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

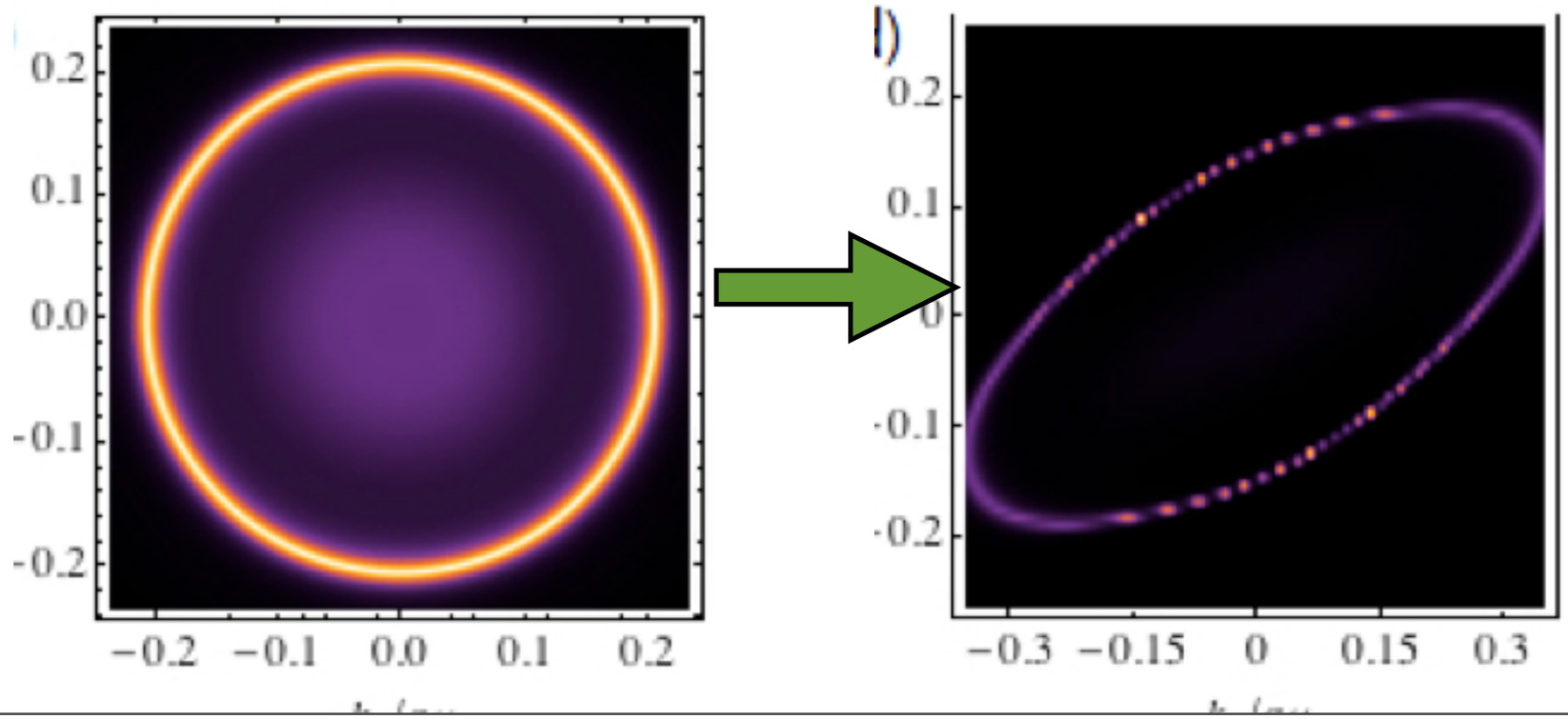
W. Lv, W. Lee, F. Kruger, Z. Leong, J. Tranquada

