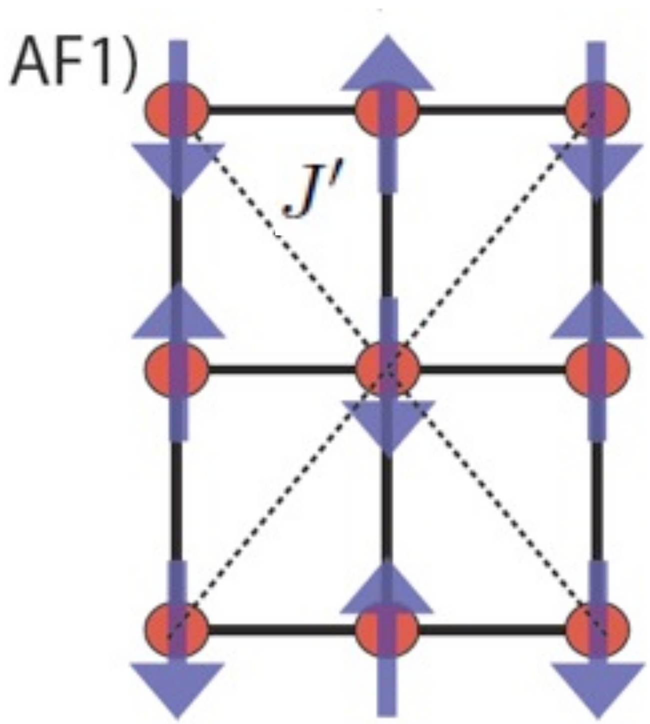
$T < T_{SPT}$



$$t_b > t_a$$

$$J \sim \frac{t^2}{U}$$

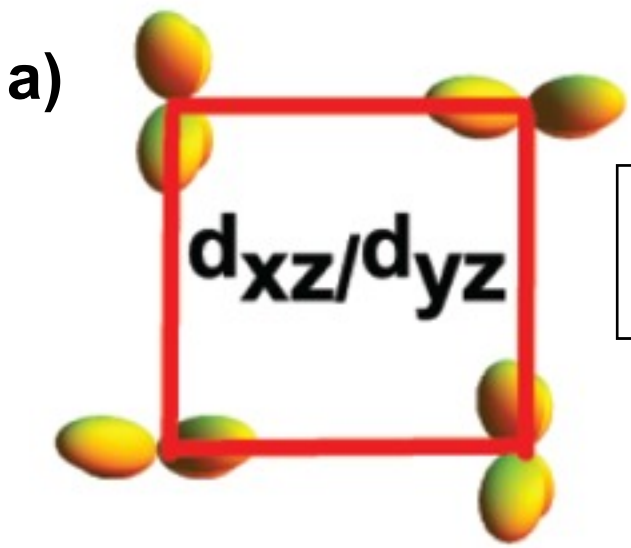
$$J_b > J_a$$



$$E_1 = -2J_a + 4J'$$

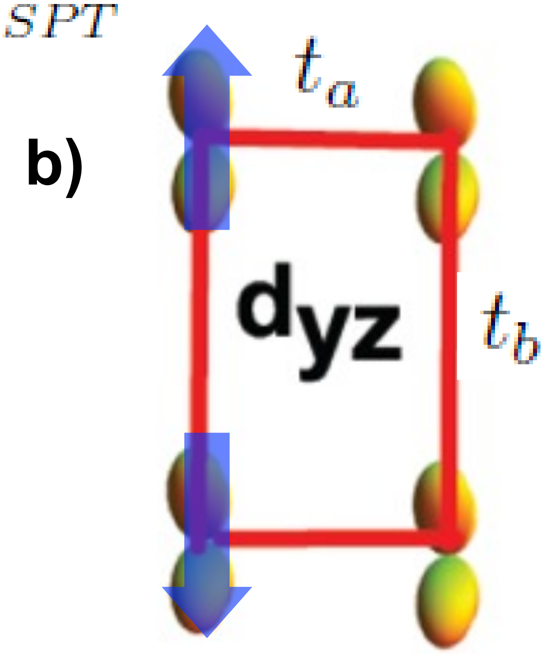
SPT-induced Collinear AF

$T > T_{SPT}$

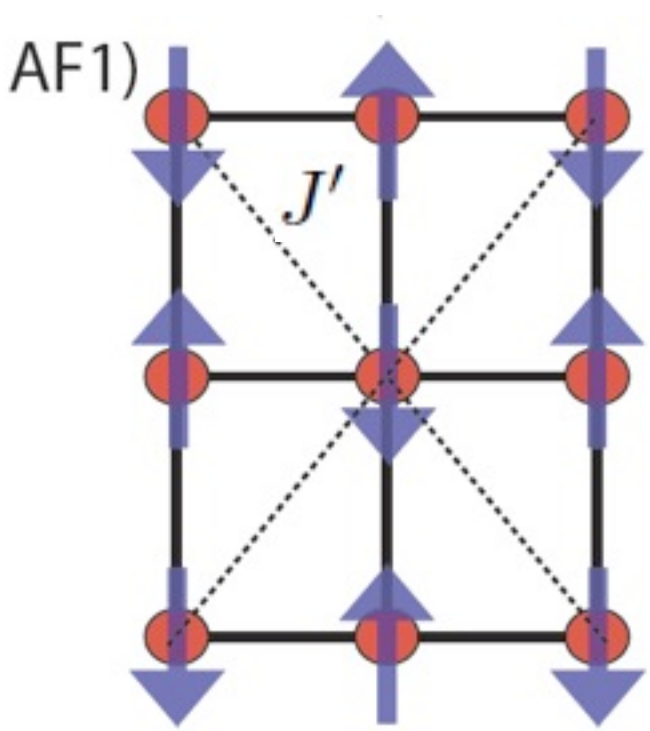


spin disordered

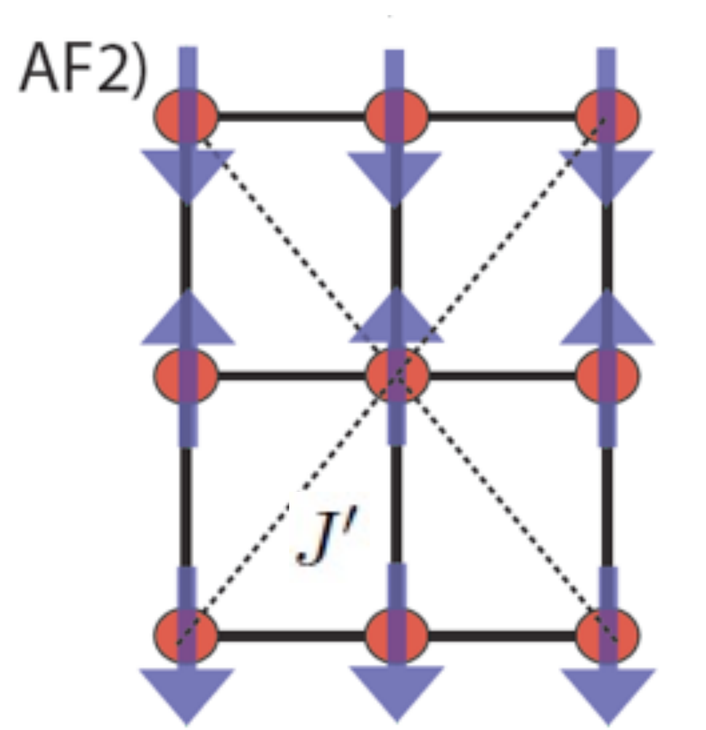
$T < T_{SPT}$



$$t_b > t_a$$
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$



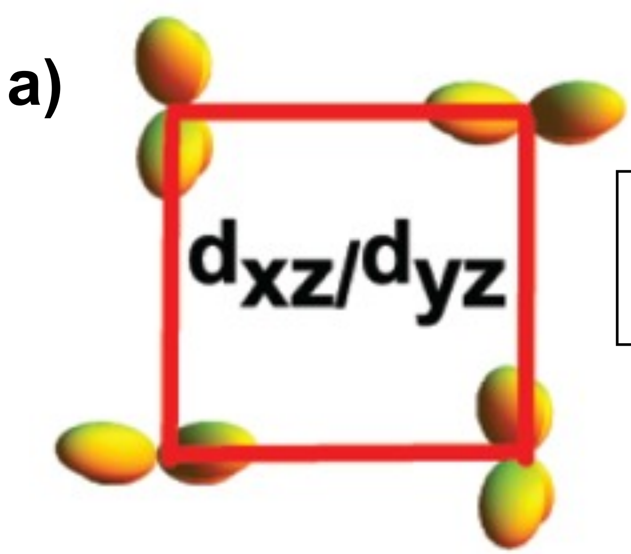
$$E_1 = -2J_a + 4J'$$



$$E_2 = +2J_a - 4J'$$

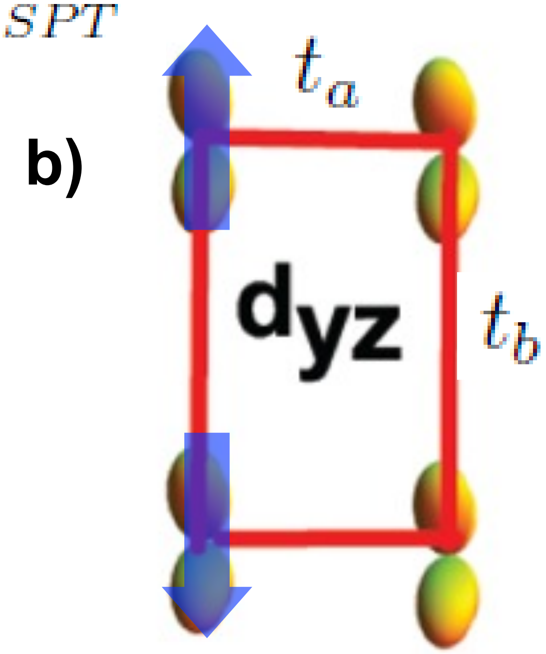
SPT-induced Collinear AF

$T > T_{SPT}$

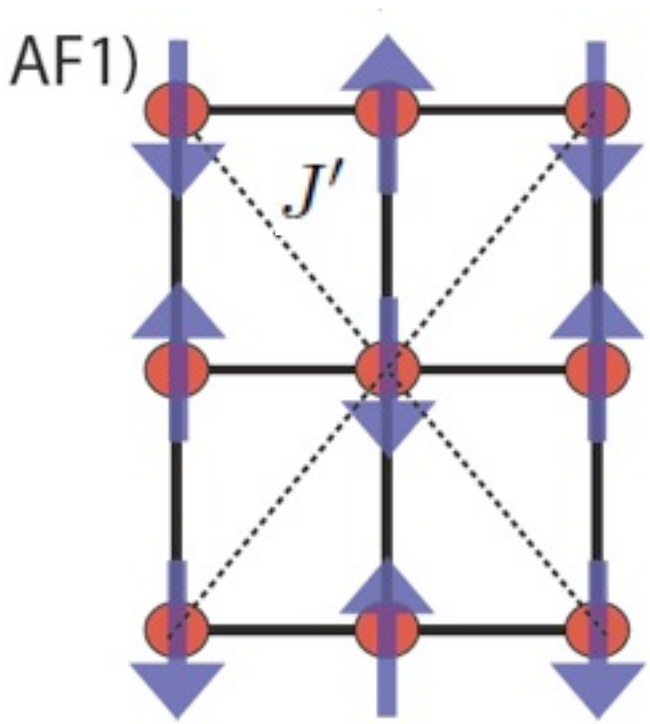


spin disordered

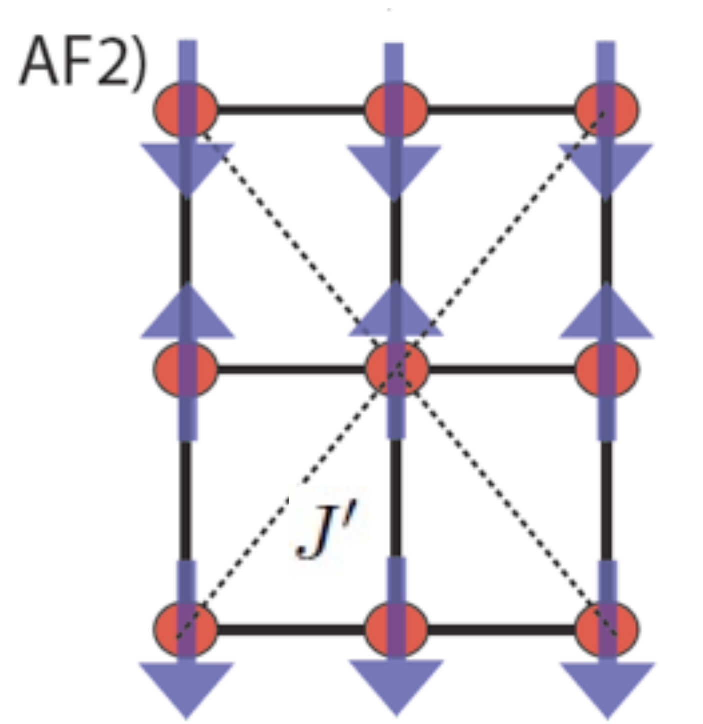
$T < T_{SPT}$



$$t_b > t_a$$
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$



$$E_1 = -2J_a + 4J'$$



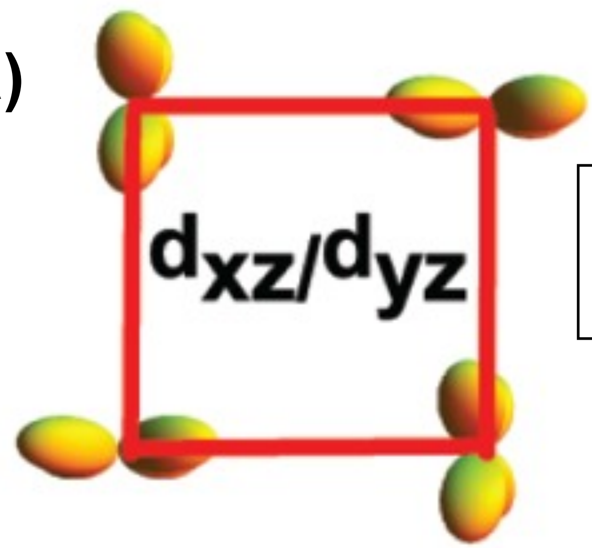
$$E_2 = +2J_a - 4J'$$

$$J' > \frac{J_a}{2}$$

SPT-induced Collinear AF

$T > T_{SPT}$

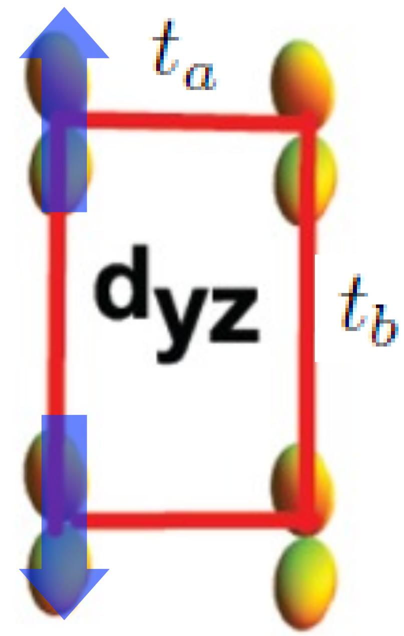
a)



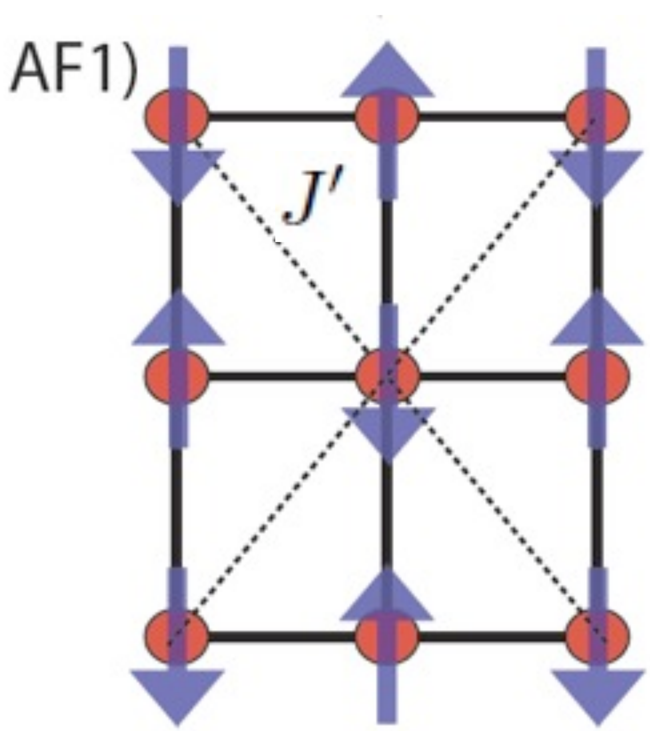
spin disordered

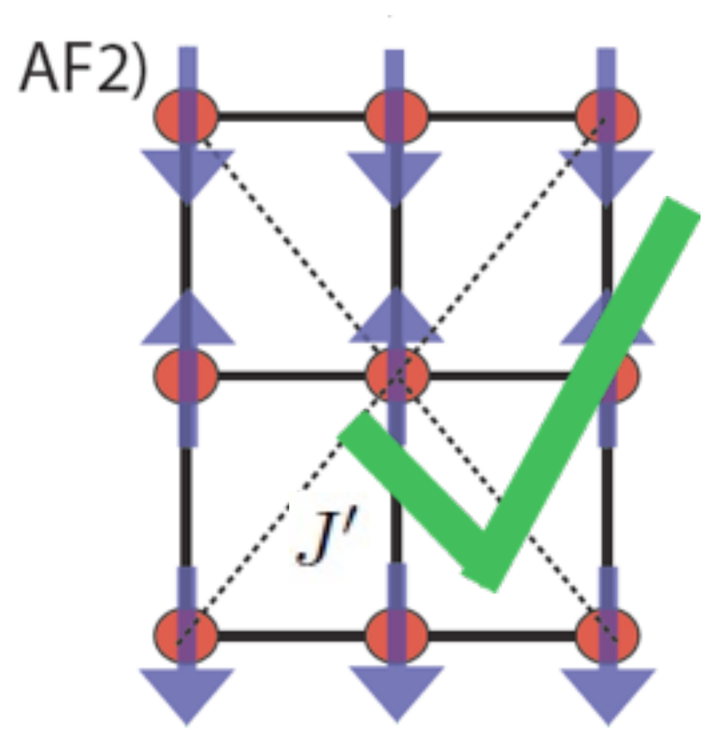
$T < T_{SPT}$

b)



$$t_b > t_a$$
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$





$$J' > \frac{J_a}{2}$$

$$E_1 = -2J_a + 4J'$$

$$E_2 = +2J_a - 4J'$$

SPT-induced magnetism

$$H_{\mathrm{SO}} = J_{\mathrm{SPT}} \sum_{\langle i,j \rangle} M_i M_j + \sum_{\langle\langle i,j \rangle\rangle} J_2 \left(M_i, M_j \right) \mathbf{S}_i \cdot \mathbf{S}_\mathbf{j}$$
$$+ \sum_i J_{1x} \left(M_i, M_{i+\hat{x}} \right) \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}}$$
$$+ \sum_i J_{1y} \left(M_i, M_{i+\hat{y}} \right) \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}}$$

$$J_{1x} \left(M_i, M_j \right) = \delta_{M_i, M_j} \left(J_{1b} \delta_{M_i,1} + J_{1a} \delta_{M_i,-1} \right)$$
$$J_{1y} \left(M_i, M_j \right) = \delta_{M_i, M_j} \left(J_{1a} \delta_{M_i,1} + J_{1b} \delta_{M_i,-1} \right)$$
$$J_2 \left(M_i, M_j \right) = \delta_{M_i, M_j} J_2$$

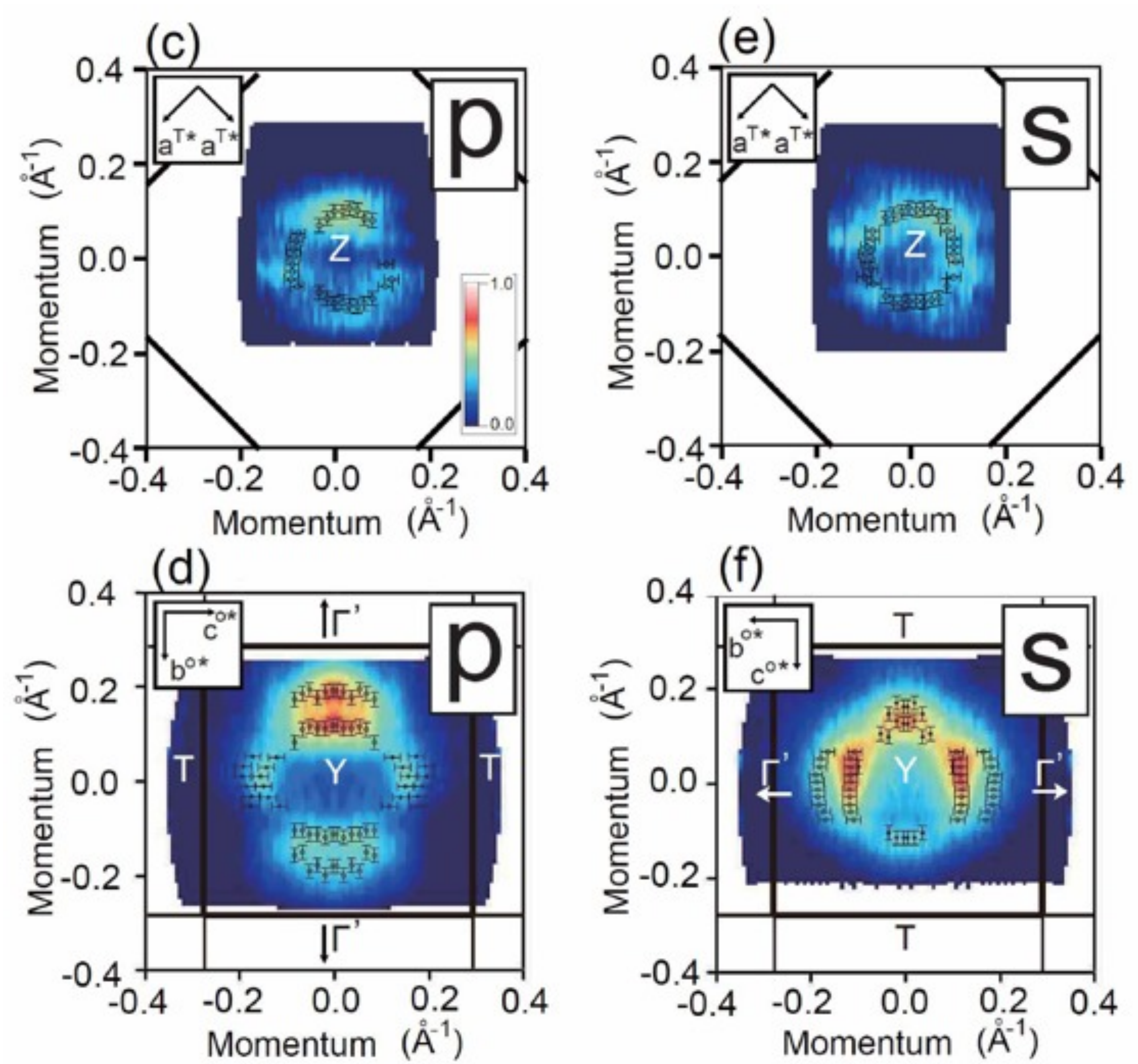
$$M_i = \pm 1, i = d_{yz}, d_{xz}$$

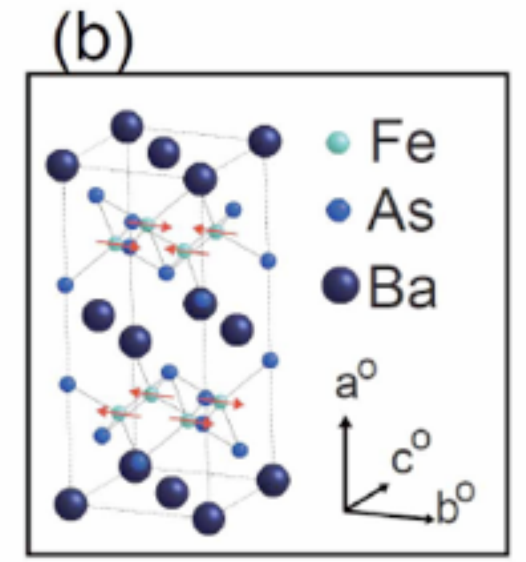
122 Fe-Fe is shorter: J_{1b} is enhanced

