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

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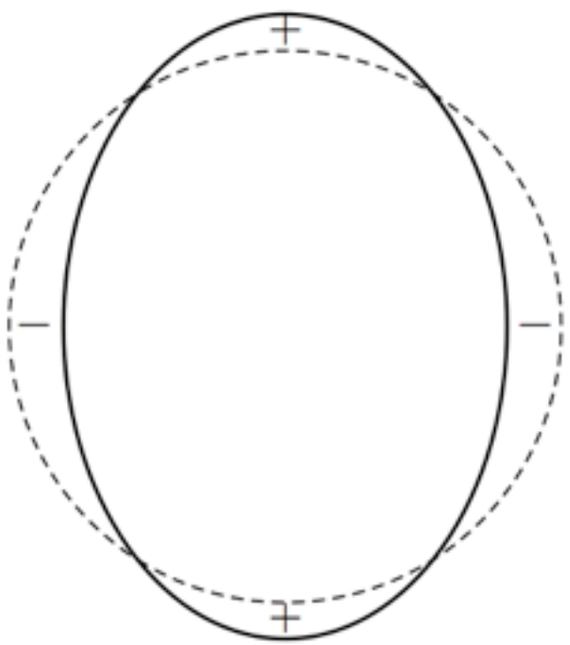
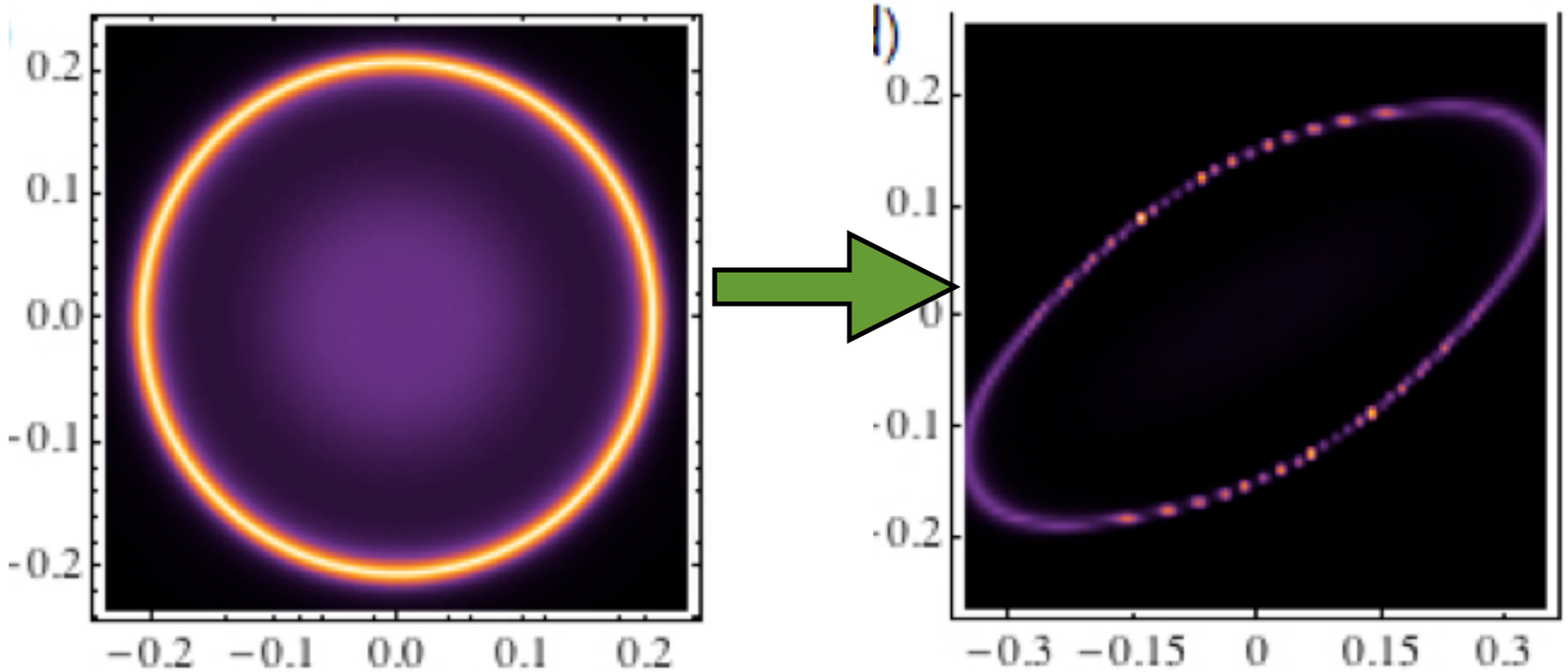
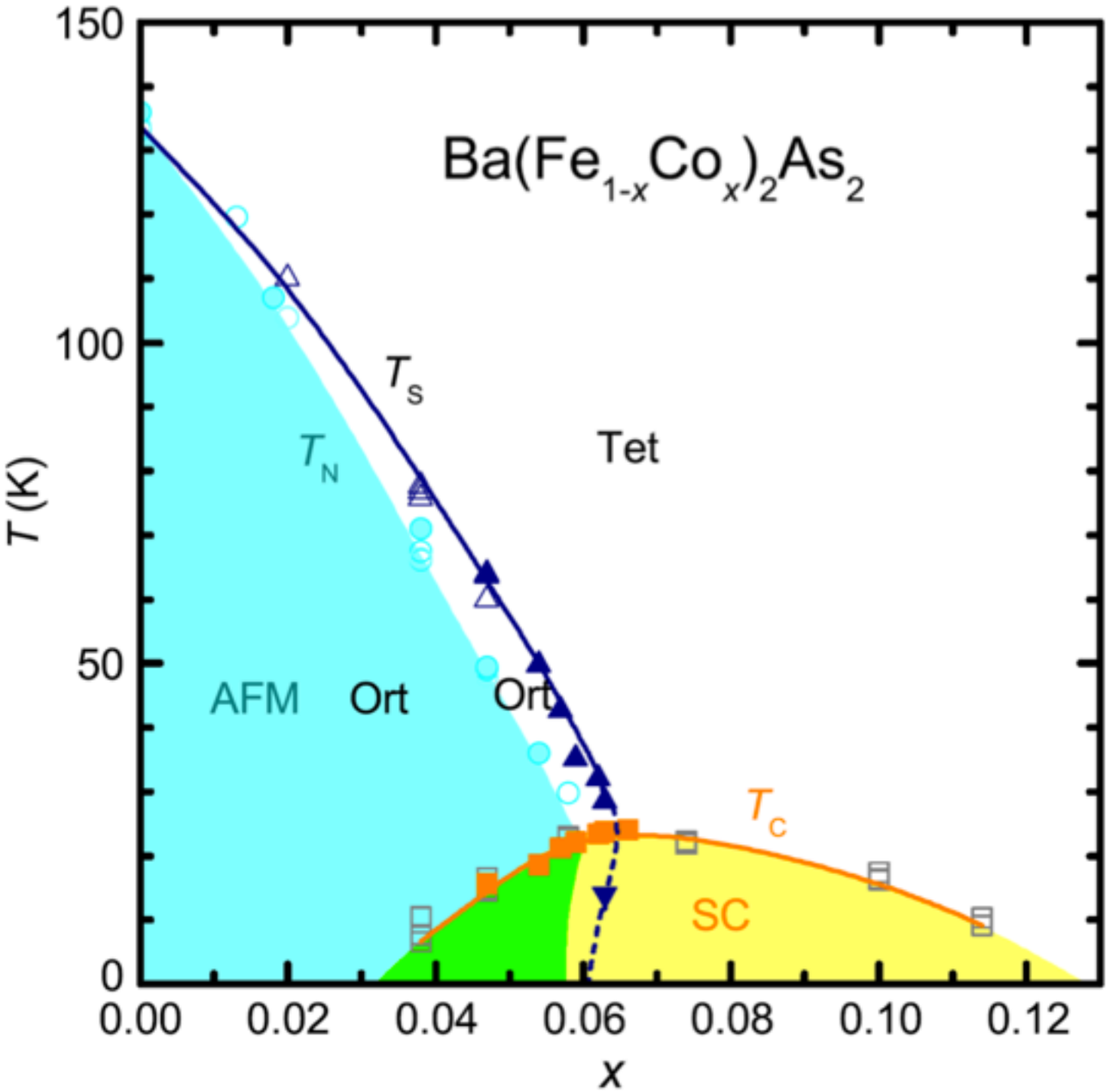




- *Phase Diagram*



S. Nandi, et al. PRL (2010)

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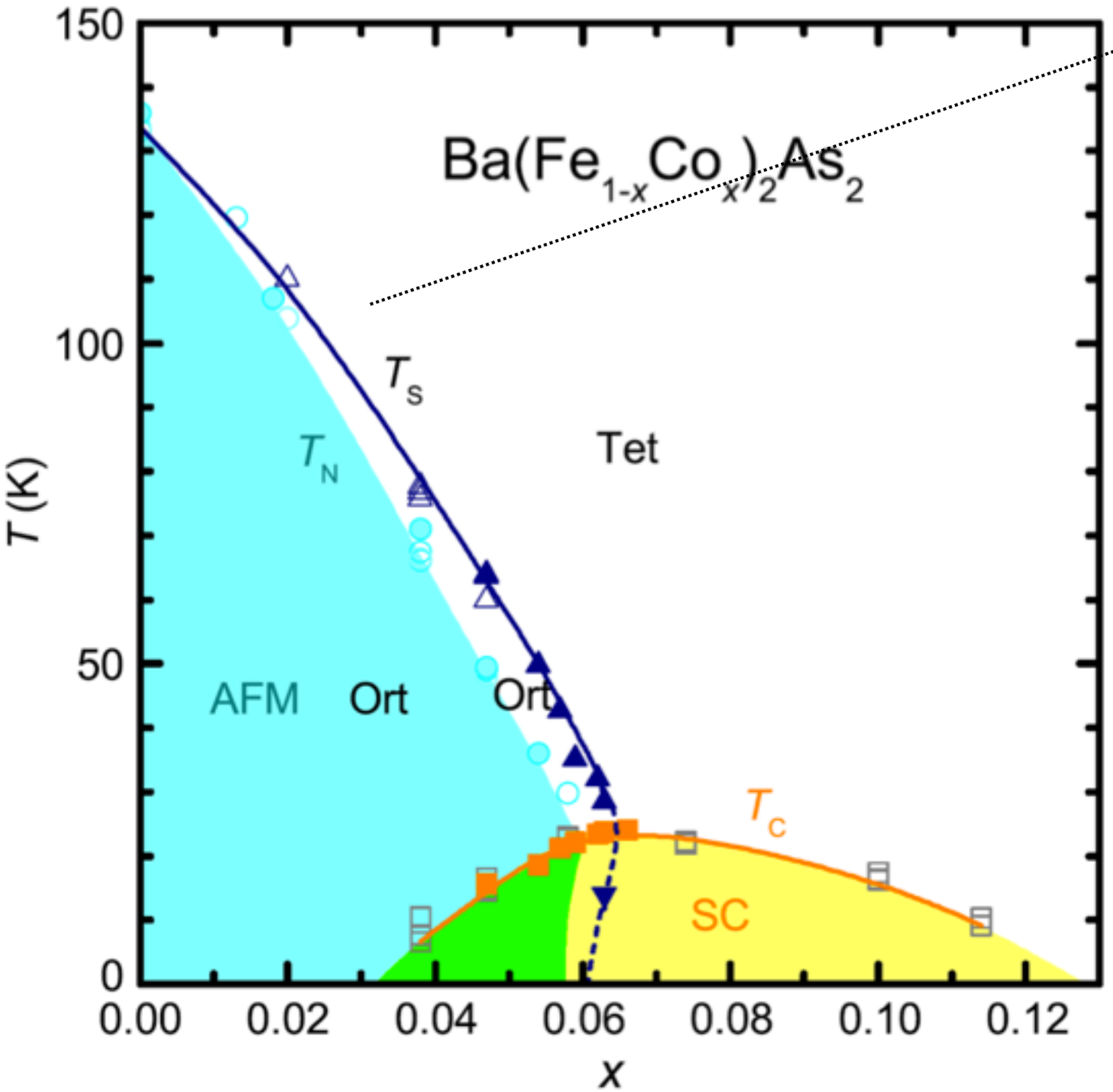

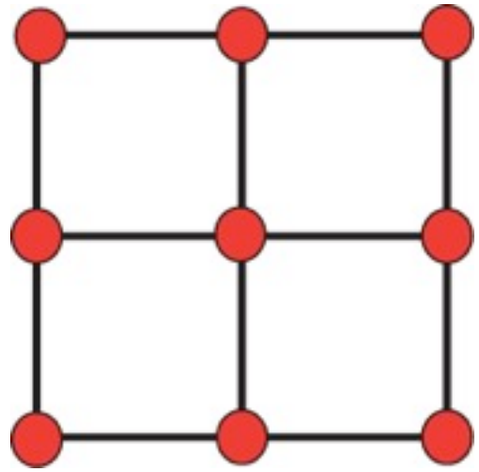

S. Nandi, et al. PRL (2010)

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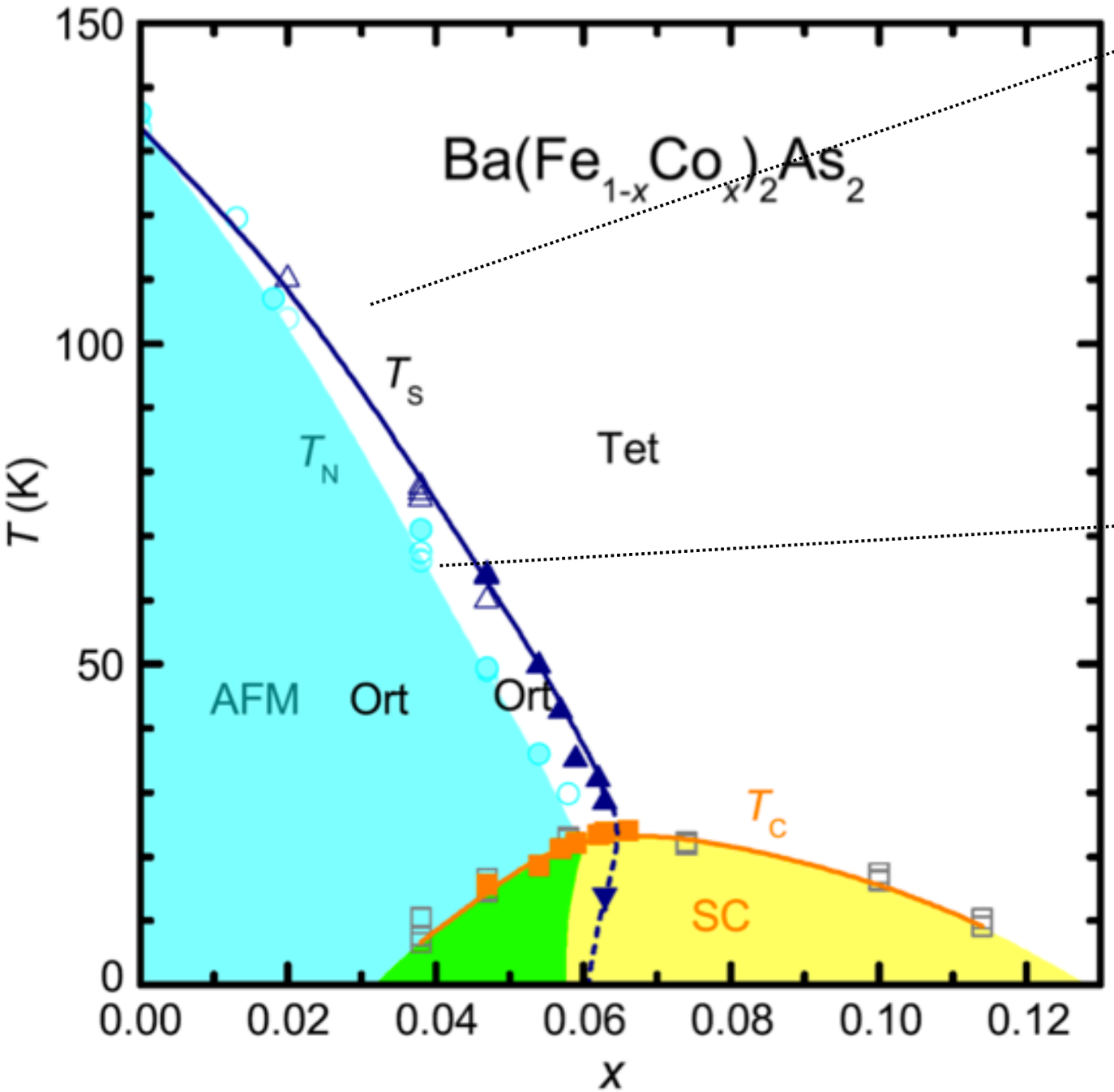
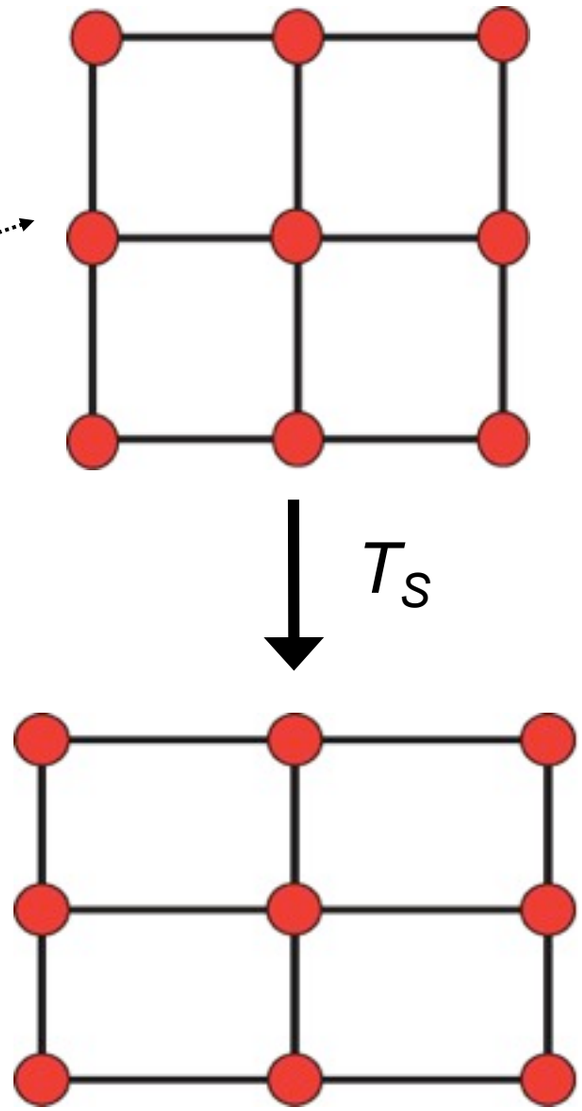
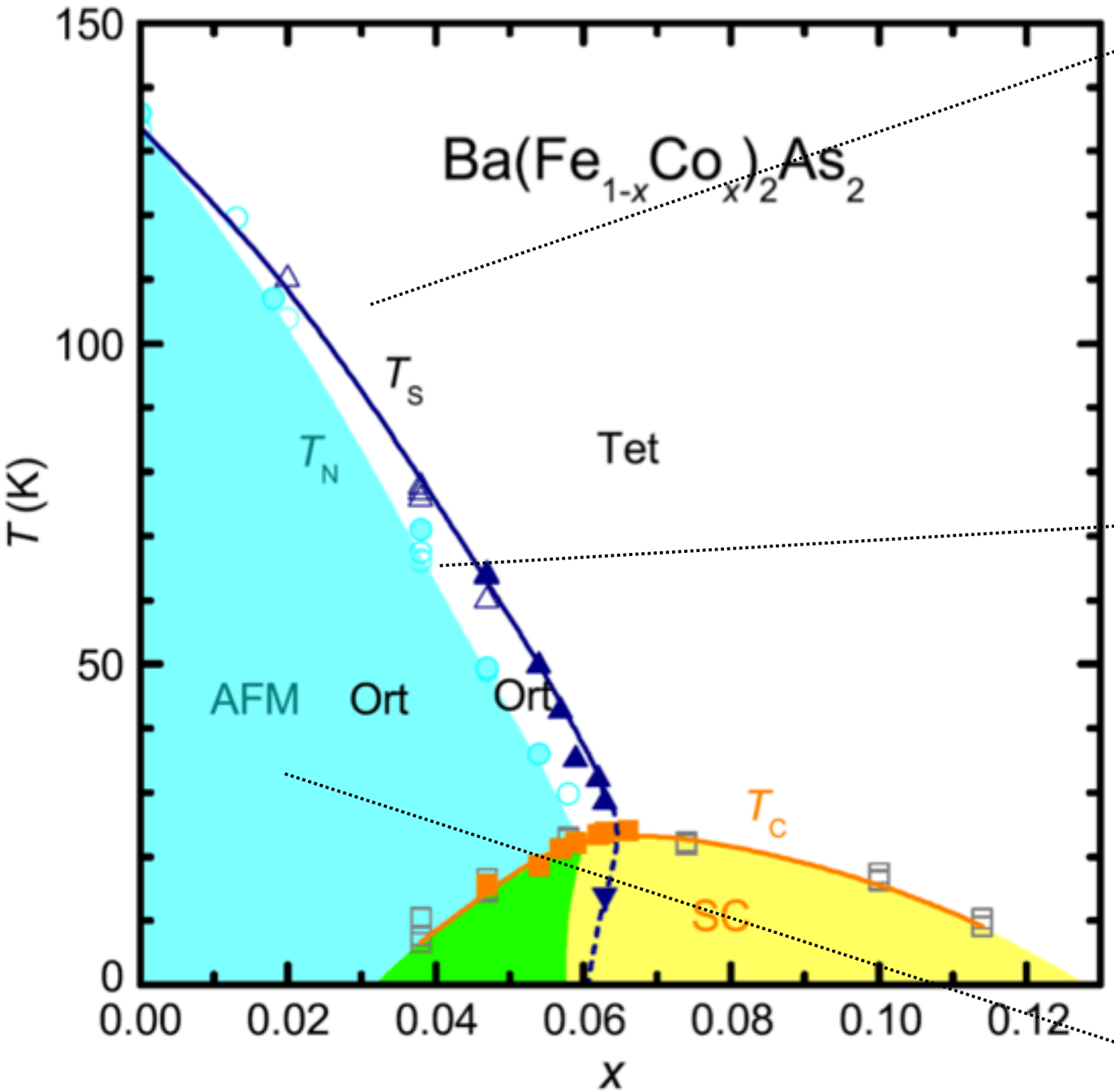
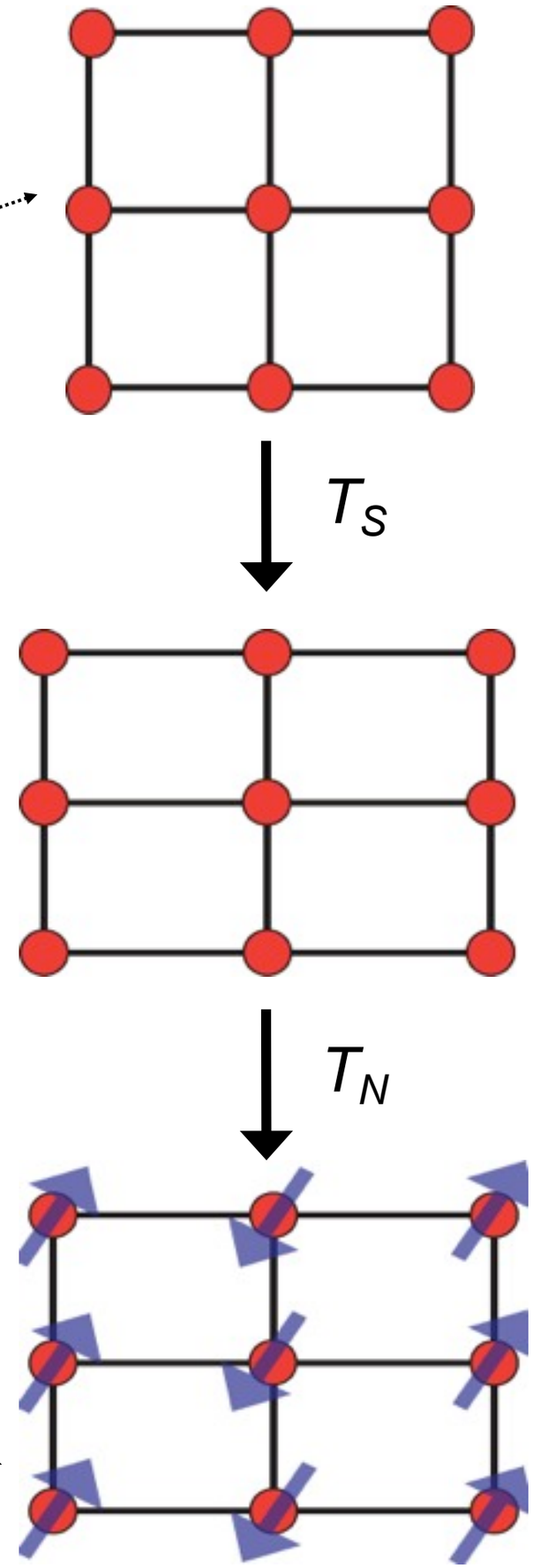




S. Nandi, et al. PRL (2010)

- *Phase Diagram*





S. Nandi, et al. PRL (2010)

What is new with Fe-based superconductors?