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

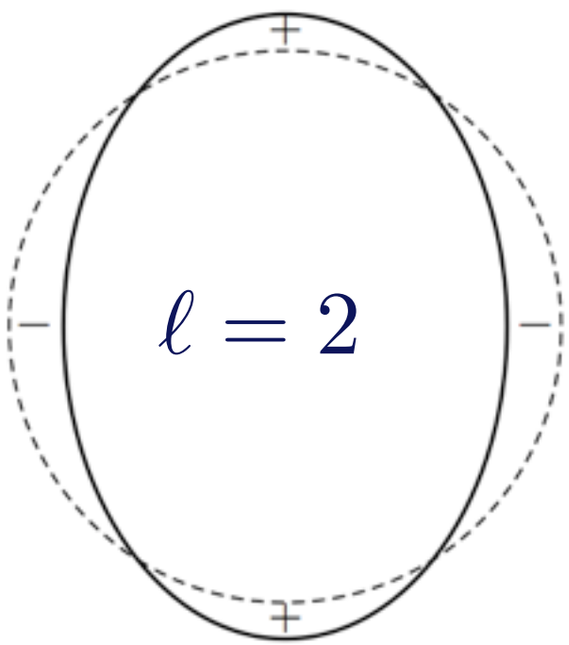
Thanks to: DOE (EFRC)+BNL