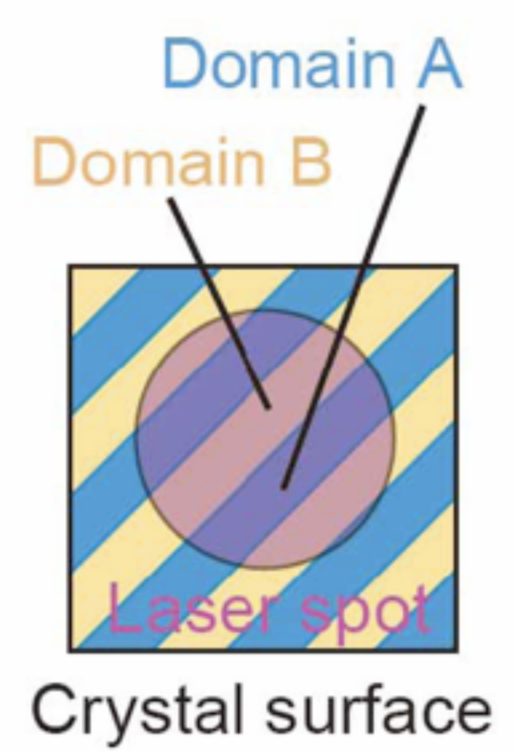
Orbital-polarized Fermi surface in antiferromagnetic state of $BaFe_2As_2$

Shimojima, et al.
arXiv:0904.1632

- **Polarized ARPES**



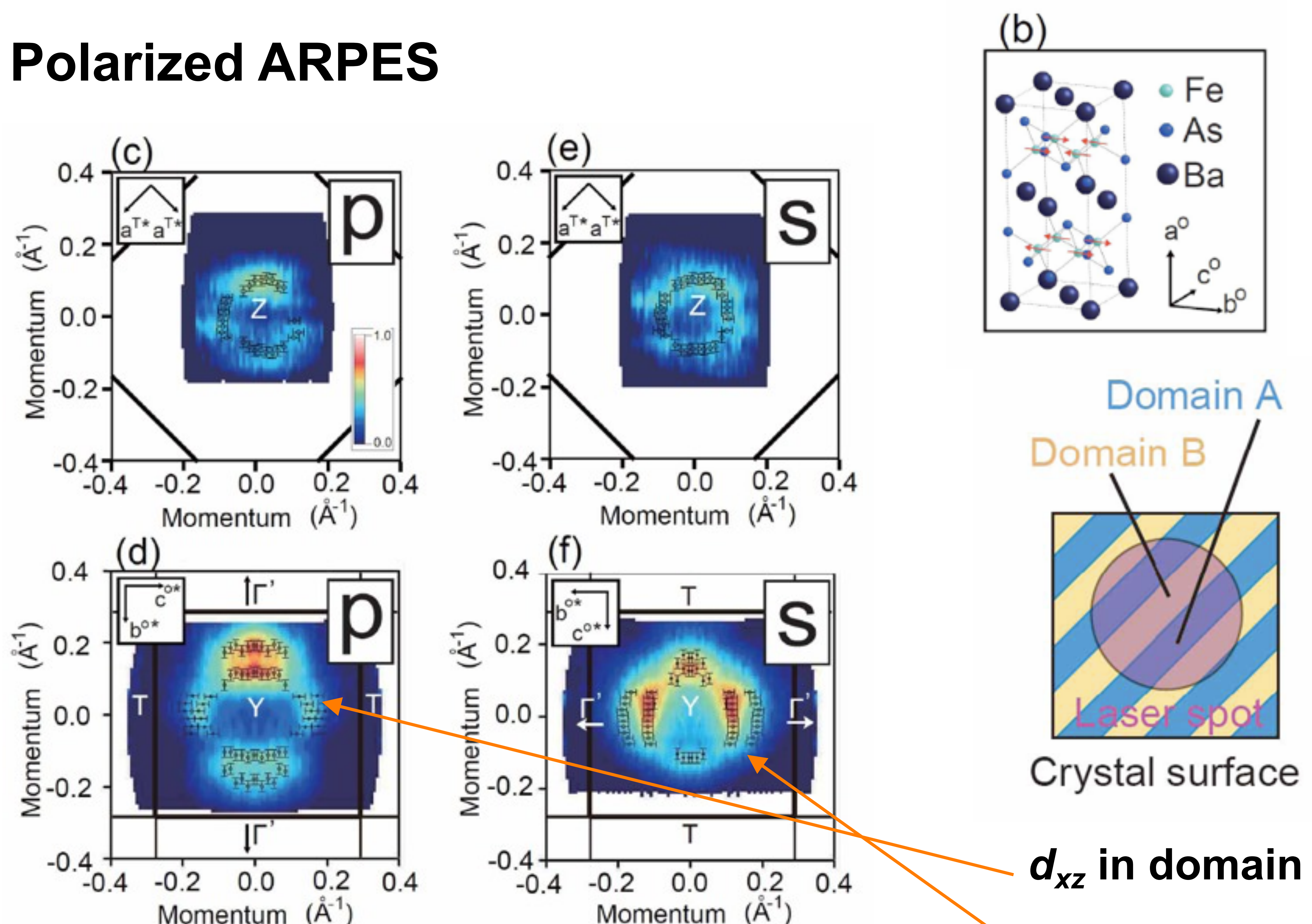




Orbital-polarized Fermi surface in antiferromagnetic state of $BaFe_2As_2$

Shimojima, et al.
arXiv:0904.1632

- **Polarized ARPES**



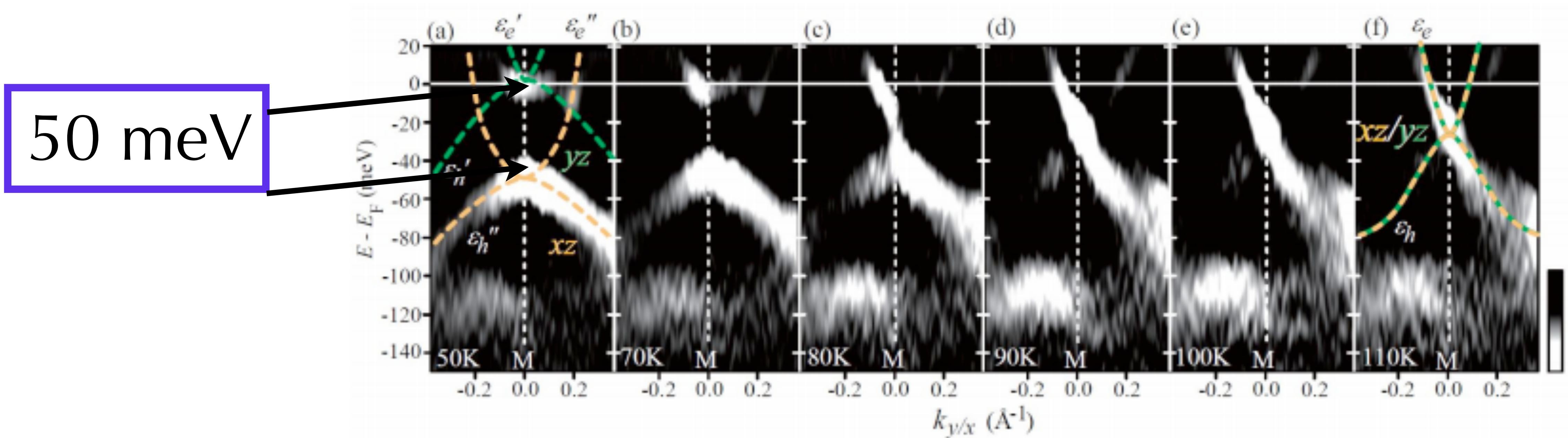
***d$_{xz}$* in domain A**

***d$_{xz}$* in domain B**

Lifting of *xz/yz* orbital degeneracy at the structural transition in detwinned FeSe

T. Shimojima[1,*], Y. Suzuki[1], T. Sonobe[1], A. Nakamura[1], M. Sakano[1], J. Omachi[2], K. Yoshioka[3], M. Kuwata-Gonokami[2,3], K. Ono[4], H. Kumigashira[4], A. E. Böhmer[5], F. Hardy[5], T. Wolf[5], C. Meingast[5], H. v. Löhneysen[5,6], H. Ikeda[7], K. Ishizaka[1]

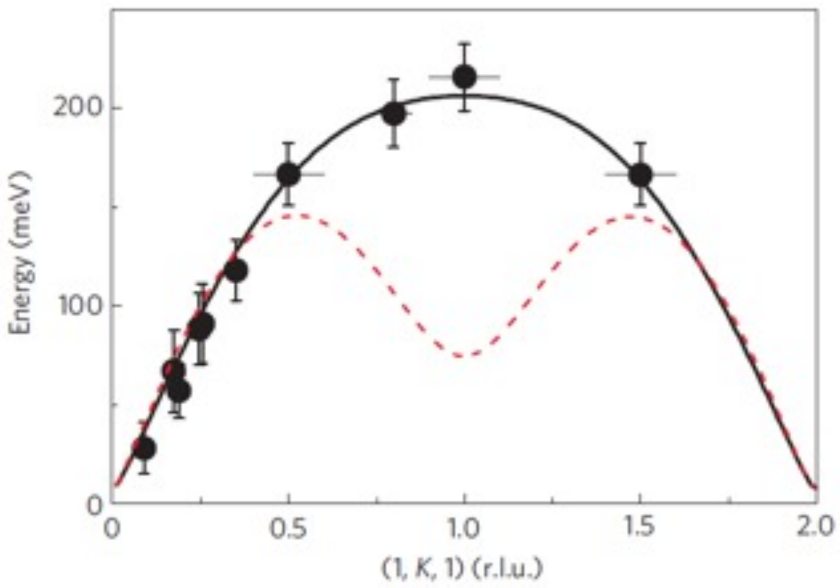
[1]*Quantum-Phase Electronics Center(QPEC) and Department of Applied Physics, University of Tokyo, Bunkyo, Tokyo 113-8656, Japan.*
[2]*Photon Science Center, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
[3]*Department of Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*
[4]*KEK, Photon Factory, Tsukuba, Ibaraki 305-0801, Japan.*
[5]*Institut für Festkörperphysik, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany*
[6]*Physikalisches Institut, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany*
[7]*Department of Physics, Kyoto University, Kyoto 606-8502, Japan.*

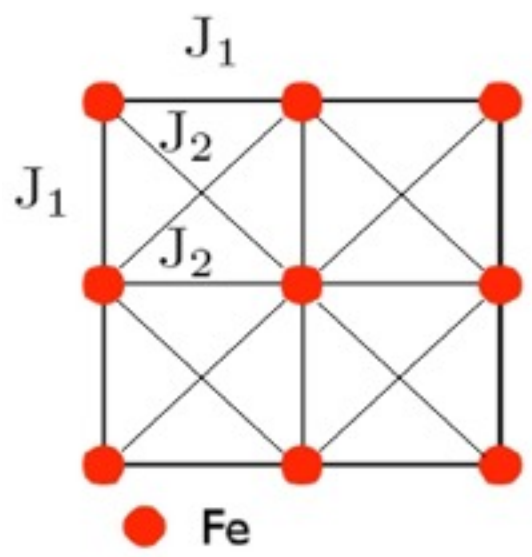


as in Na111 and Ba122

• *Inelastic neutron scattering*

Experimental Puzzle 1?





J. Zhao, *et al.* Nature Physics (2009)

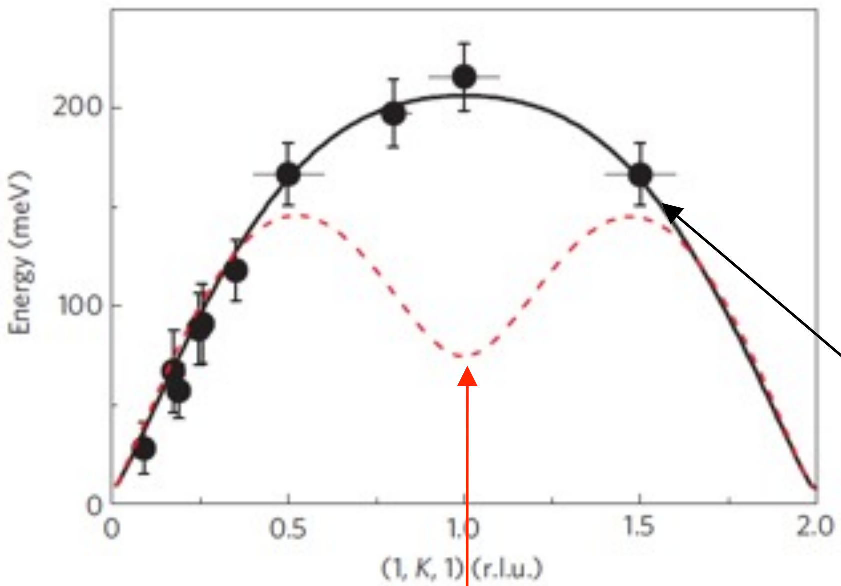
$$SJ_1^a = 27\,\mathrm{meV}$$
$$SJ_1^b = 25\,\mathrm{meV}$$
$$SJ_2 = 36\,\mathrm{meV}$$

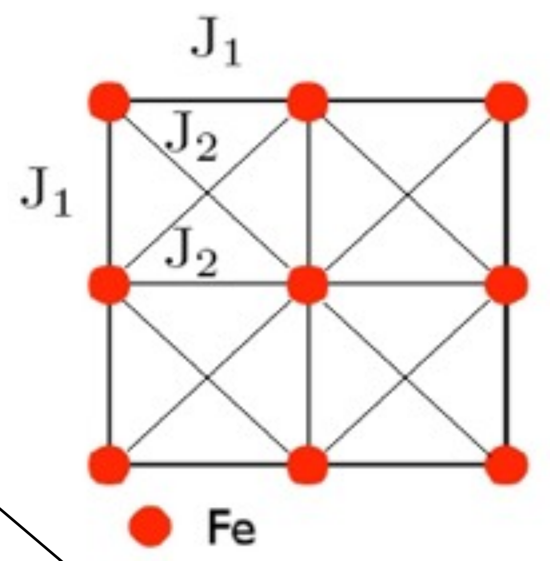
$$SJ_1^a = 49.9 \pm 9.9\,\mathrm{meV}$$
$$SJ_1^b = -5.7 \pm 4.5\,\mathrm{meV}$$
$$SJ_2 = 18.9 \pm 3.4\,\mathrm{meV}$$

Why is the magnetism frustrated?

• *Inelastic neutron scattering*

Experimental Puzzle 1?





J. Zhao, *et al.* Nature Physics (2009)

$$SJ_1^a = 27\,\text{meV}$$
$$SJ_1^b = 25\,\text{meV}$$
$$SJ_2 = 36\,\text{meV}$$

$$SJ_1^a = 49.9 \pm 9.9\,\text{meV}$$
$$SJ_1^b = -5.7 \pm 4.5\,\text{meV}$$
$$SJ_2 = 18.9 \pm 3.4\,\text{meV}$$

Why is the magnetism frustrated?

Double-Exchange Model

$$\mathcal{H}_{\mathrm{loc}} = \frac{J_1}{S^2} \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \frac{J_2}{S^2} \sum_{\langle\langle i,j \rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

unlike manganites

$$\nu J_H \ll \infty$$

Double-Exchange Model

$$\mathcal{H}_{\rm loc} = \frac{J_1}{S^2}\sum_{\langle i,j\rangle} \boldsymbol{S}_i\cdot\boldsymbol{S}_j + \frac{J_2}{S^2}\sum_{\langle\langle i,j\rangle\rangle} \boldsymbol{S}_i\cdot\boldsymbol{S}_j$$

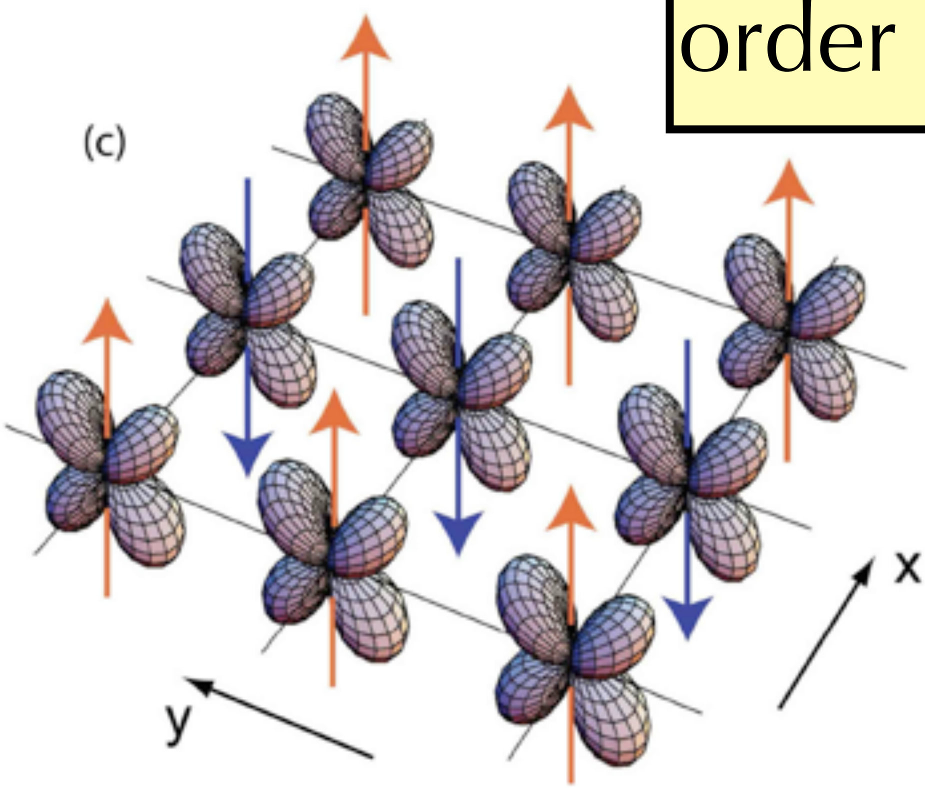
$$\mathcal{H}_{\rm it} = -\sum_{ij,\alpha\beta,\nu} t_{ij}^{\alpha\beta} c_{i\alpha\nu}^{\dagger} c_{j\beta\nu} + \frac{V}{2}\sum_{i,\alpha\neq\beta,\nu\nu'} \hat{n}_{i\alpha\nu}\hat{n}_{i\beta\nu'}$$

$$\mathcal{H}_{\rm H}^{(0)} = -\frac{J_{\rm H}}{2}\sum_{k,\alpha,\nu} \nu\tilde{c}_{k\alpha\nu}^{\dagger}\tilde{c}_{k\alpha\nu}$$