What is new with Fe-based superconductors?

d^6 not d^9

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multi-orbital physics

d^6 not d^9

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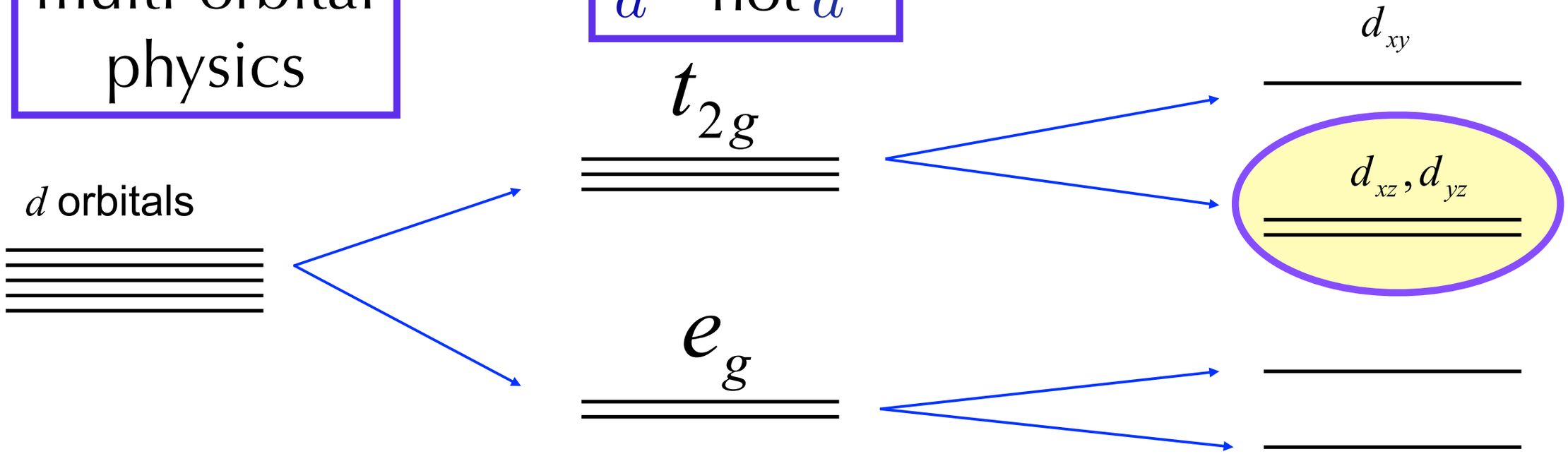
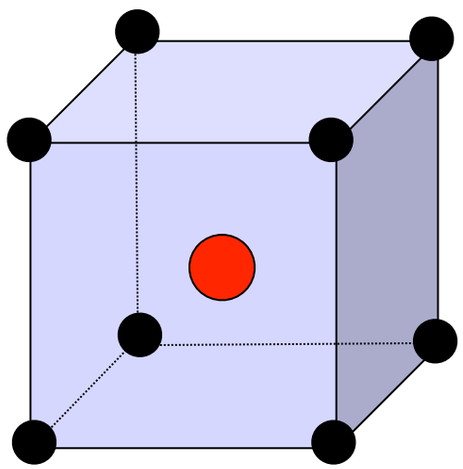
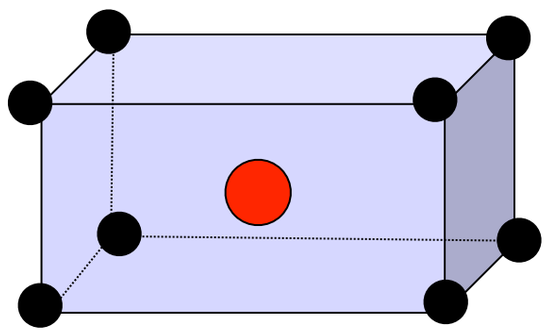


atom



cubic symmetry
(a=b=c)



tetragonal symmetry
(a=b≠c)

Who is in the Driver's Seat?

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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)
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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

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

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

Why Do I care?

Why Do I care?

cuprates

d^9

no orbital
degree of freedom

Why Do I care?

cuprates

d^9

no orbital
degree of freedom

pnictides

d^6

orbital degeneracy

Why Do I care?

cuprates

d^9

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no orbital
degree of freedom

orbital degeneracy

is the orbital degree of freedom important?

subtle problem

$$O(3) \times Z_2$$

subtle problem

$$O(3) \times Z_2 \rightarrow (\pi, 0), (0, \pi)$$

subtle problem

$$O(3) \times Z_2$$

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

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

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

} magnetic fluctuations

subtle problem

$O(3) \times Z_2$

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

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} magnetic fluctuations

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

structural transition

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

} nematic

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

subtle problem

$O(3) \times Z_2$

orbitals

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

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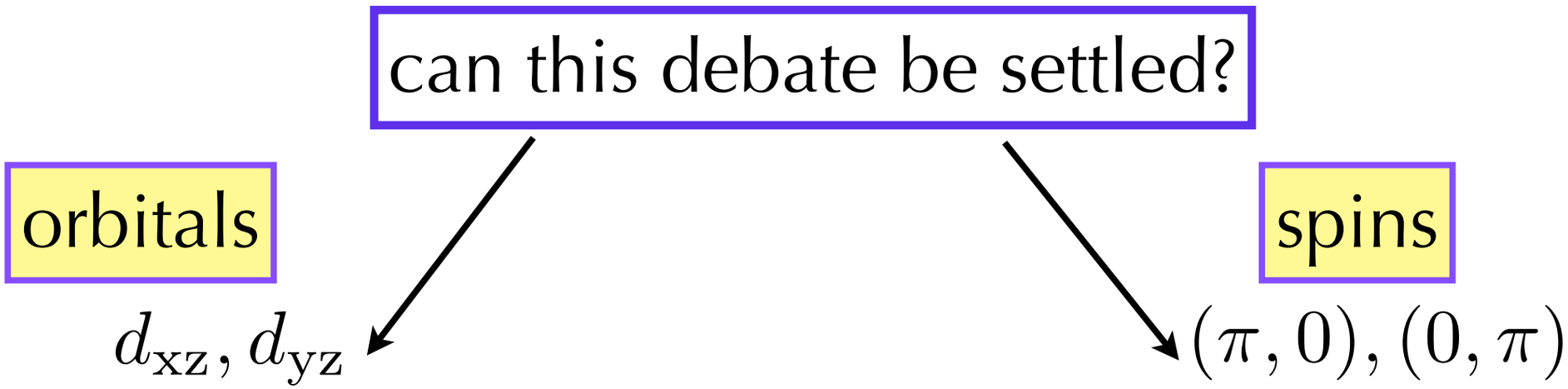
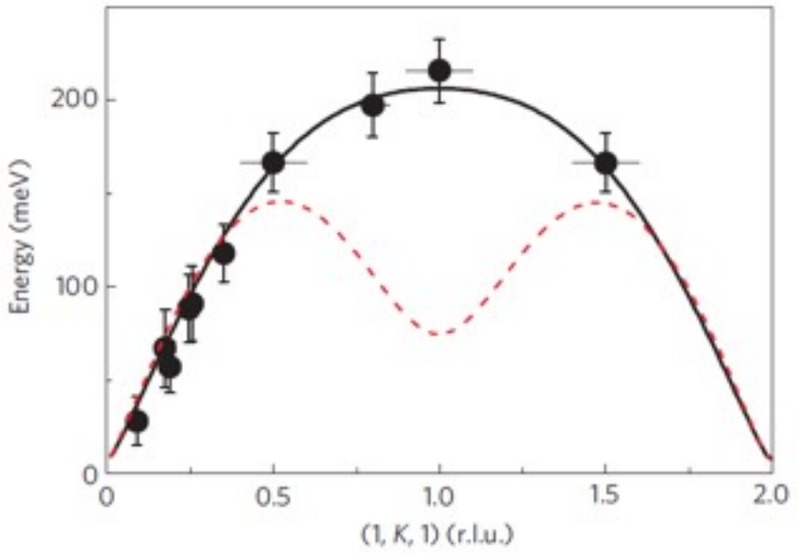
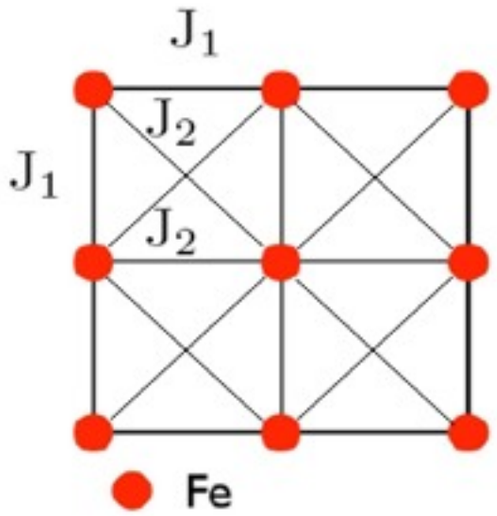

can this debate be settled?
orbitals
spins
d_{xz}, d_{yz}
$(\pi, 0), (0, \pi)$

Experimental Puzzle 1?

- *Inelastic neutron scattering*





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

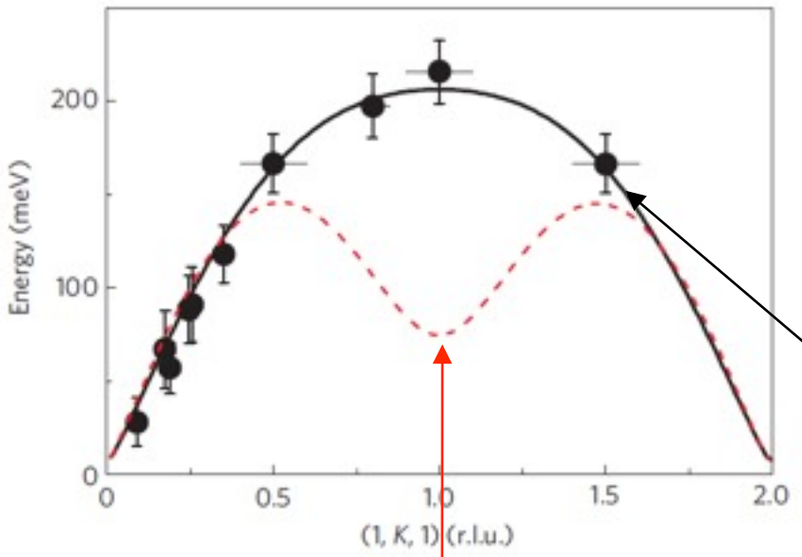
$$
\begin{aligned}
SJ_1^a &= 27\,\text{meV} \\
SJ_1^b &= 25\,\text{meV} \\
SJ_2 &= 36\,\text{meV}
\end{aligned}
$$

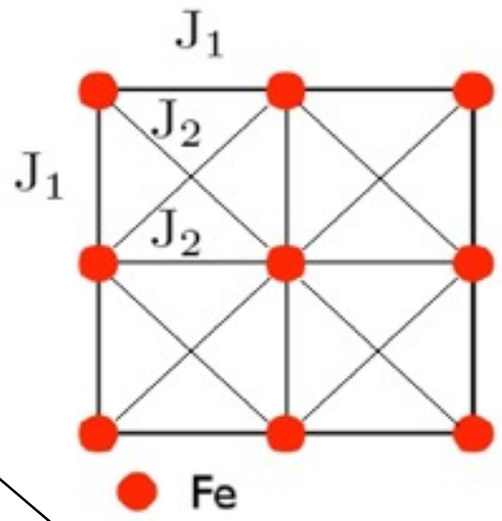
$$
\begin{aligned}
SJ_1^a &= 49.9 \pm 9.9\,\text{meV} \\
SJ_1^b &= -5.7 \pm 4.5\,\text{meV} \\
SJ_2 &= 18.9 \pm 3.4\,\text{meV}
\end{aligned}
$$

Why is the magnetism frustrated?

Experimental Puzzle 1?

- *Inelastic neutron scattering*





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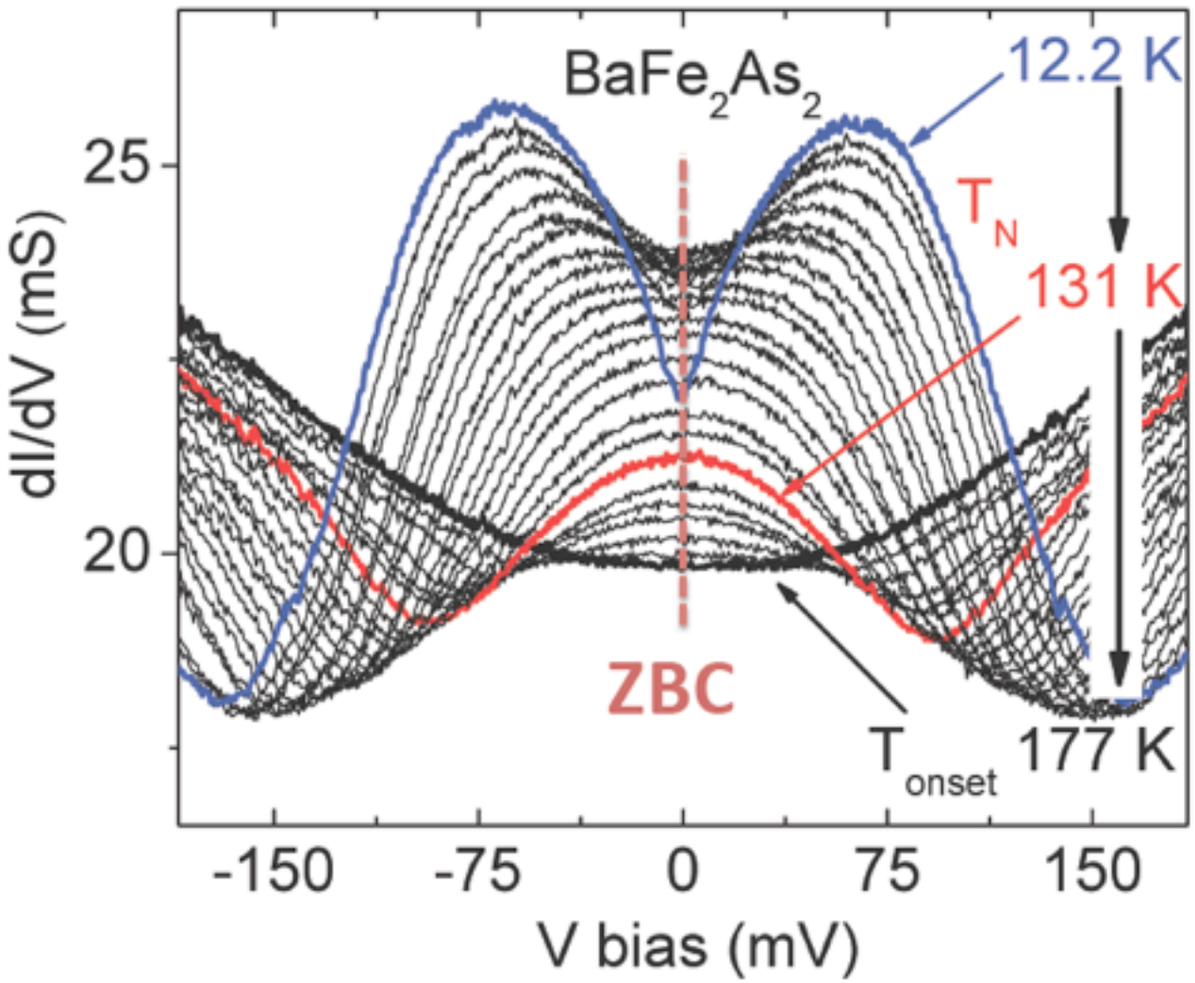
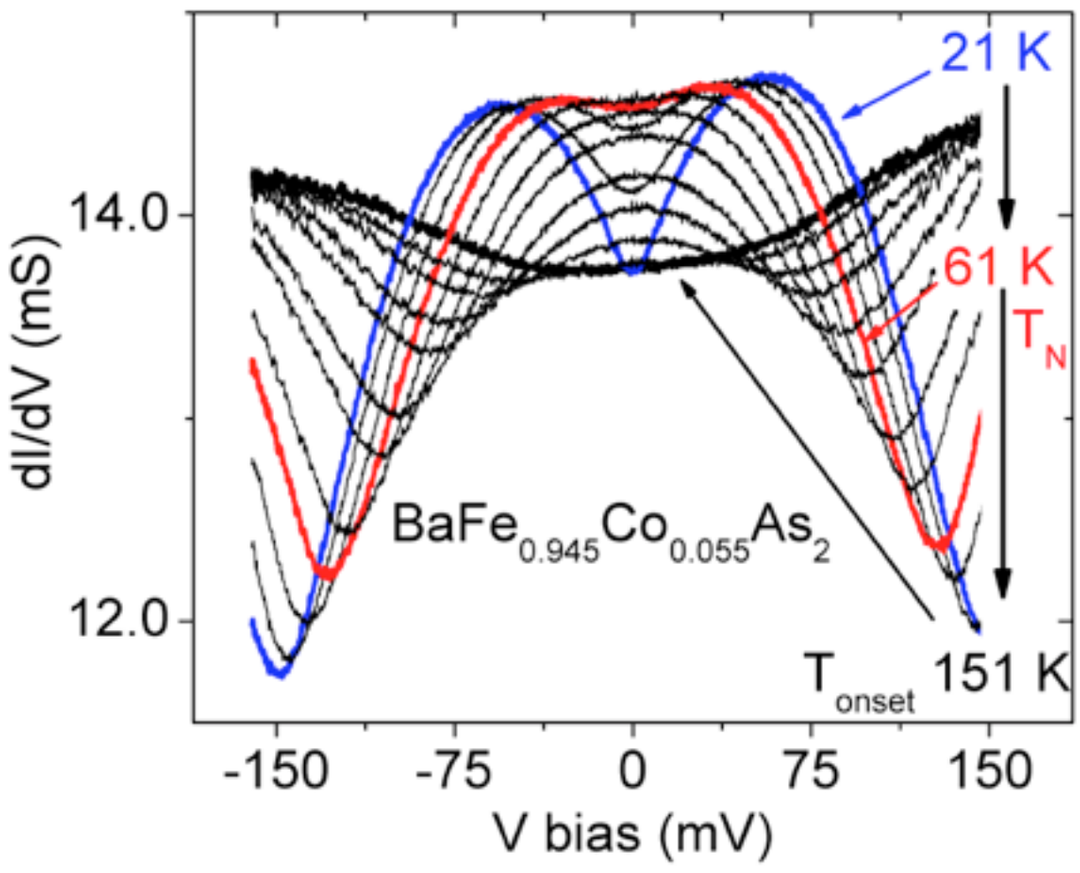
Why is the magnetism frustrated?

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

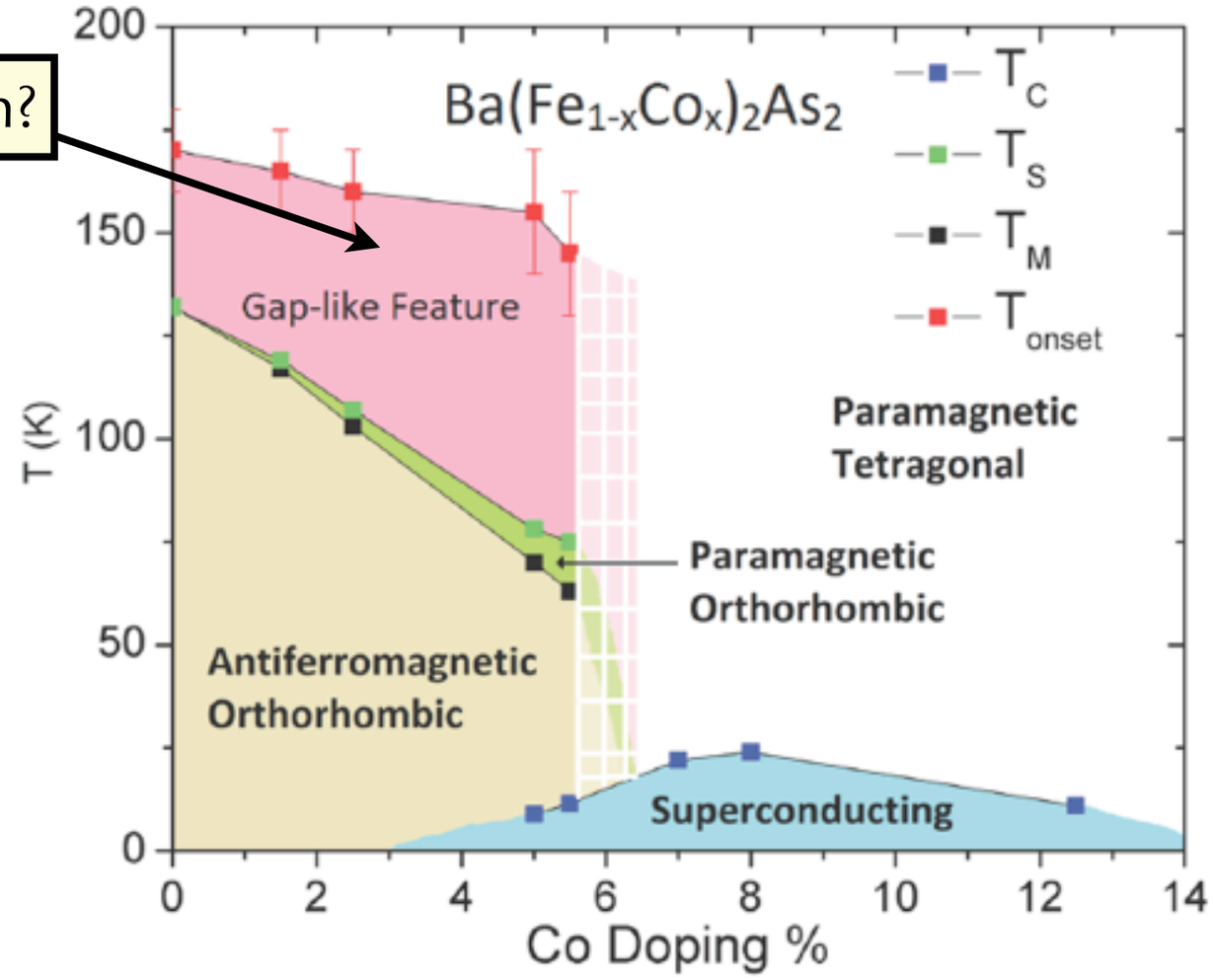




H. Ahram, L. Greene, ... (UIUC)

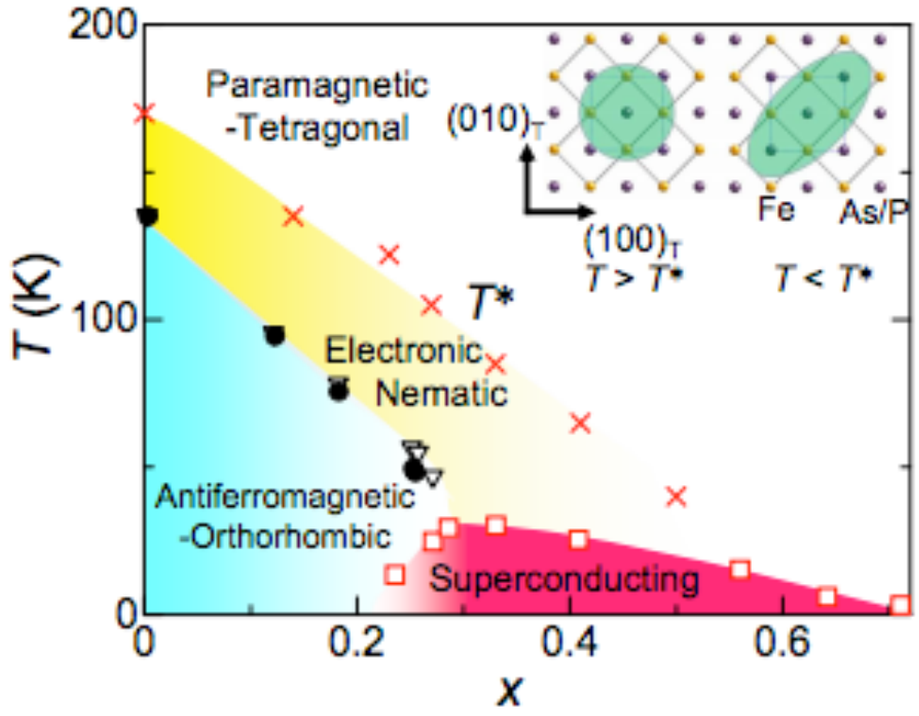
Crossover into a strongly correlated state on the underdoped side of the phase diagram

origin?