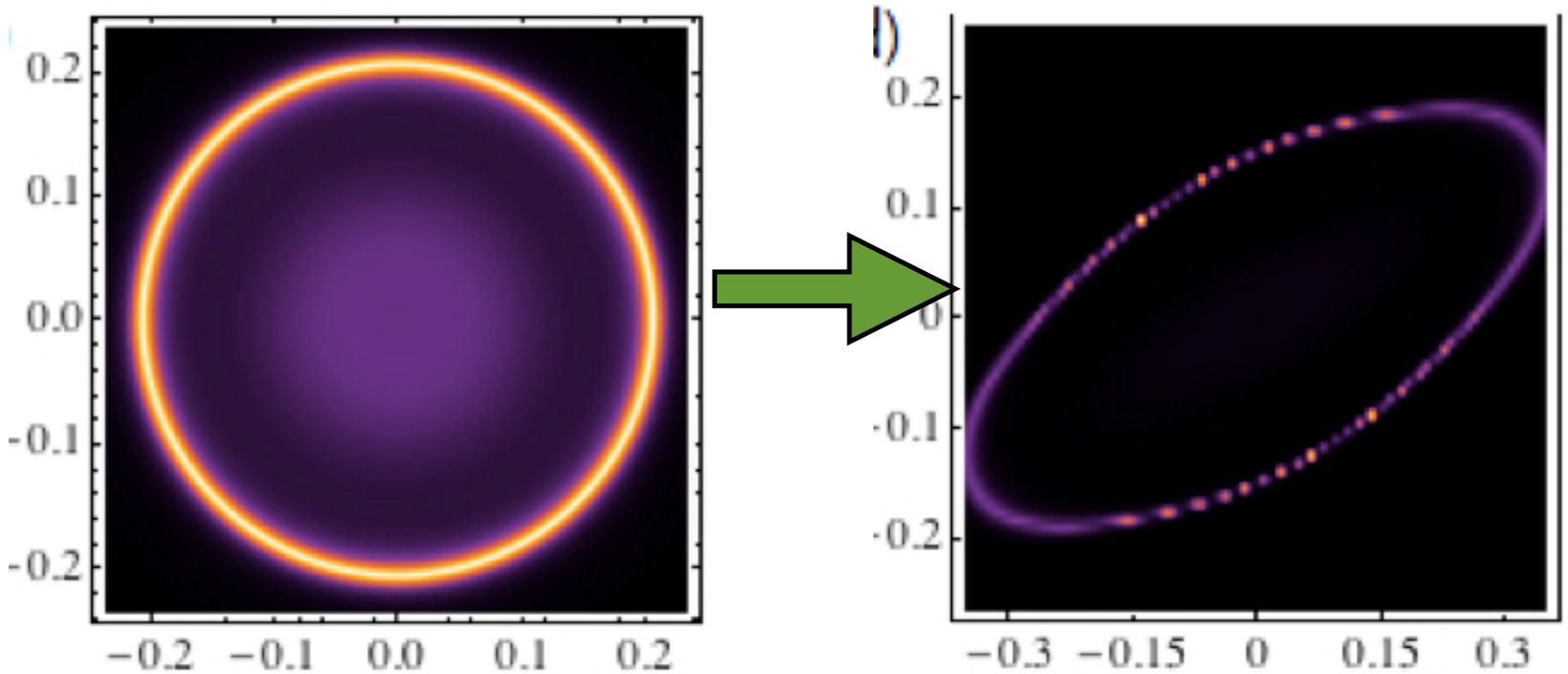


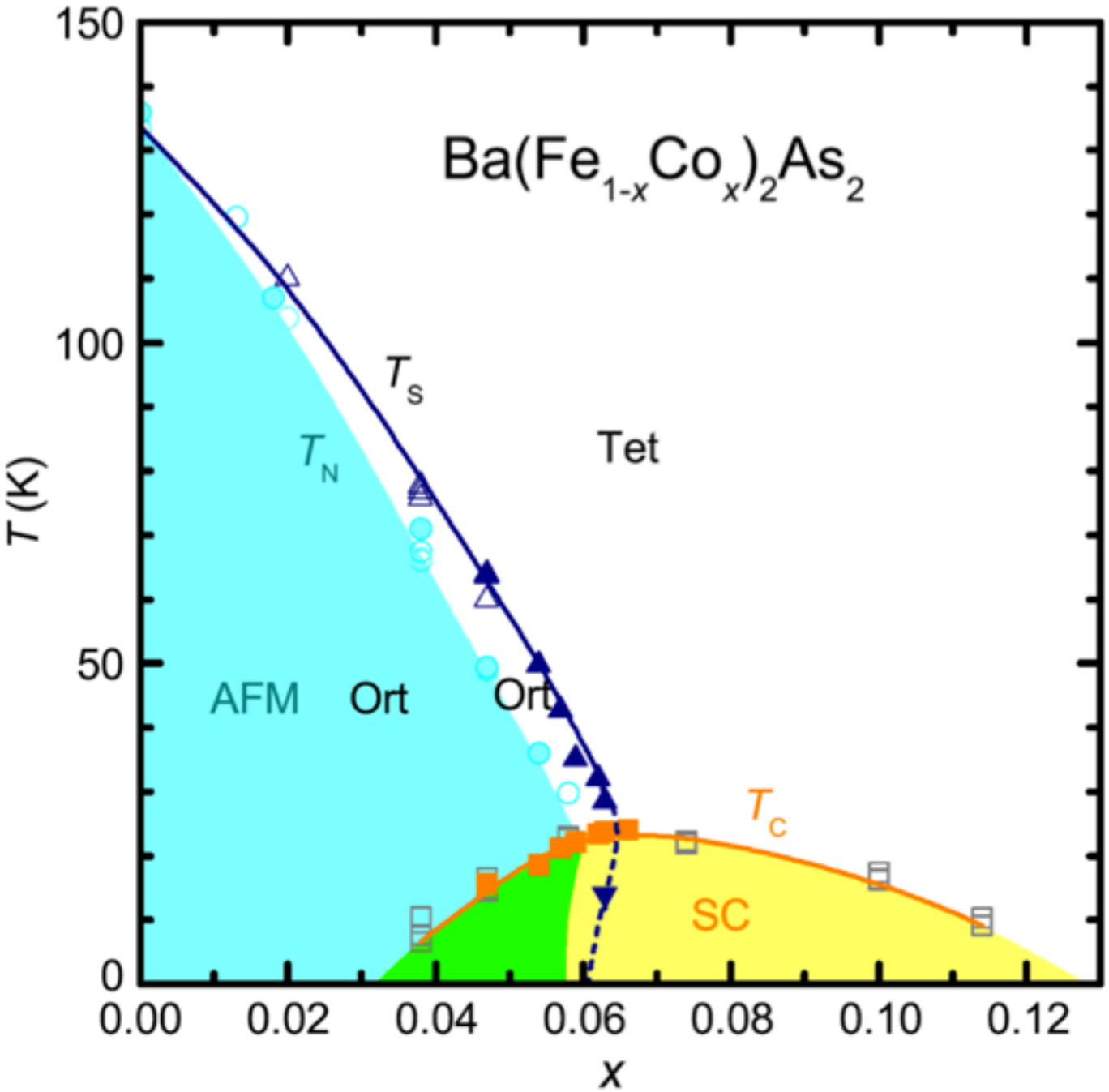
Spin or Orbital-based Physics in the Fe-based Superconductors?