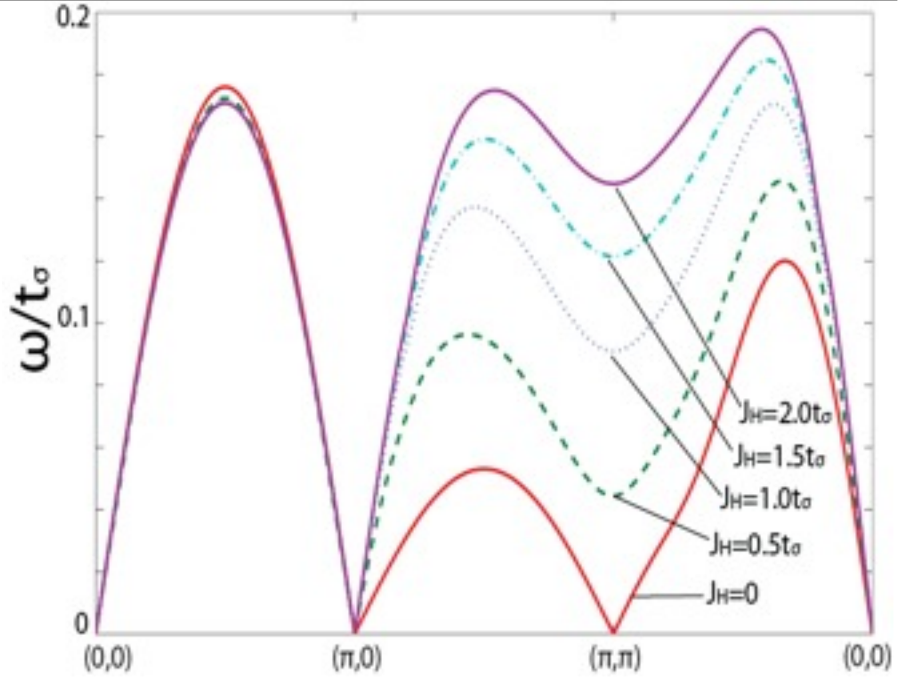
unlike manganites

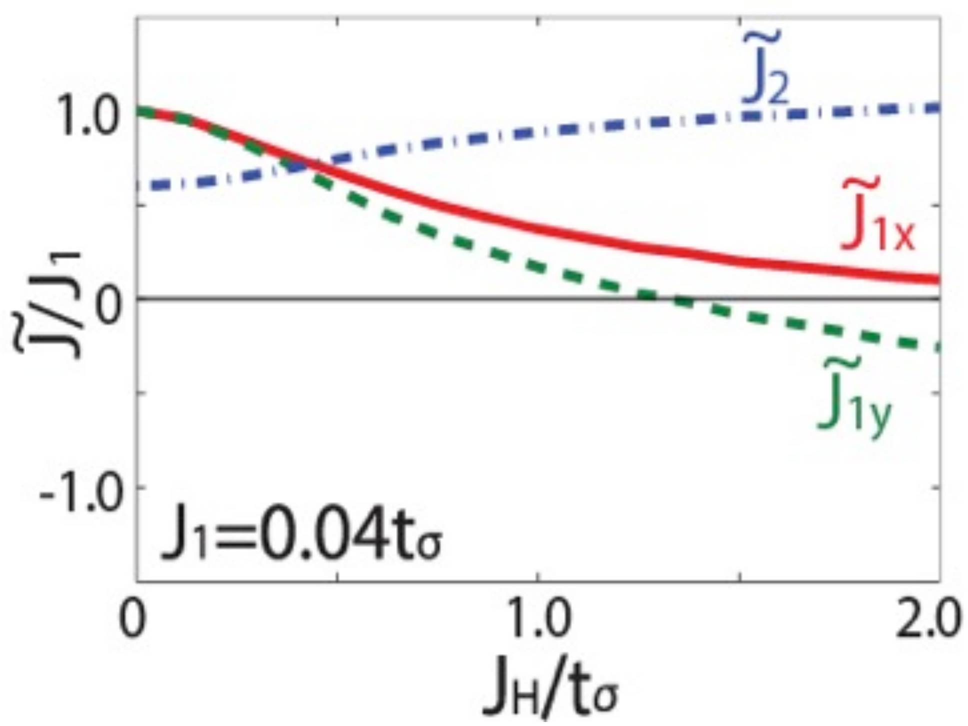
$$\nu J_H \ll \infty$$

answer: emergent ferro-orbital order from Hund coupling

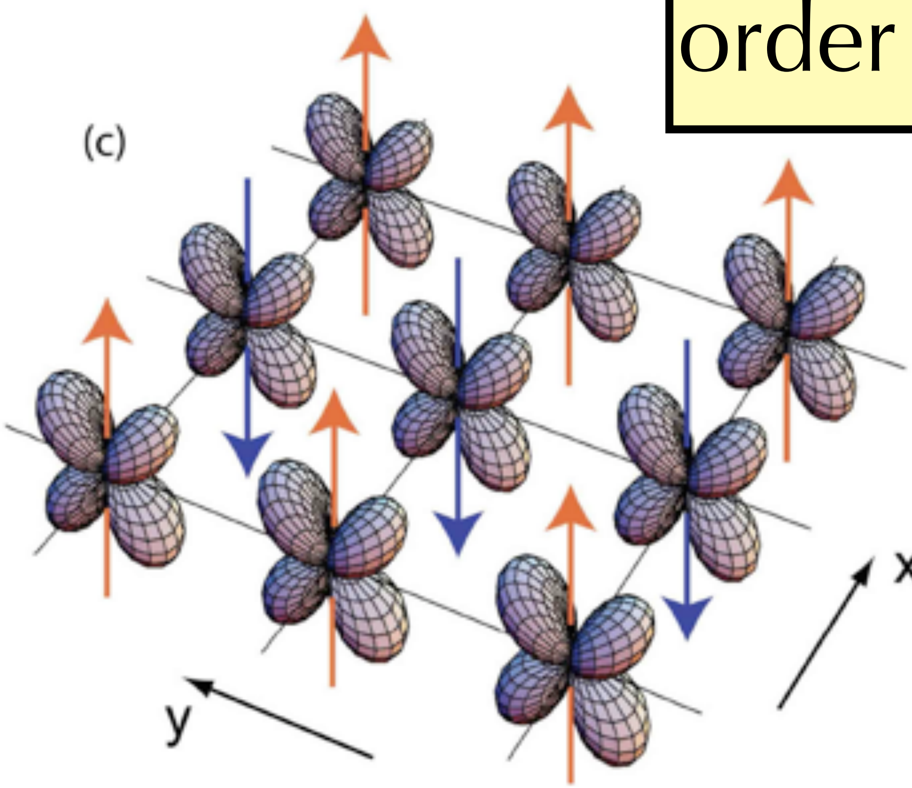


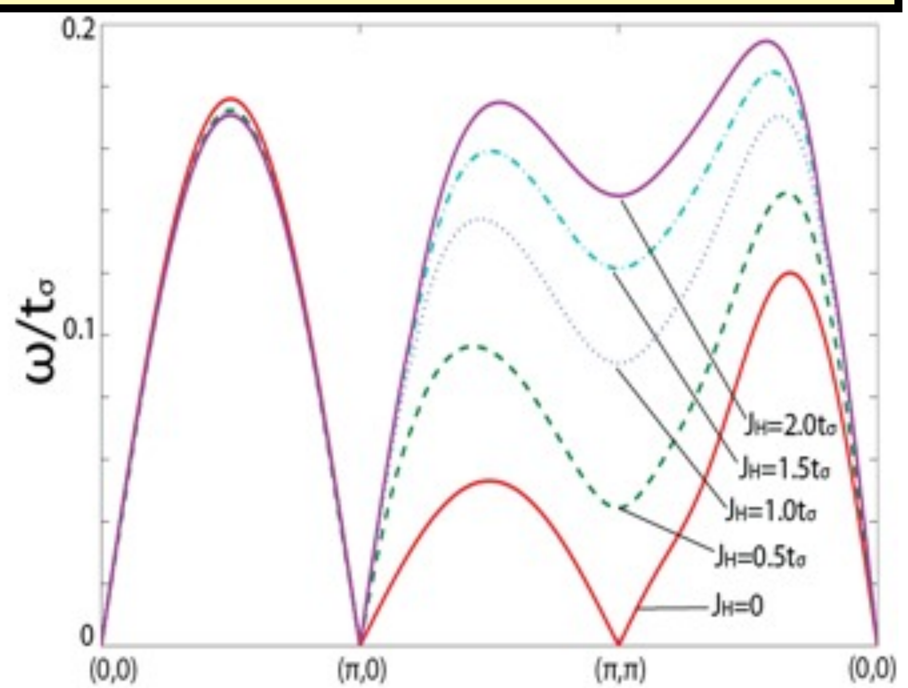
WL, FK, PP, Phys. Rev. B, vol. 82, p. 045125 (2010)



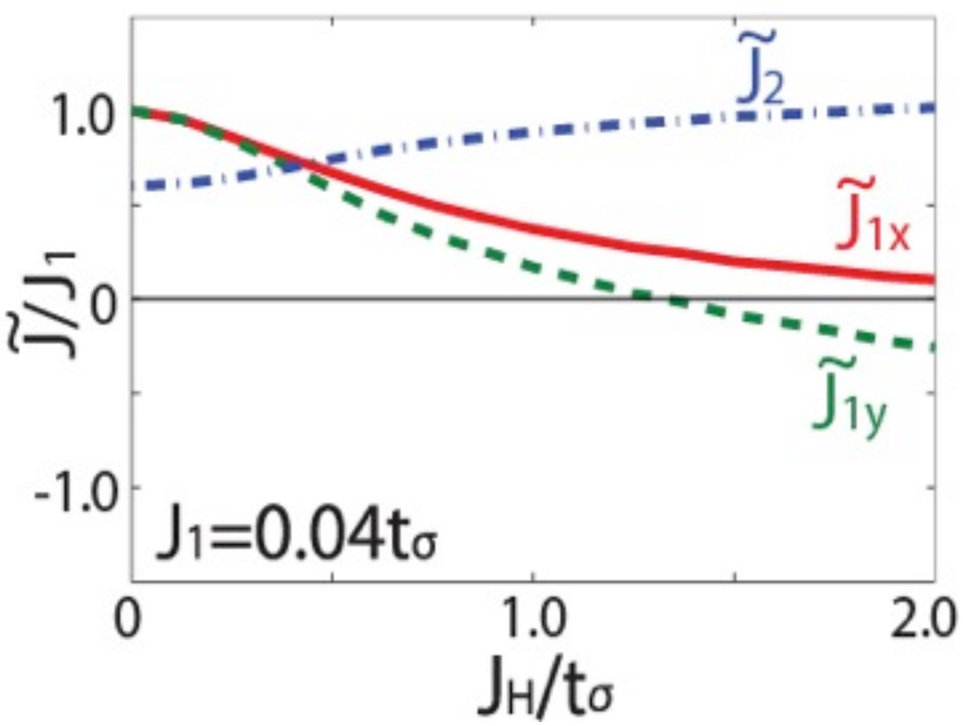


answer: emergent ferro-orbital order from Hund coupling



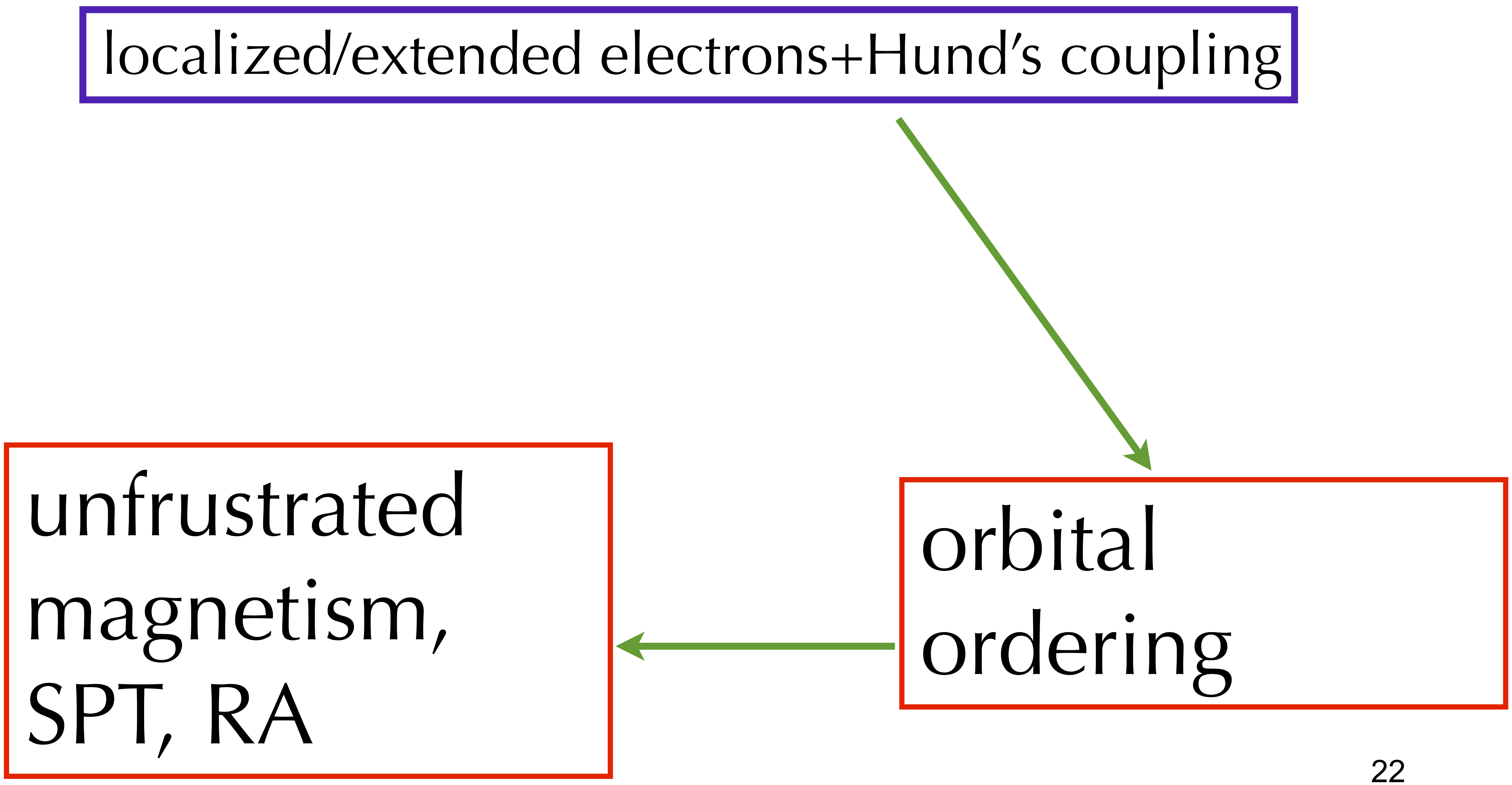


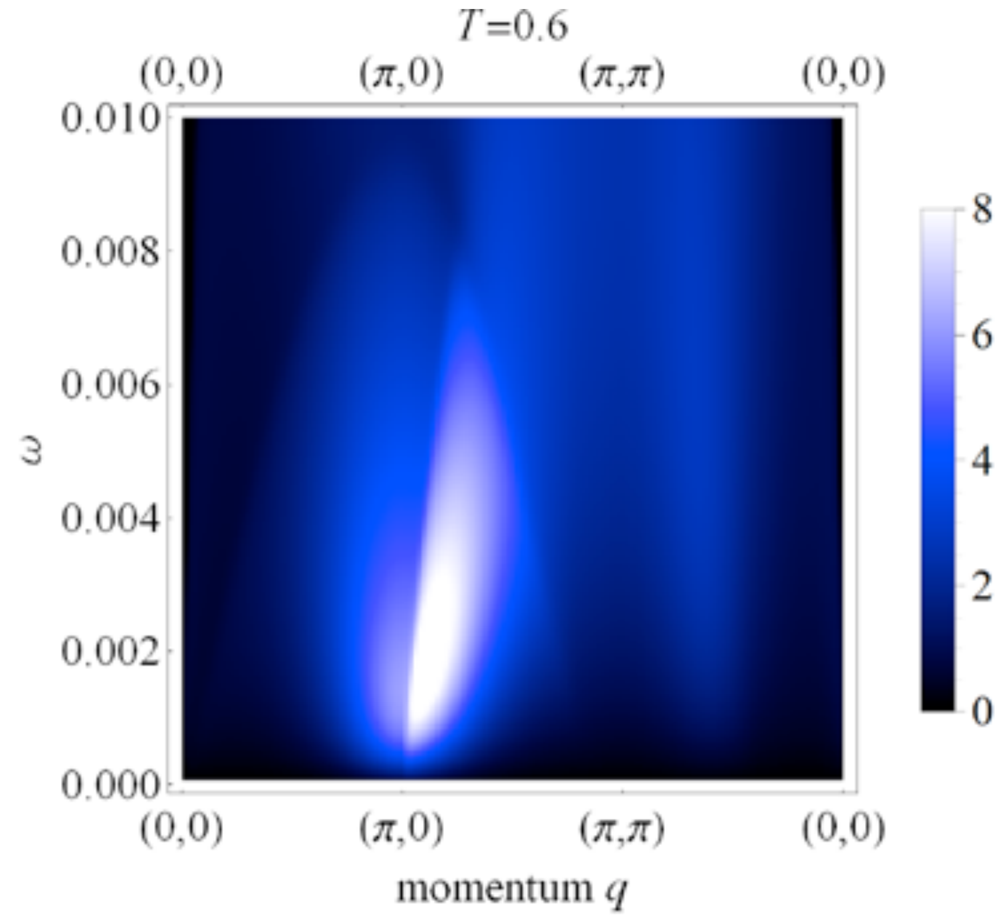
WL, FK, PP, Phys. Rev. B, vol. 82, p. 045125 (2010)



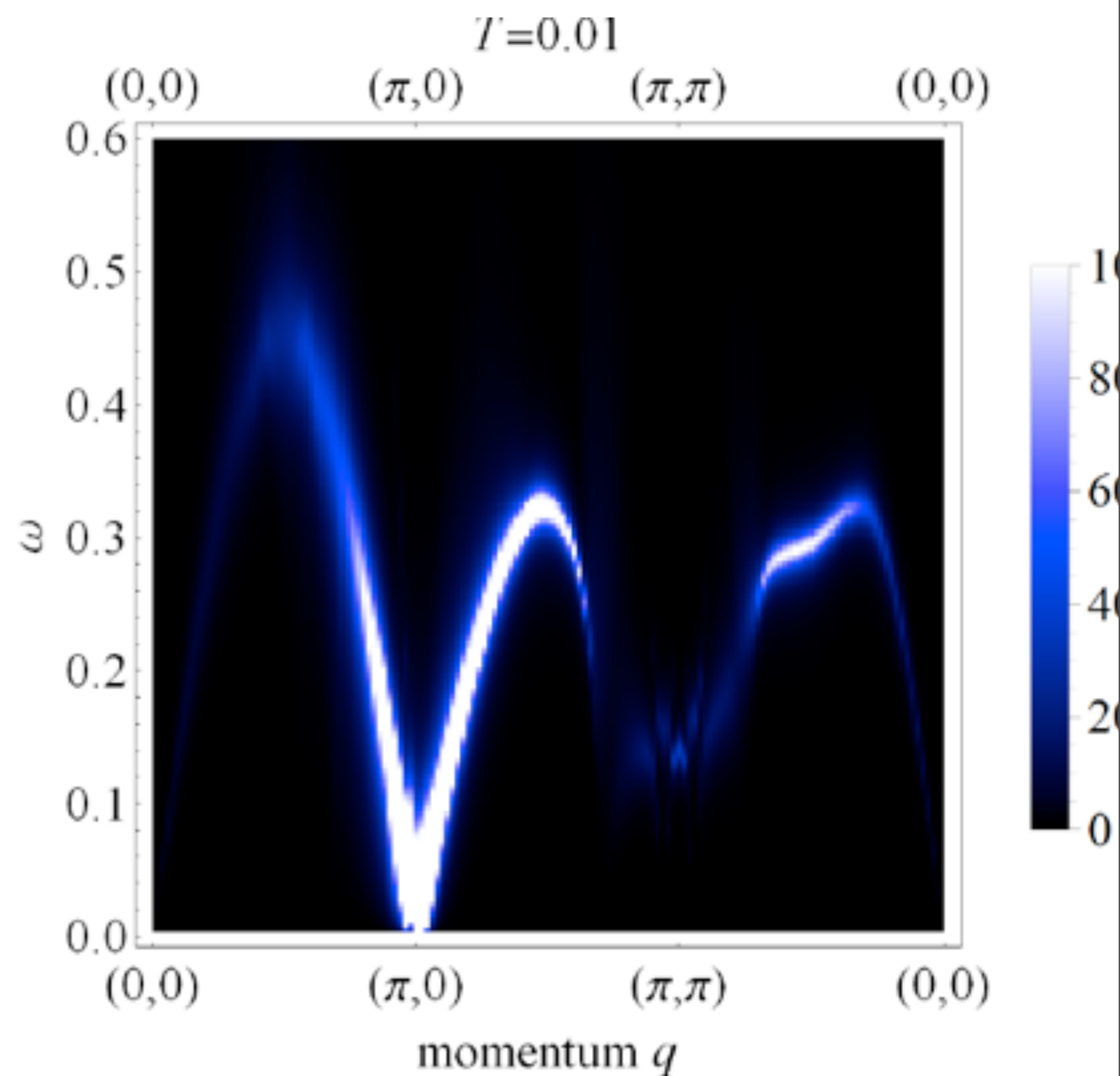
- *Comparison with experiments*:

$$J_{\rm H} \sim t_\sigma \sim 1\,{\rm eV} \quad \tilde{J} \sim 0.01\,t_\sigma \sim 10\,{\rm meV}$$

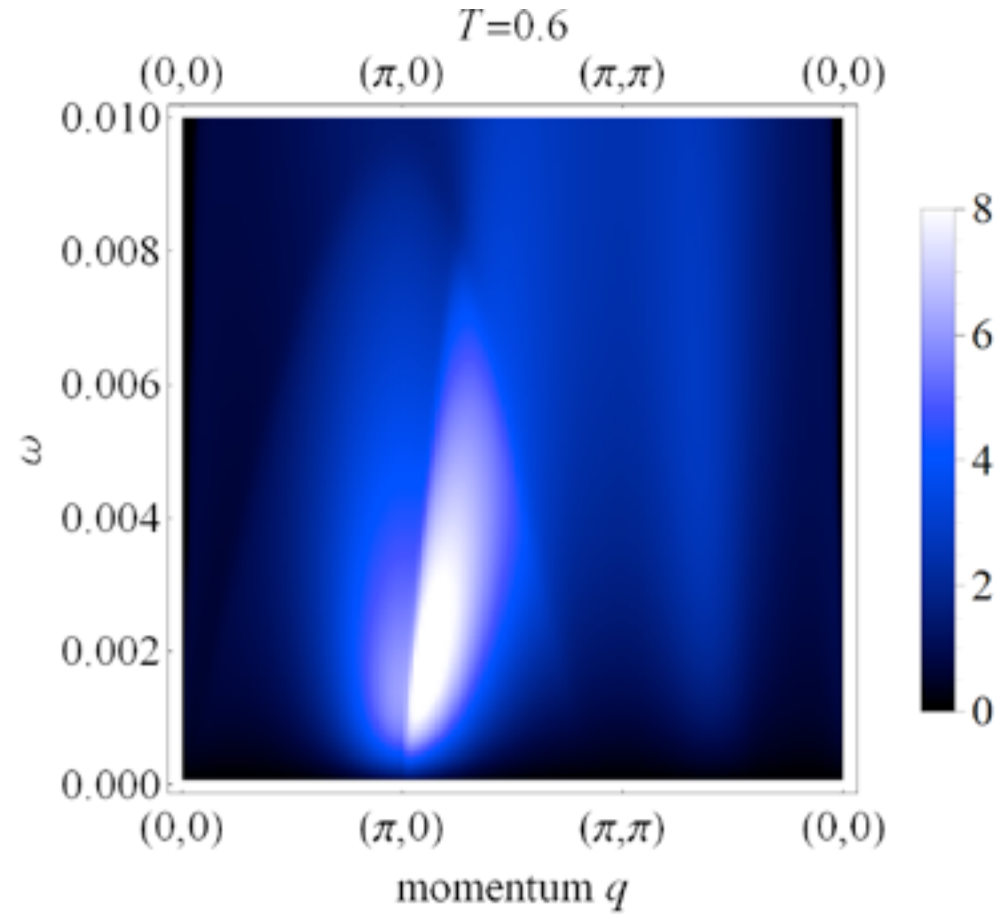

localized/extended electrons+Hund's coupling
orbital ordering
unfrustrated magnetism, SPT, RA