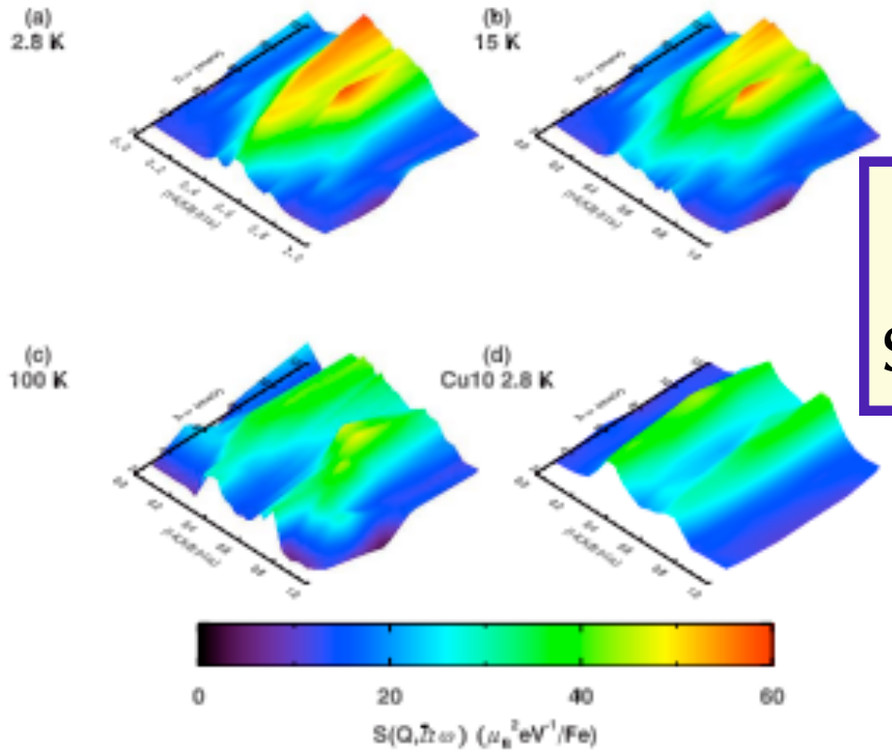
Greene, et al.

Nature 486, 382–385 (2012)



Matsuda, et al.

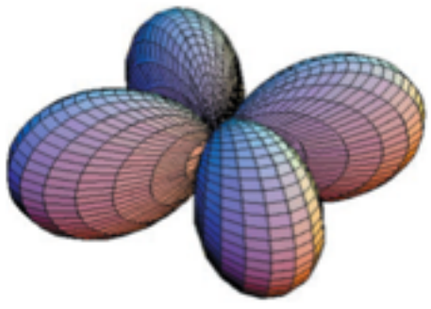
Experimental puzzle 3: What is the origin of the incommensurate-commensurate transition



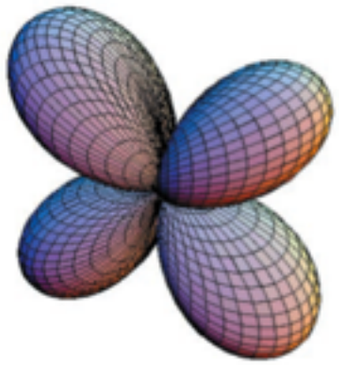
something besides spin degree of freedom

Orbital Ordering

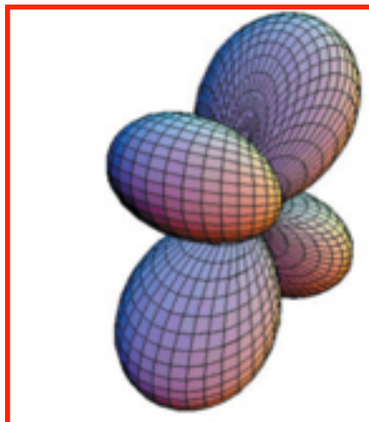
t_{2g}



xy



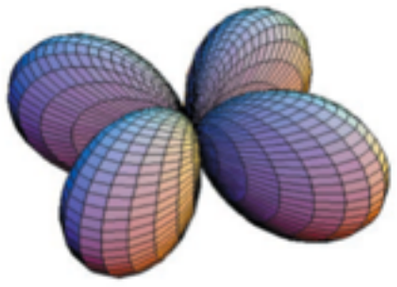
yz



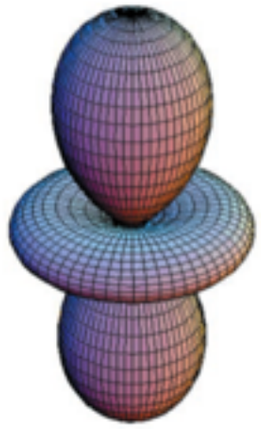
zx

only d_yz and d_xz break rotational symmetry in xy plane.

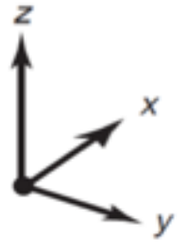
e_g



x^2-y^2



$3z^2-r^2$

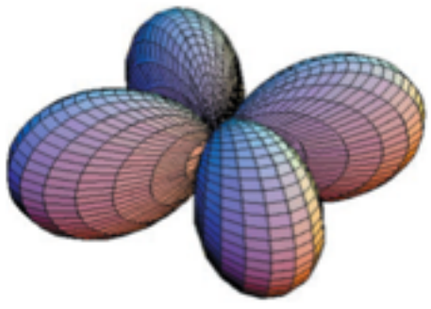


Orbital Ordering

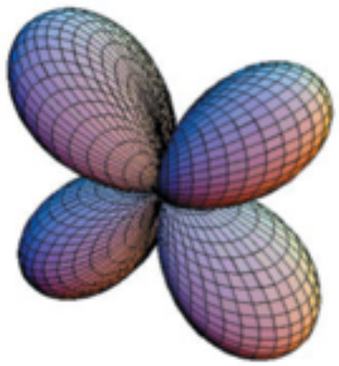
unequal occupancy of d_{xz} and d_{yz}

drive the structural transition, magnetism, ...

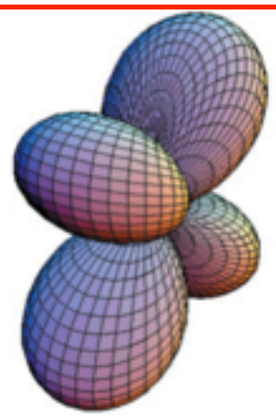
t_{2g}



xy

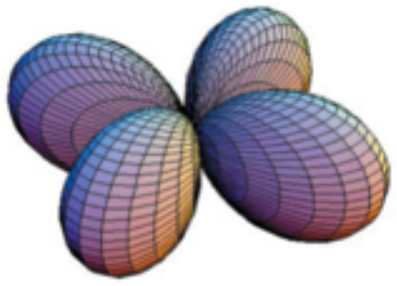


yz

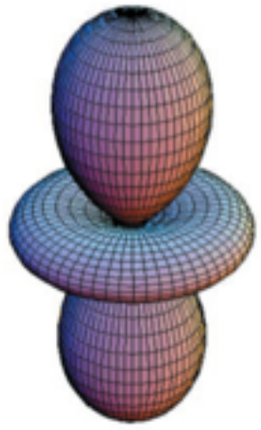


zx

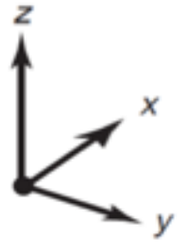
e_g



x^2-y^2



$3z^2$-r^2

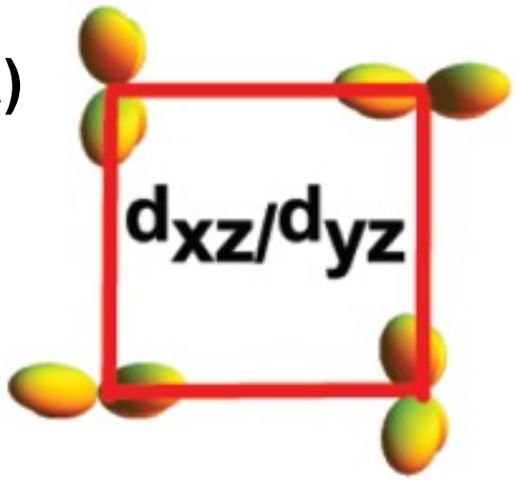


only d_yz and d_xz break rotational symmetry in xy plane.

structural transition

$T > T_{SPT}$

a)



b)

$T < T_{SPT}$

c)

Lv, Wu, PP, 2009

structural transition

$T > T_{SPT}$

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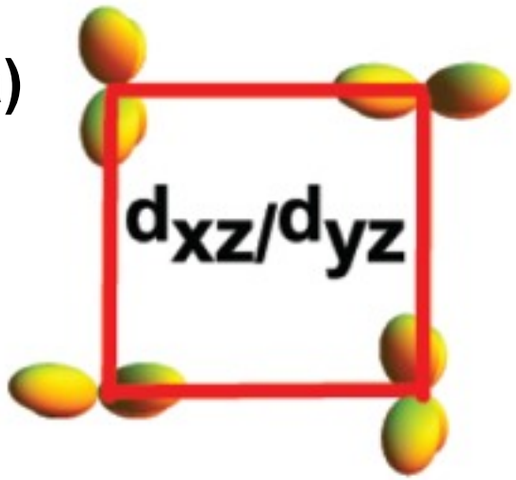

b)

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c)

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:

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

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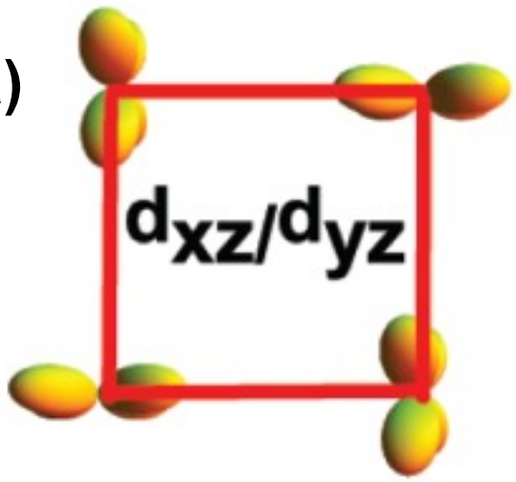

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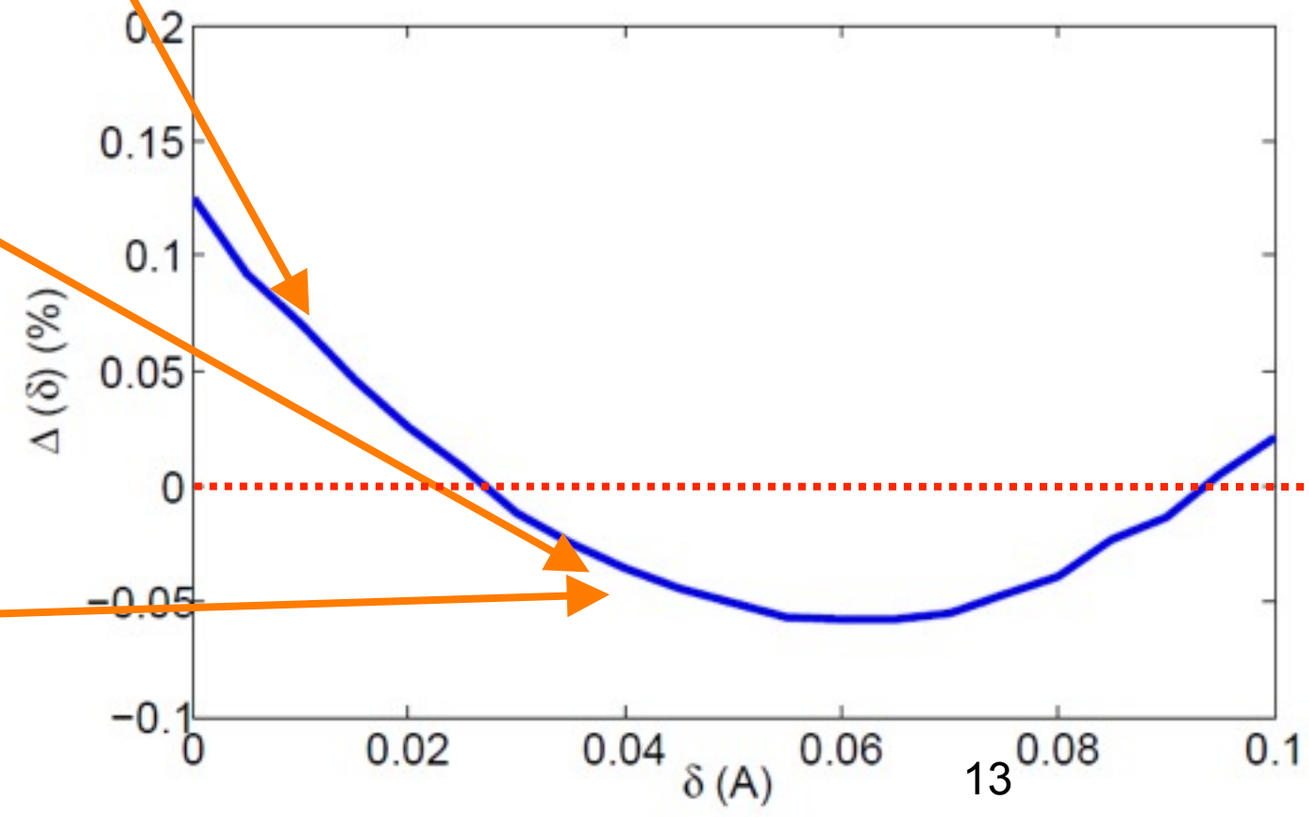

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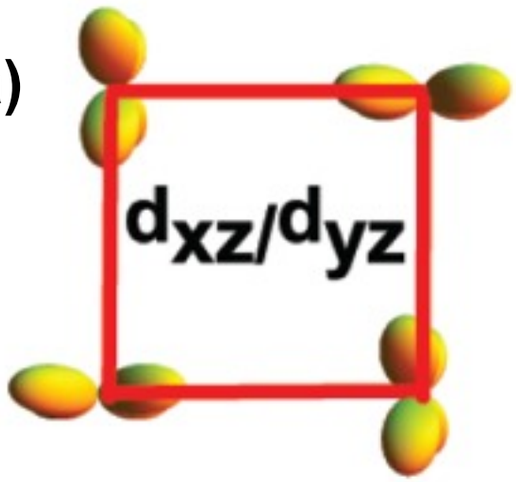
$T > T_{SPT}$

a)



b)

$T < T_{SPT}$

c)

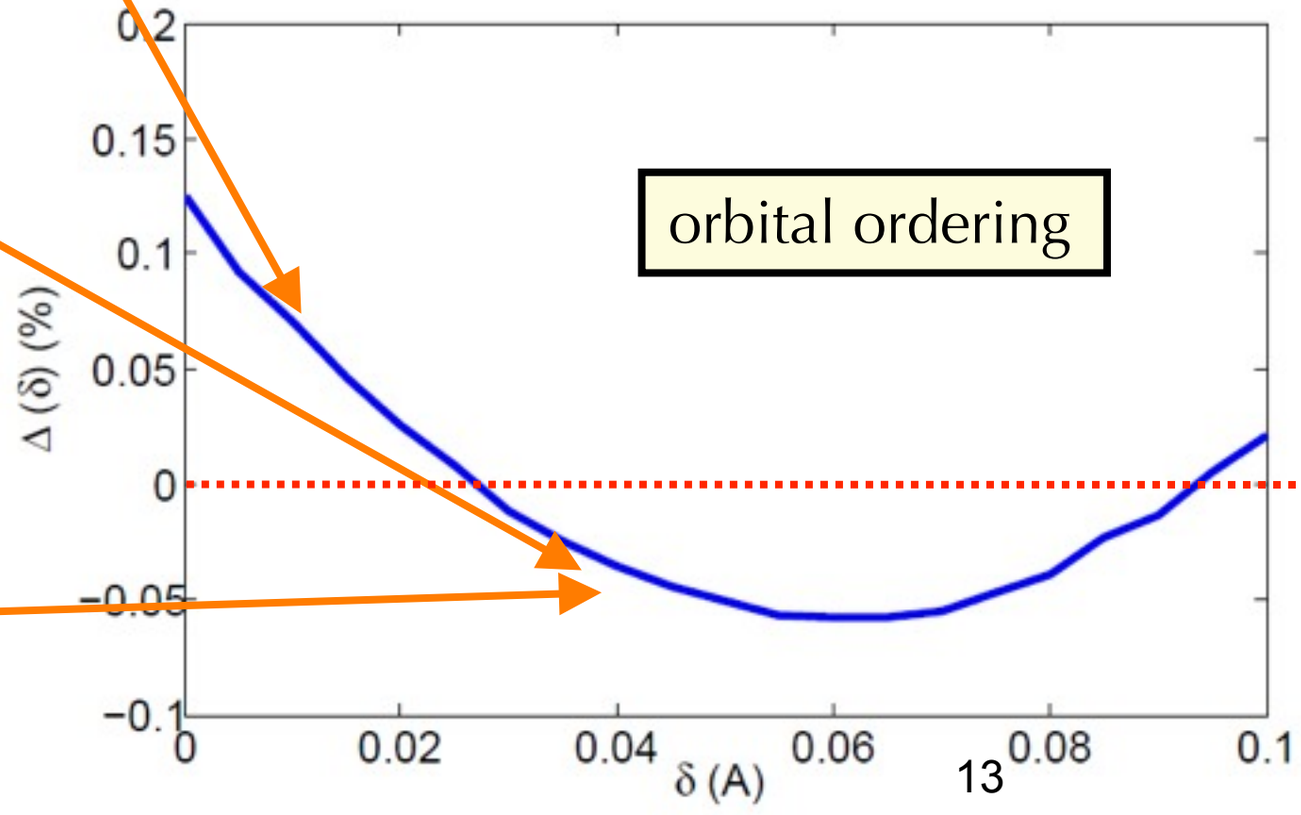
Lv, Wu, PP, 2009

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:

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



orbital ordering

SPT in Ising Universality Class

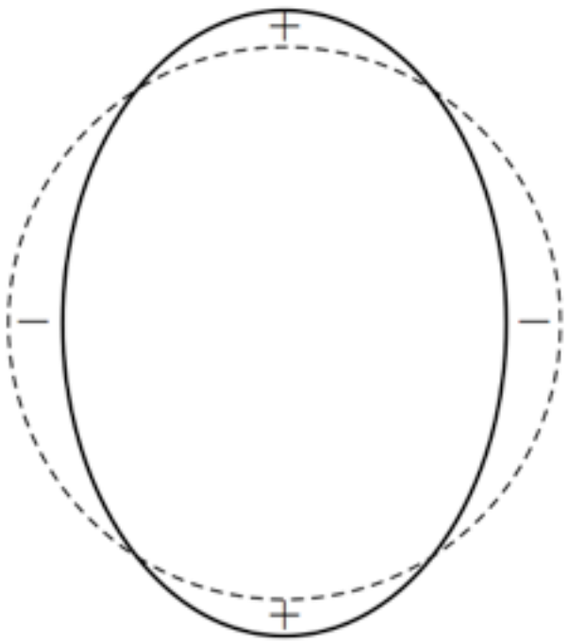
$$H_{\mathrm{SPT}} = -J_{\mathrm{SPT}} \sum_{\langle i,j \rangle} M_i M_j$$

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

structural transition=nematic?

structural transition=nematic?

electron nematic



continuous symmetry breaking

goldstone boson

structural transition=nematic?

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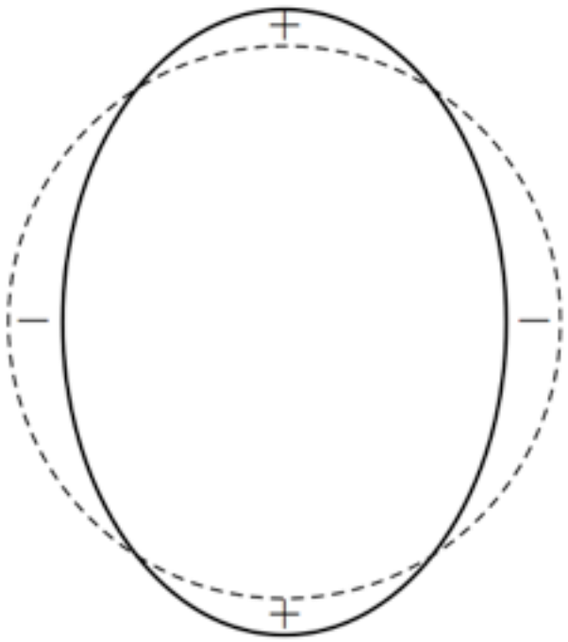

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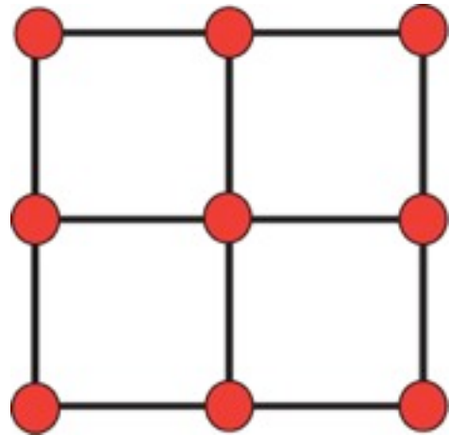


C_4

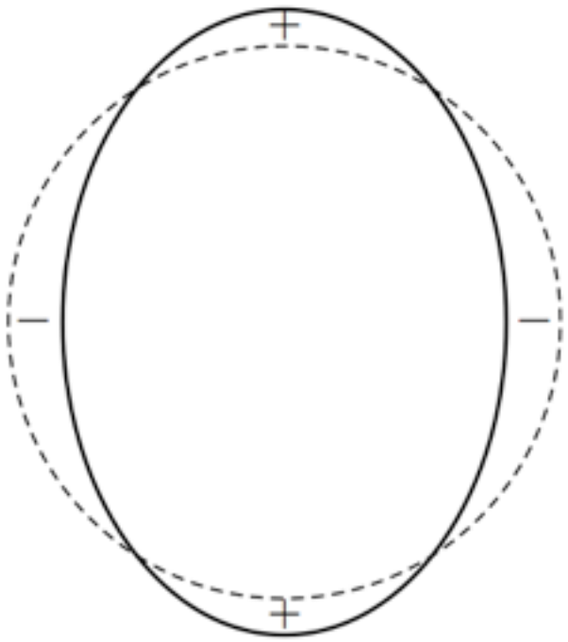
T_s

C_2

no goldstone boson

structural transition=nematic?

electron nematic



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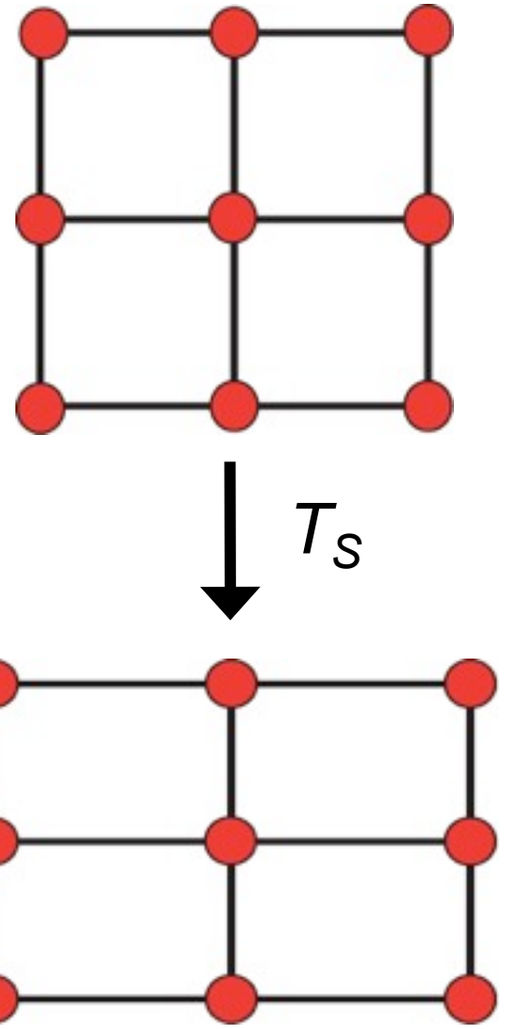

no goldstone boson

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

$T > T_{SPT}$

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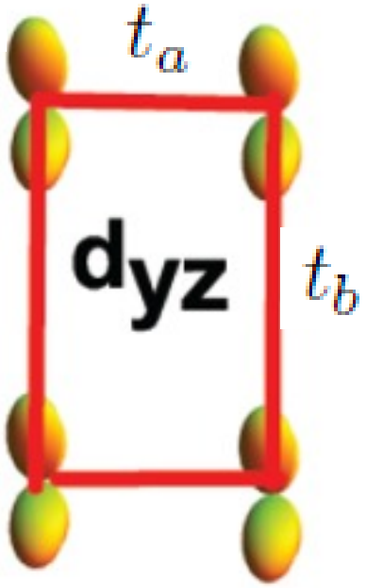
spin disordered

$T < T_{SPT}$

b)



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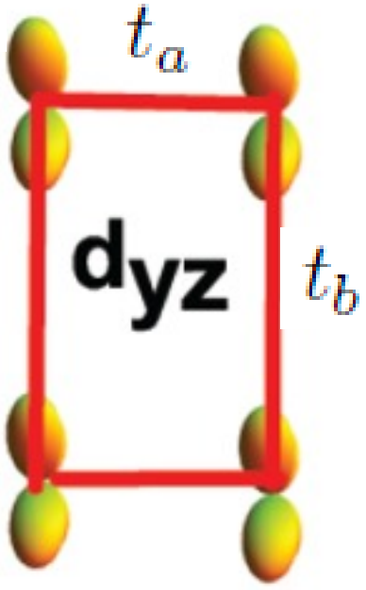

$$t_b > t_a$$

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

$$J_b > J_a$$

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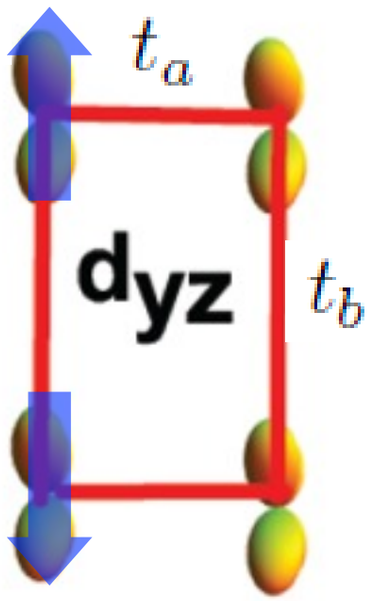