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

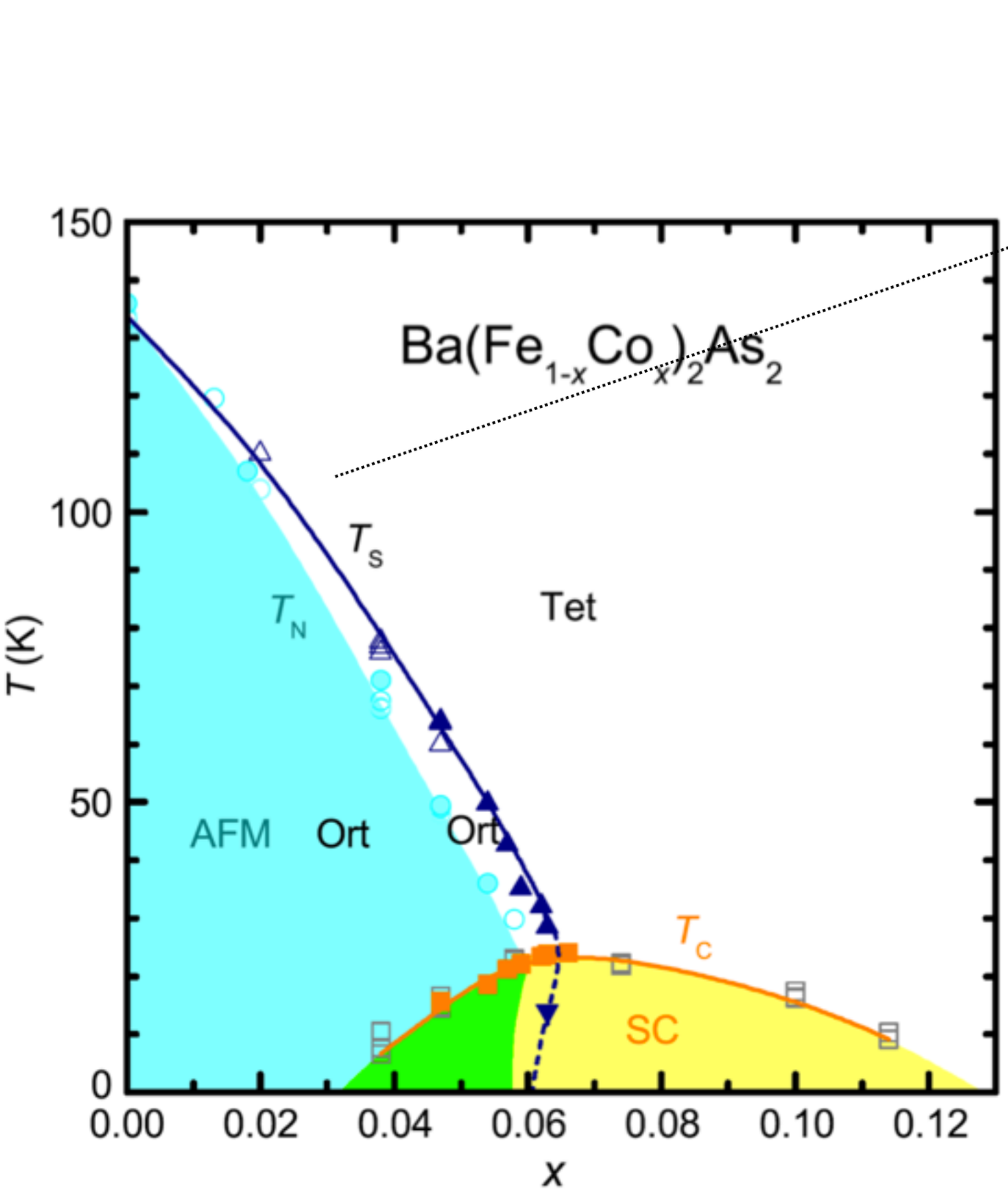
Thanks to: DOE (EFRC)+BNL