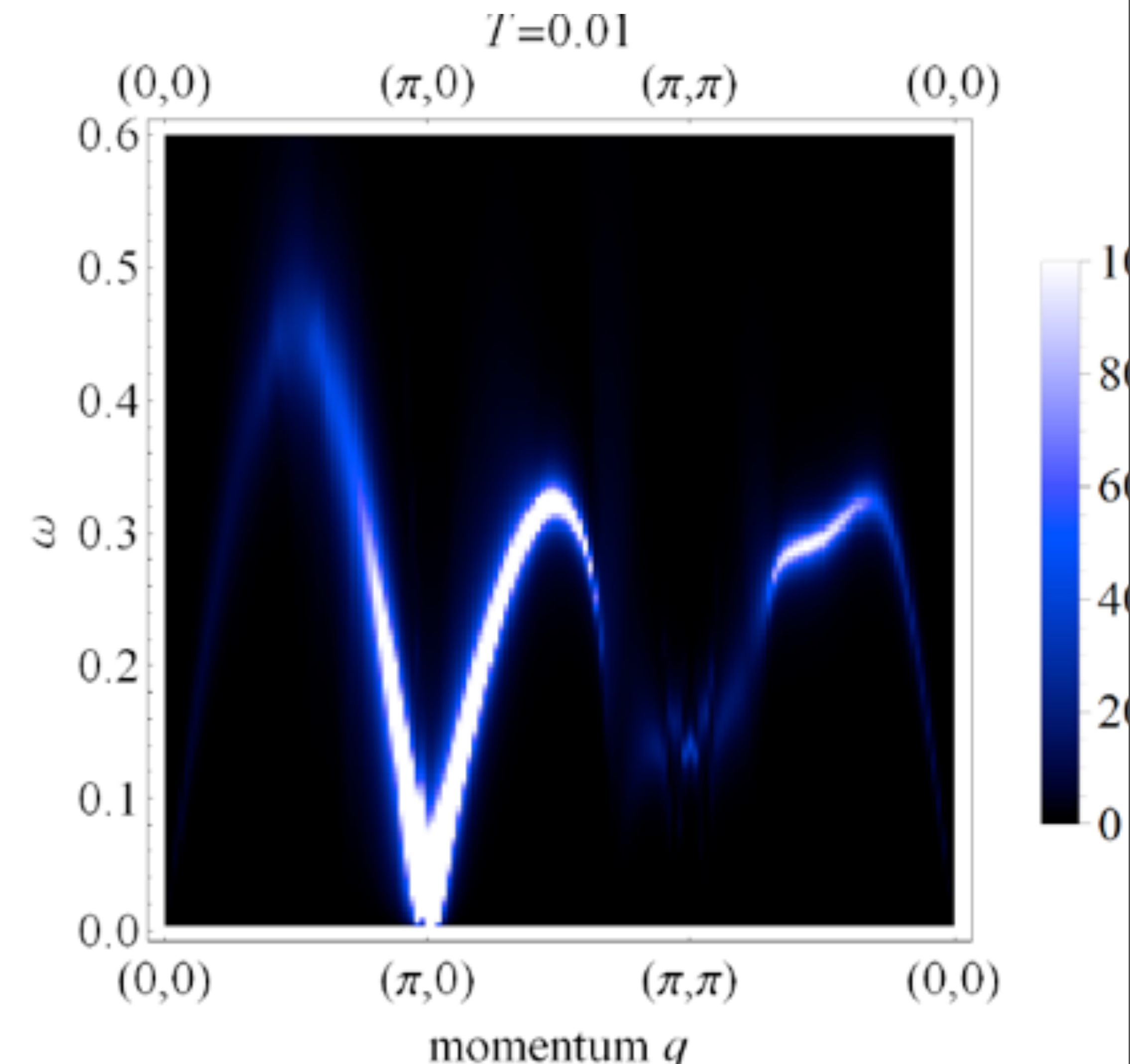
high T
paramagnetic state



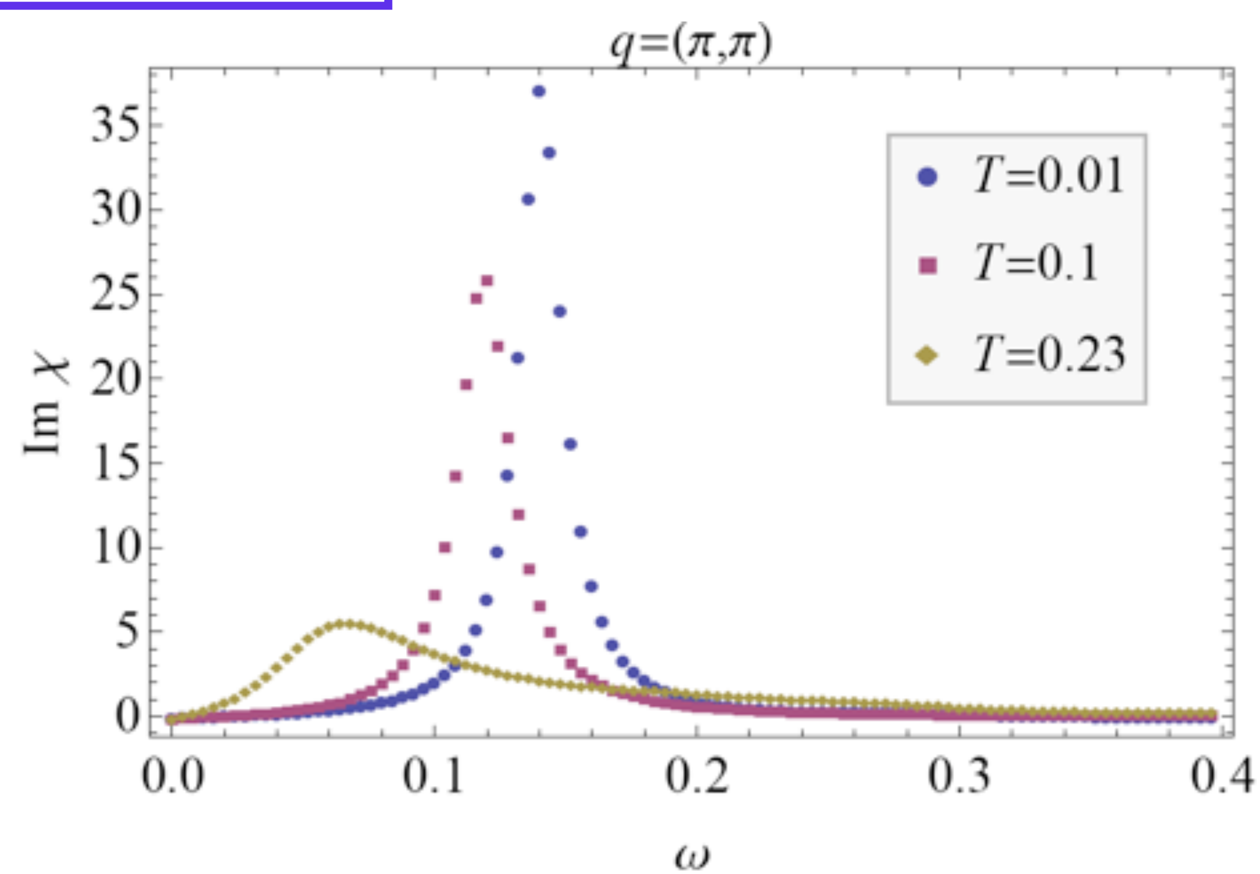
low T
ordered state



high T
paramagnetic state



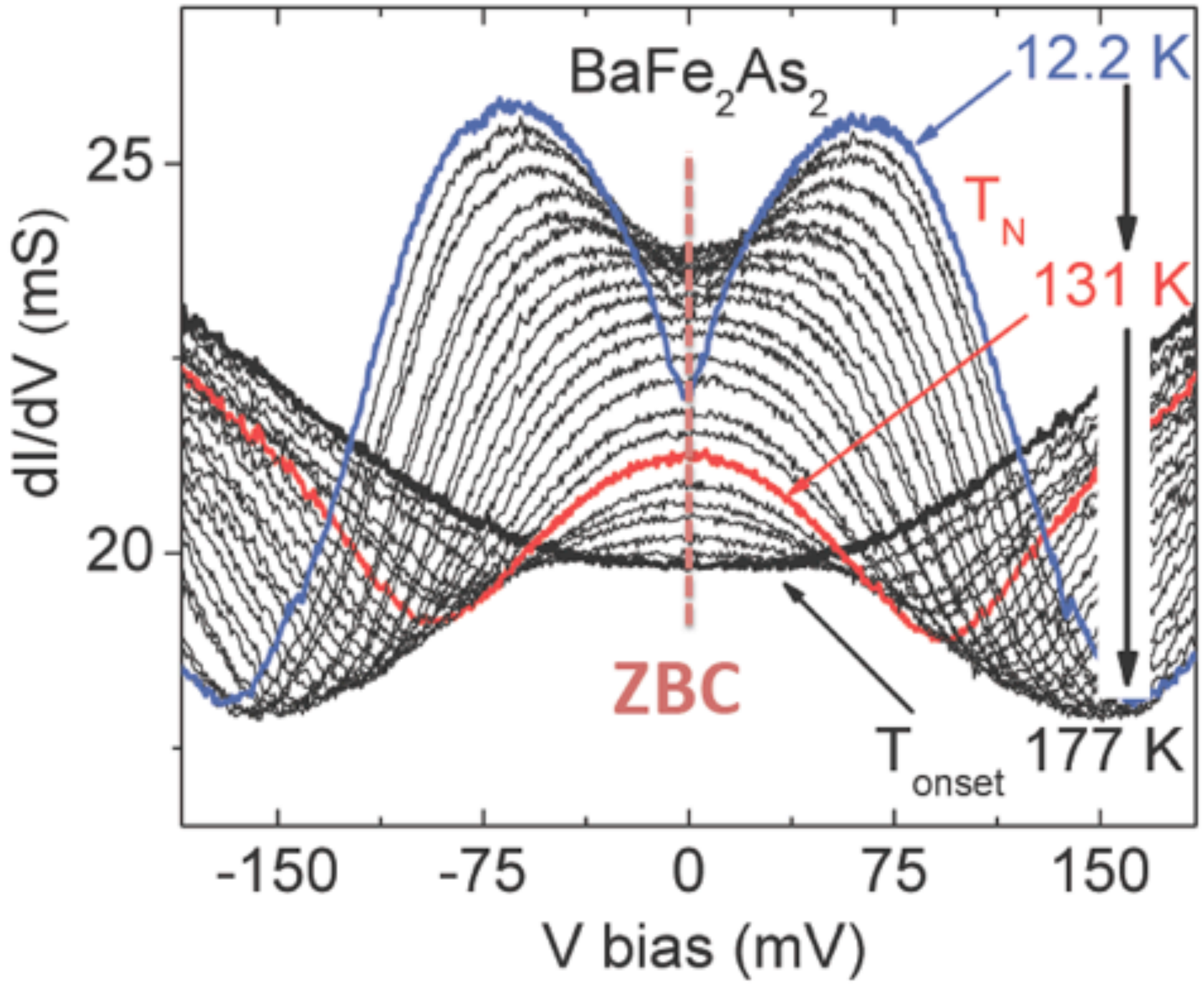
low T
ordered state

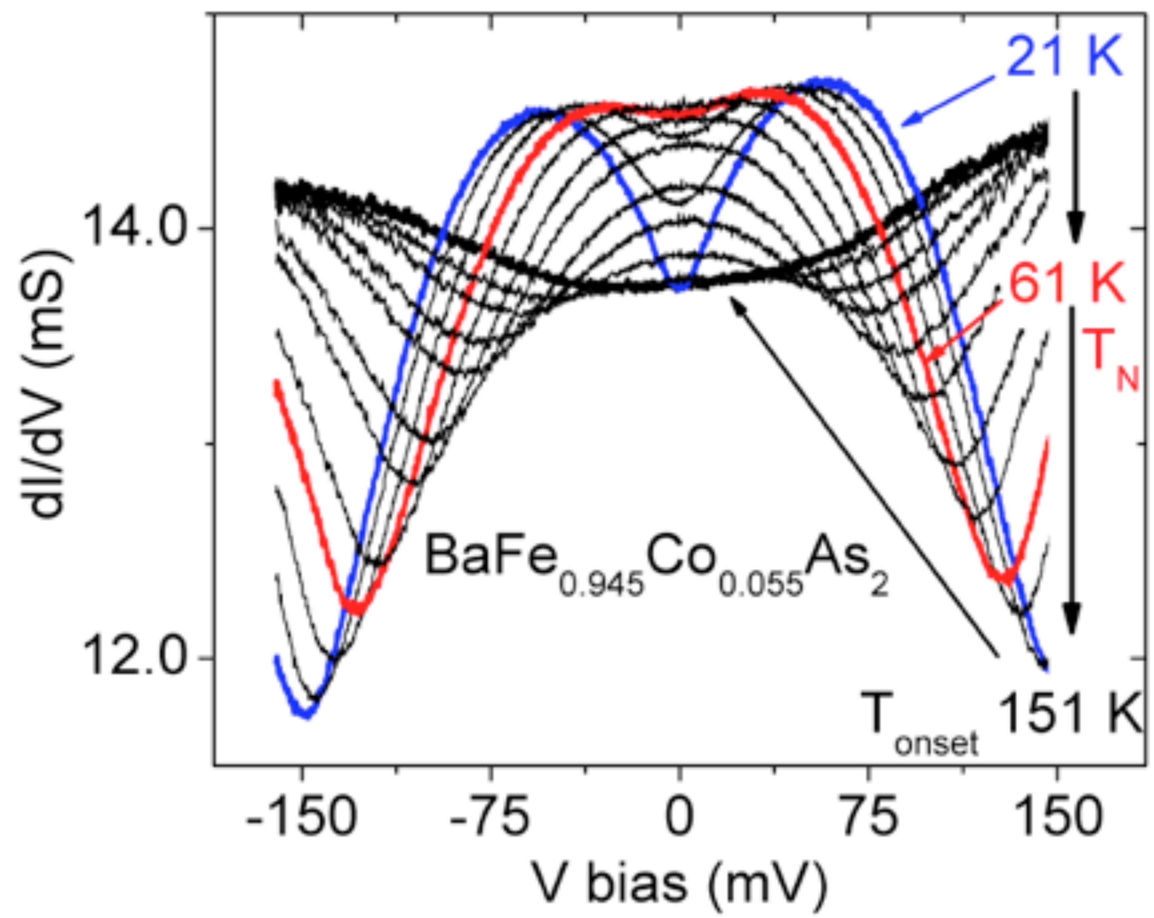


prediction:
Landau damping
increases
as T increases

Z. Leong, et al,
PRB, xxx,2014

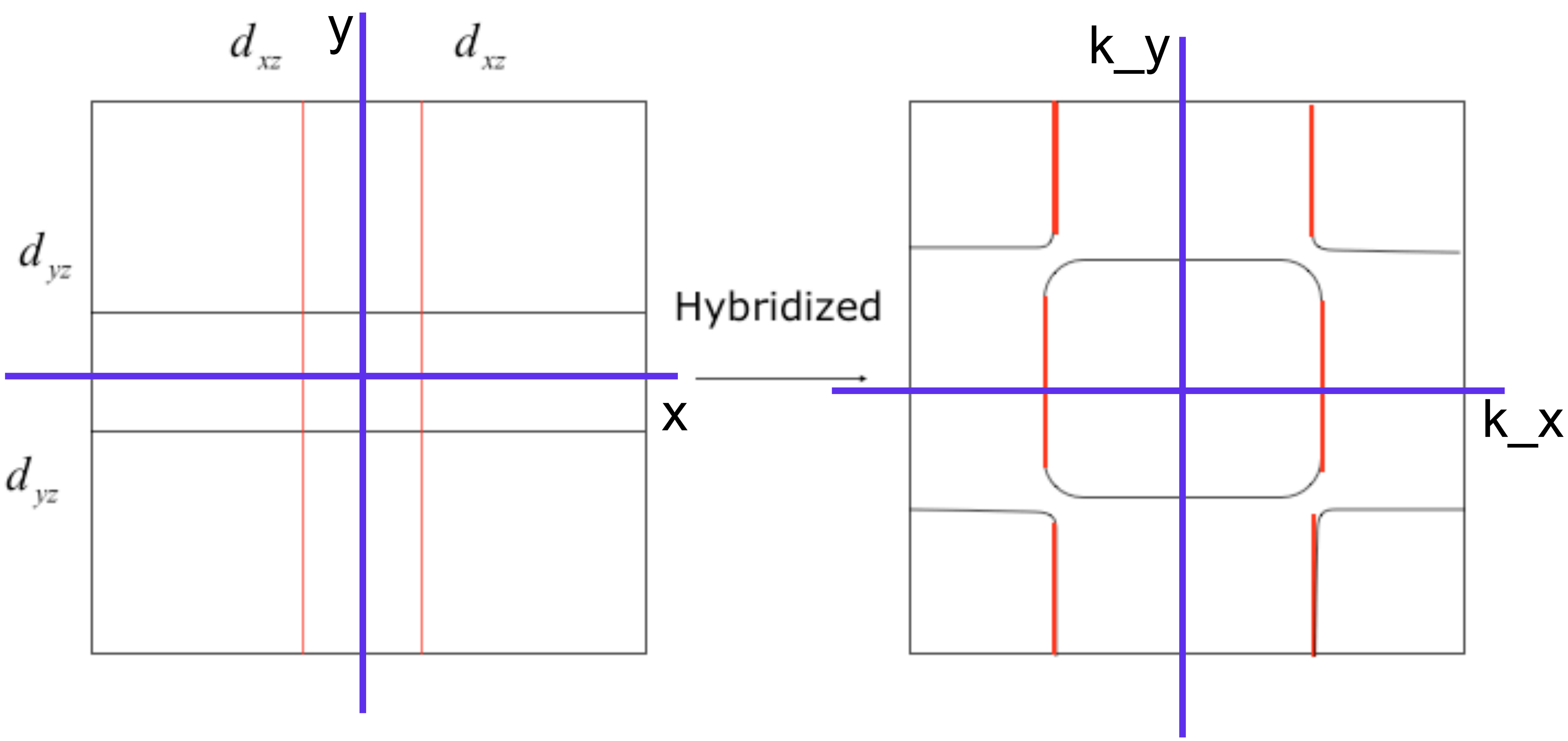
Experimental puzzle 2: What is the origin of the excess conductance above the structural transition?