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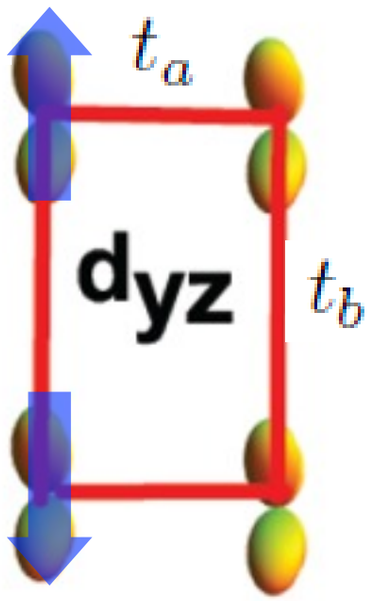

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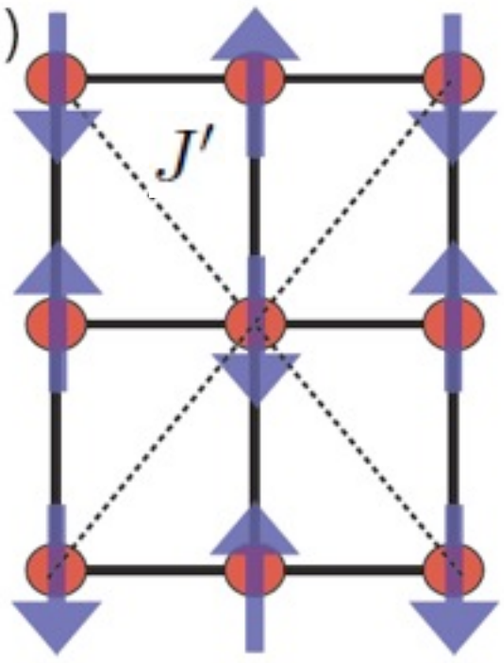
AF1)



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

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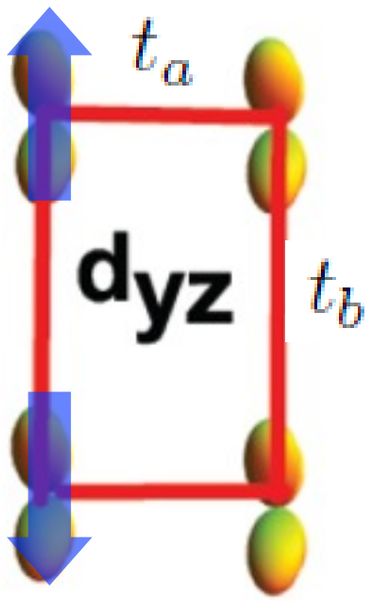
$T < T_{SPT}$

b)



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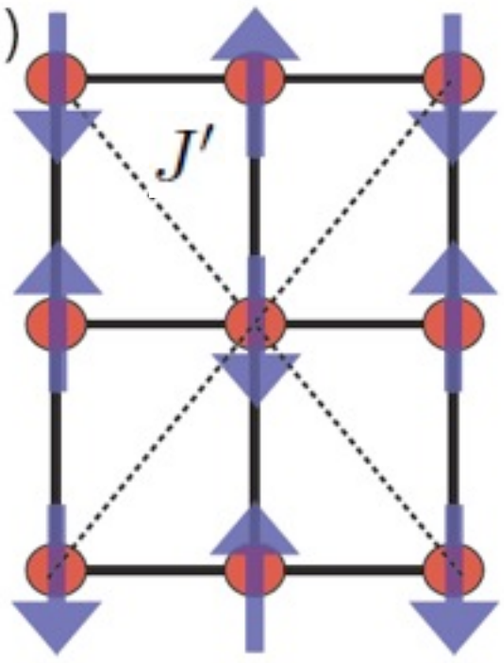

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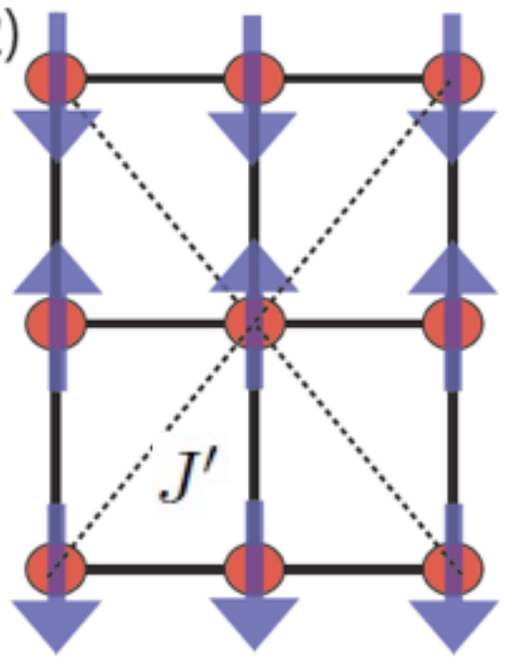
AF2)



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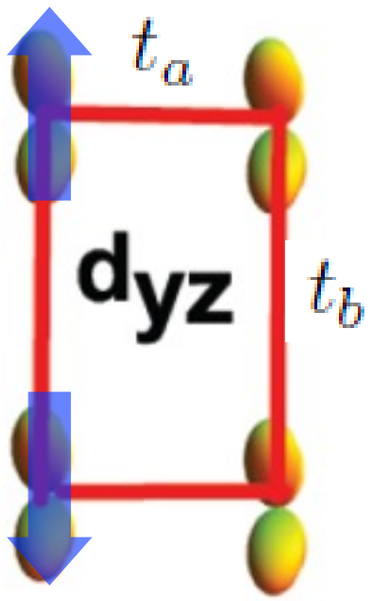

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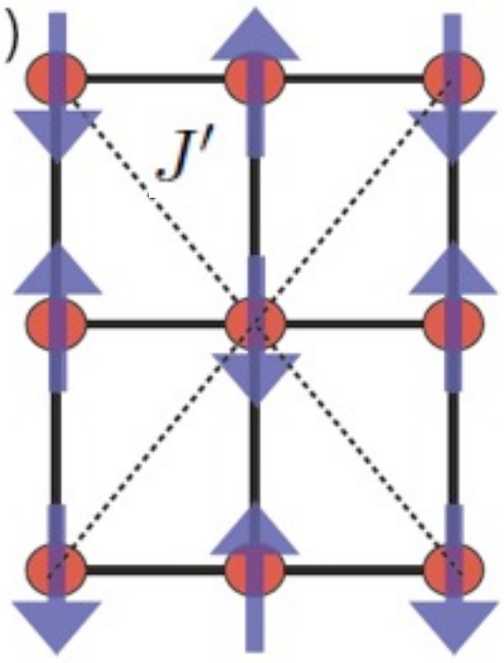

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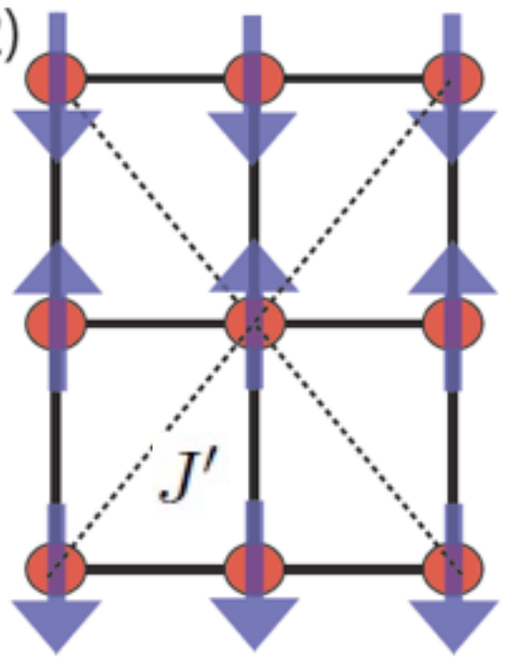

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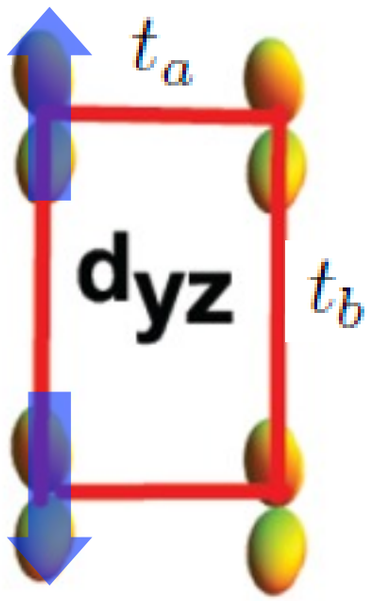

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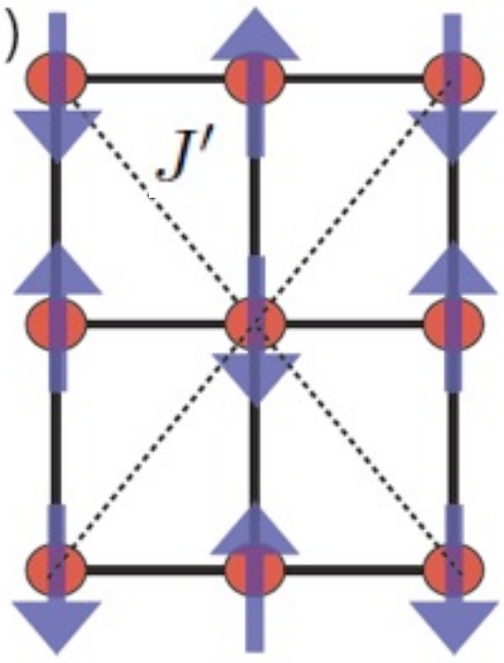

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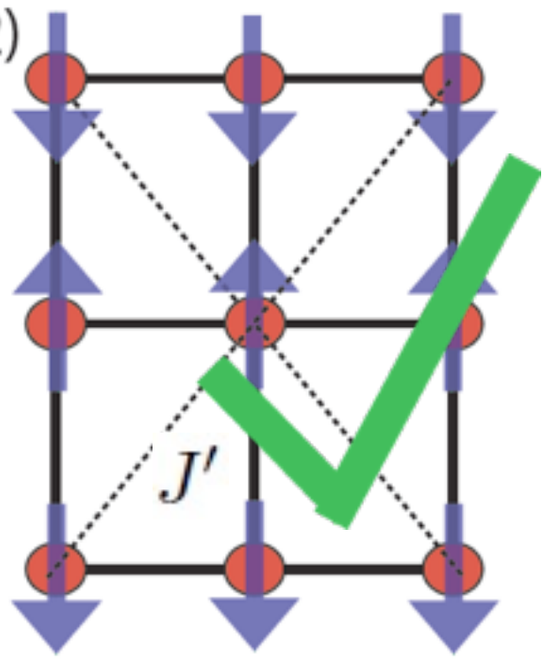


$$E_2 = +2J_a - 4J'$$

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

SPT-induced magnetism

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

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

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

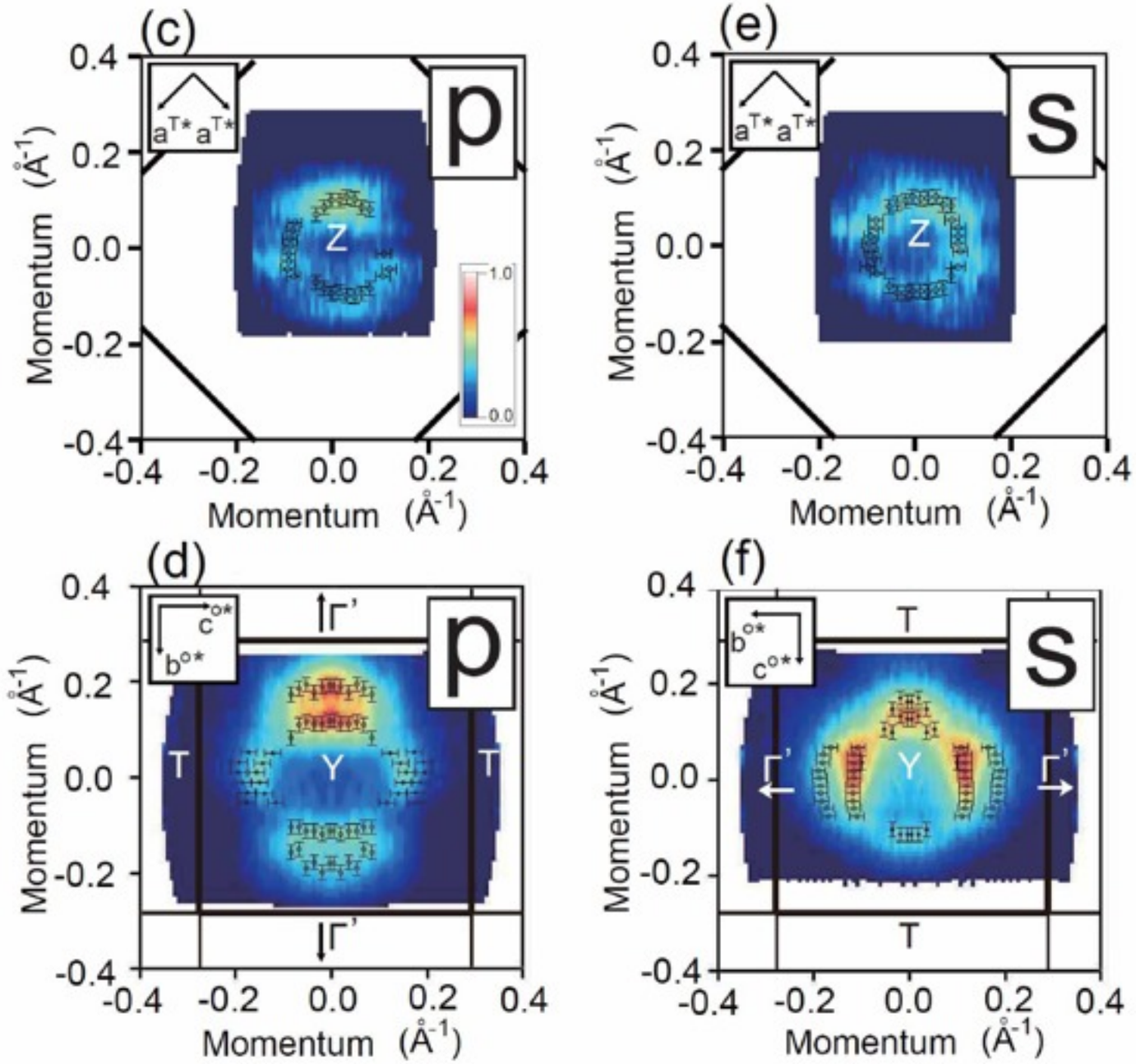
122 Fe-Fe is shorter: J_{1b} is enhanced

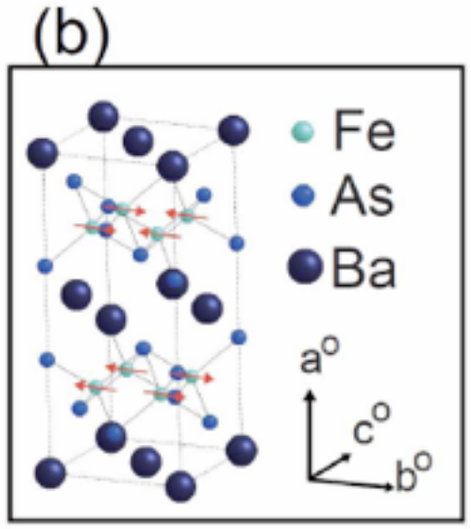
Orbital-polarized Fermi surface in antiferromagnetic state of

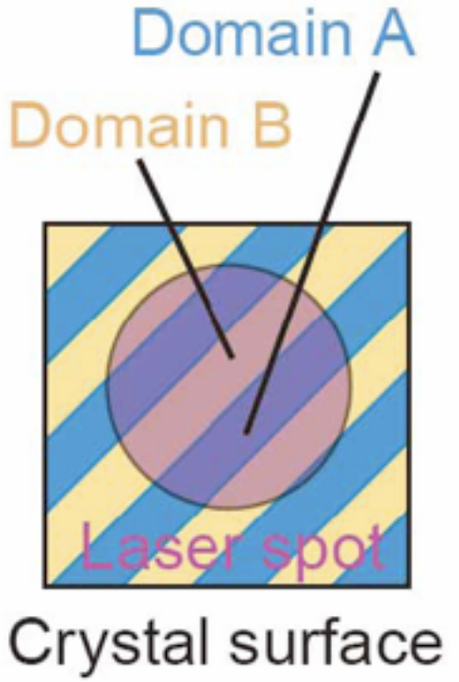
$BaFe_2As_2$

Shimojima, et al.
arXiv:0904.1632

- **Polarized ARPES**







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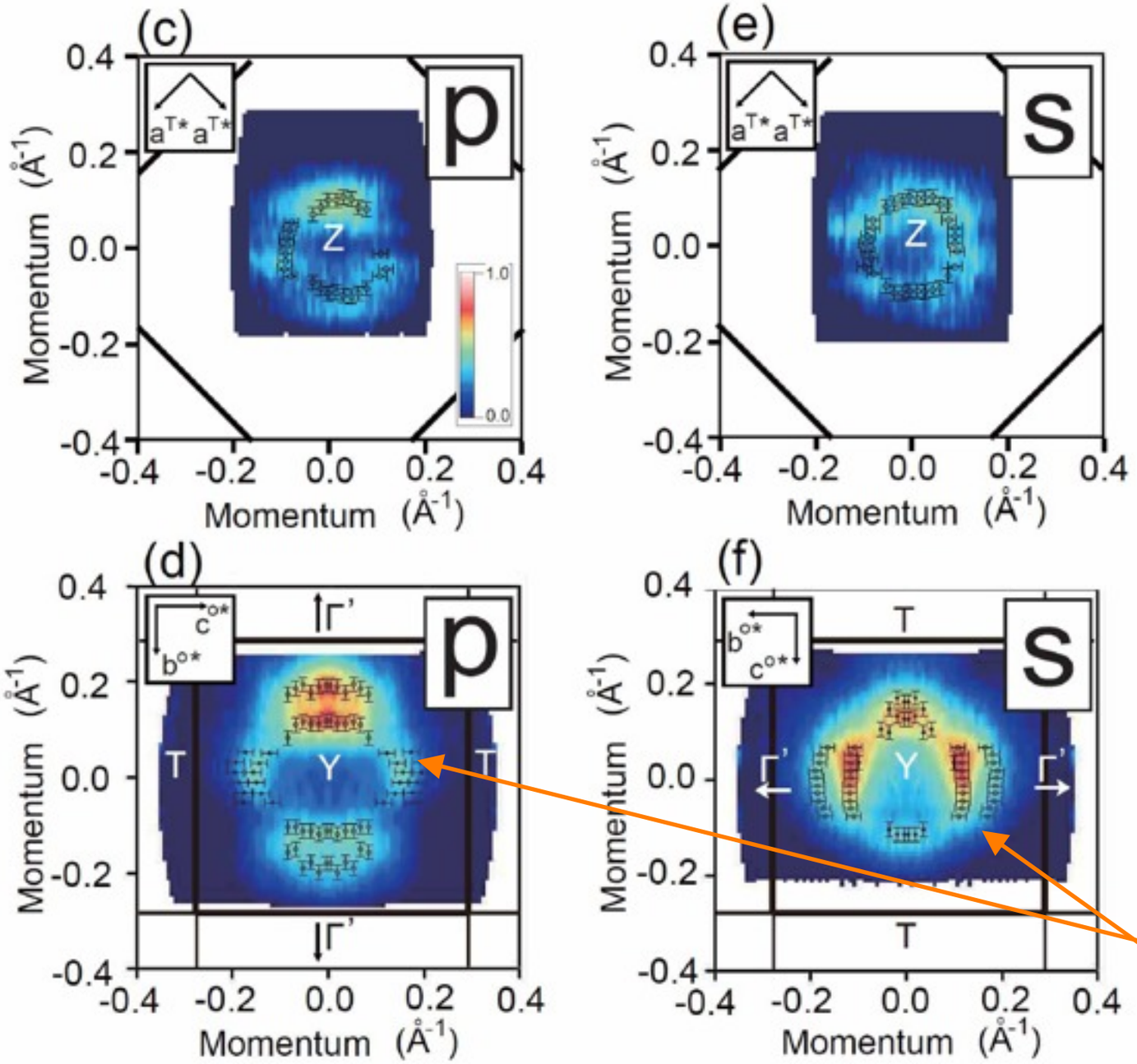
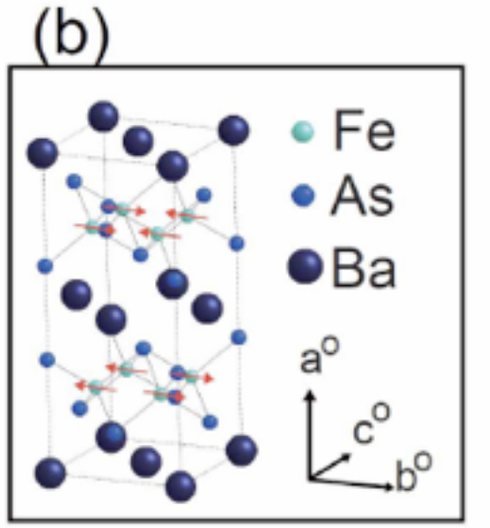
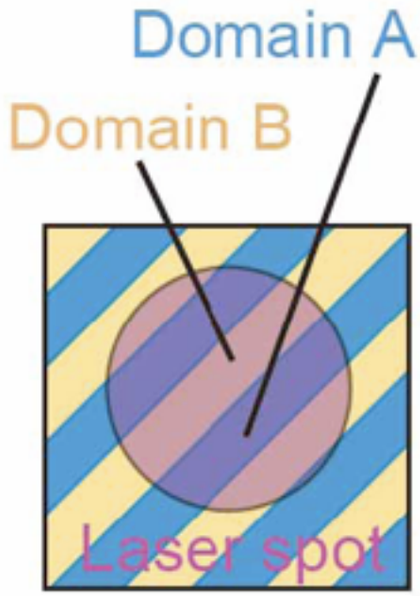
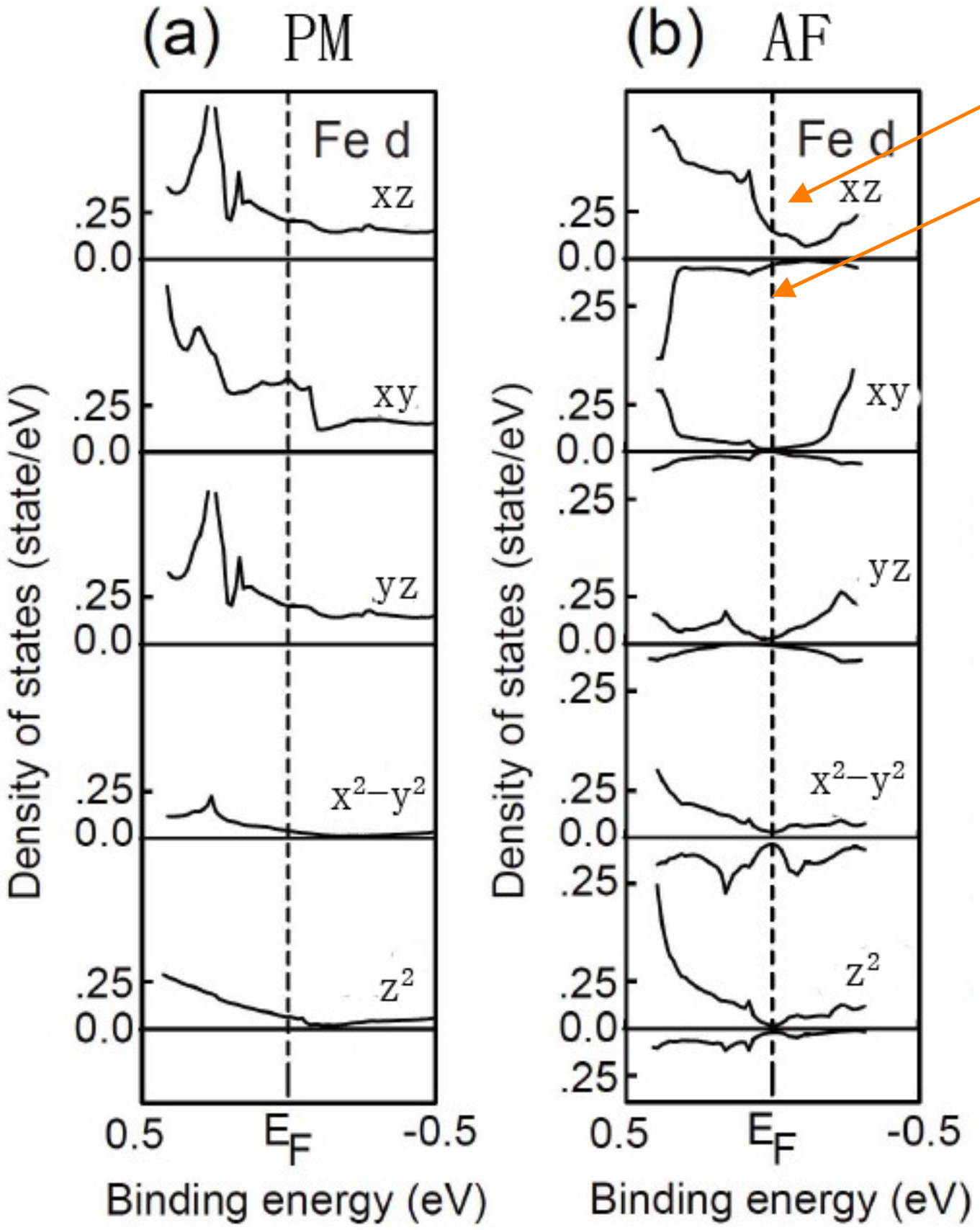






d_{xz} in domain A

d_{xz} in domain B



(a) PM state:

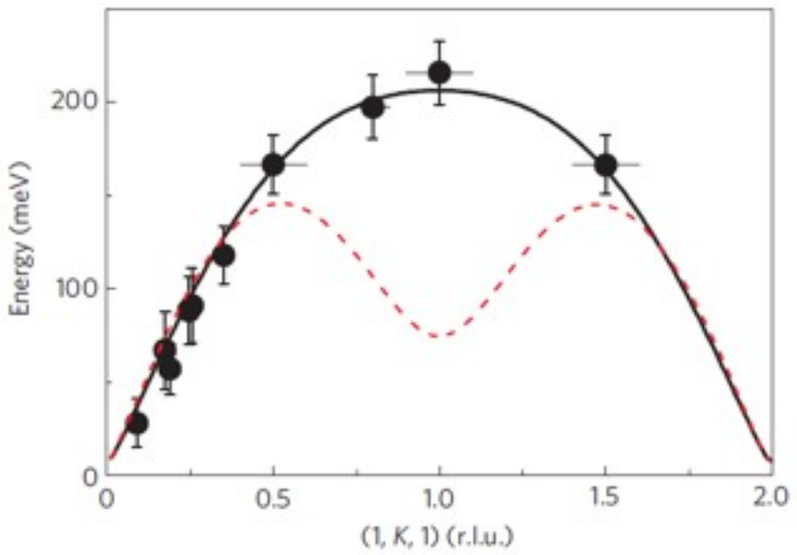
1. d_{xz}, d_{yz} degenerate
2. Fermi surface is composed by multiple orbitals

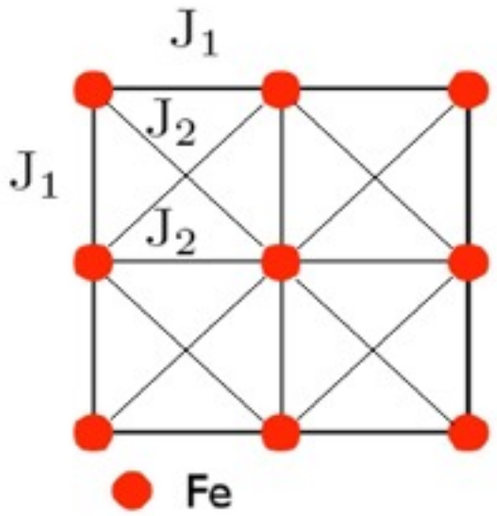
(b) AF state:

1. Localized moment is formed by d_{xz}
2. Fermi surface is orbital-polarized

- *Inelastic neutron scattering*

Experimental Puzzle 1?