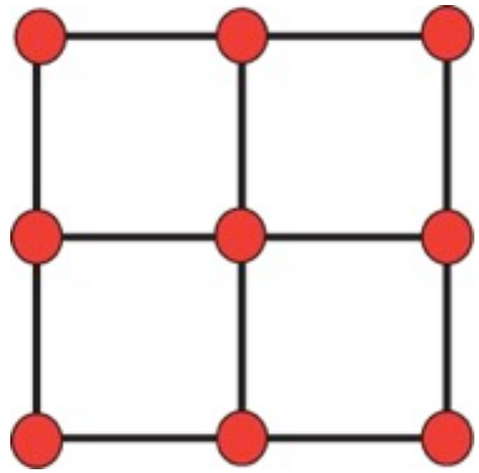




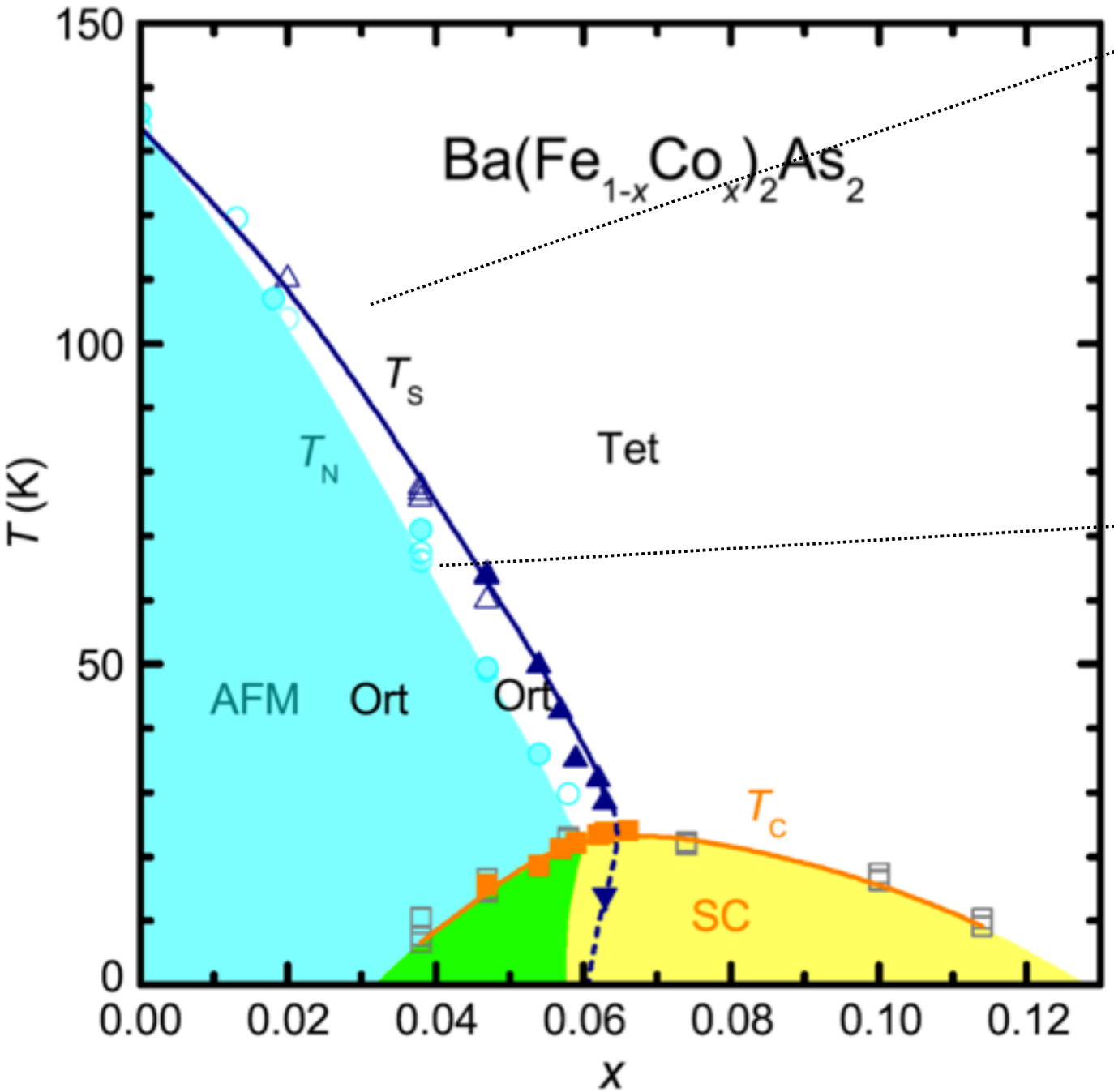


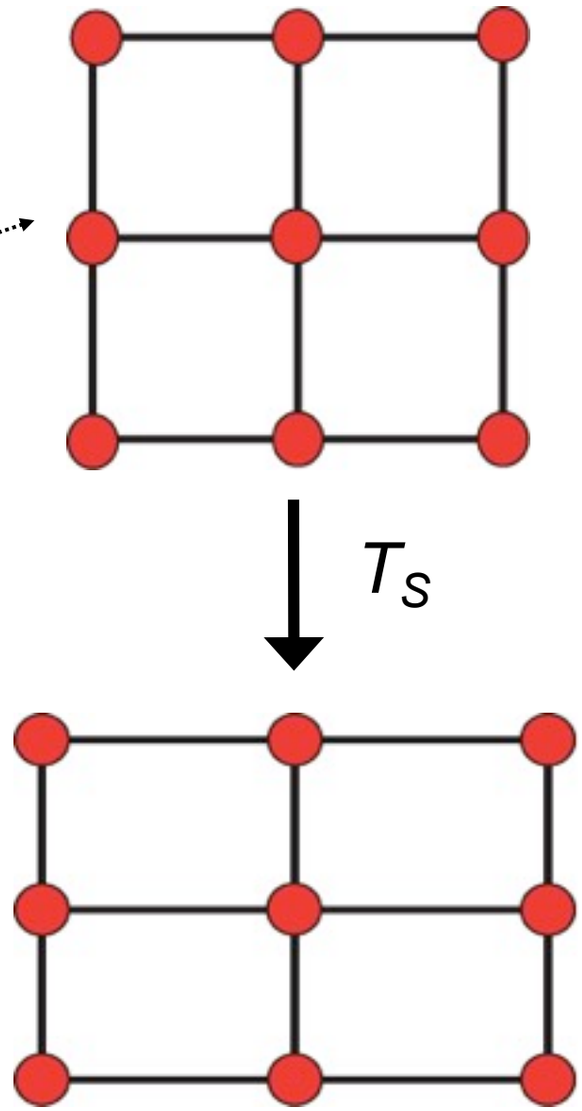
S. Nandi, et al. PRL (2010)