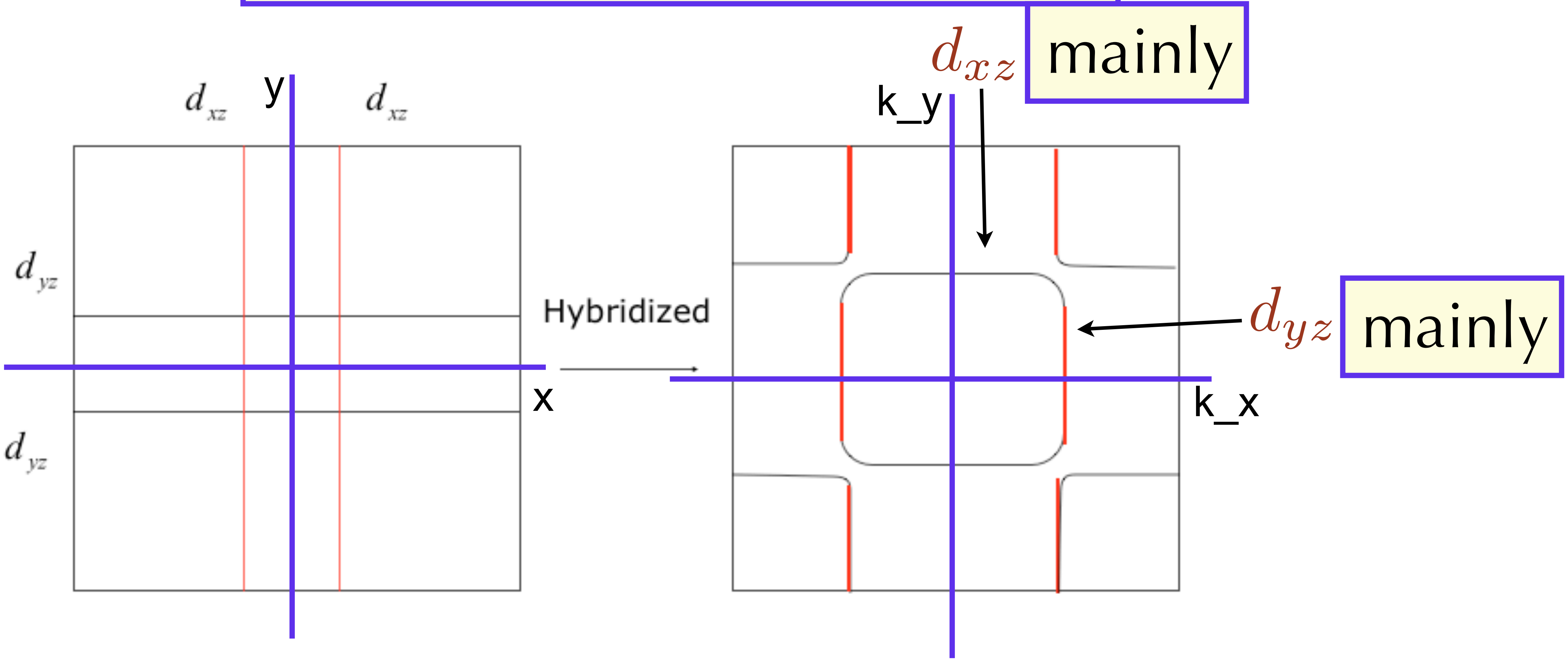


H. Ahram, L. Greene, ... (UIUC)

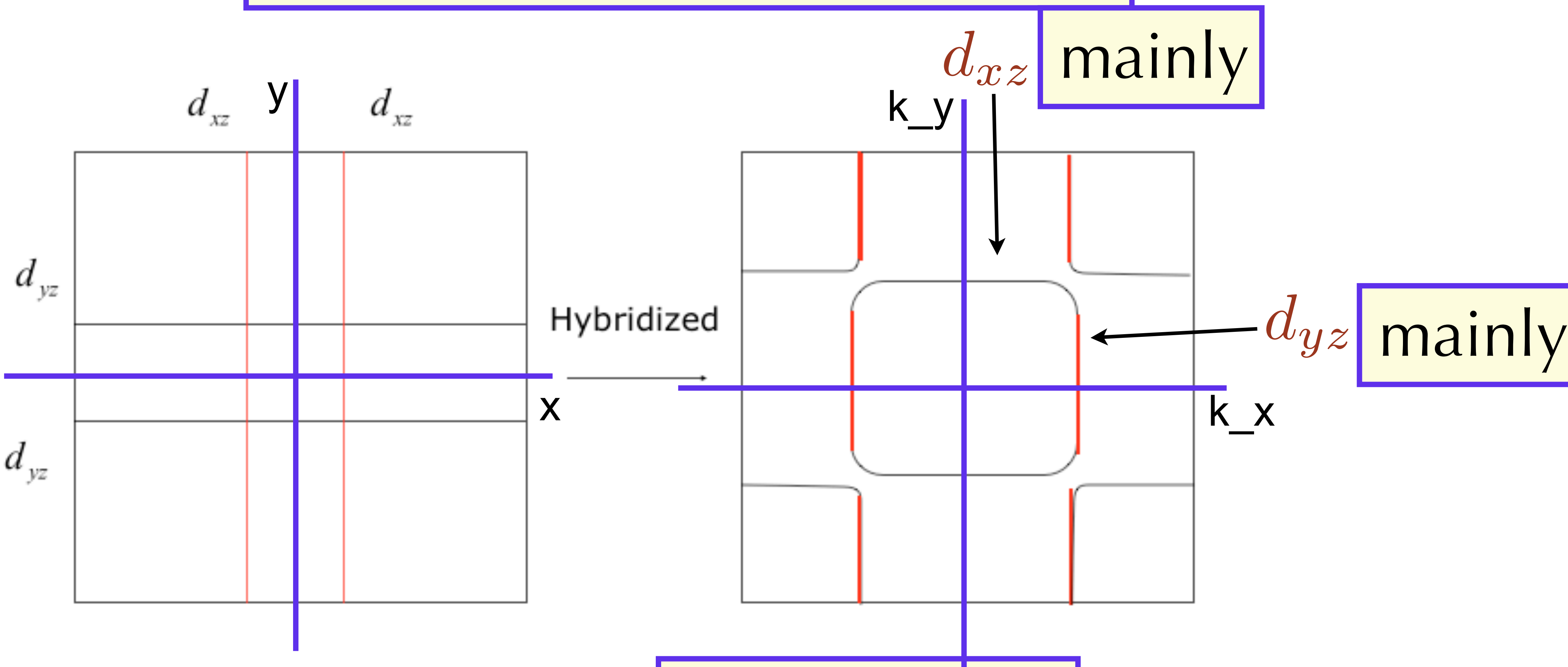
Fermi surface in Brillouin zone



Fermi surface in Brillouin zone



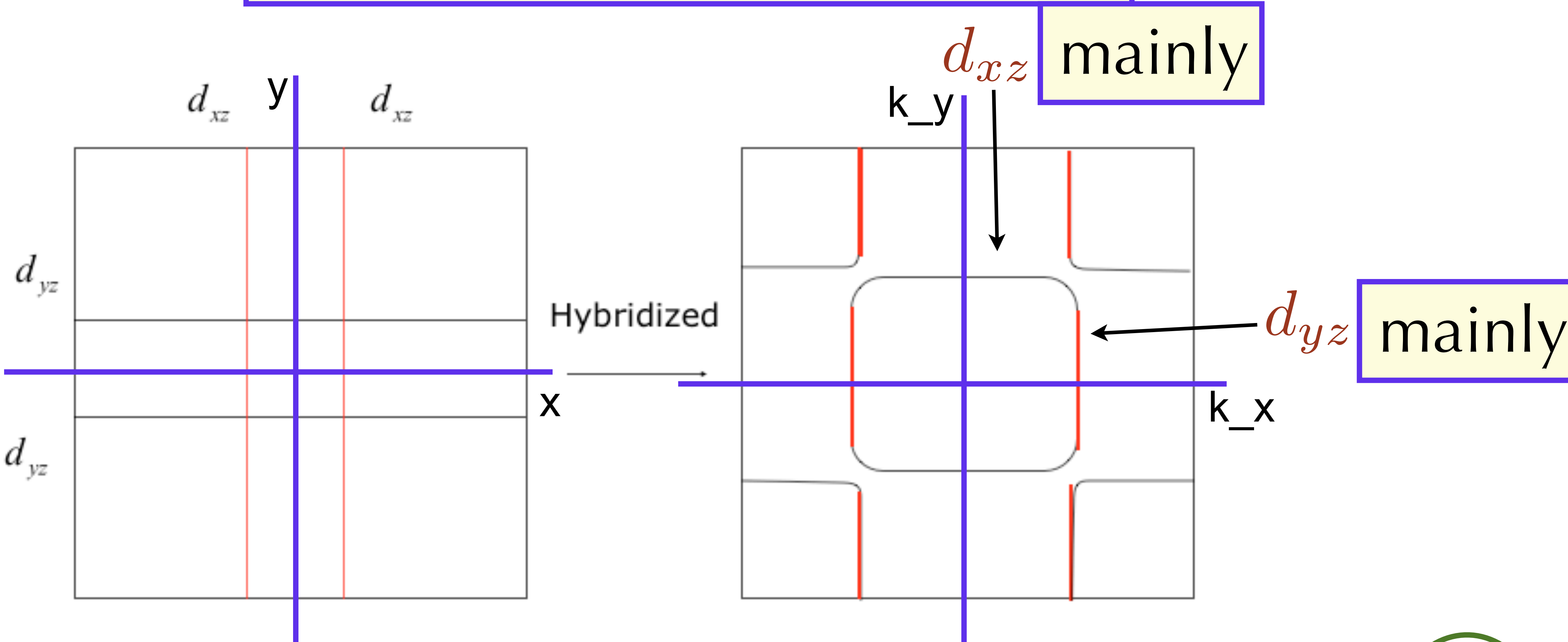
Fermi surface in Brillouin zone



on-site interaction

anisotropic in hybridized basis

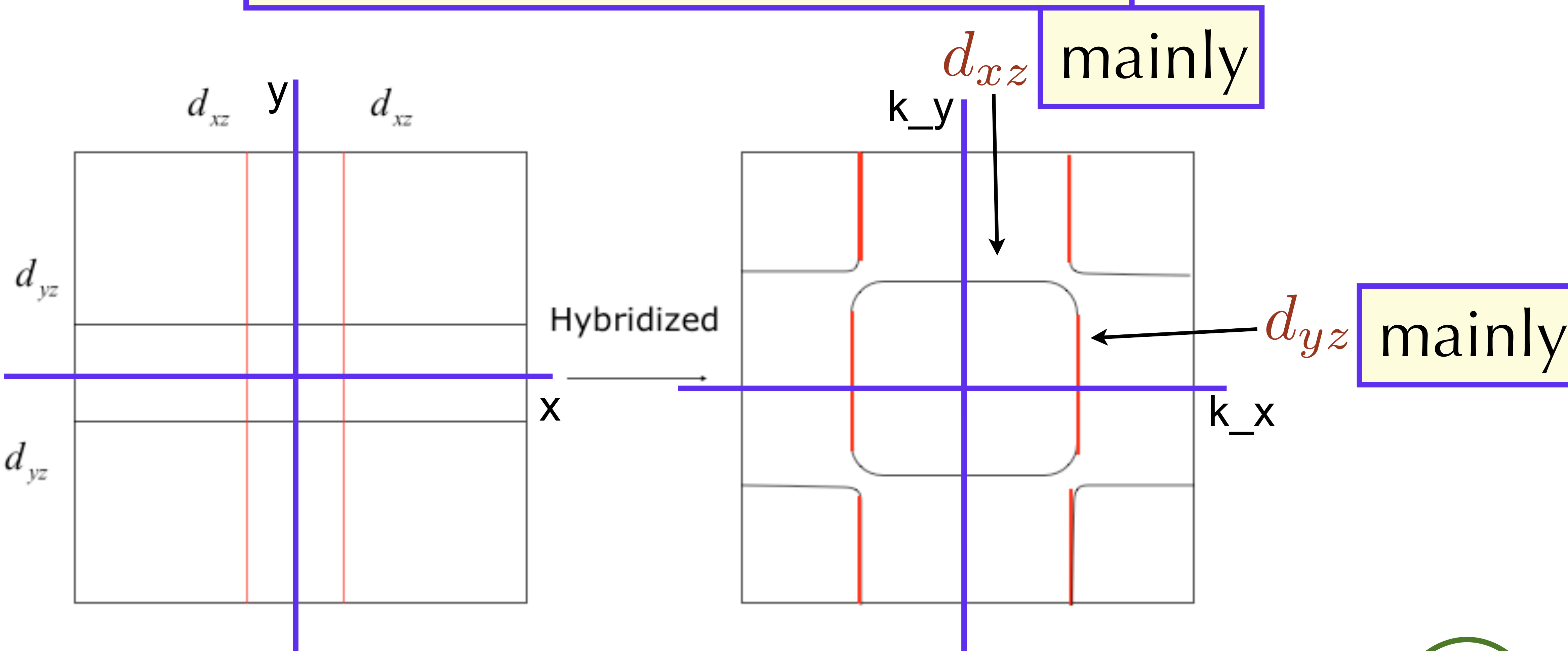
Fermi surface in Brillouin zone



on-site interaction

anisotropic in hybridized basis

Fermi surface in Brillouin zone



on-site interaction → anisotropic in hybridized basis →

orbital ordering in multi-orbital system = nematic order

Multiorbital Hubbard Model

$$H = H_t + H_I$$

$$H_t = -\sum_{i,j} \sum_{a,b} \sum_{\sigma} t_{ij}^{ab} \left(c_{ia\sigma}^{+} c_{jb\sigma} + h.c. \right)$$

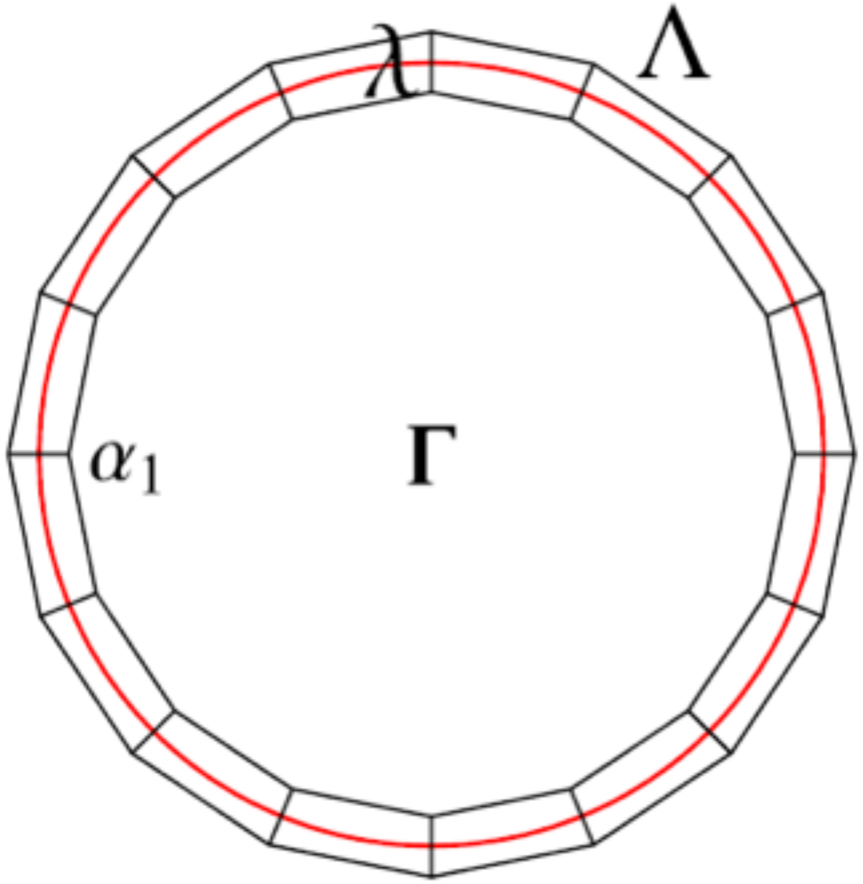
$$H_I = \sum_{ia} U n_{ia\uparrow} n_{ia\downarrow} + \sum_{i,b>a} \left(U' - \frac{J}{2} \right) n_{ia} n_{ib} - 2J \vec{S}_{ia} \times \vec{S}_{ib} + J \left(c_{ia\uparrow} c_{ia\downarrow} c_{ib\downarrow}^{+} c_{ib\uparrow}^{+} + h.c. \right)$$

$$U' = U - 2J$$

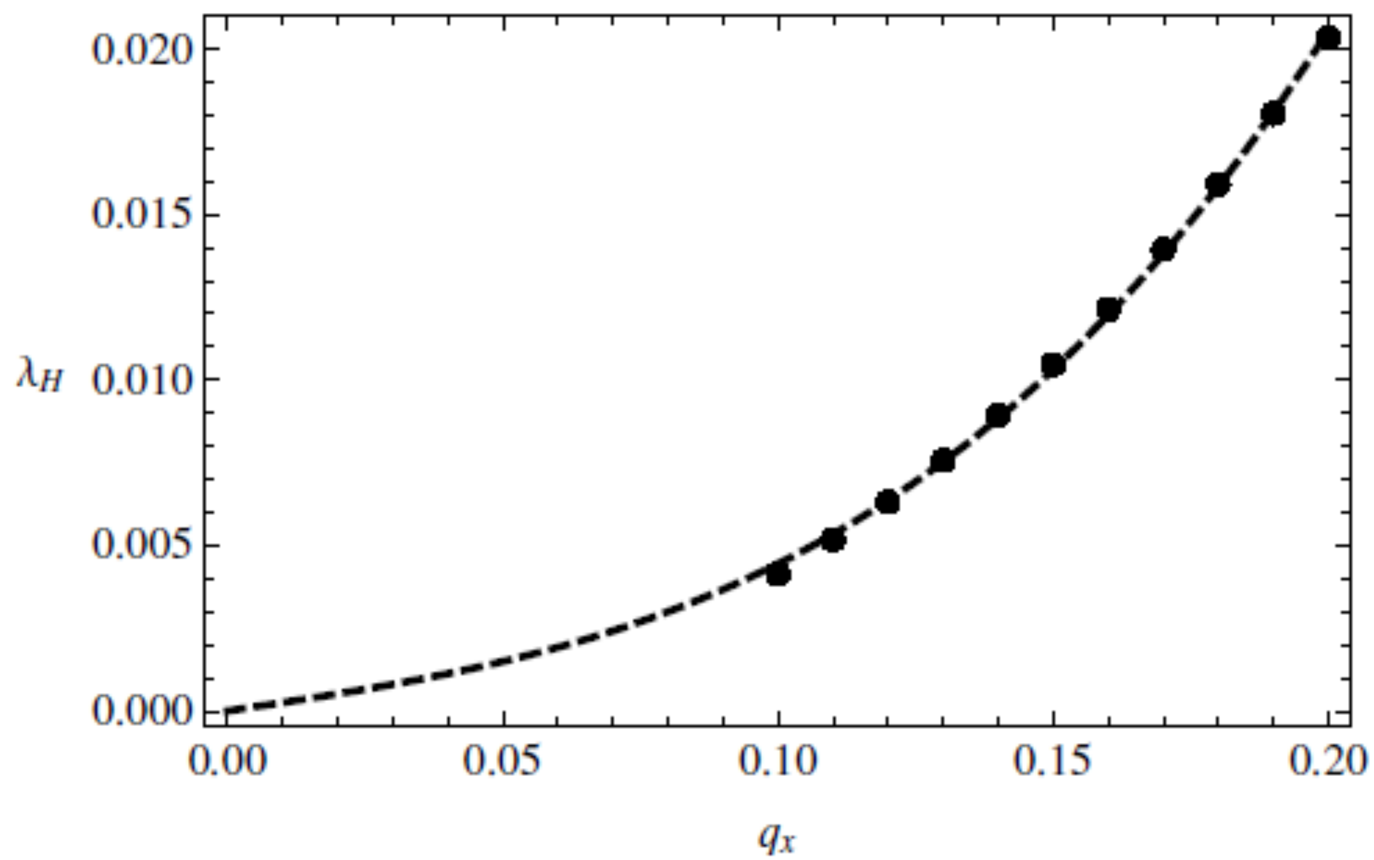
Theoretical approaches:

- Multidimensional Bosonization for two-orbital model
- Generalized RPA for realistic five orbital model

z=3 Overdamped Mode in Two-Orbital Model at Orbital Ordering QCP

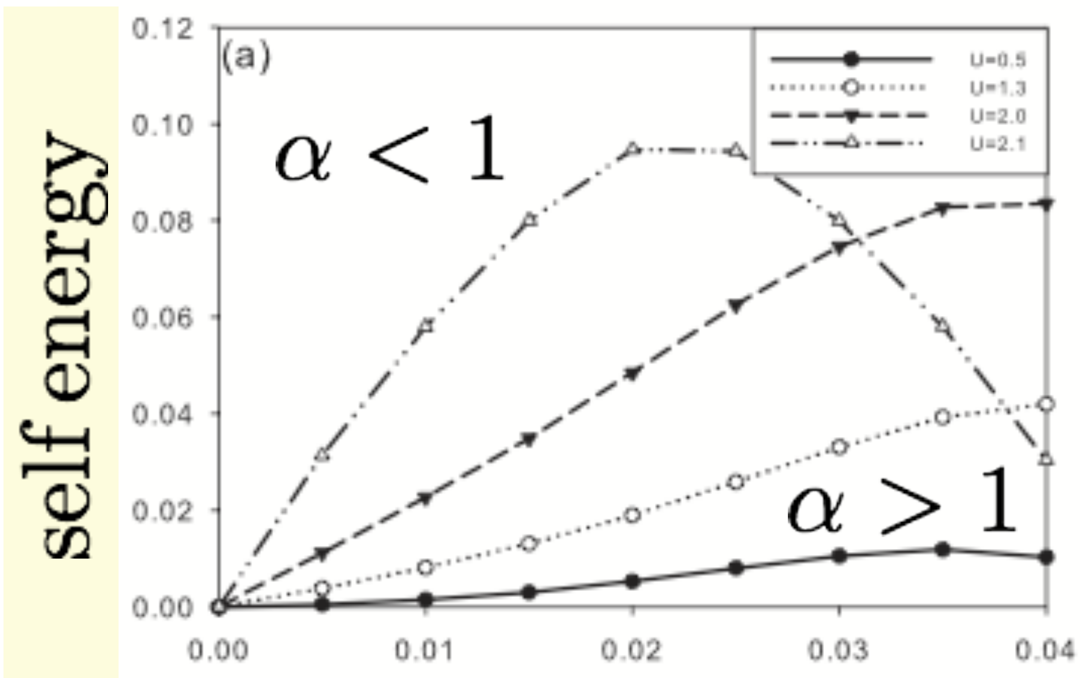


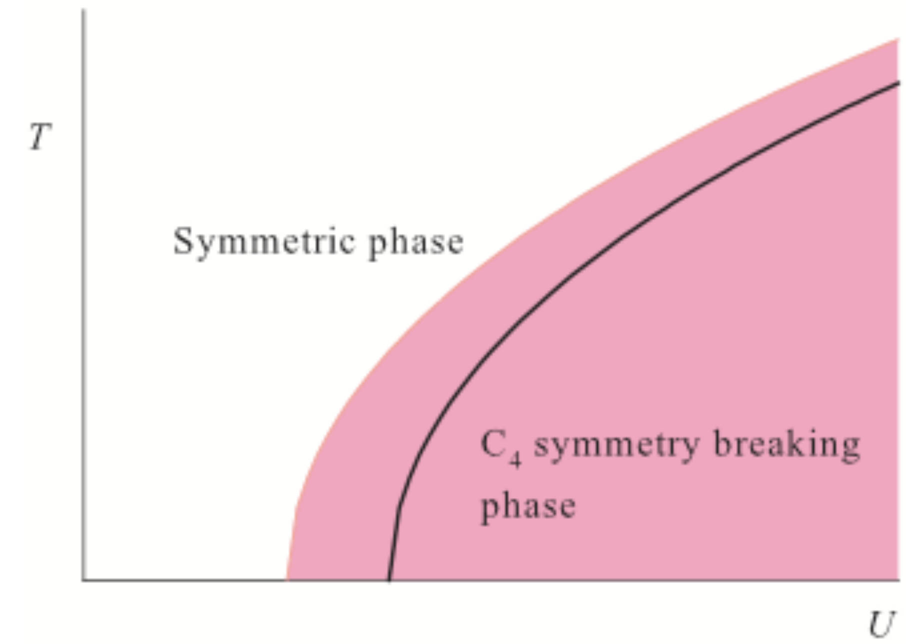
Patches for multidimensional bosonization



$$\frac{\omega}{q} = i\frac{\lambda_H}{q} \propto iq^2$$

Self-Energy with One Loop Corrections (2-band model)

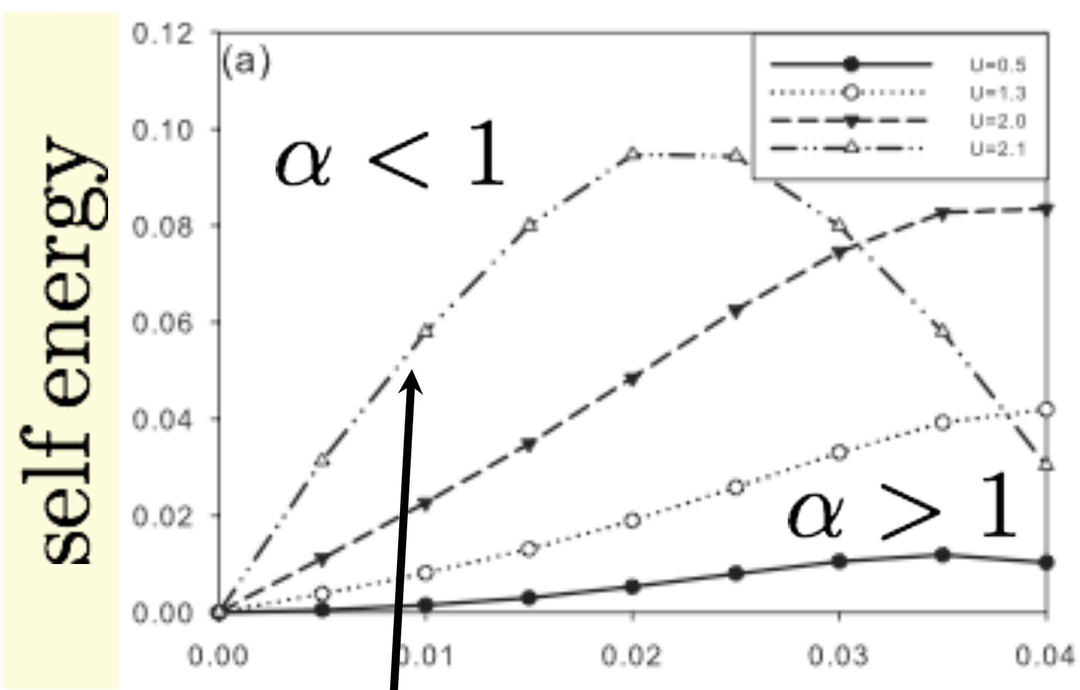


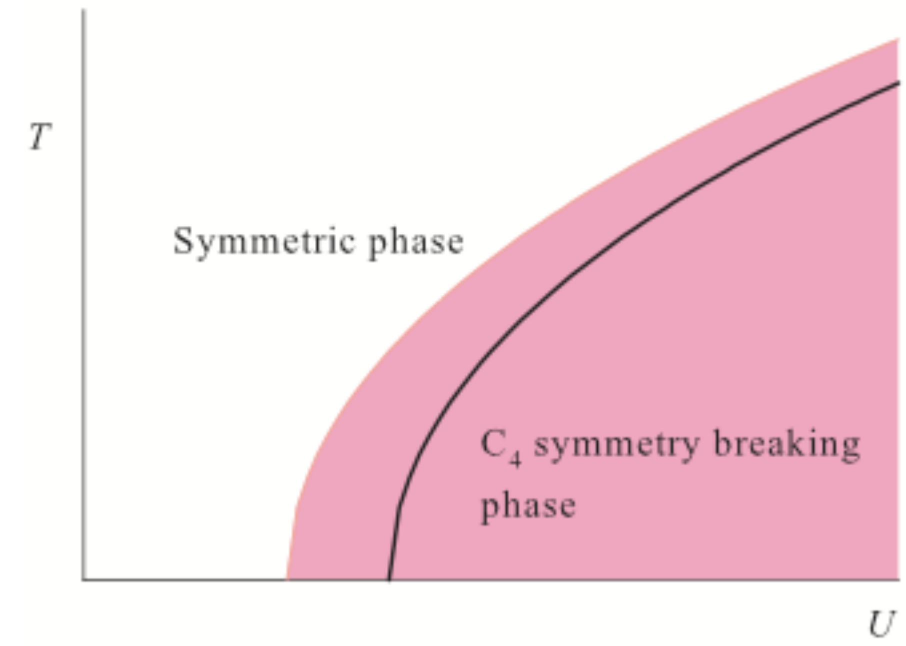


$$\frac{1}{\tau} = \mathrm{Im}\Sigma(k_F,\omega) = a\omega^{\alpha} + \ldots$$

Wei-Cheng Lee, and Philip W. Phillips, Phys. Rev. B **86**, 245113 (2012)

Self-Energy with One Loop Corrections (2-band model)



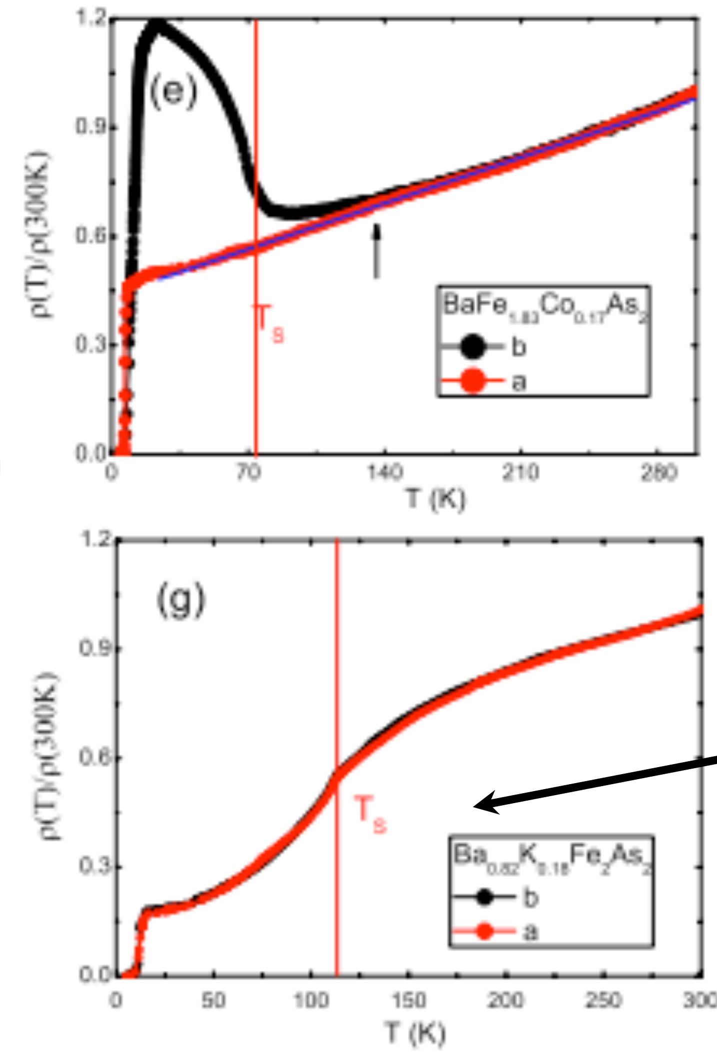


P. Johnson, ARPES possible experiment

$$\frac{1}{\tau} = \mathrm{Im}\Sigma(k_F, \omega) = a\omega^{\alpha} + \ldots$$

Wei-Cheng Lee, and Philip W. Phillips, Phys. Rev. B **86**, 245113 (2012)

resistivity anisotropy and NFL are linked



prediction:
no ZBC in hole-doped pnictides!
(future work)