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

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

$$
\begin{aligned}
SJ_1^a &= 49.9 \pm 9.9\,\text{meV} \\
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Why is the magnetism frustrated?

- *Inelastic neutron scattering*

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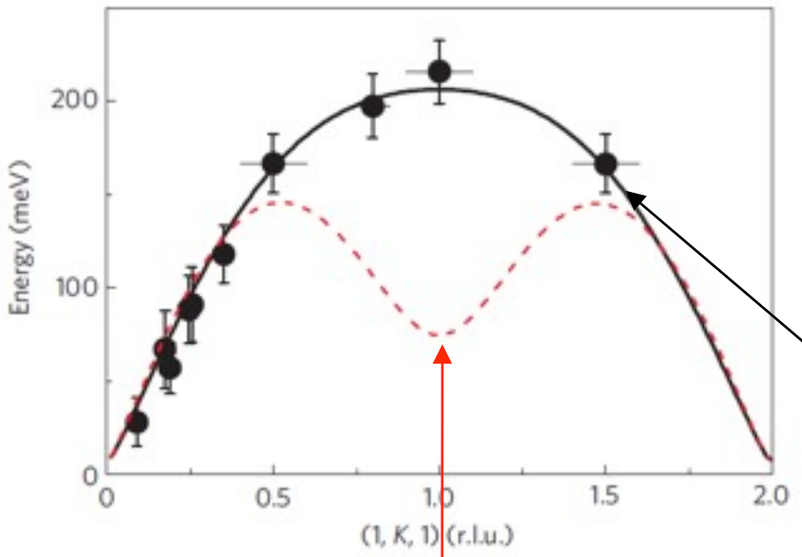

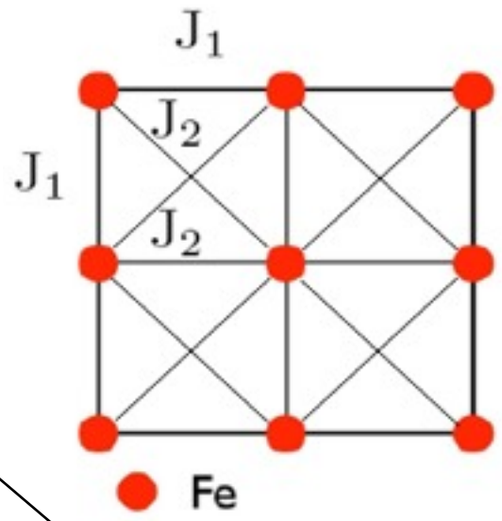

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Why is the magnetism frustrated?

Double-Exchange Model

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

unlike manganites

$$\nu J_H \ll \infty$$

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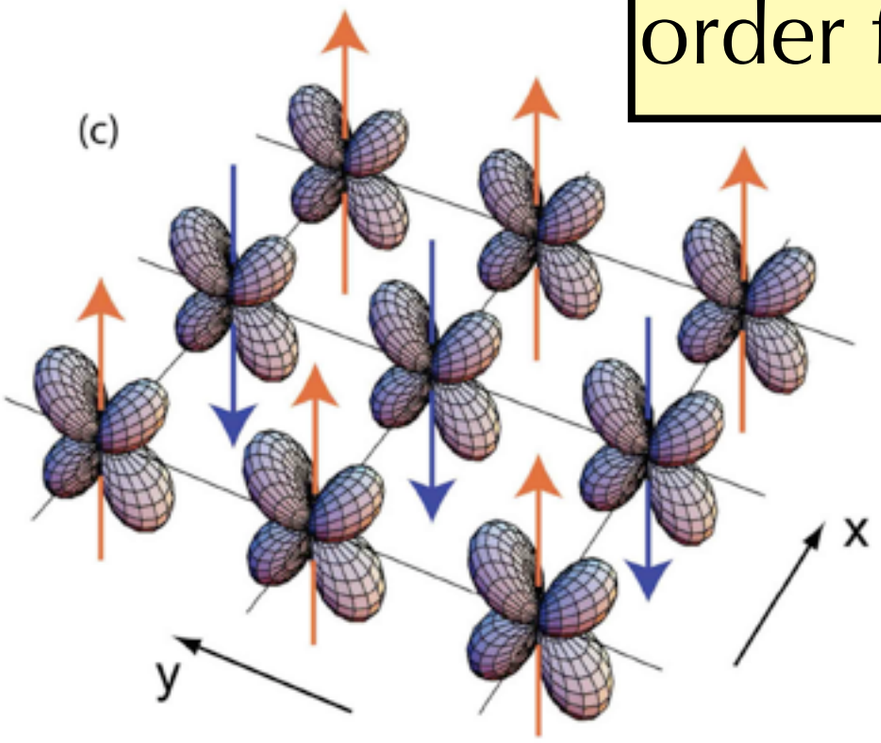
$$\mathcal{H}_{\rm it} = - \sum_{ij,\alpha\beta,\nu} t_{ij}^{\alpha\beta} c_{i\alpha\nu}^{\dagger} c_{j\beta\nu} + \frac{V}{2} \sum_{i,\alpha\neq\beta,\nu\nu'} \hat{n}_{i\alpha\nu} \hat{n}_{i\beta\nu'}$$

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

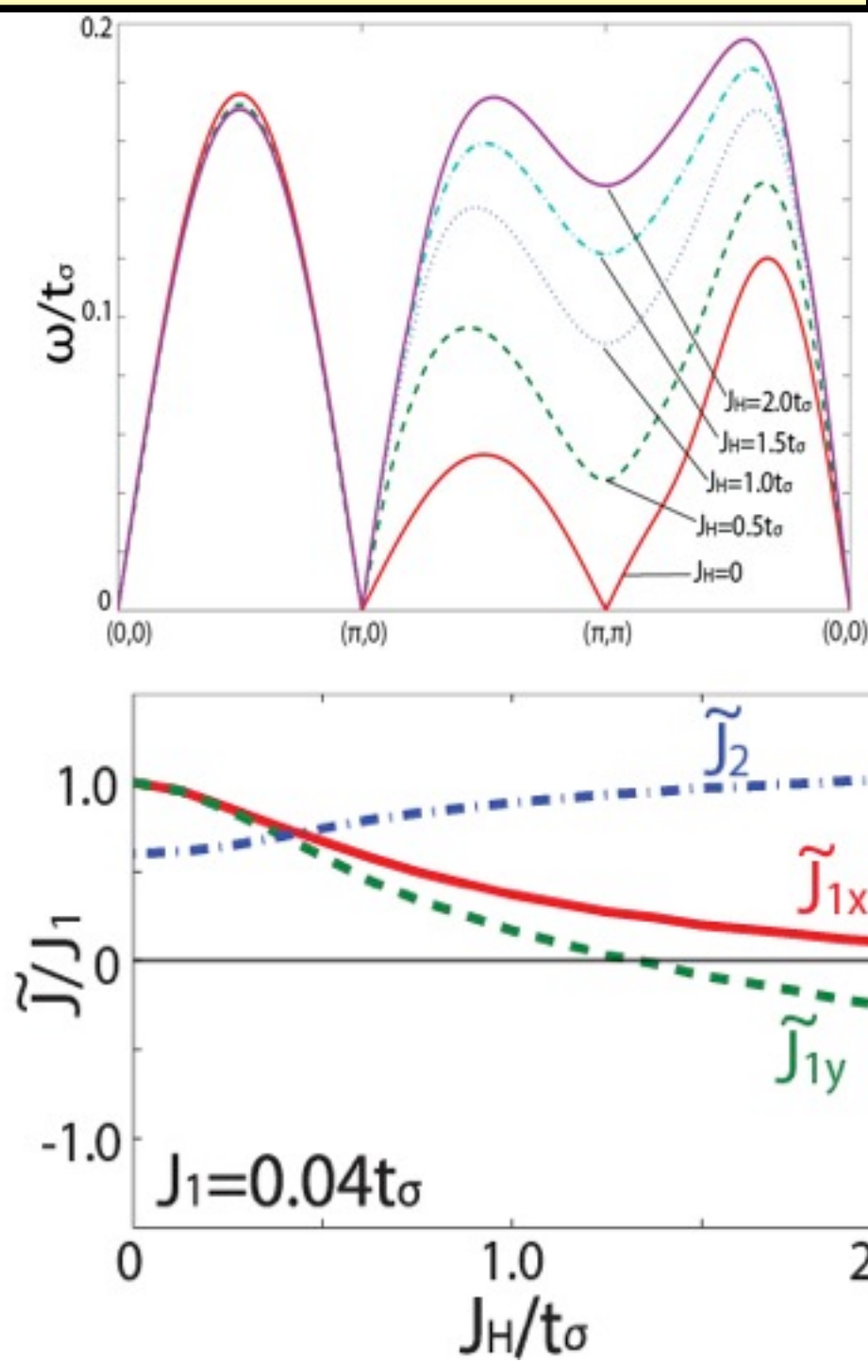
unlike manganites

$$\nu J_H \ll \infty$$

answer: emergent ferro-orbital order from Hund coupling



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



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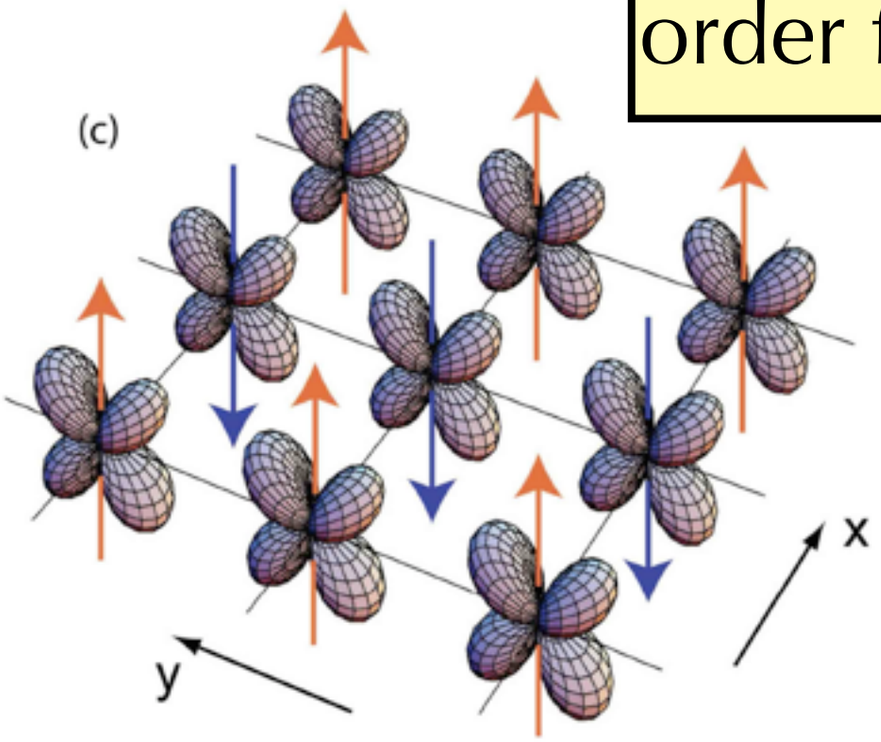
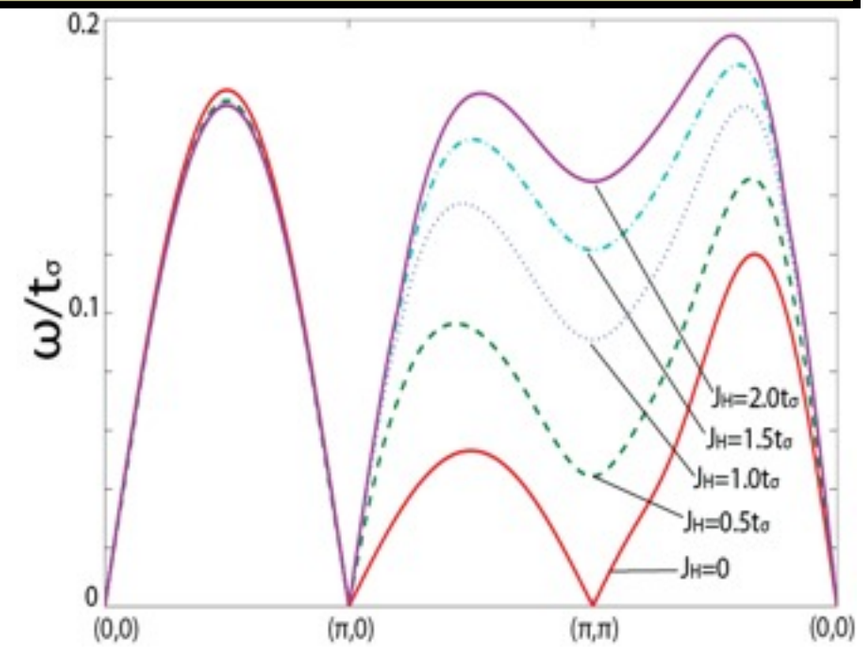
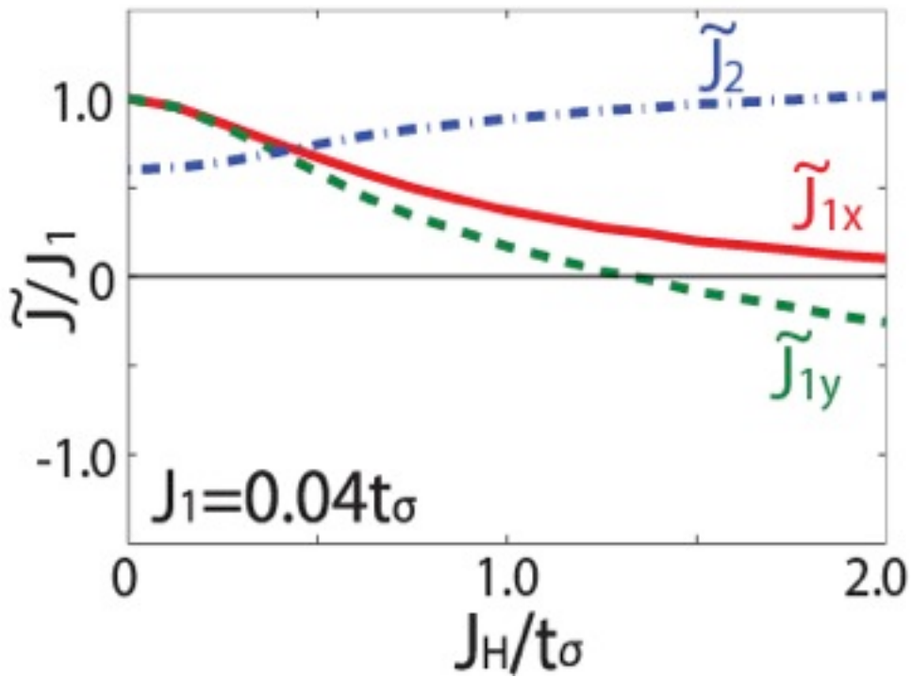


WL, FK, PP, Phys. Rev. B, vol. 82, p. 045125 (2010)

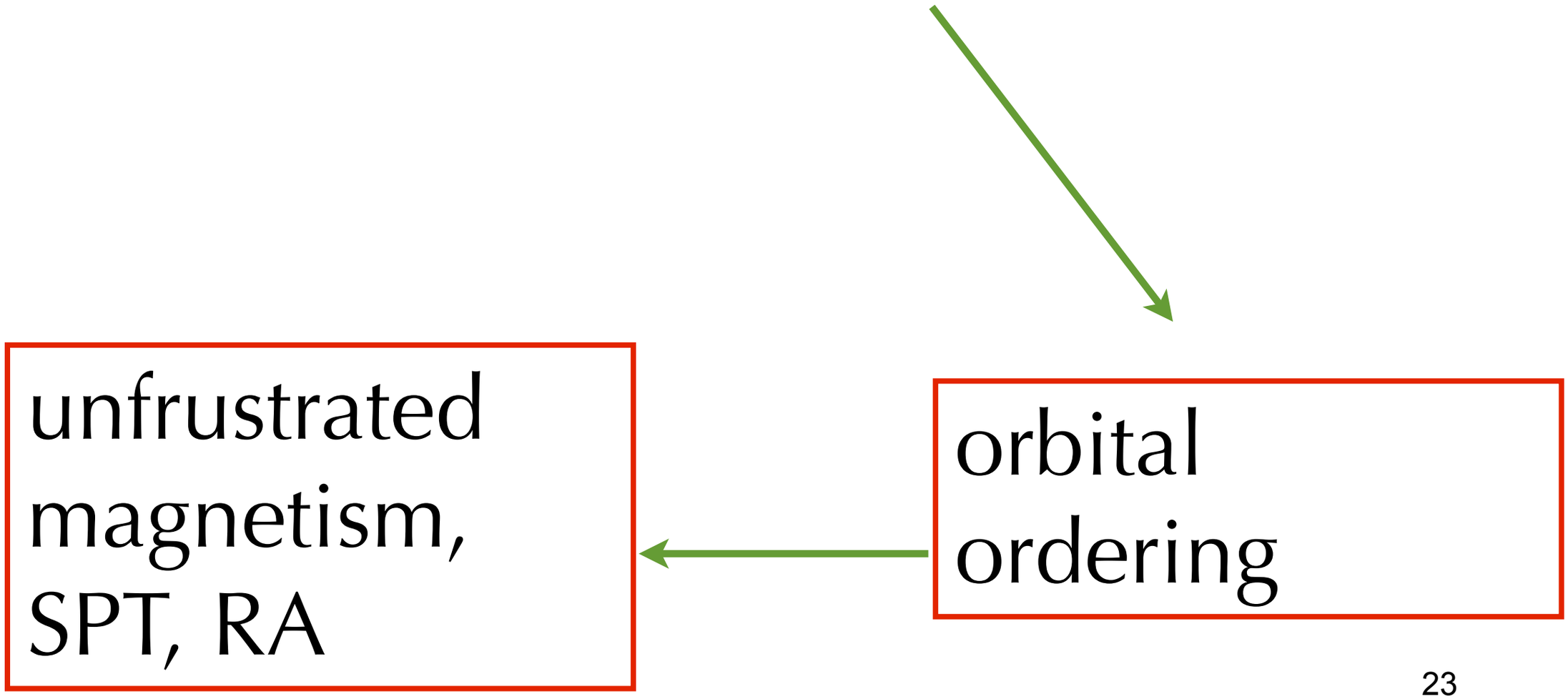
- *Comparison with experiments*:

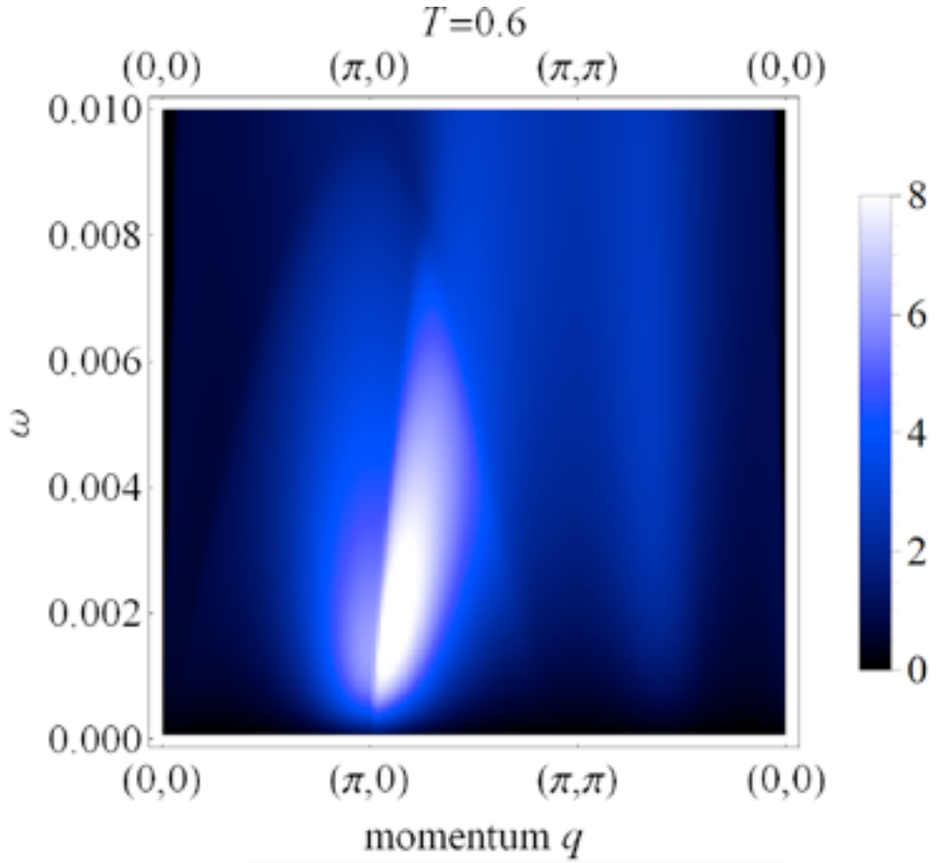
$$J_{\mathrm{H}} \sim t_\sigma \sim 1\,\mathrm{eV} \quad \tilde{J} \sim 0.01\,t_\sigma \sim 10\,\mathrm{meV}$$