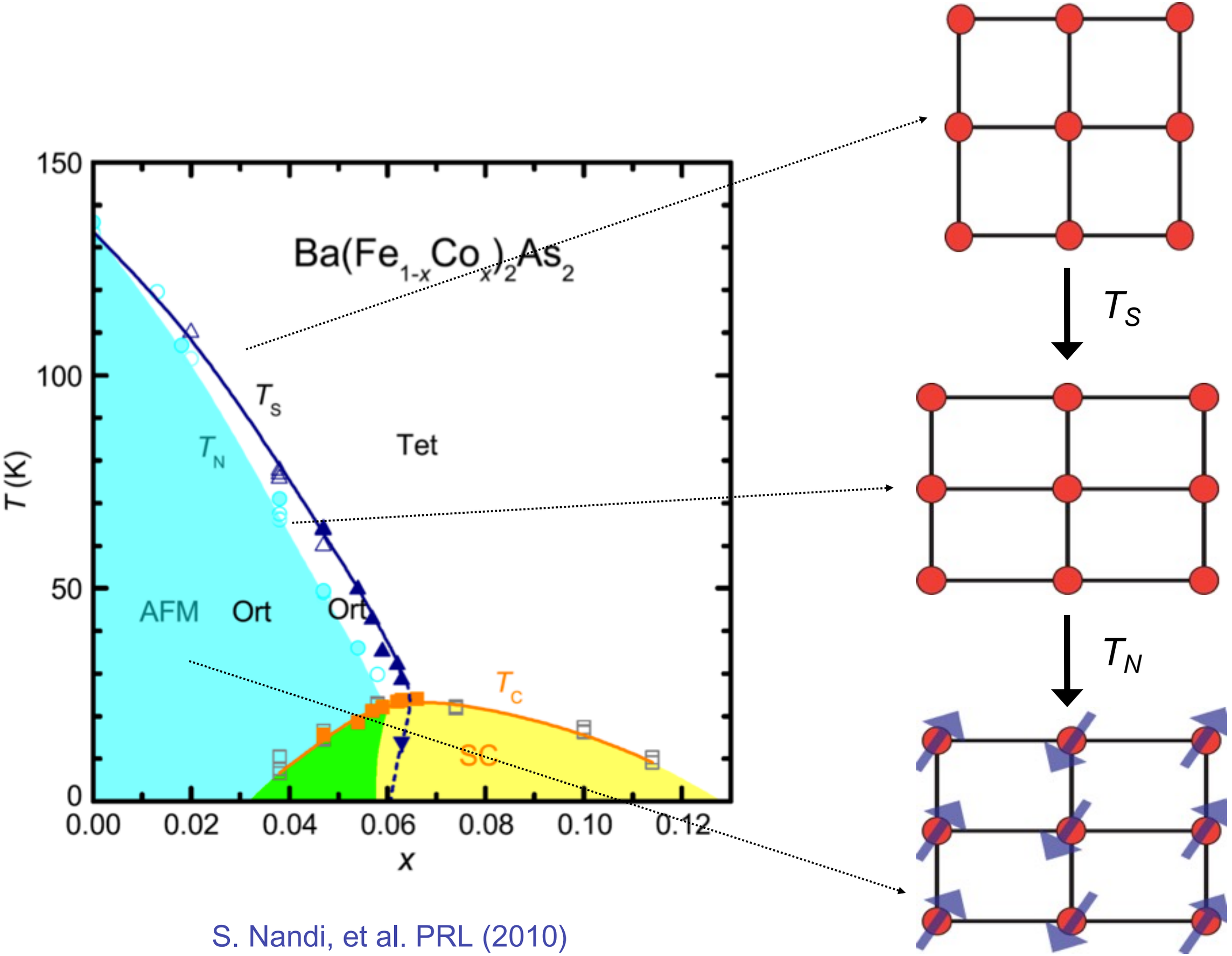


S. Nandi, et al. PRL (2010)





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)
……

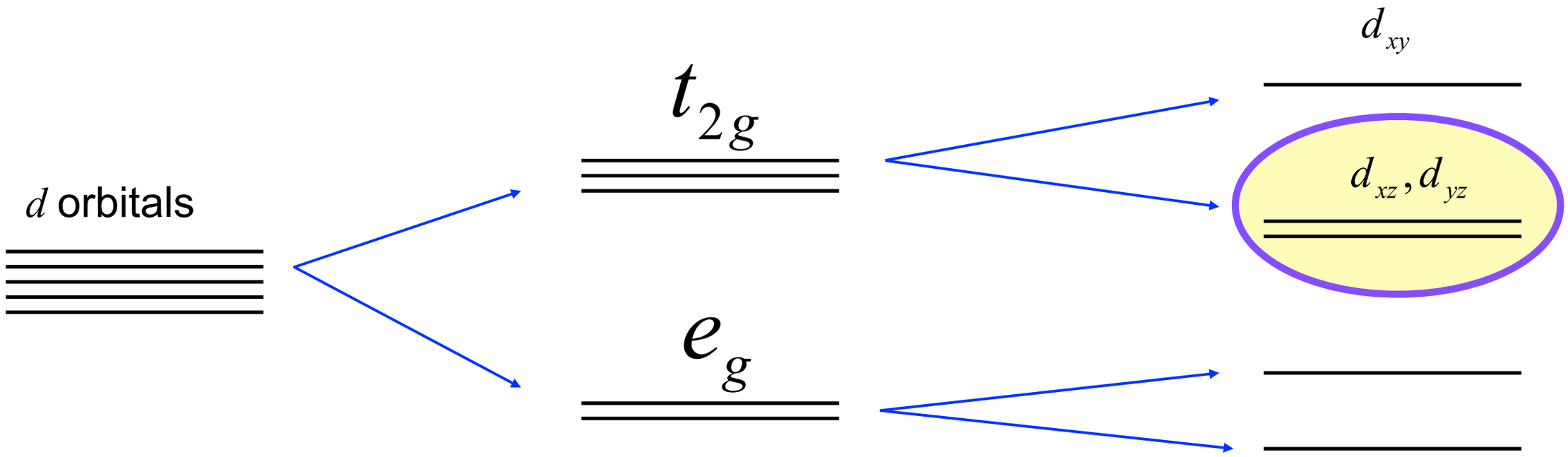
spin order

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

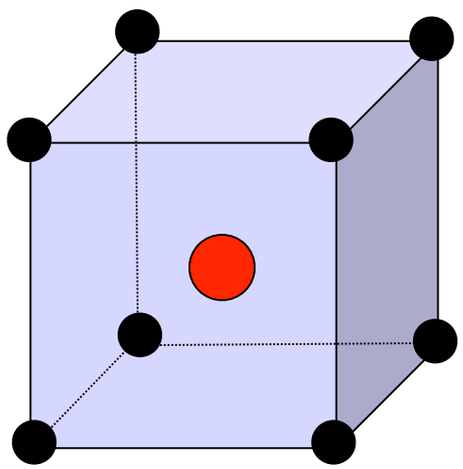
Nematic order in iron superconductors – who is in the driver's seat?

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

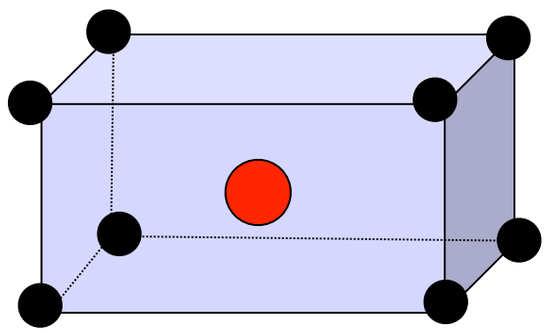
What is new with Fe-based superconductors?