PRL **107**, 067001 (2011) PHYSICAL REVIEW LETTERS week ending 5 AUGUST 2011

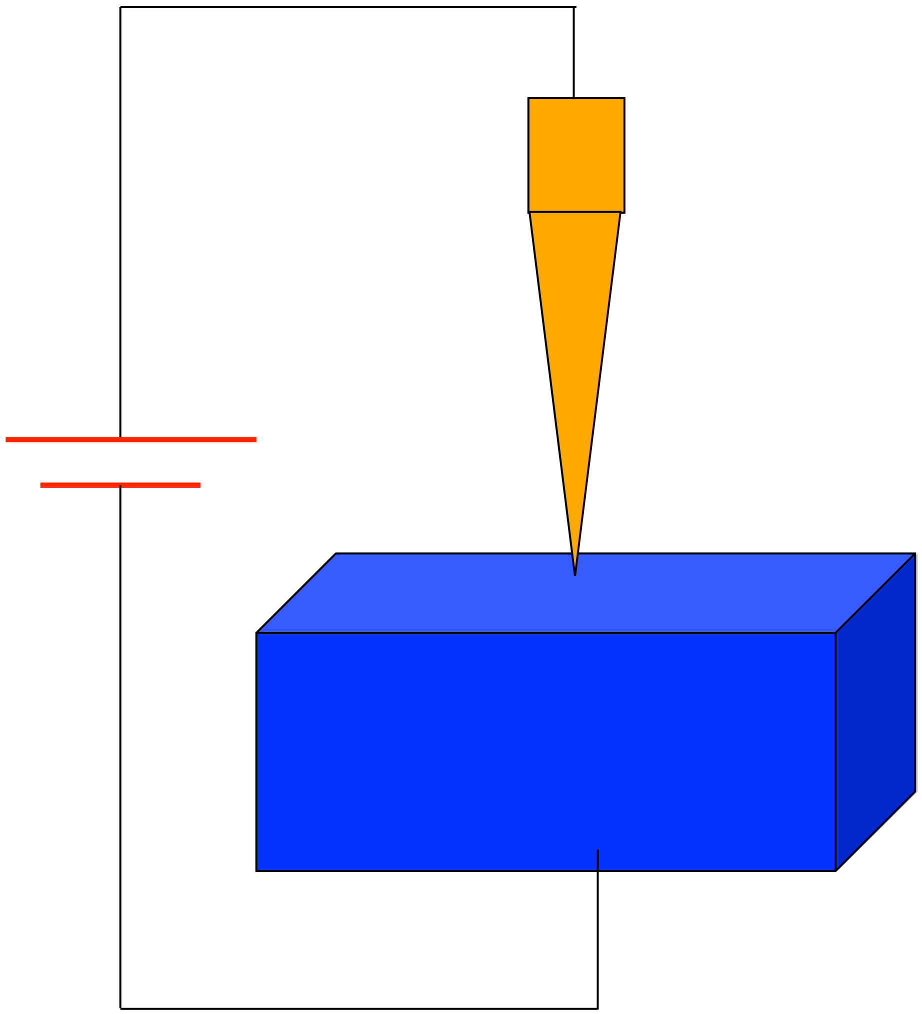
Measurements of the Anisotropic In-Plane Resistivity of Underdoped FeAs-Based Pnictide Superconductors

J. J. Ying,[1] X. F. Wang,[1] T. Wu,[1] Z. J. Xiang,[1] R. H. Liu,[1] Y. J. Yan,[1] A. F. Wang,[1] M. Zhang,[1] G. J. Ye,[1] P. Cheng,[1] J. P. Hu,[2] and X. H. Chen[1,*]

[1]*Hefei National Laboratory for Physical Science at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China*
[2]*Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA*

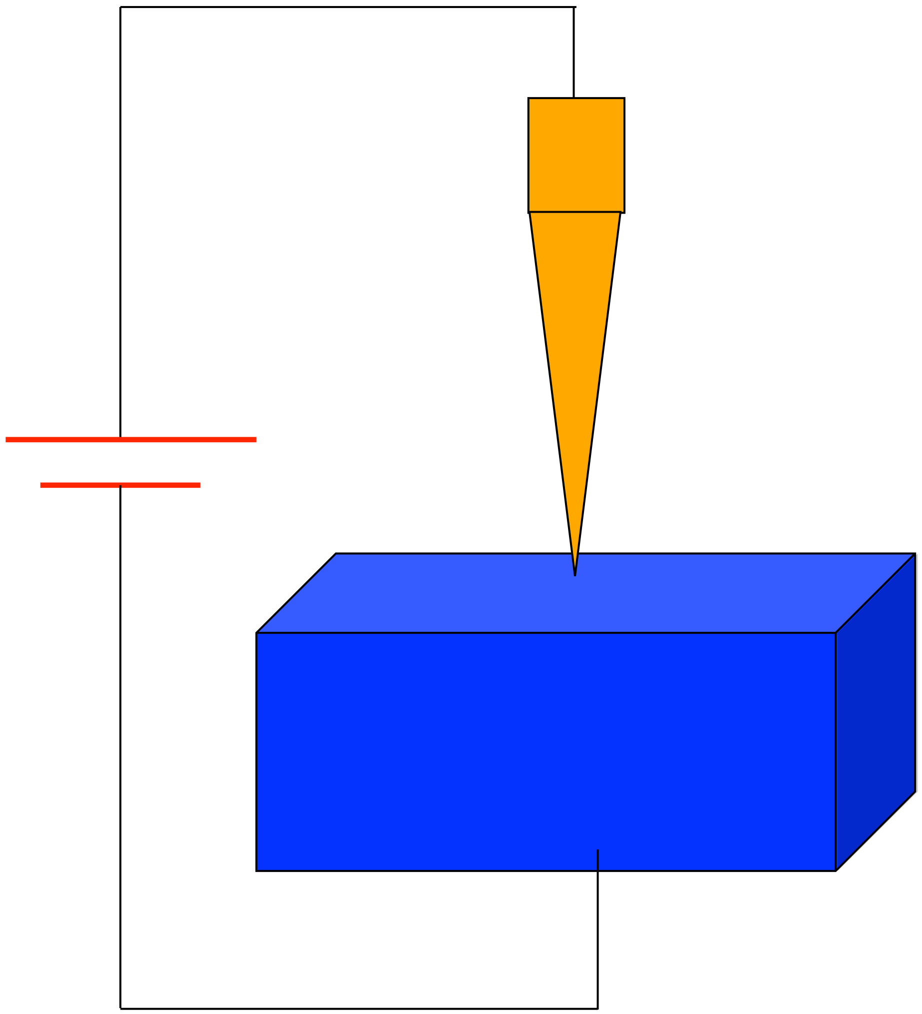
(Received 13 December 2010; published 2 August 2011)

Point Contact Spectroscopy



Wei-Cheng Lee, *et. al.,* submitted, PNAS.

Point Contact Spectroscopy

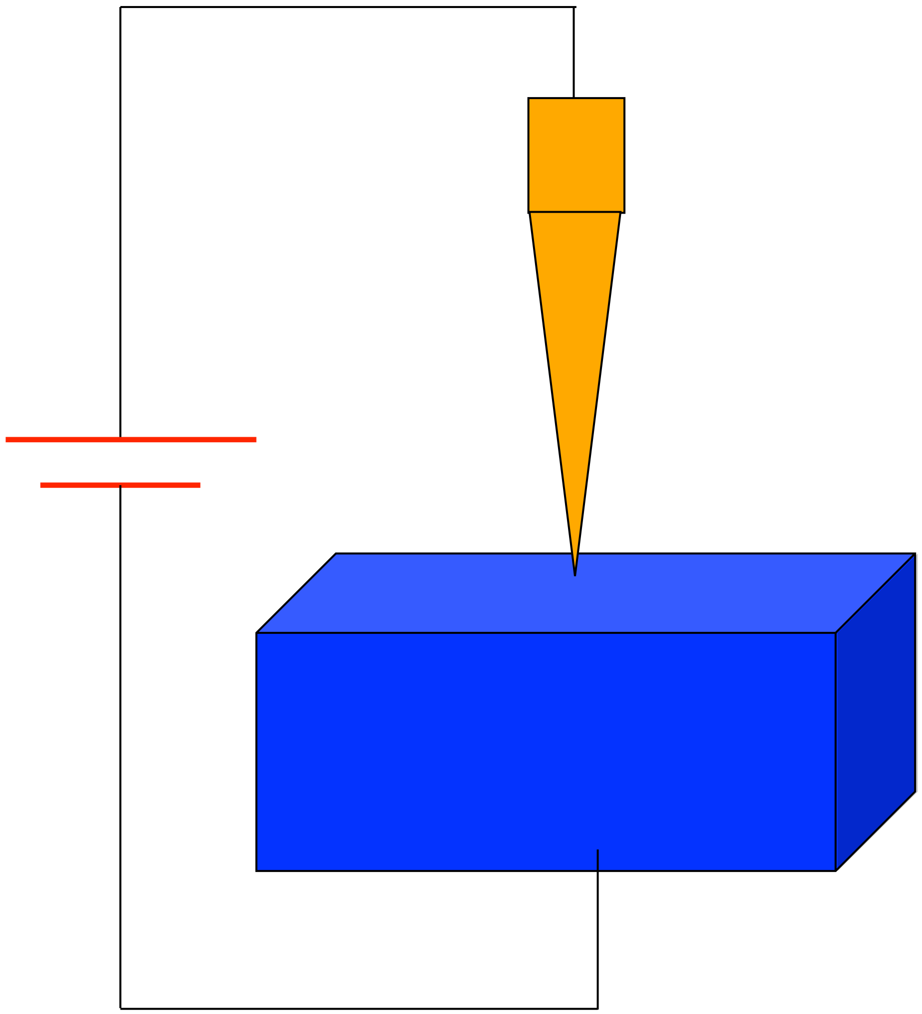


Using Keldysh formalism, for small voltage bias,

$$\frac{dI}{dV} \propto \int dk\, T(k, eV)\, \mathrm{Im}\, G(k, eV)$$

Wei-Cheng Lee, *et. al.,* submitted, PNAS.

Point Contact Spectroscopy



Using Keldysh formalism, for small voltage bias,

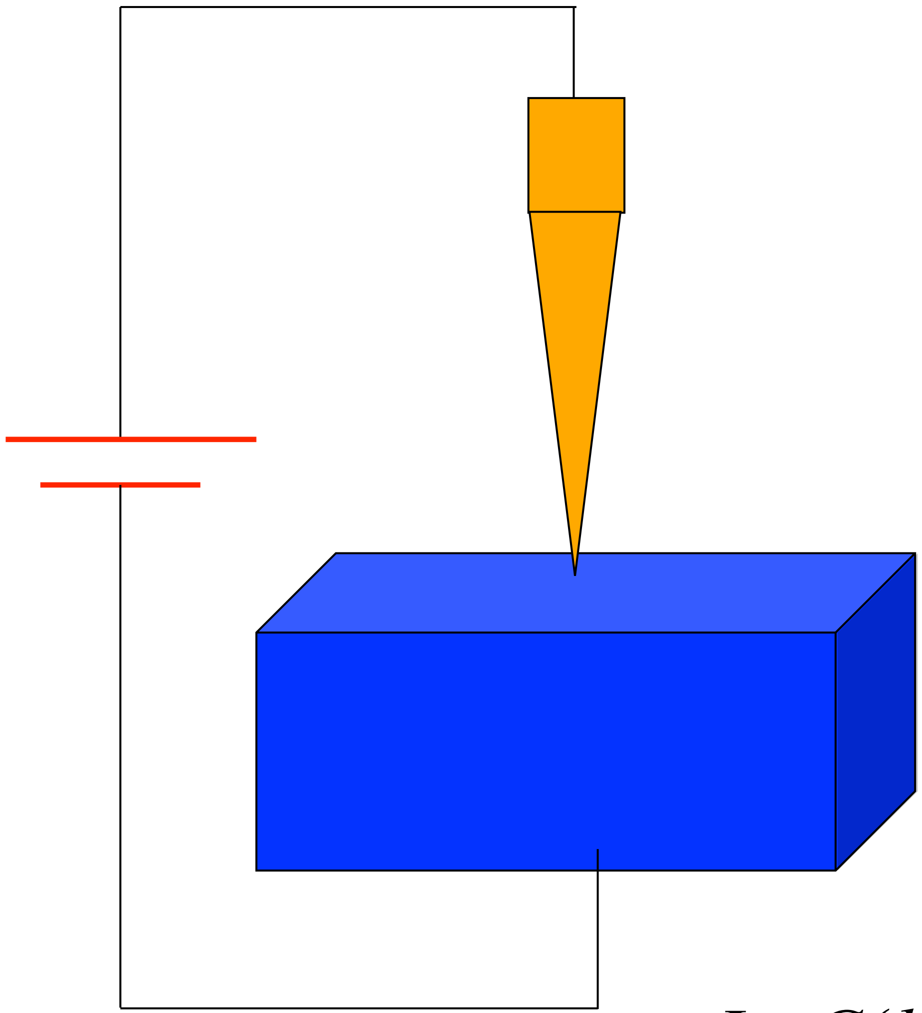
$$\frac{dI}{dV} \propto \int dk\, T(k,eV)\, \mathrm{Im}\, G(k,eV)$$

For metals

$$T(k,eV) \sim v_k, \mathrm{Im}\, G(k,eV) = \delta(\varepsilon_k - eV), \frac{dI}{dV} = const.$$

Wei-Cheng Lee, *et. al.,* submitted, PNAS.

Point Contact Spectroscopy



Using Keldysh formalism, for small voltage bias,

$$\frac{dI}{dV} \propto \int dk\, T(k,eV)\, \mathrm{Im}\, G(k,eV)$$

For metals

$$T(k,eV) \sim v_k, \mathrm{Im}\, G(k,eV) = \delta(\varepsilon_k - eV), \frac{dI}{dV} = const.$$

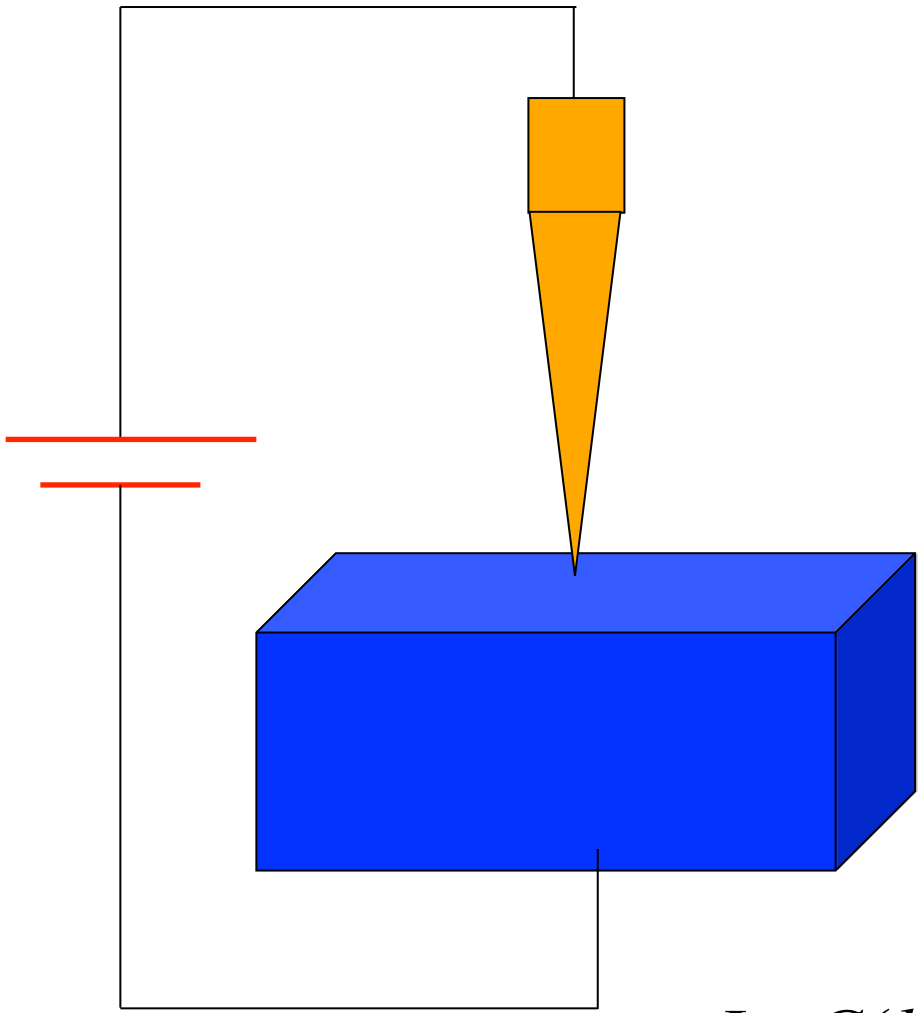
For non-Fermi liquid due to nematic QCP,

$$\mathrm{Im}\, G(k,eV) \neq \delta(\varepsilon_k - eV),$$

$$\frac{dI}{dV} \propto \int d\vec{k}\, \mathrm{Im}\, G(k,eV) = const. + A(eV/E_F)^{2/3} \ln(eV/E_F)$$

Wei-Cheng Lee, *et. al.,* submitted, PNAS.

Point Contact Spectroscopy



Using Keldysh formalism, for small voltage bias,

$$\frac{dI}{dV} \propto \int dk\, T(k,eV)\, \mathrm{Im}\, G(k,eV)$$

For metals

$$T(k,eV) \sim v_k, \mathrm{Im}\, G(k,eV) = \delta(\varepsilon_k - eV), \frac{dI}{dV} = const.$$

For non-Fermi liquid due to nematic QCP,

$$\mathrm{Im}\, G(k,eV) \neq \delta(\varepsilon_k - eV),$$

$$\frac{dI}{dV} \propto \int d\vec{k}\, \mathrm{Im}\, G(k,eV) = const. + A(eV/E_F)^{2/3} \ln(eV/E_F)$$

a peak at eV=0!!!

M. J. Lawler, et. al., Phys. Rev. B 73, 085101 (2006).

Wei-Cheng Lee, *et. al.,* submitted, PNAS.

Incommensurate-to-Commensurate Transformation in $Fe_{1-x}Ni_xTe_{0.5}Se_{0.5}$

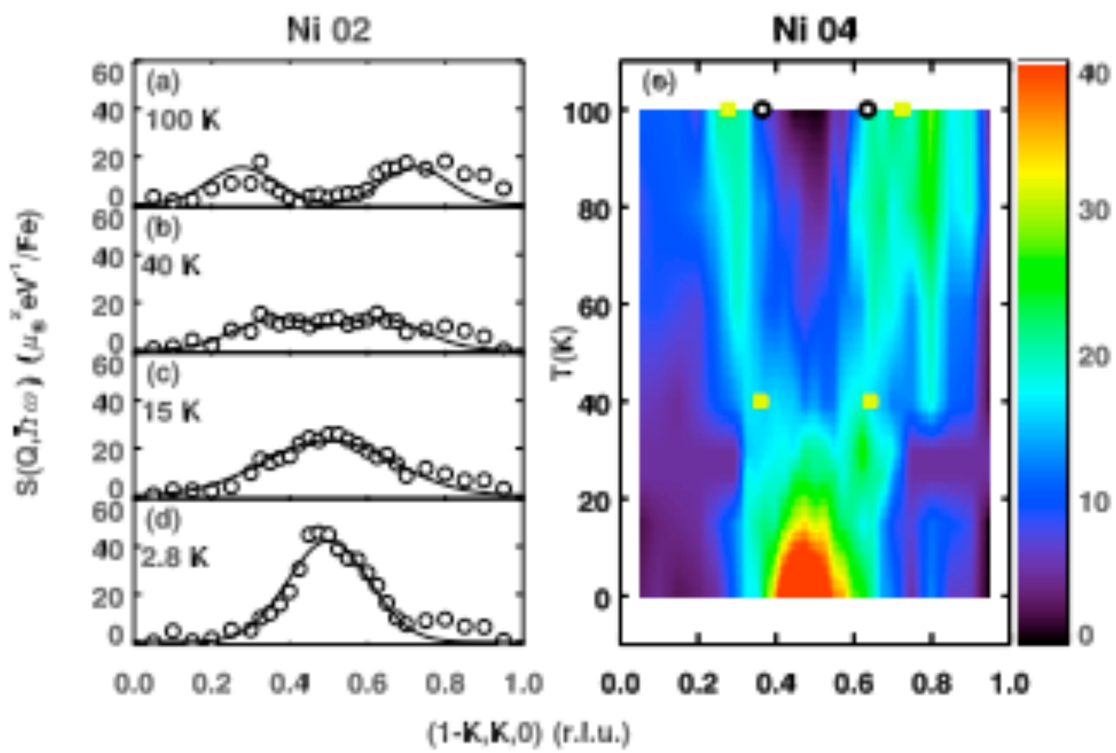
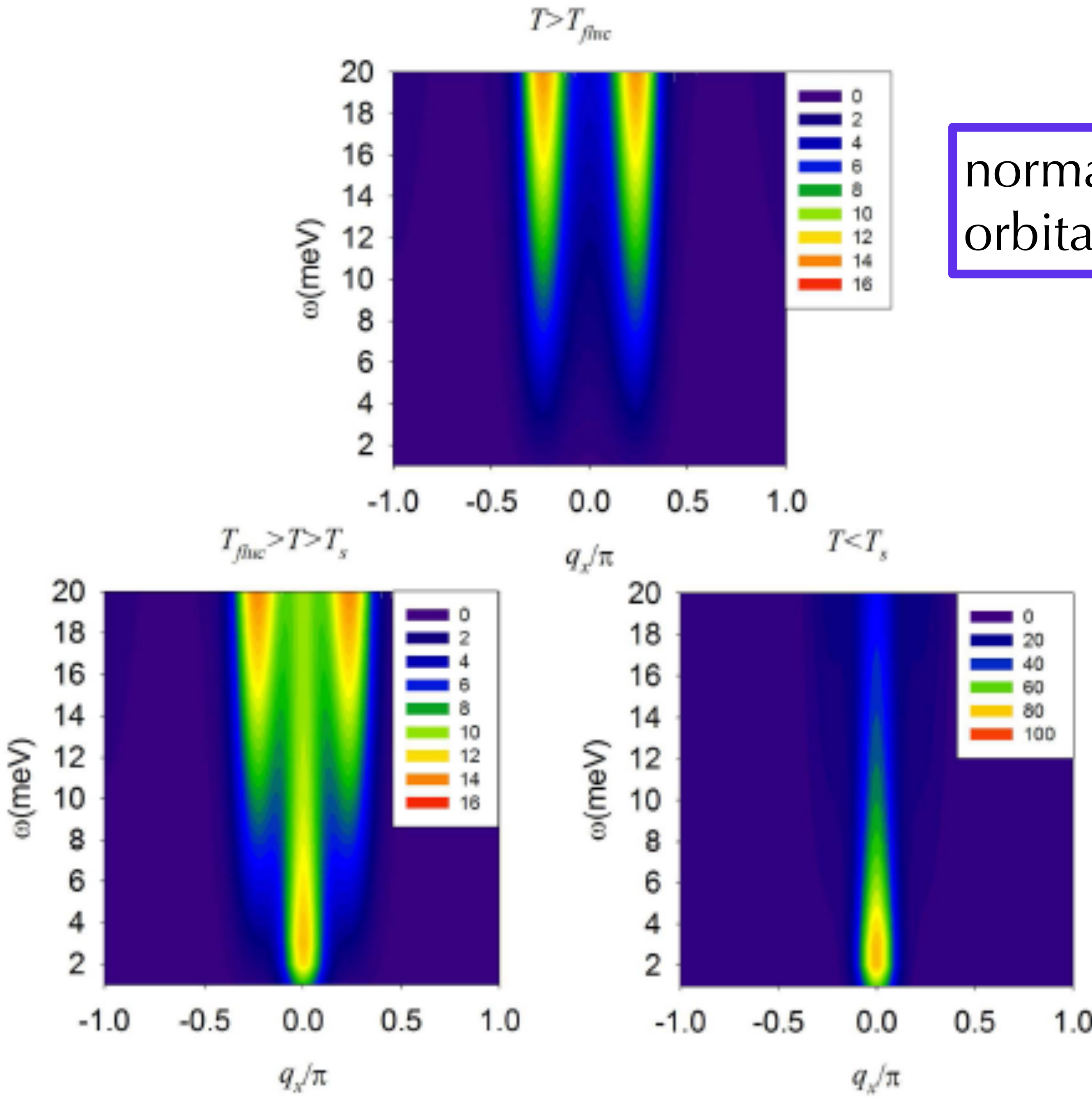


FIG. 4. (Color online) Thermal evolution of the magnetic scattering at $\hbar\omega = 5$ meV. The data are measured through $\mathbf{Q}_{AF}$ along the transverse direction for the Ni02 sample at (a) 100 K, (b) 40 K, (c) 15 K, (d) 2.8 K, and (e) for the Ni04 sample plotted as an intensity contour map in temperature–wave-vector space. The data have been smoothed. The yellow and black symbols in (e) denote the corresponding peak positions for the Ni02 sample (yellow squares) and for a superconducting $Fe_{1+\delta}Te_{0.35}Se_{0.65}$ sample [16].