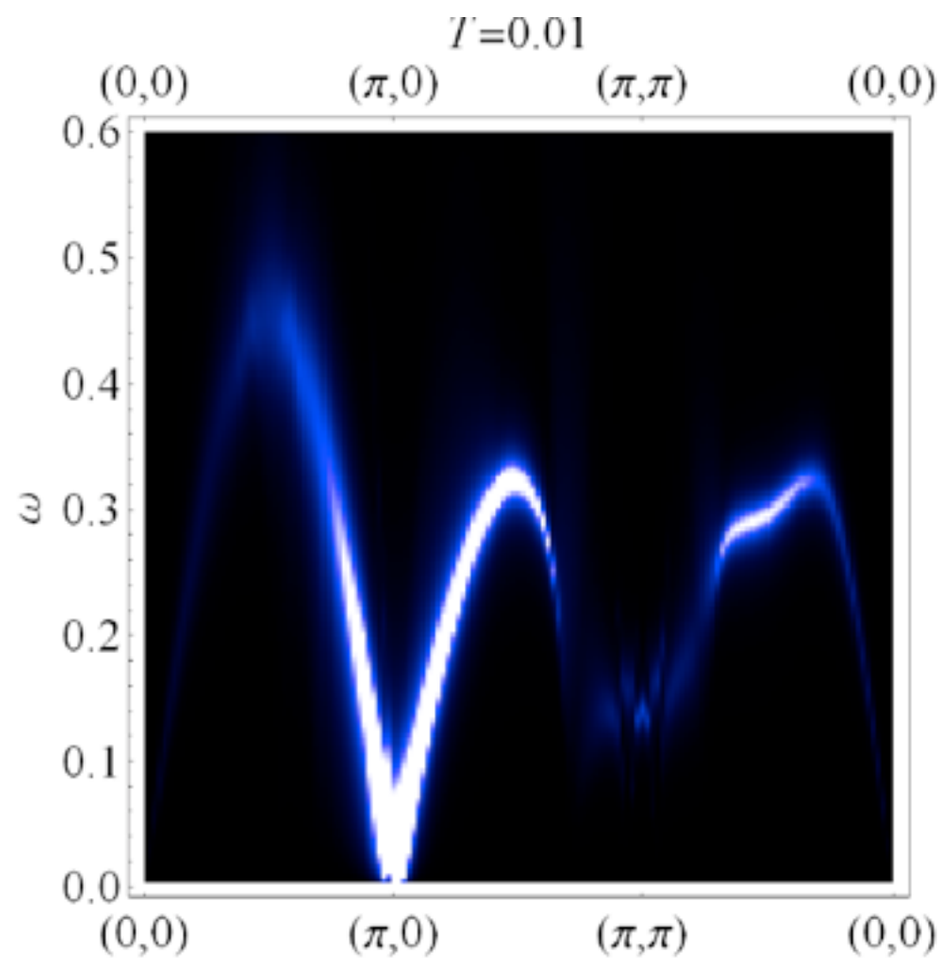


localized/extended electrons+Hund's coupling

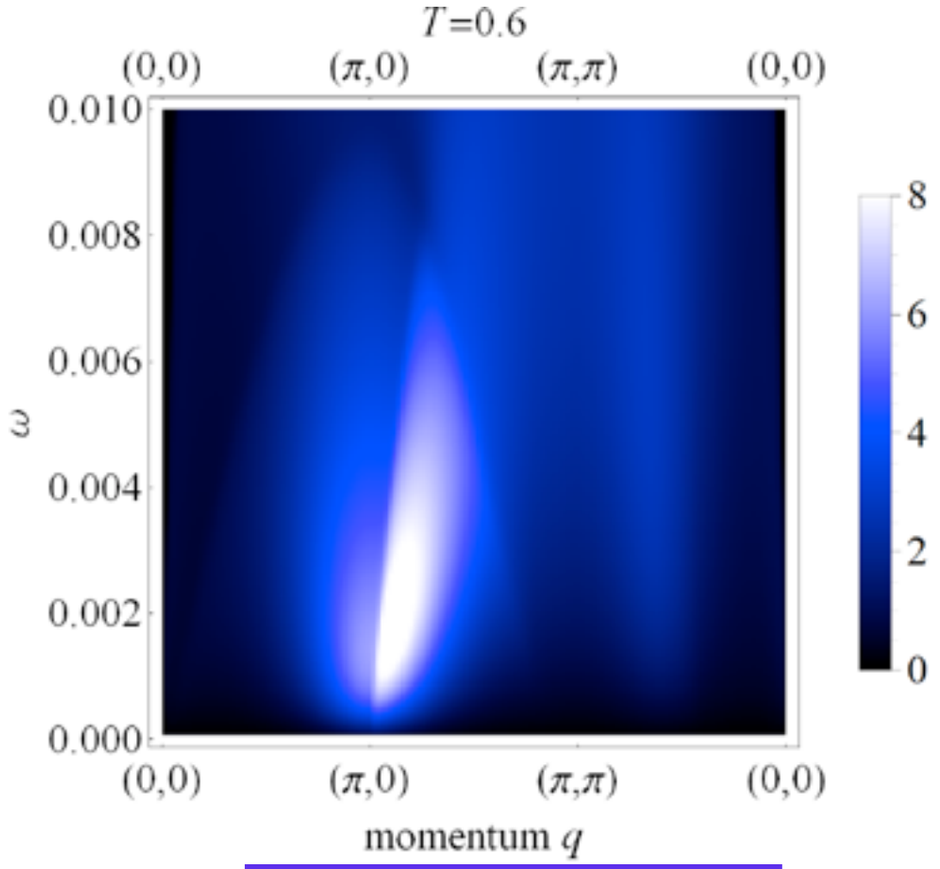




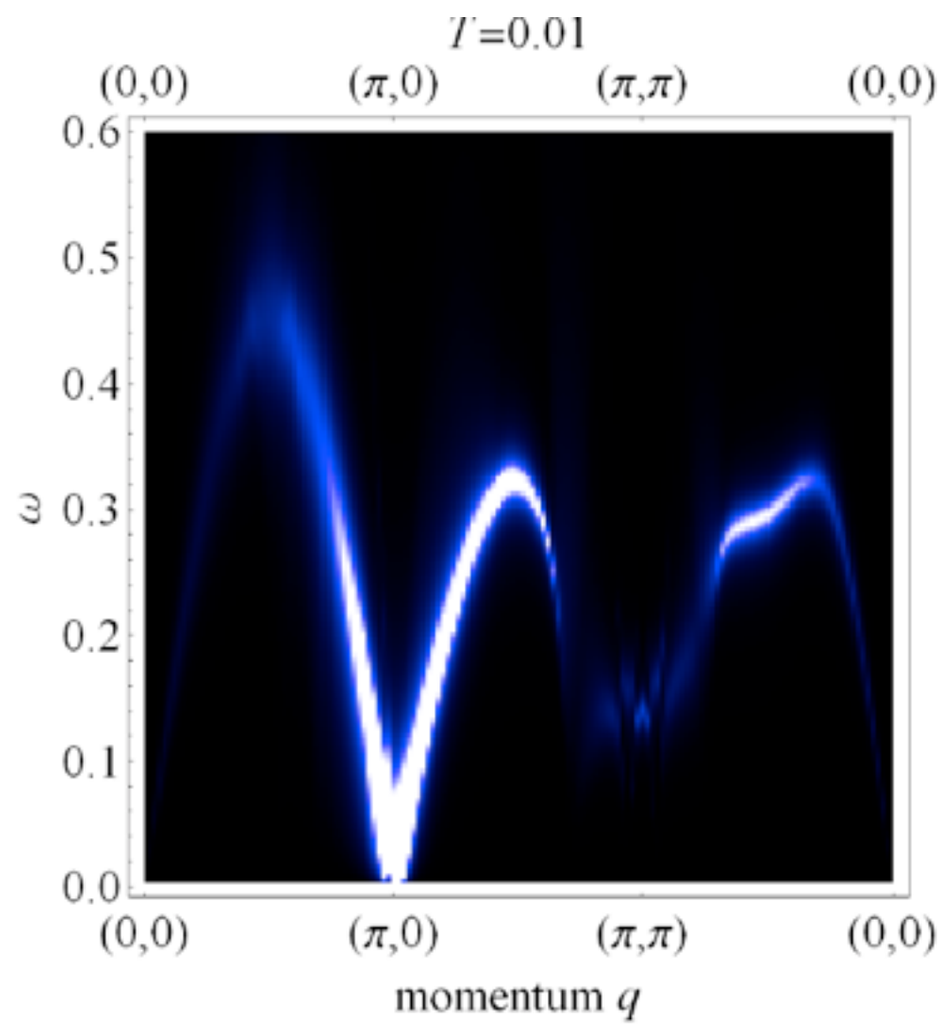
high T
paramagnetic state



low T
ordered state

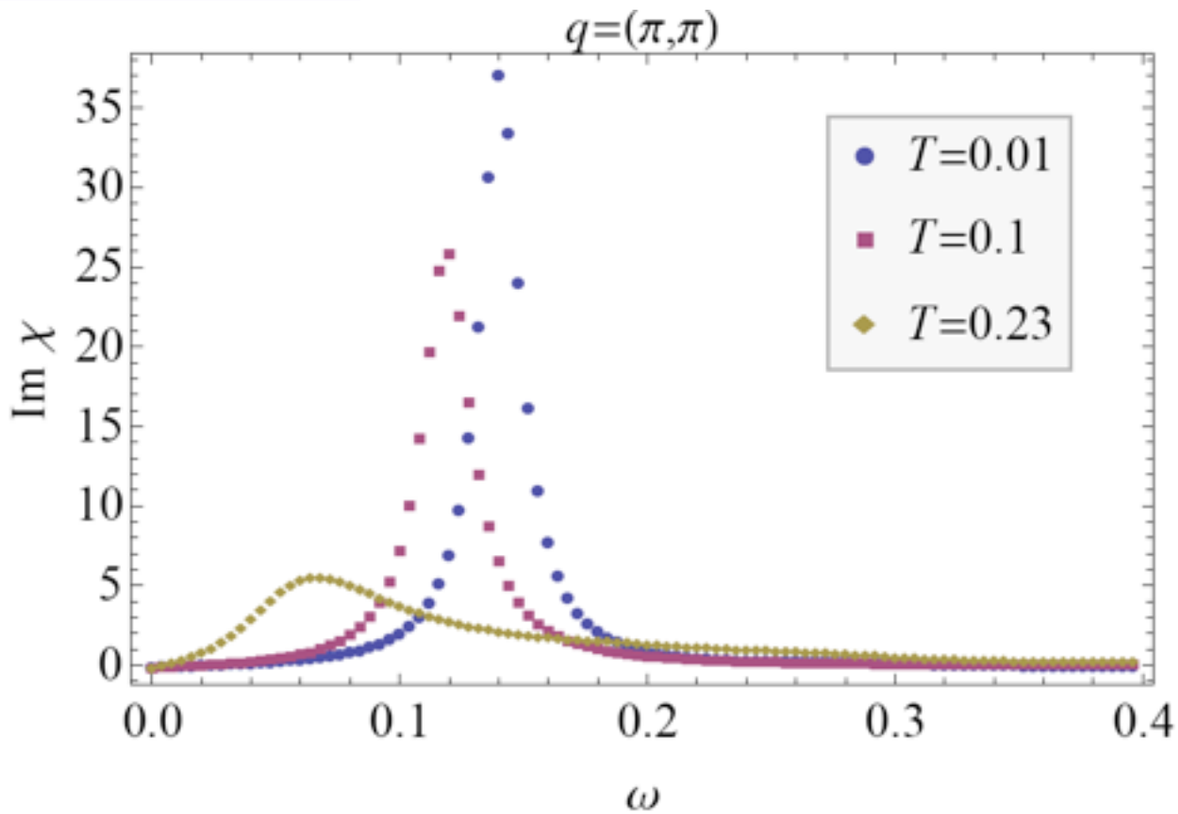


high T
paramagnetic state



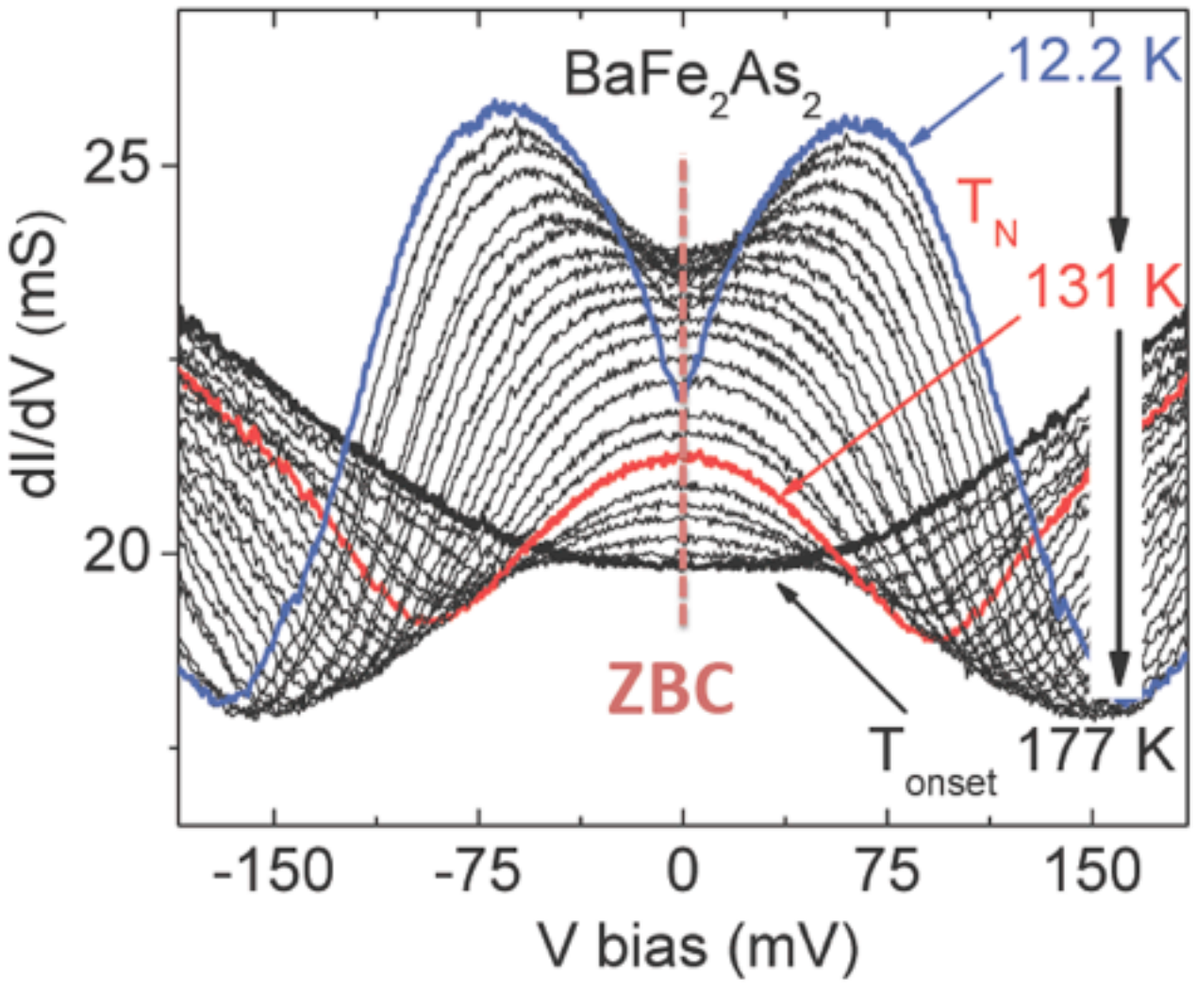
low T
ordered state

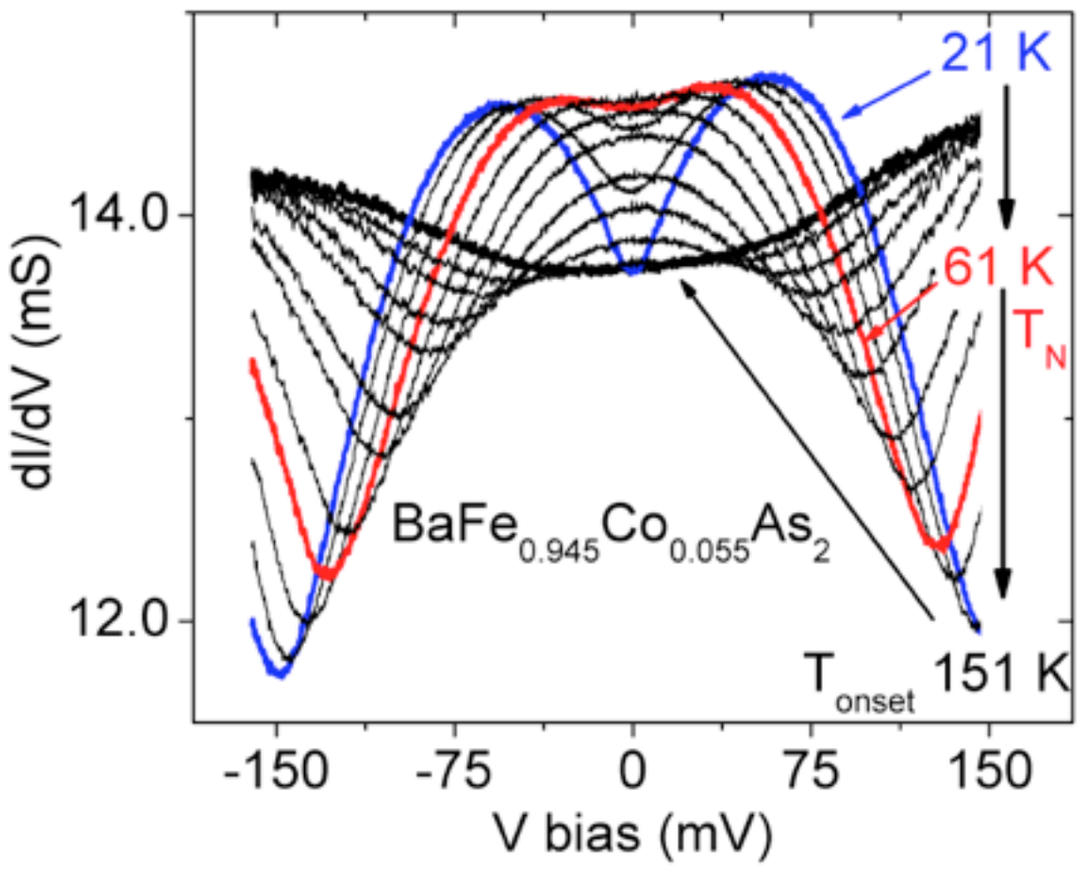
prediction:
Landau damping
increases
as T increases



Z. Leong, et al,
to be submitted

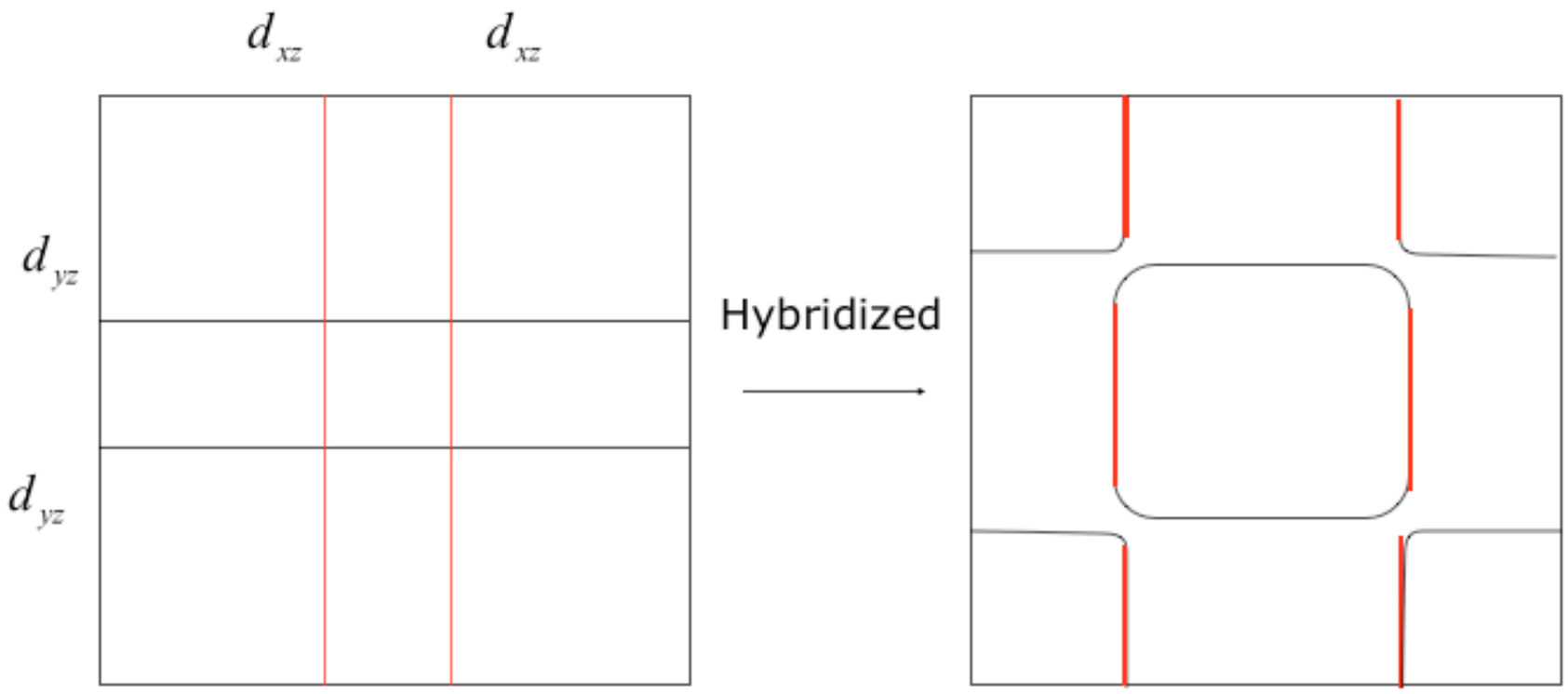
Experimental puzzle 2: What is the origin of the excess conductance above the structural transition?