atom



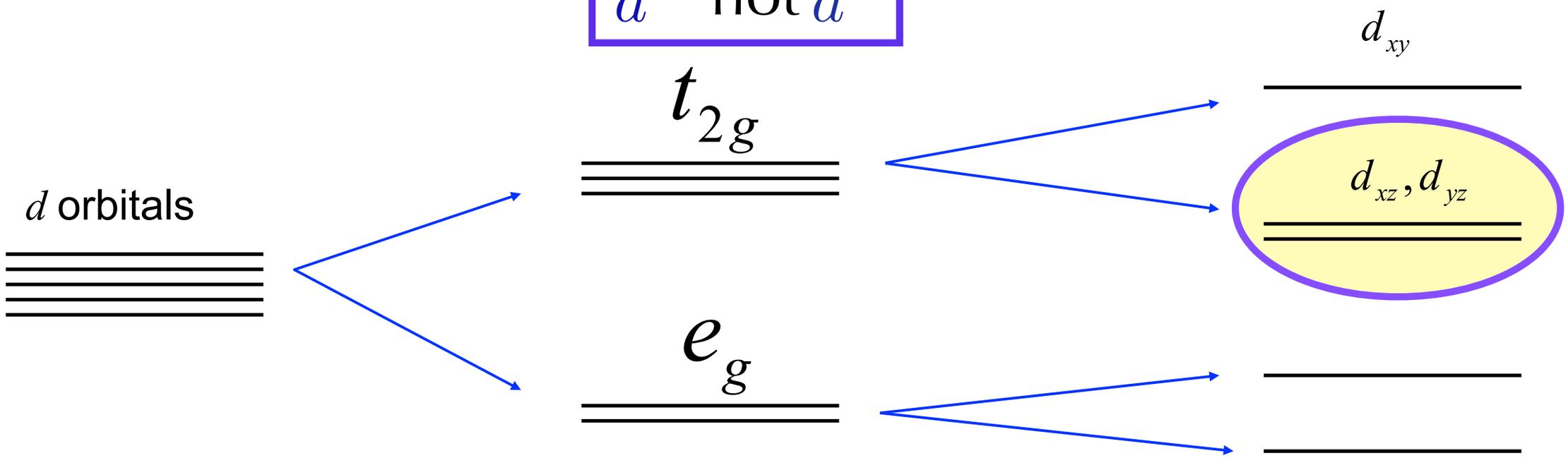
cubic symmetry
(a=b=c)

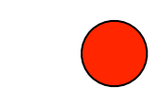


tetragonal symmetry
(a=b≠c)

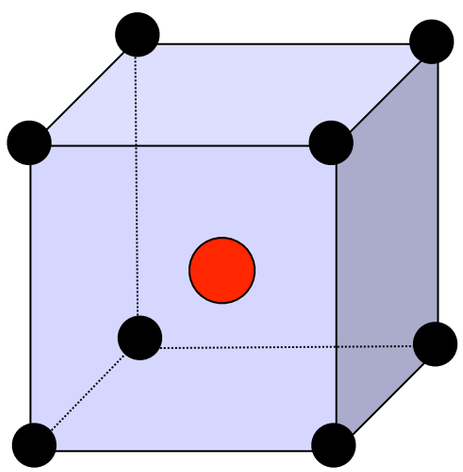
What is new with Fe-based superconductors?

d^6 not d^9

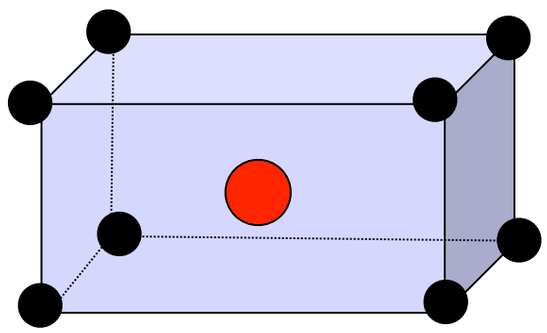




atom



cubic symmetry
(a=b=c)