Z. Xu, *et. al.*, Phys. Rev. Lett. **109**, 227002 (2012)

RPA + Gaussian Fluctuations

normal state without orbital fluctuations



Fluctuating orbital order (modeled by Gaussian fluctuation model)

Orbital ordered state

Holography: requirements for Pomeranchuk problem

Holography: requirements for Pomeranchuk problem

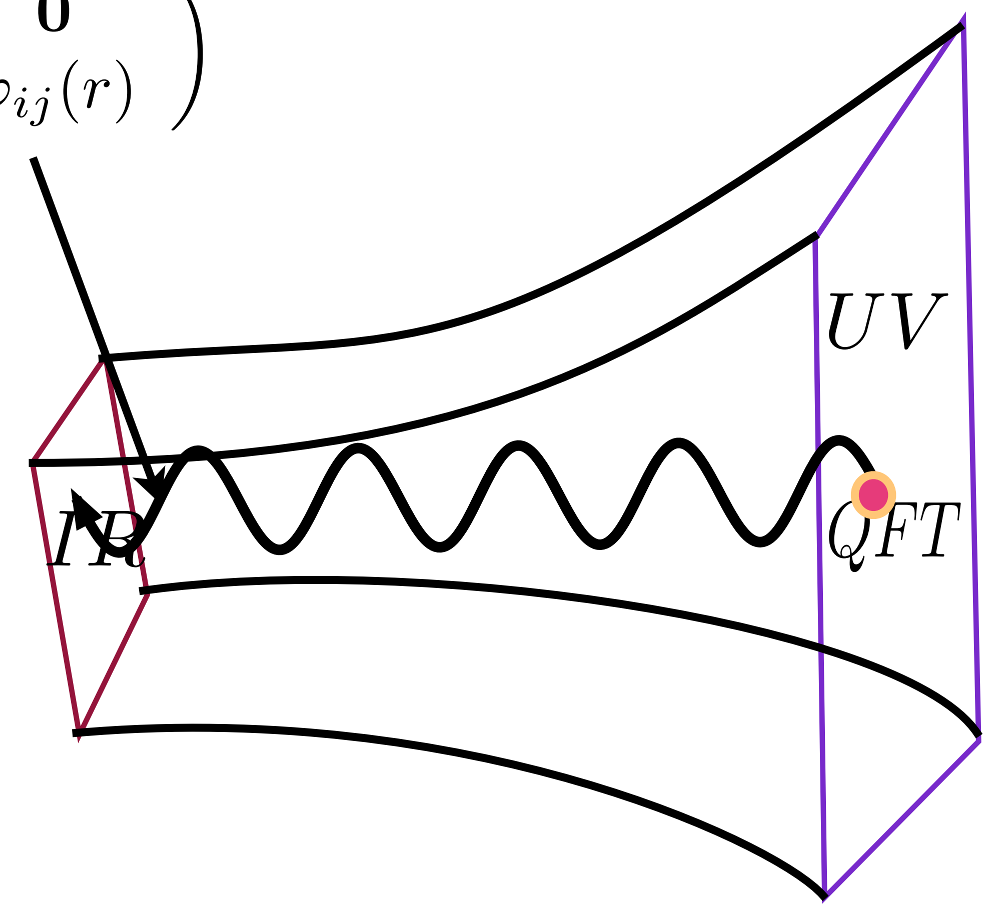
spin-2 field

$$\varphi_{\mu\nu}(r) = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \varphi_{ij}(r) \end{pmatrix}$$

Holography: requirements for Pomeranchuk problem

spin-2 field

$$\varphi_{\mu\nu}(r) = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \varphi_{ij}(r) \end{pmatrix}$$



Holography: requirements for Pomeranchuk problem

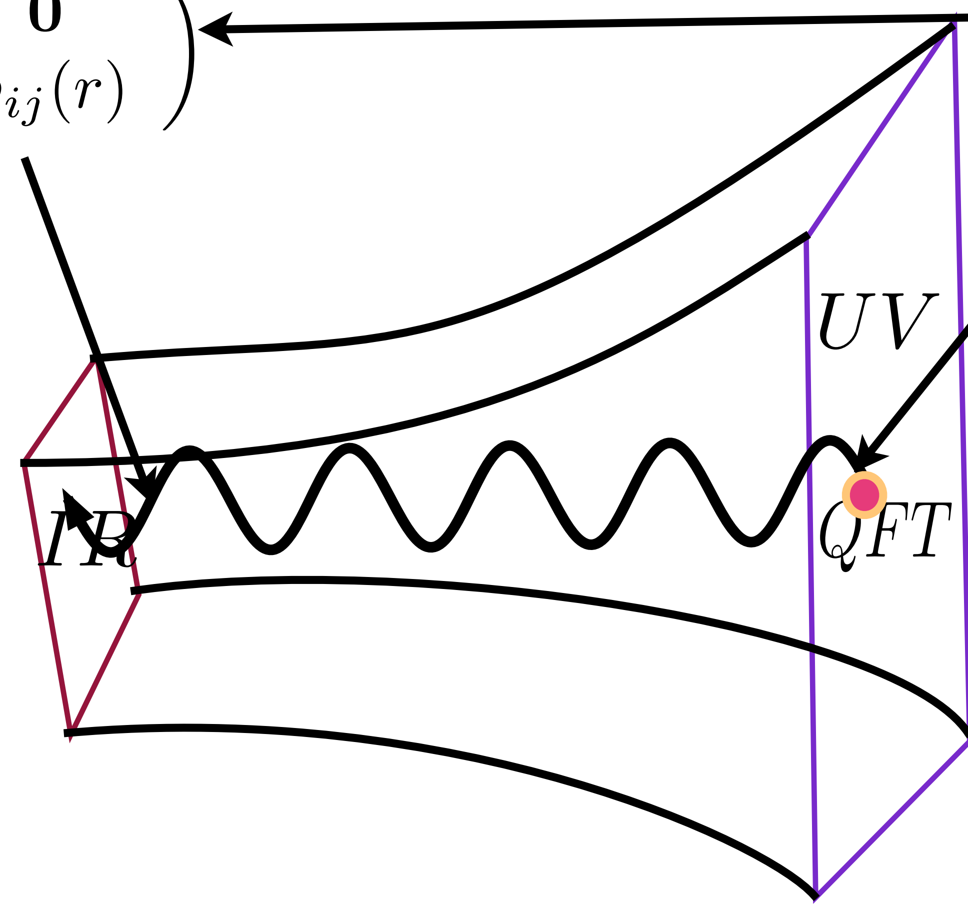
spin-2 field

$$\varphi_{\mu\nu}(r) = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \varphi_{ij}(r) \end{pmatrix}$$

$\mathcal{O}_{ij}$

nematic
order
parameter

$\langle \mathcal{O}_{ij} \rangle \neq 0$



Holography: requirements for Pomeranchuk problem

spin-2 field

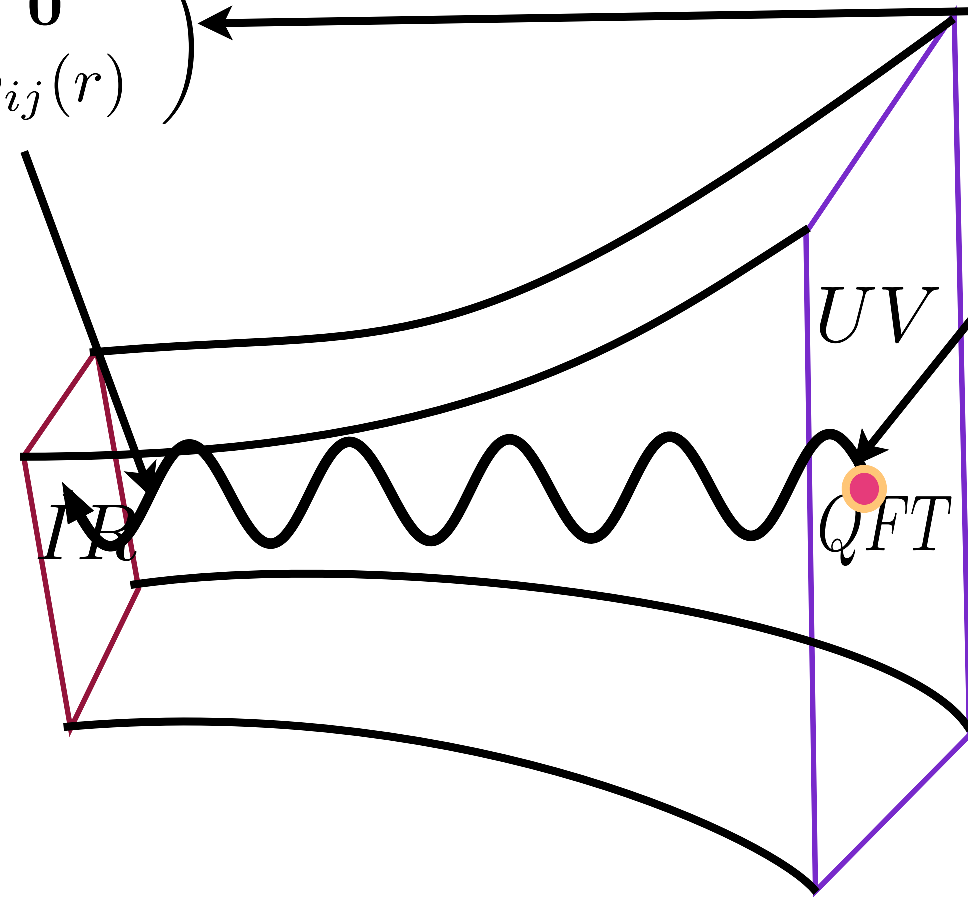
$$\varphi_{\mu\nu}(r) = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \varphi_{ij}(r) \end{pmatrix}$$

$\mathcal{O}_{ij}$

nematic order parameter

$\langle \mathcal{O}_{ij} \rangle \neq 0$

spontaneously!



Holography: requirements for Pomeranchuk problem

spin-2 field

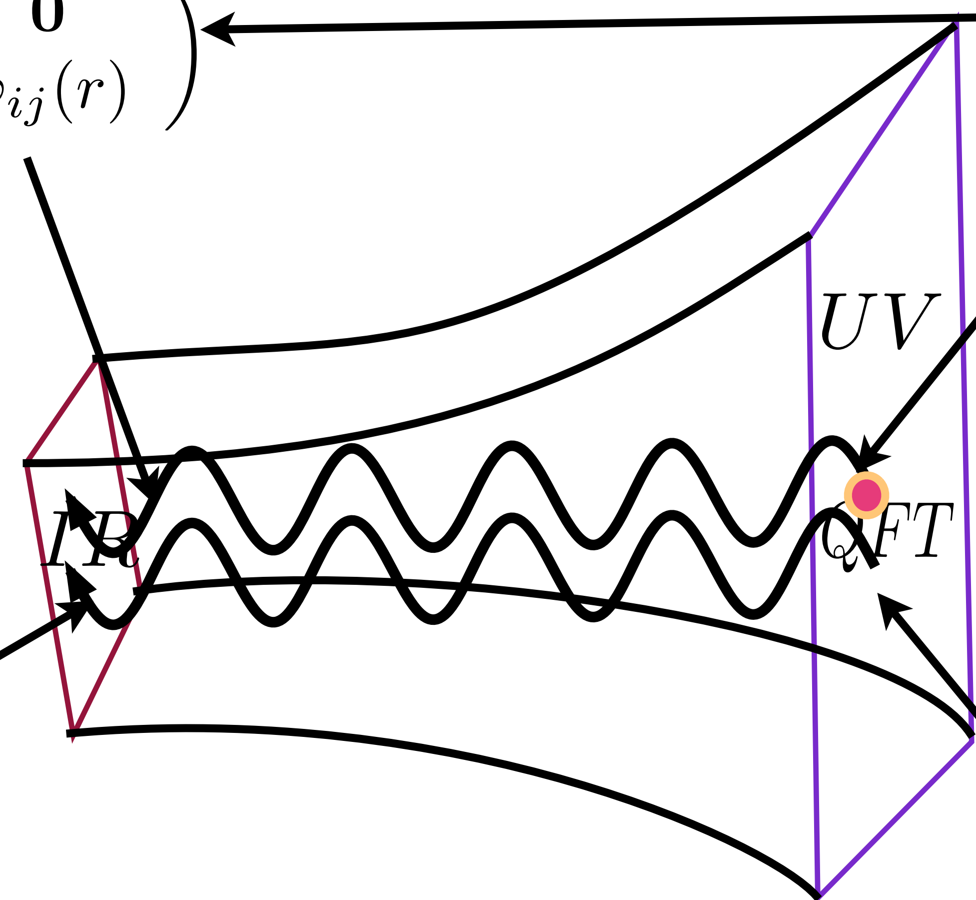
$$\varphi_{\mu\nu}(r) = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \varphi_{ij}(r) \end{pmatrix}$$

$\mathcal{O}_{ij}$

nematic order parameter

$\langle \mathcal{O}_{ij} \rangle \neq 0$

spontaneously!



ψ

spinor field

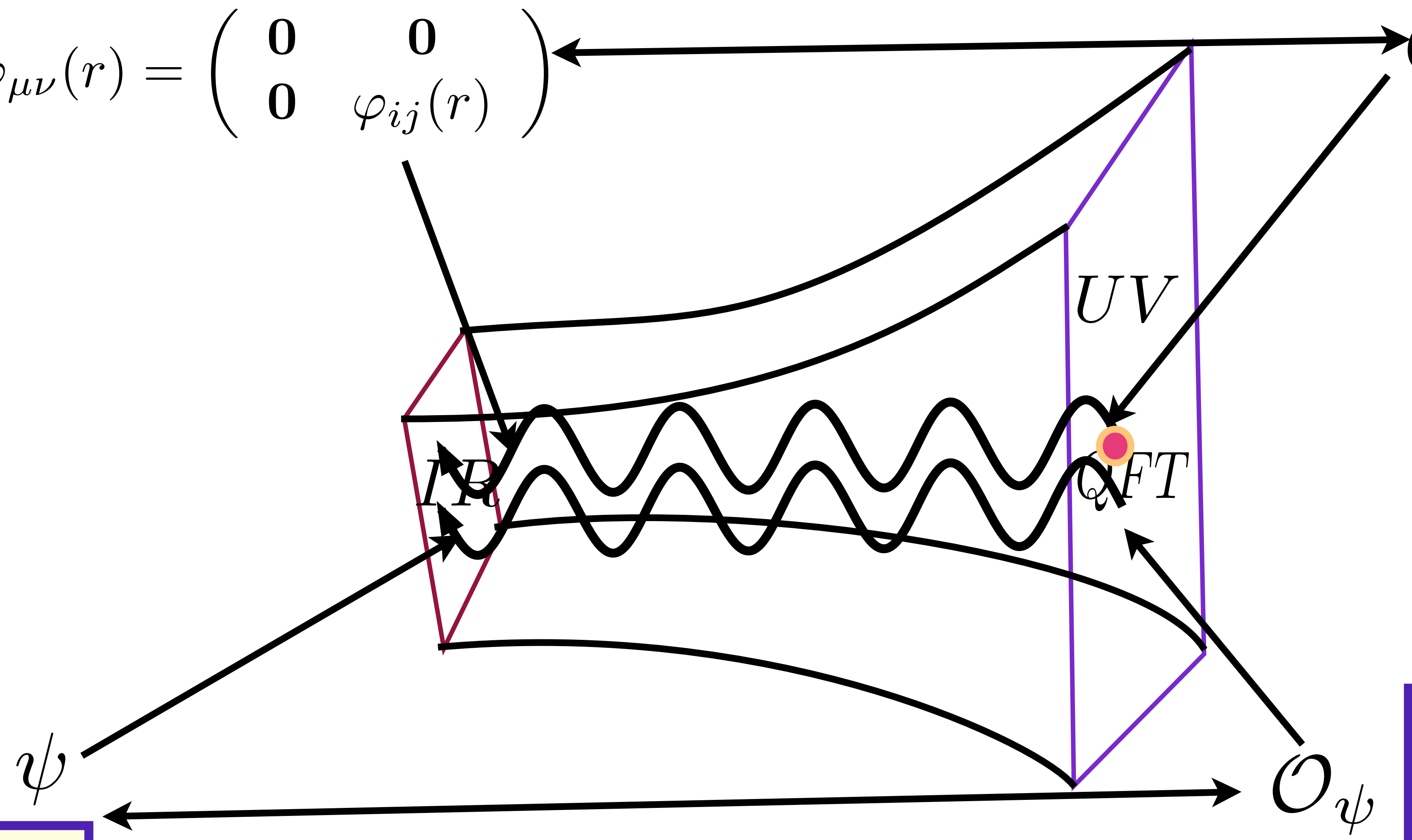
$\mathcal{O}_{\psi}$

boundary spinor operator

Holography: requirements for Pomeranchuk problem

spin-2 field

$$\varphi_{\mu\nu}(r) = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \varphi_{ij}(r) \end{pmatrix}$$



nematic order parameter

$\langle \mathcal{O}_{ij} \rangle \neq 0$

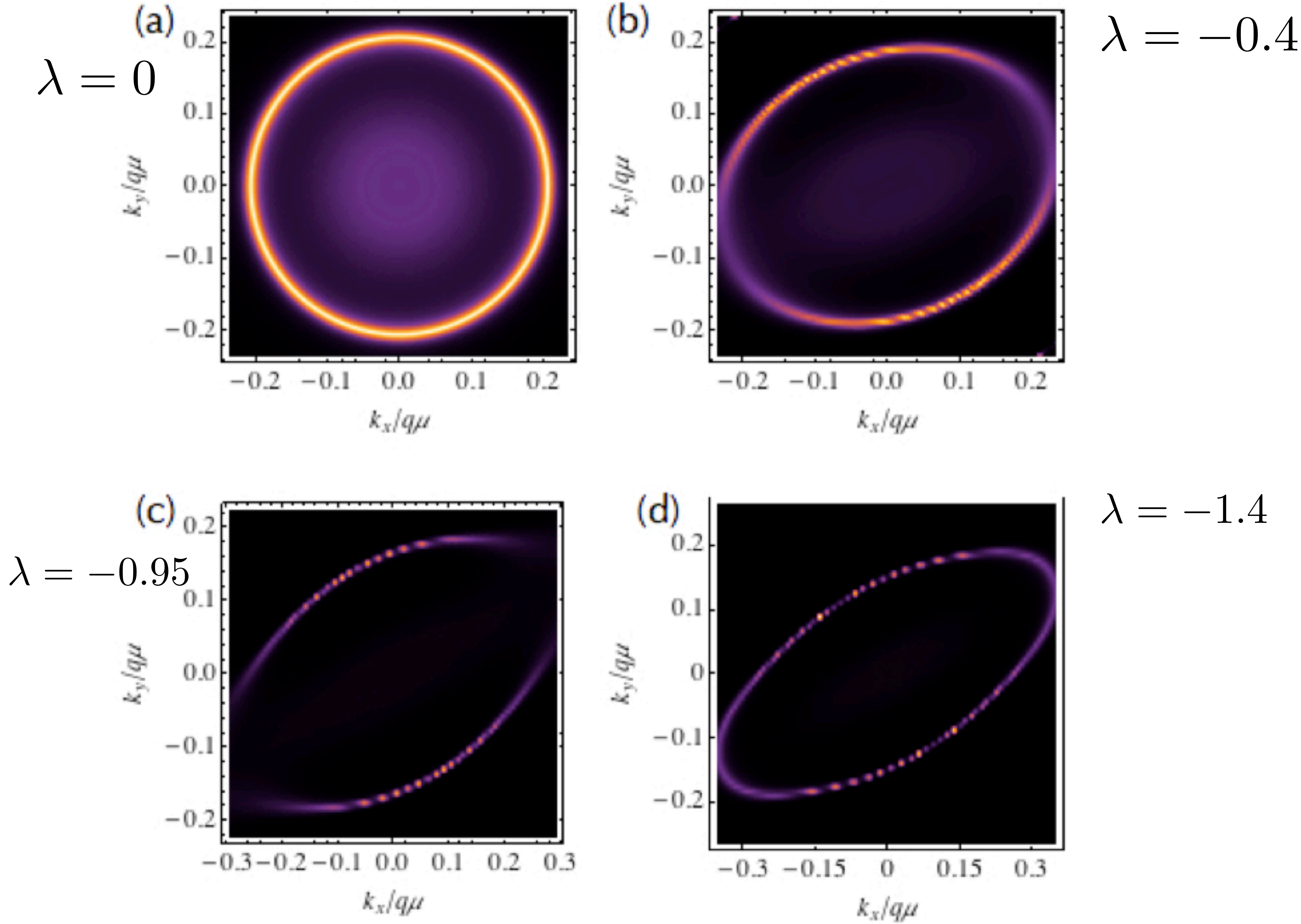
spontaneously!