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

Fermi surface in Brillouin zone



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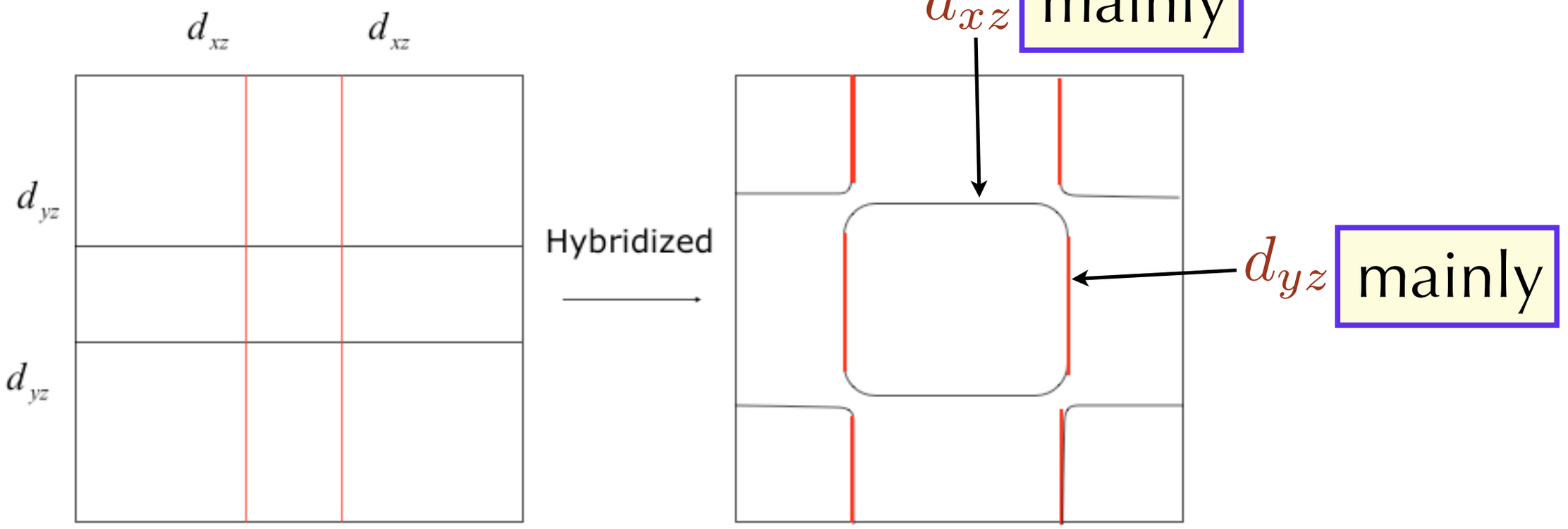

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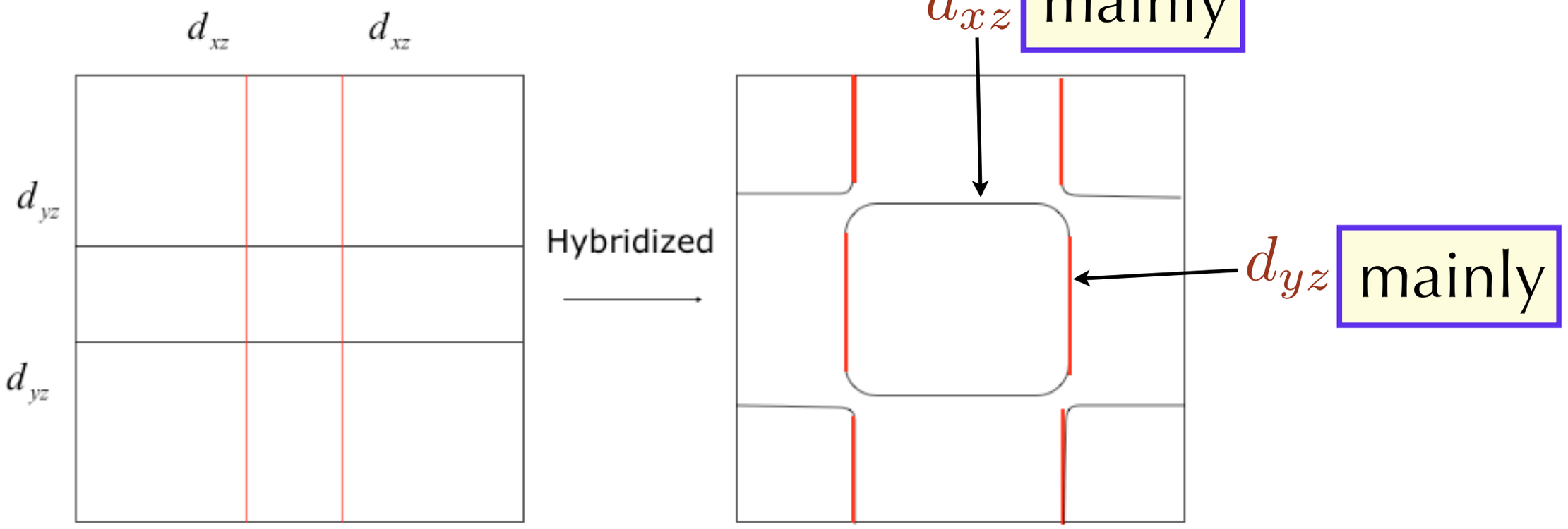
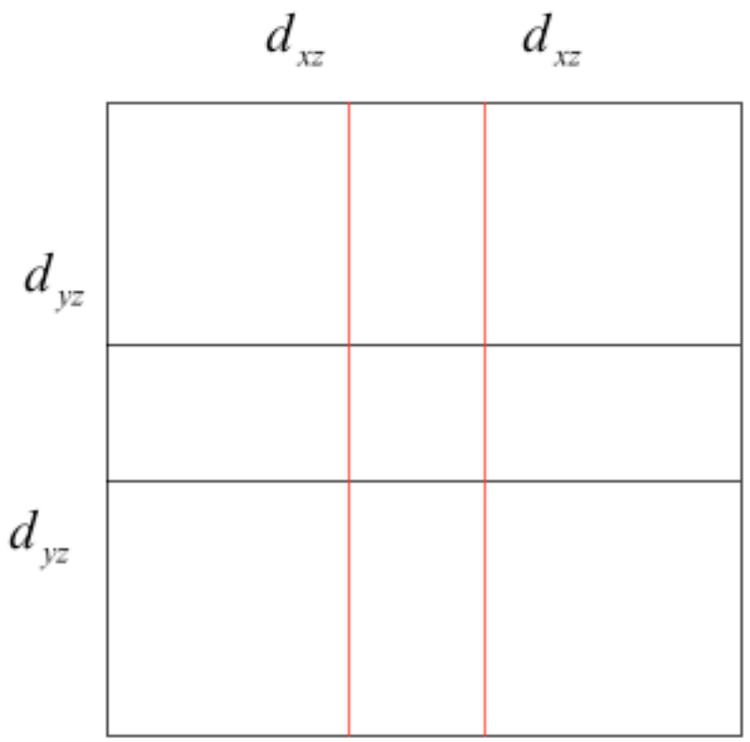


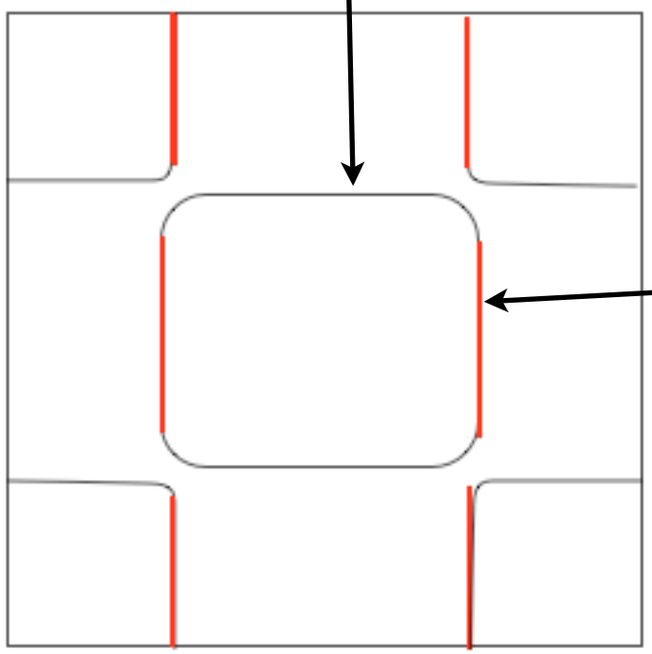
on-site interaction

anisotropic in hybridized basis

Fermi surface in Brillouin zone



Hybridized

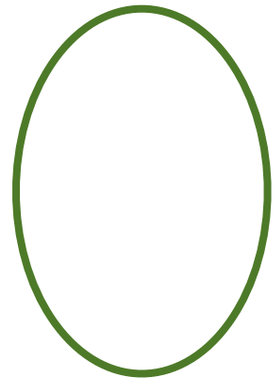


d_{xz} mainly

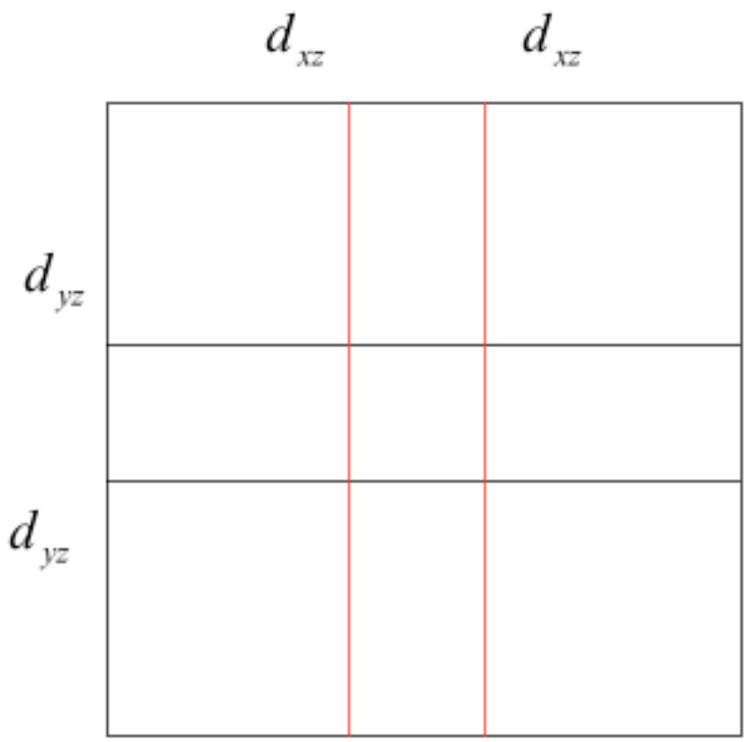
d_{yz} mainly

on-site interaction

anisotropic in hybridized basis



Fermi surface in Brillouin zone



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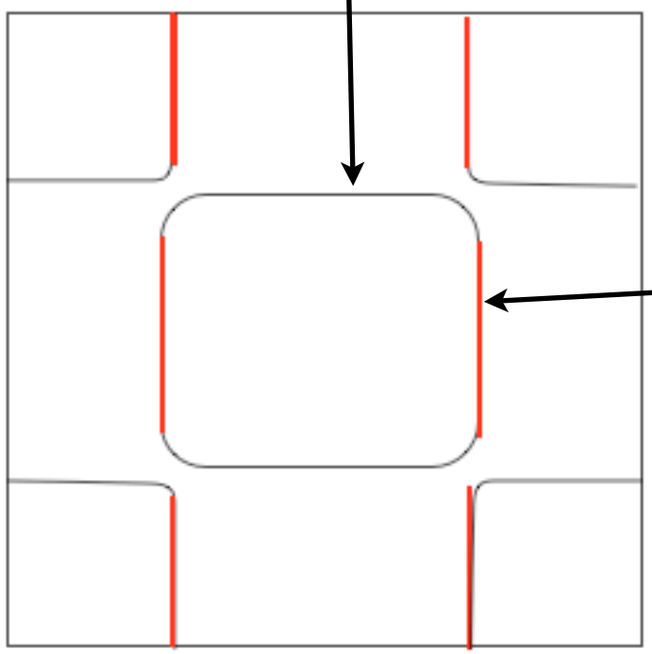

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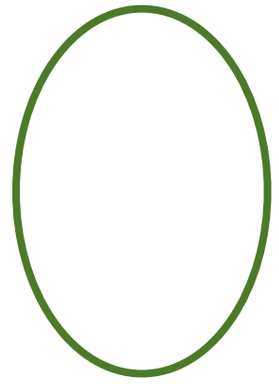


orbital ordering in multi-orbital system = nematic order

Multiorbital Hubbard Model

$$H = H_t + H_I$$

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

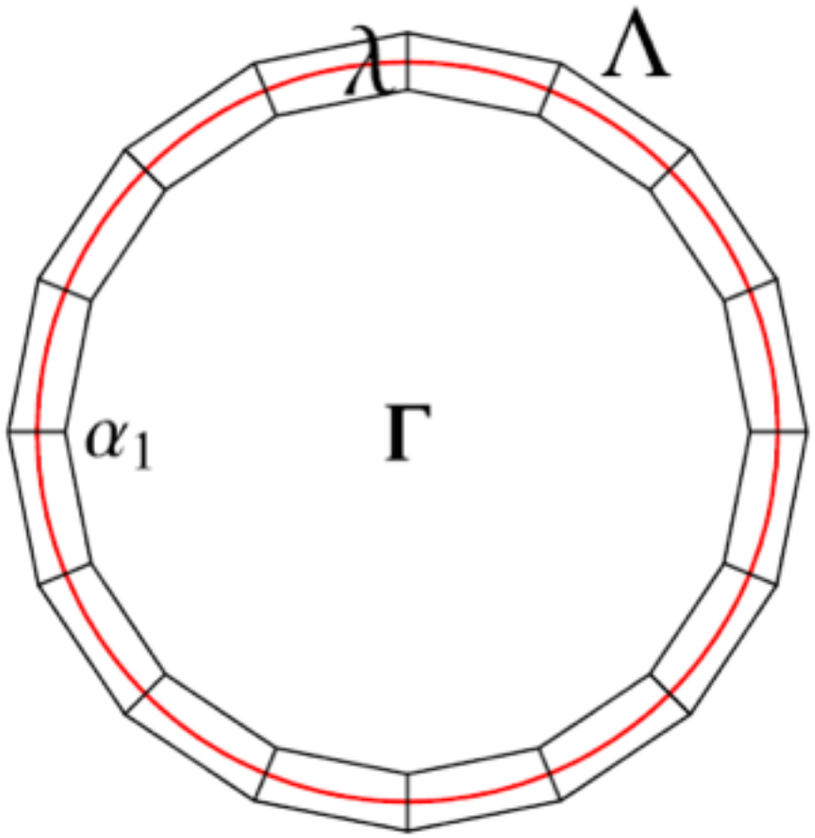
$$H_I = \sum_{ia} U n_{ia\uparrow} n_{ia\downarrow} + \sum_{i,b>a}\left(U' - \frac{J}{2}\right) n_{ia} n_{ib} - 2J\vec{S}_{ia}\times\vec{S}_{ib} + J\left(c_{ia\uparrow} c_{ia\downarrow} c_{ib\downarrow}^{+} c_{ib\uparrow}^{+} + h.c.\right)$$

$$U' = U - 2J$$

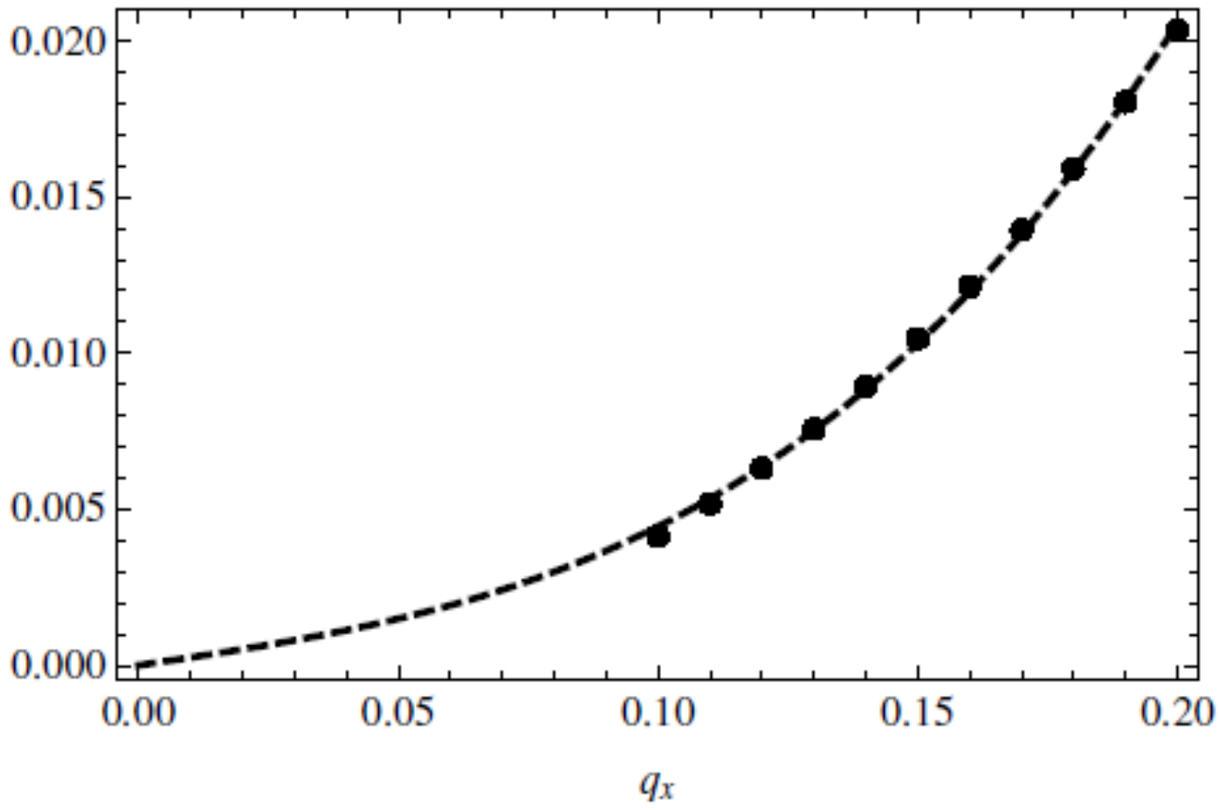
Theoretical approaches:

- 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

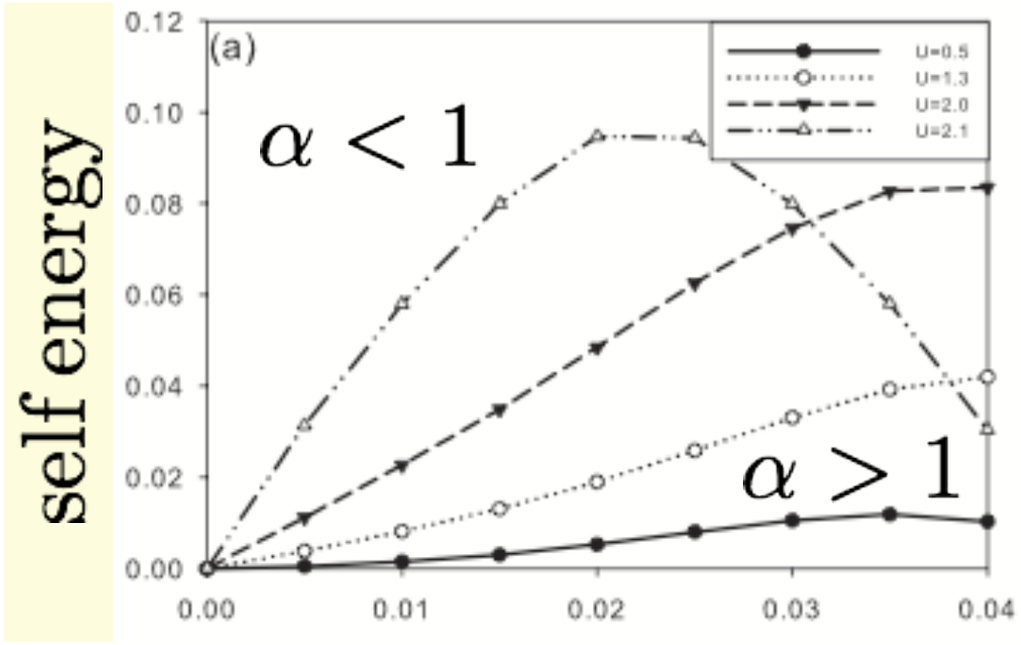


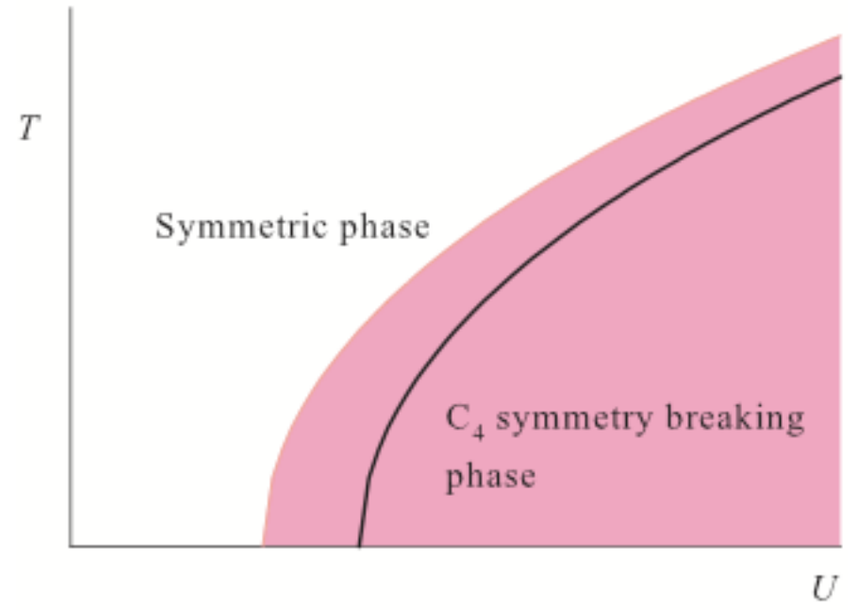
Patches for multidimensional bosonization



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

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

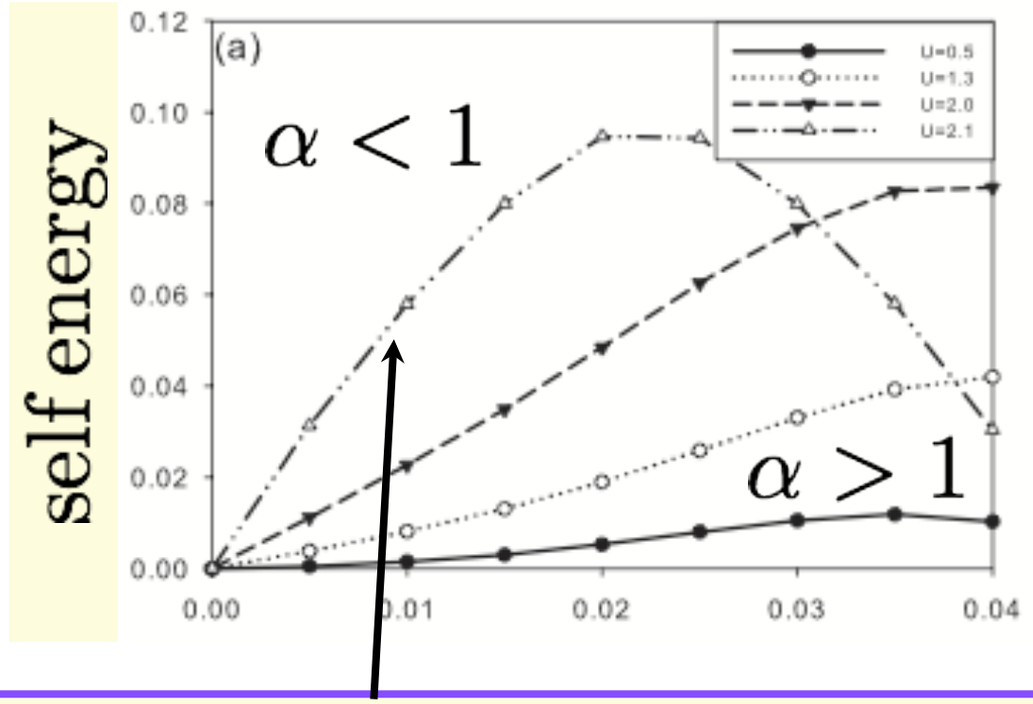


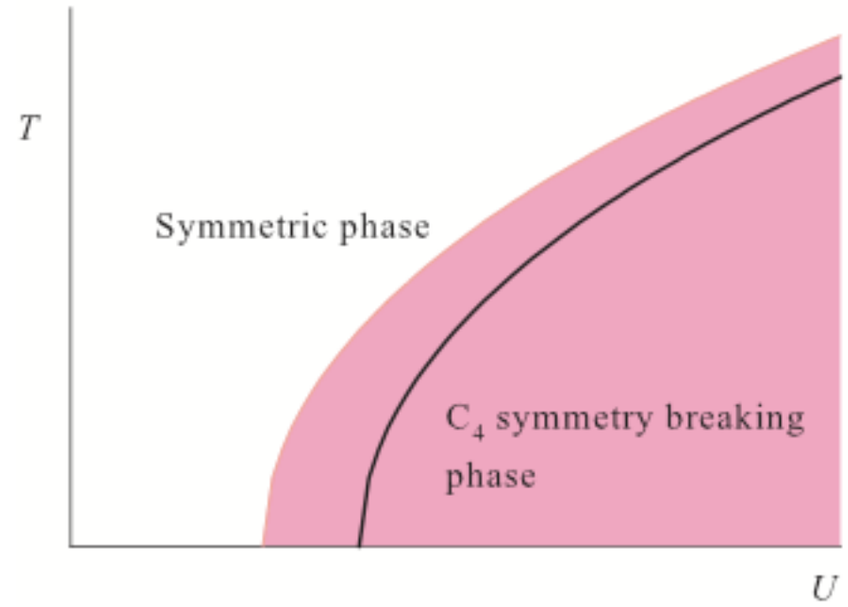


$$\frac{1}{\tau} = \mathrm{Im}\,\Sigma(k_F, \omega) = a\omega^{\alpha} + \ldots$$

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

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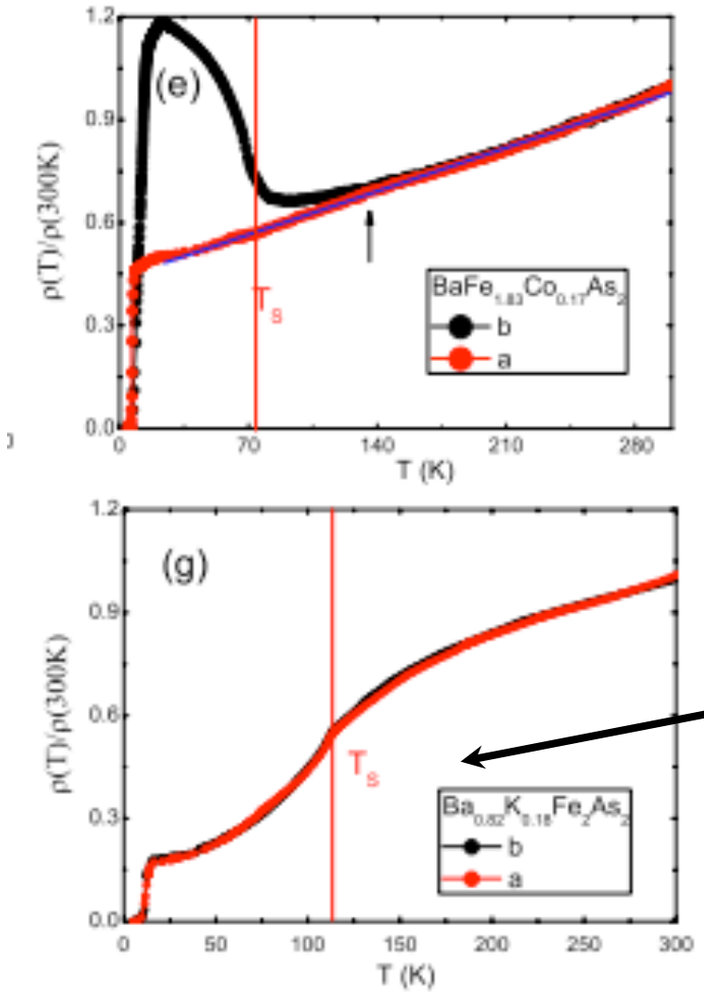
Wei-Cheng Lee, and Philip W. Phillips, Phys. Rev. B **86**, 245113 (2012)