spinor field

boundary spinor operator

gauge field

$$A = \mu\left(1 - \frac{r_0}{r}\right)dt \xrightarrow{r \to \infty} \mu$$



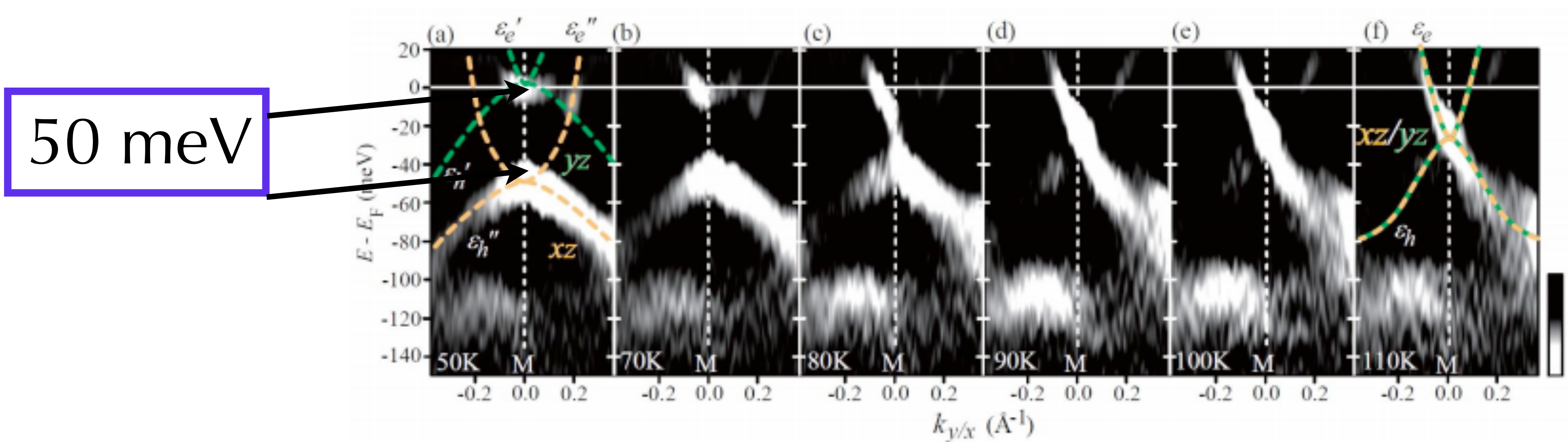
(a)
$\lambda = 0$
(b)
$\lambda = -0.4$
(c)
$\lambda = -0.95$
(d)
$\lambda = -1.4$
$k_y/q\mu$
$k_x/q\mu$

Puzzle #4

Lifting of *xz/yz* orbital degeneracy at the structural transition in detwinned FeSe

T. Shimojima[1,*], Y. Suzuki[1], T. Sonobe[1], A. Nakamura[1], M. Sakano[1], J. Omachi[2], K. Yoshioka[3], M. Kuwata-Gonokami[2,3], K. Ono[4], H. Kumigashira[4], A. E. Böhmer[5], F. Hardy[5], T. Wolf[5], C. Meingast[5], H. v. Löhneysen[5,6], H. Ikeda[7], K. Ishizaka[1]

[1]*Quantum-Phase Electronics Center(QPEC) and Department of Applied Physics, University of Tokyo, Bunkyo, Tokyo 113-8656, Japan.*
[2]*Photon Science Center, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
[3]*Department of Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*
[4]*KEK, Photon Factory, Tsukuba, Ibaraki 305-0801, Japan.*
[5]*Institut für Festkörperphysik, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany*
[6]*Physikalisches Institut, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany*
[7]*Department of Physics, Kyoto University, Kyoto 606-8502, Japan.*



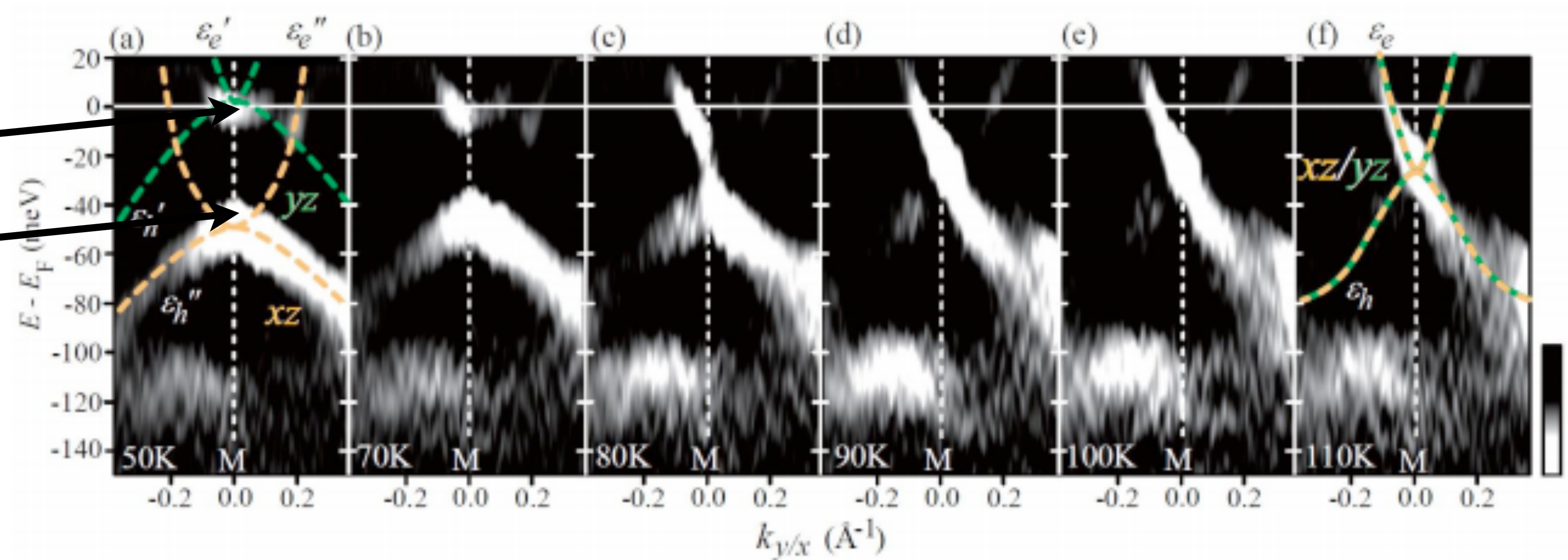
Puzzle #4

Lifting of *xz/yz* orbital degeneracy at the structural transition in detwinned FeSe

T. Shimojima[1,*], Y. Suzuki[1], T. Sonobe[1], A. Nakamura[1], M. Sakano[1], J. Omachi[2], K. Yoshioka[3], M. Kuwata-Gonokami[2,3], K. Ono[4], H. Kumigashira[4], A. E. Böhmer[5], F. Hardy[5], T. Wolf[5], C. Meingast[5], H. v. Löhneysen[5,6], H. Ikeda[7], K. Ishizaka[1]

[1]Quantum-Phase Electronics Center(QPEC) and Department of Applied Physics, University of Tokyo, Bunkyo, Tokyo 113-8656, Japan.
[2]Photon Science Center, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
[3]Department of Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan
[4]KEK, Photon Factory, Tsukuba, Ibaraki 305-0801, Japan.
[5]Institut für Festkörperphysik, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany
[6]Physikalisches Institut, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany
[7]Department of Physics, Kyoto University, Kyoto 606-8502, Japan.

50 meV



what about NMR below T_s?

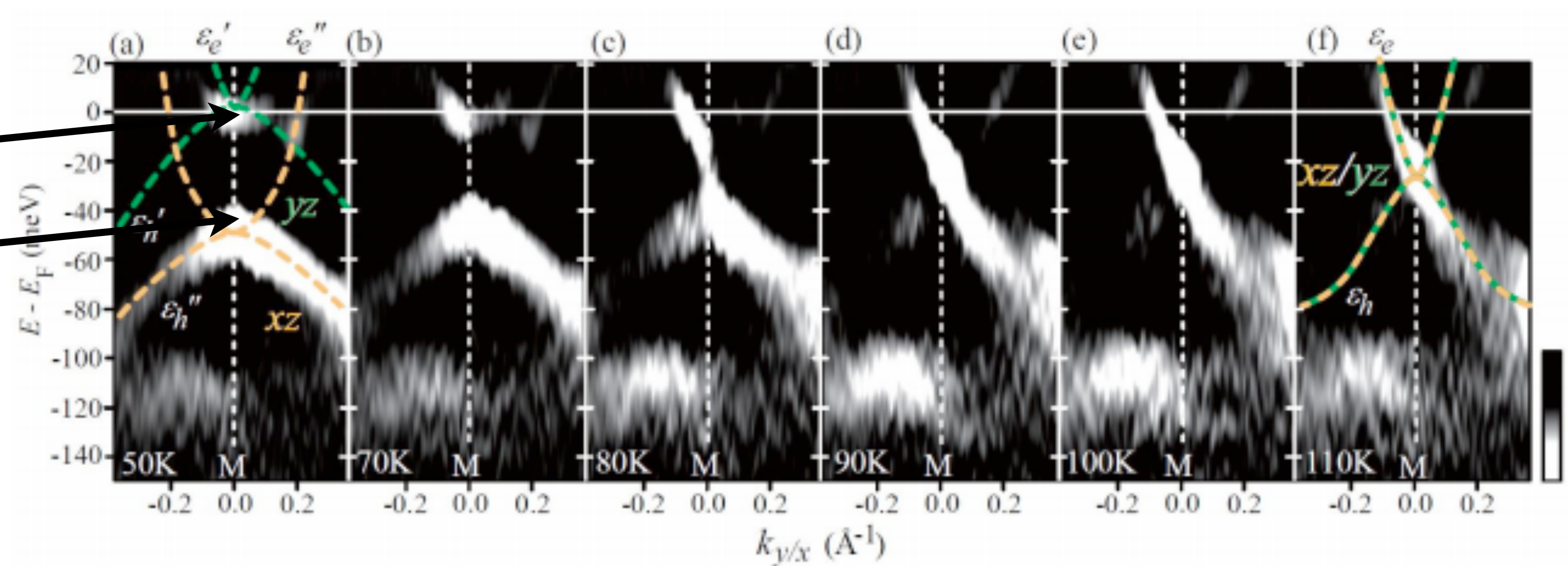
Puzzle #4

Lifting of *xz/yz* orbital degeneracy at the structural transition in detwinned FeSe

T. Shimojima[1,*], Y. Suzuki[1], T. Sonobe[1], A. Nakamura[1], M. Sakano[1], J. Omachi[2],
K. Yoshioka[3], M. Kuwata-Gonokami[2,3], K. Ono[4], H. Kumigashira[4], A. E. Böhmer[5],
F. Hardy[5], T. Wolf[5], C. Meingast[5], H. v. Löhneysen[5,6], H. Ikeda[7], K. Ishizaka[1]

[1]*Quantum-Phase Electronics Center(QPEC) and Department of Applied Physics, University of Tokyo, Bunkyo, Tokyo 113-8656, Japan.*
[2]*Photon Science Center, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
[3]*Department of Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*
[4]*KEK, Photon Factory, Tsukuba, Ibaraki 305-0801, Japan.*
[5]*Institut für Festkörperphysik, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany*
[6]*Physikalisches Institut, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany*
[7]*Department of Physics, Kyoto University, Kyoto 606-8502, Japan.*

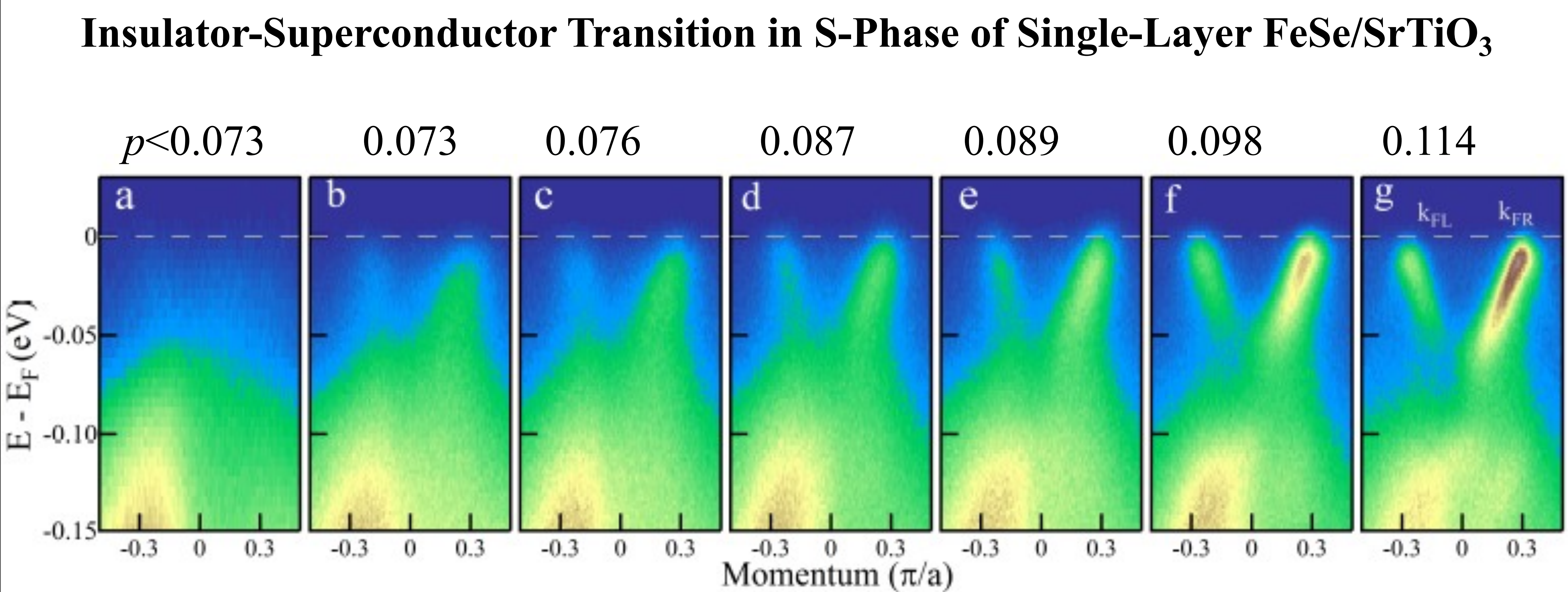
50 meV



what about NMR below T_s?

shear modulus in manganites?

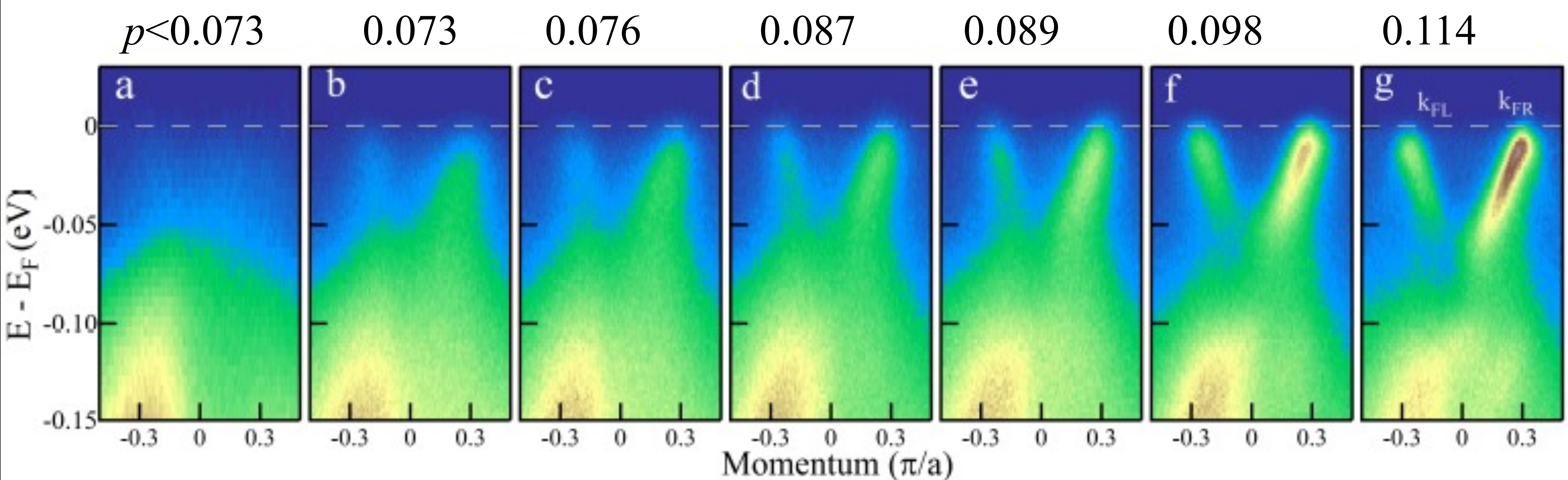
what really are the `pnictides'?



J. F. He, X. J. Zhou et al., arXiv:1401.7115.

what really are the `pnictides'?

Insulator-Superconductor Transition in S-Phase of Single-Layer FeSe/SrTiO$_3$



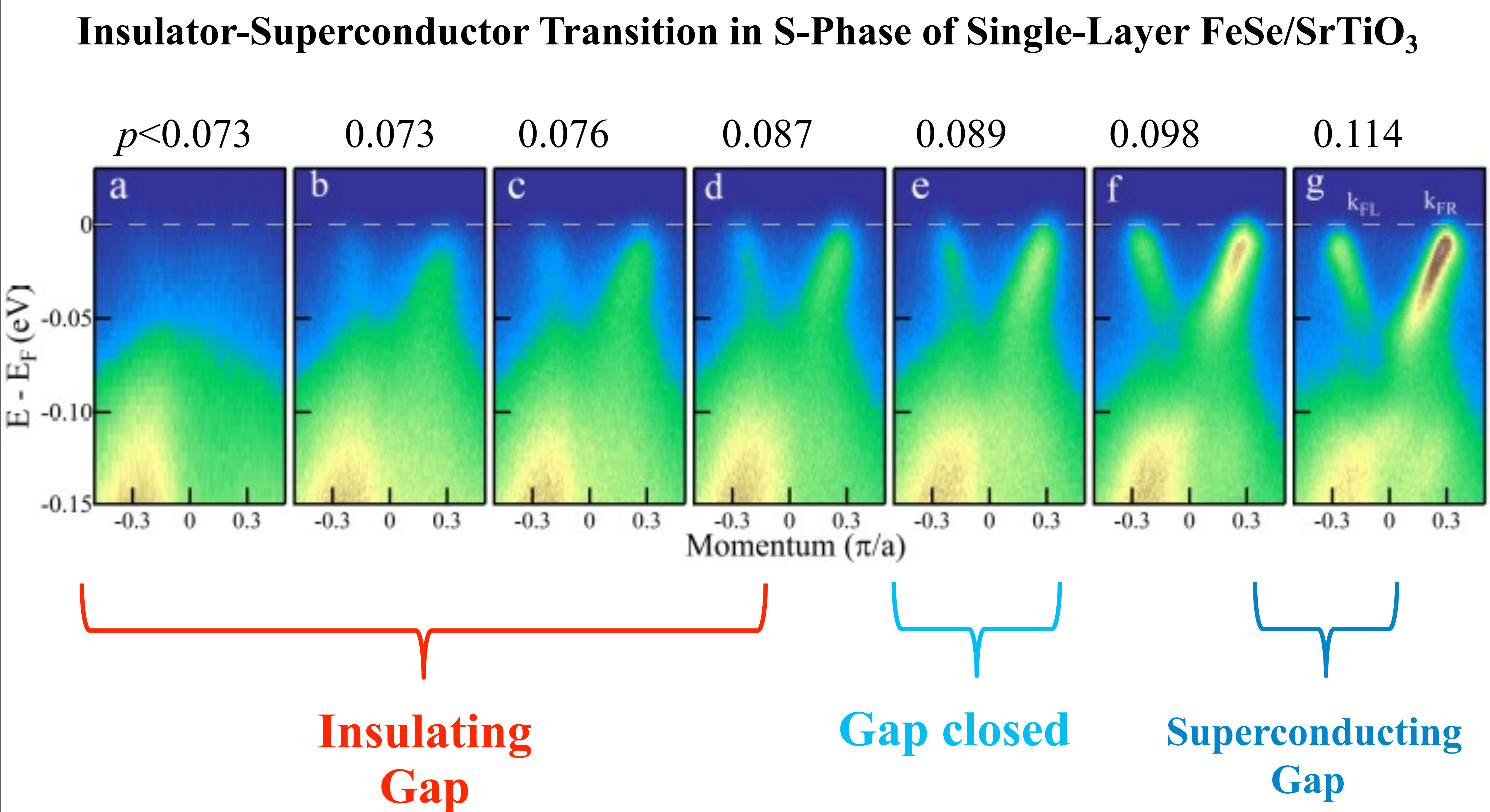
Insulating Gap

Gap closed

Superconducting Gap

J. F. He, X. J. Zhou et al., arXiv:1401.7115.

what really are the `pnictides'?



orbital-selective Mott transition

J. F. He, X. J. Zhou et al., arXiv:1401.7115.

Routes to High-T_c

$CuFeTe_2$, $Li_xNi_{1-x}O_2$, ?FeSe?

Routes to High-T_c

cuprates: one Cu spin

Mott Physics

$CuFeTe_2$, $Li_xNi_{1-x}O_2$, ?FeSe?

Routes to High-T_c

pnictides: several unapired Fe spins

bad metals

cuprates: one Cu spin

Mott Physics

CuFeTe_2, Li_xNi_{1-x}O_2, ?FeSe?

Routes to High-T_c

pnictides: several unapired Fe spins

bad metals

cuprates: one Cu spin

Mott Physics

are multi-orbital Mott systems higher T_c materials?

CuFeTe_2, Li_xNi_{1-x}O_2, ?FeSe?

Possible systems (multi-orbital Mott systems) ?

Simple

$NiO_{1-x}F_x$

hole-doping a
d^8 system.
Does it superconduct?

complex
(oxychalchogenides

$A_2O_3Fe_2M_2$

A= La, Y
M=Se, S, Te

Co and Cu- based

$La_2Co_2Se_2O_3$
$Na_2OCu_4OSe_2$

Possible systems (multi-orbital Mott systems) ?

Simple

$NiO_{1-x}F_x$

hole-doping a d^8 system.
Does it superconduct?

complex
(oxychalchogenides

$A_2O_3Fe_2M_2$

A= La, Y
M=Se, S, Te

Co and Cu- based

$La_2Co_2Se_2O_3$
$Na_2OCu_4OSe_2$

Band Narrowing and Mott Localization in Iron Oxychalcogenides $La_2O_2Fe_2O(Se,S)_2$

Jian-Xin Zhu,[1] Rong Yu,[2] Hangdong Wang,[3] Liang L. Zhao,[2] M. D. Jones,[4]
Jianhui Dai,[3] Elihu Abrahams,[5] E. Morosan,[2] Minghu Fang,[3] and Qimiao Si[2]
[1] *Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2] *Department of Physics & Astronomy, Rice University, Houston, Texas 77005, USA*
[3] *Department of Physics, Zhejiang University, Hangzhou 310027, P. R. China*
[4] *University at Buffalo, SUNY, Buffalo, New York 14260, USA*
[5] *Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08855, USA**

Is this what is going on in FeSe?