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

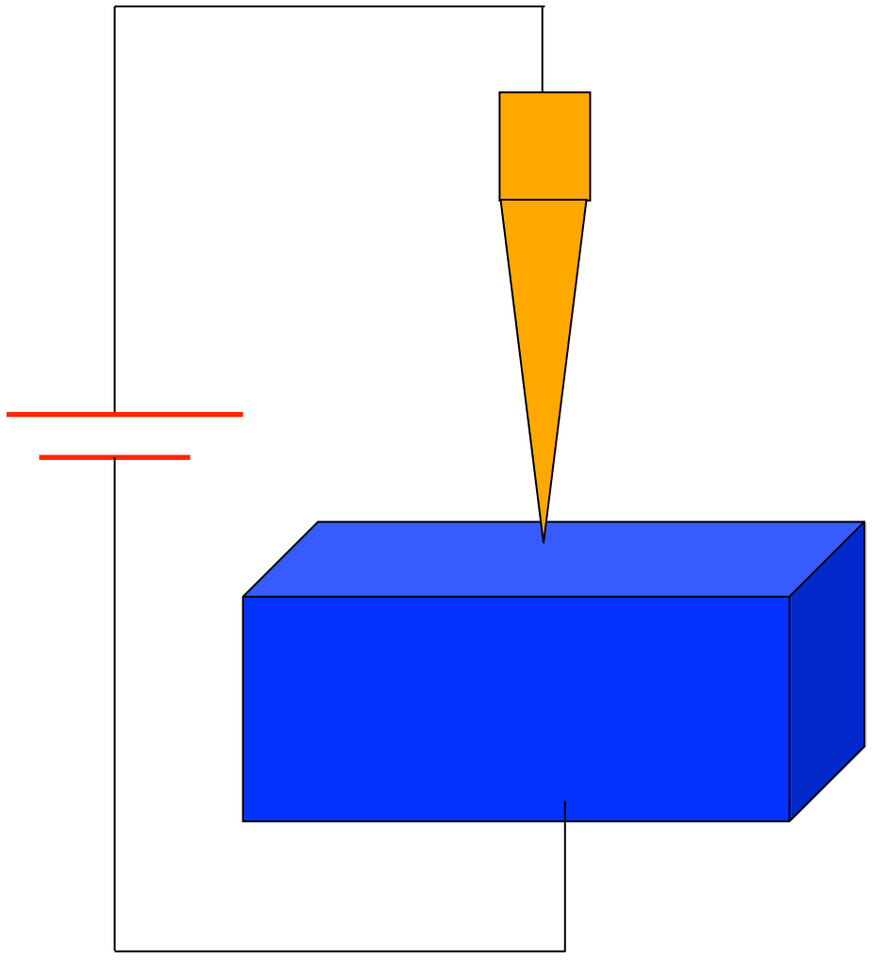
J. J. Ying,[1] X. F. Wang,[1] T. Wu,[1] Z. J. Xiang,[1] R. H. Liu,[1] Y. J. Yan,[1] A. F. Wang,[1] M. Zhang,[1] G. J. Ye,[1] P. Cheng,[1] J. P. Hu,[2] and X. H. Chen[1,*]

[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*

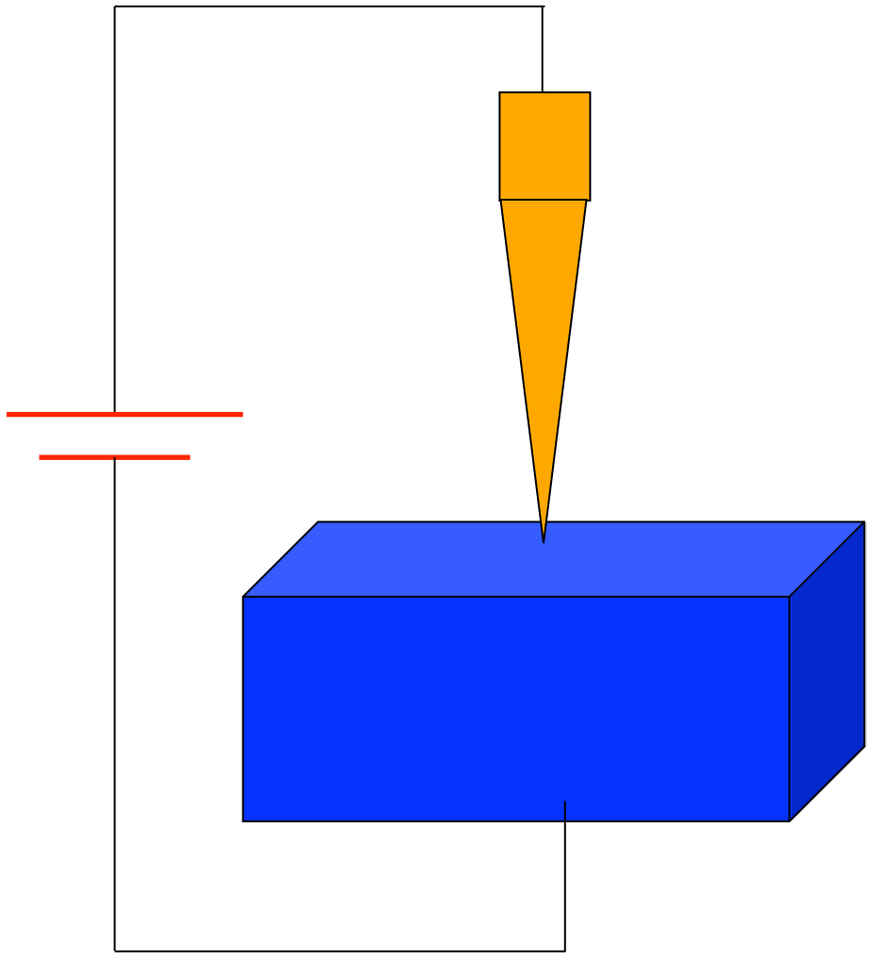
(Received 13 December 2010; published 2 August 2011)

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.

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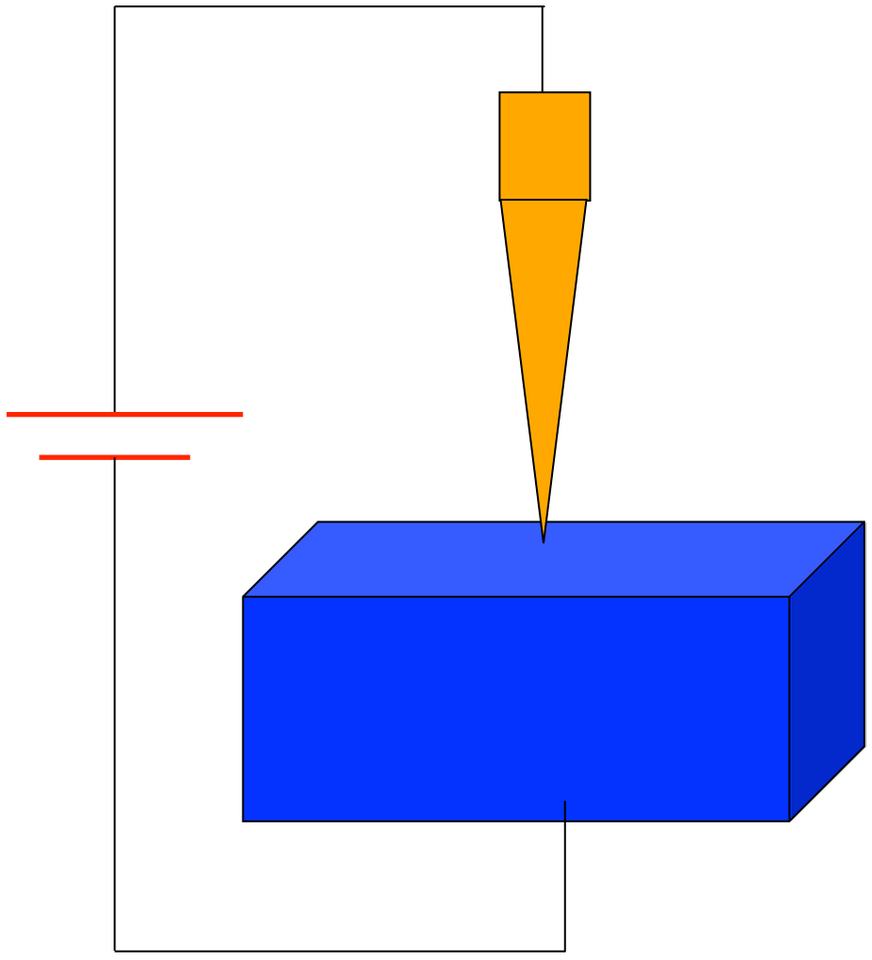

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For metals

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

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

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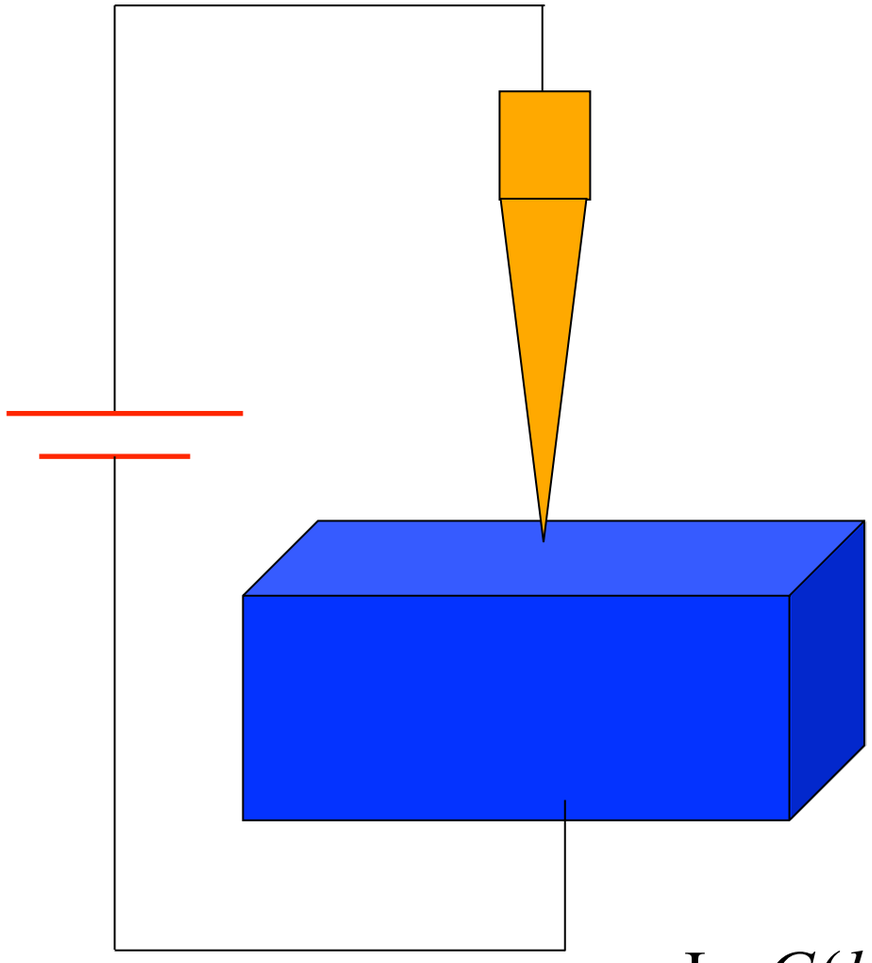

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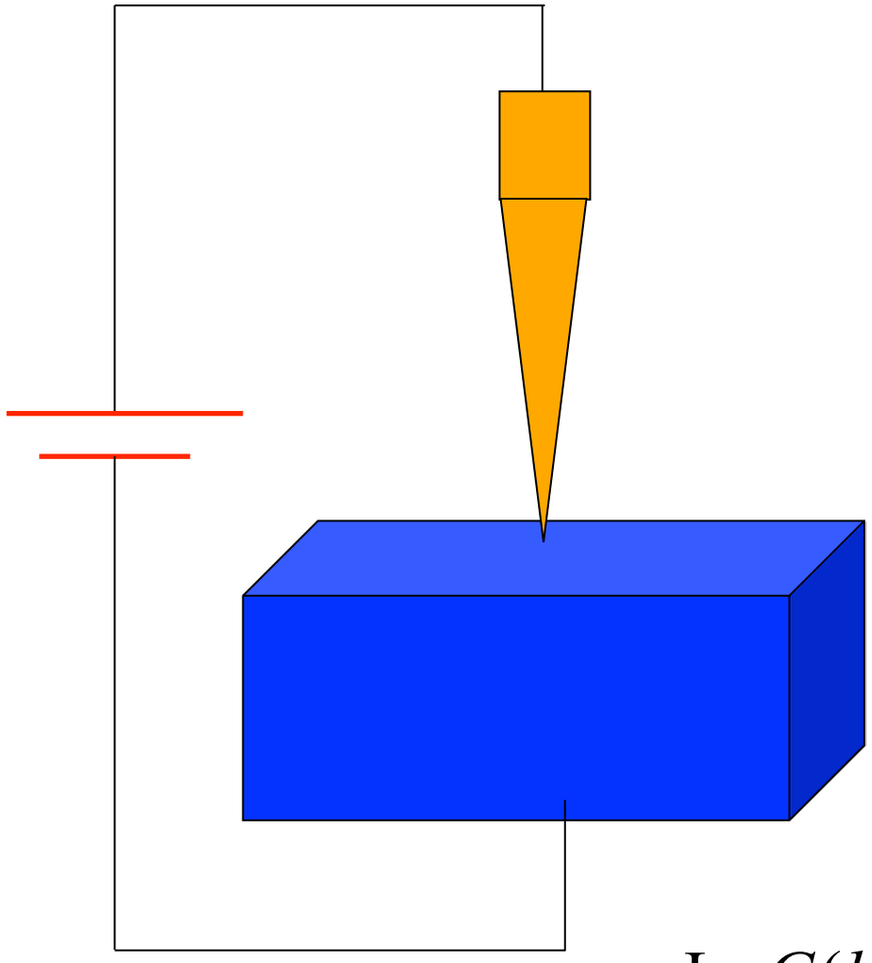
For non-Fermi liquid due to nematic QCP,

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

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

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

Point Contact Spectroscopy



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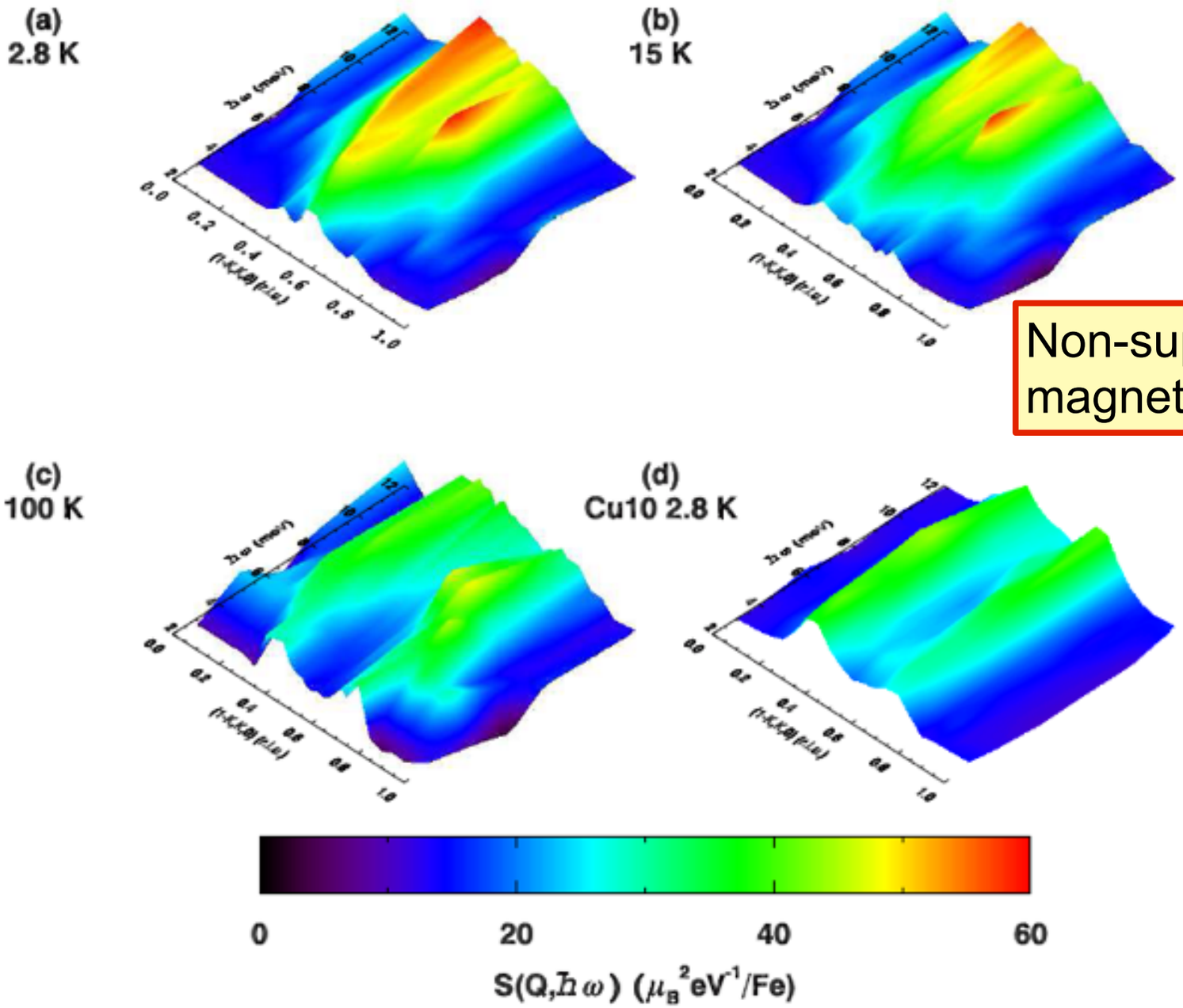
a peak at eV=0!!!

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

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

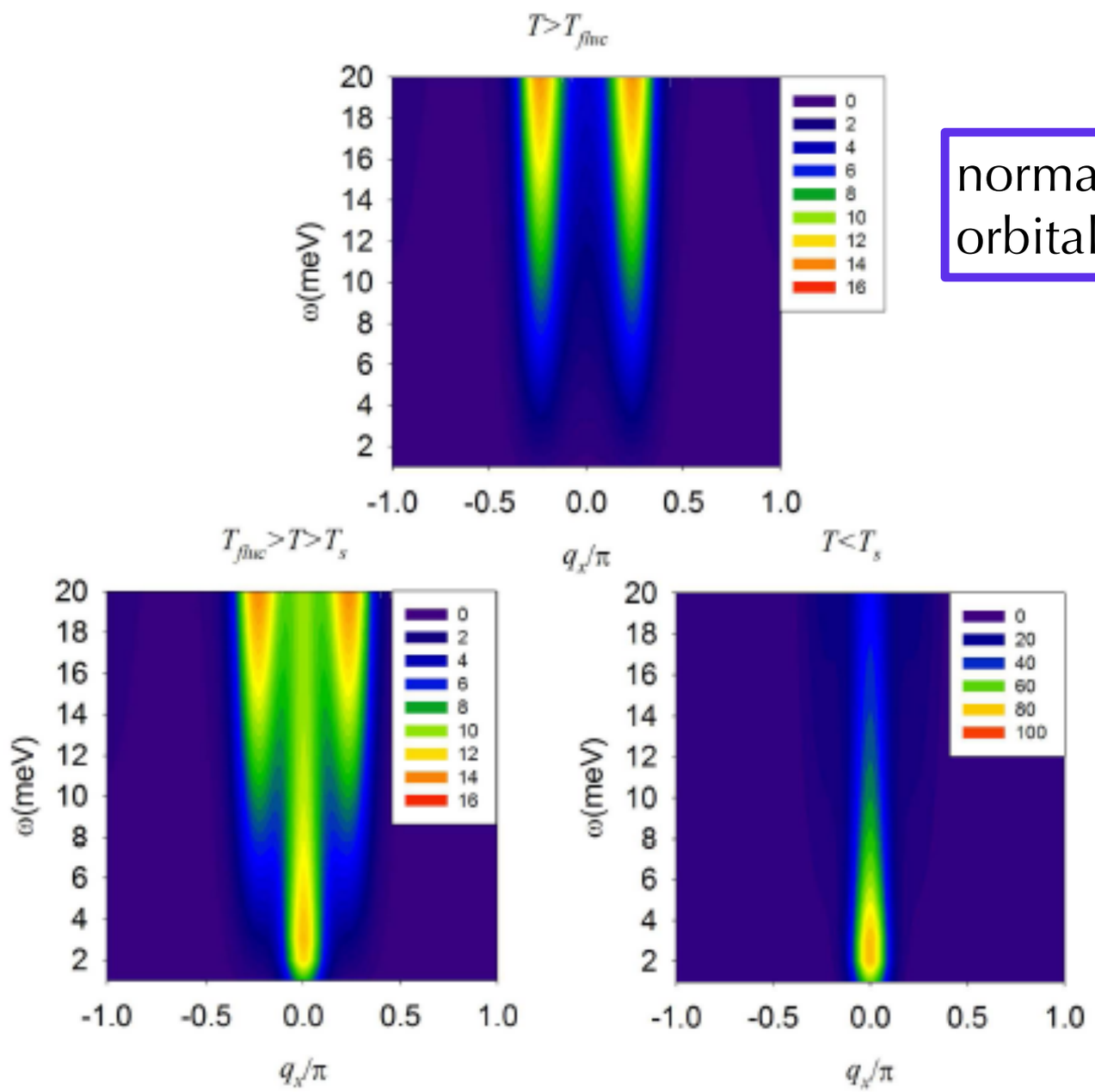
Incommensurate-to-Commensurate Transformation in $Fe_{1-x}Ni_xTe_{0.5}Se_{0.5}$



Non-superconducting - Incommensurate magnetic excitation all the time

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

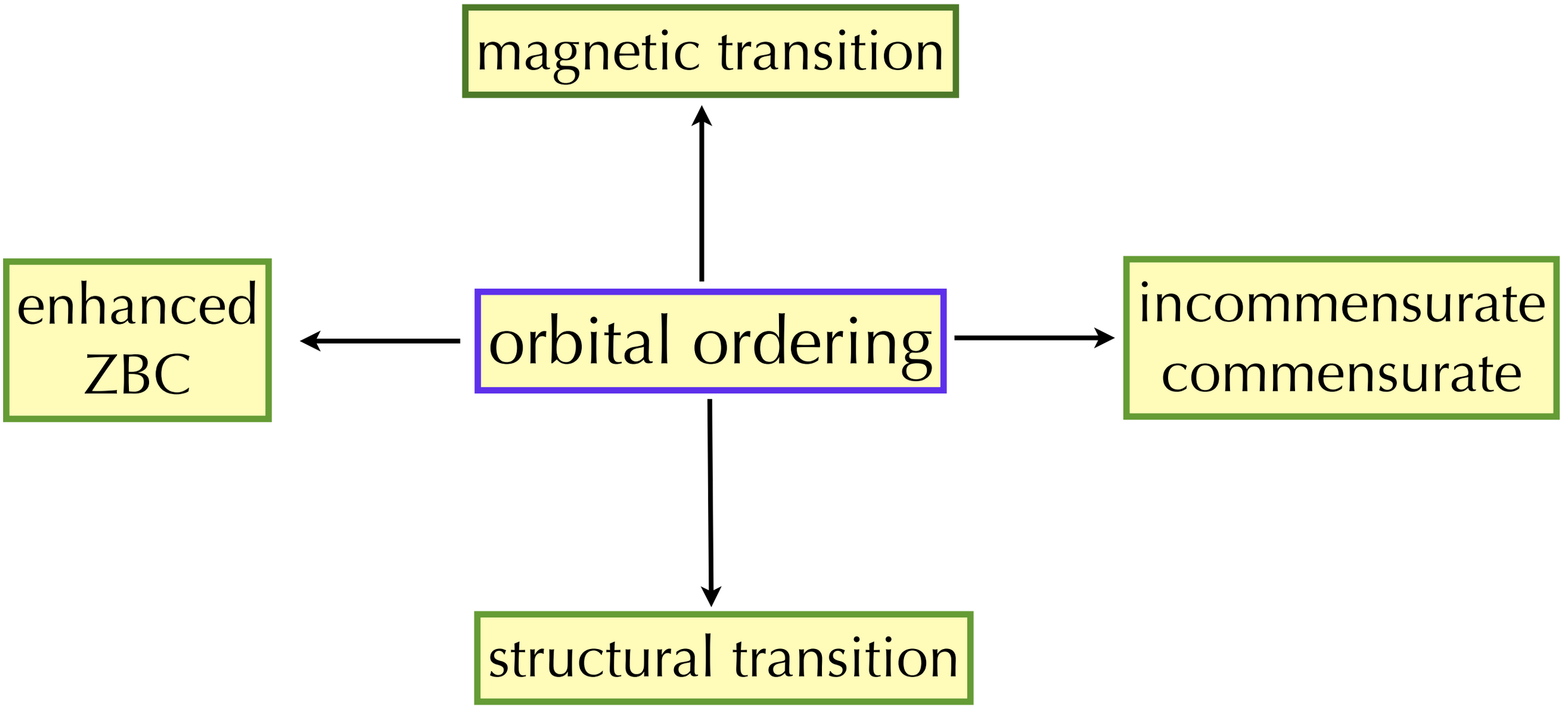
Our Theory – RPA + Gaussian Fluctuations



normal state without orbital fluctuations

Fluctuating orbital order (modeled by Gaussian fluctuation model)

Orbital ordered state


magnetic transition
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structural transition

magnetic transition

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structural transition

thanks to DOE (EFRC)