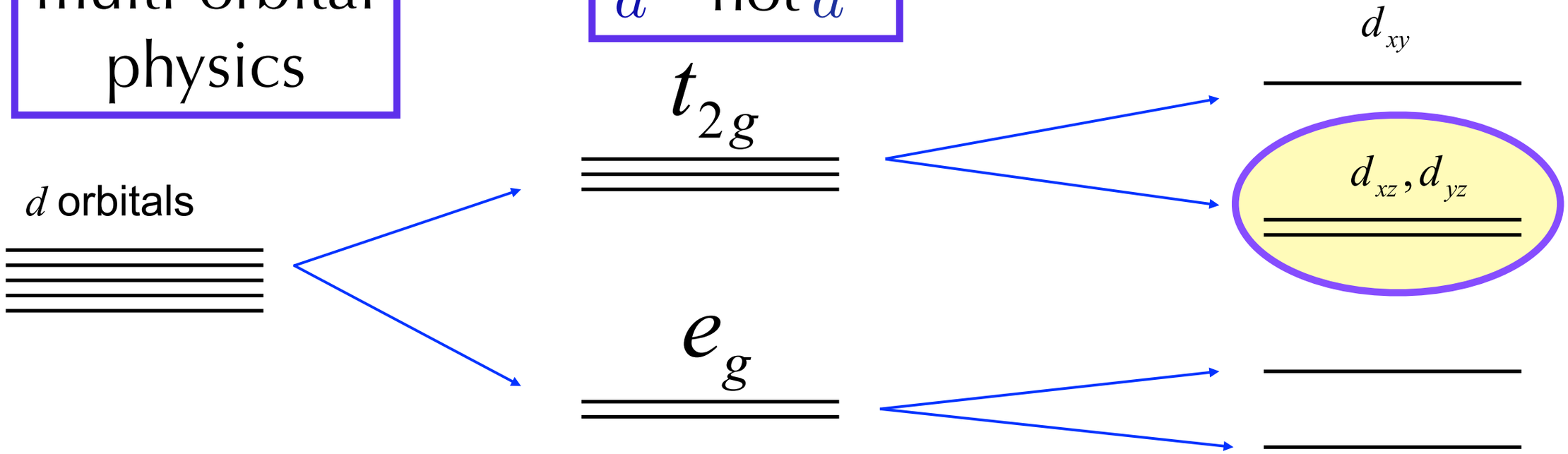


tetragonal symmetry
(a=b≠c)

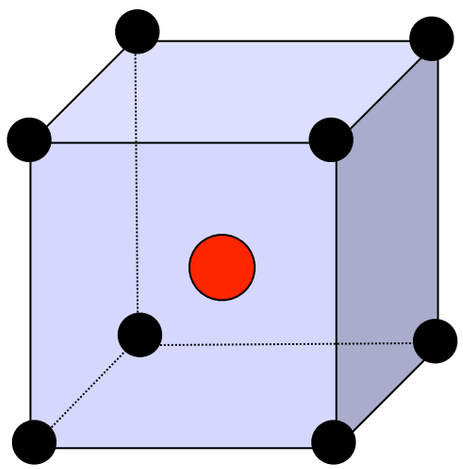
What is new with Fe-based superconductors?

multi-orbital physics

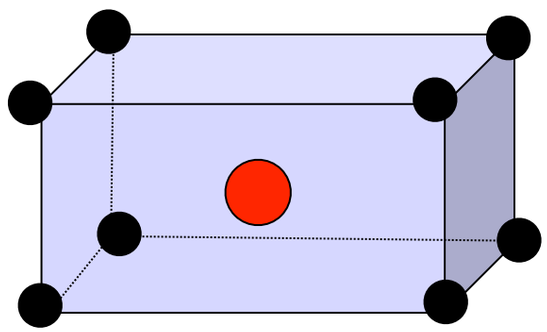
d^6 not d^9



atom



cubic symmetry
(a=b=c)



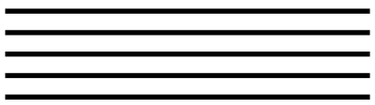
tetragonal symmetry
(a=b≠c)

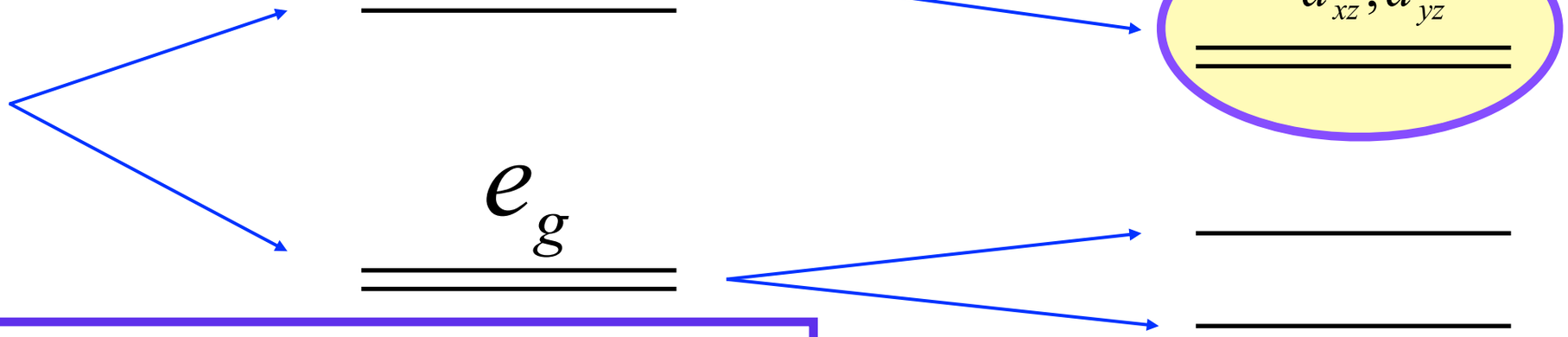
What is new with Fe-based superconductors?

multi-orbital physics

d^6 not d^9

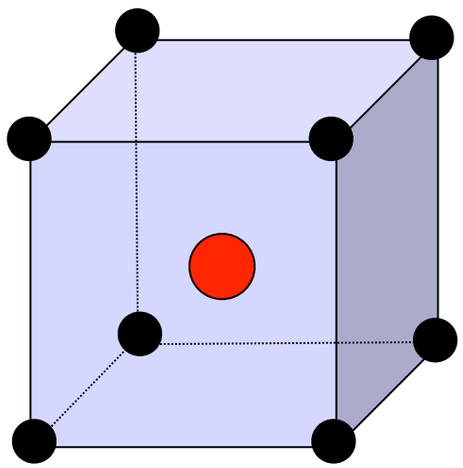
d orbitals



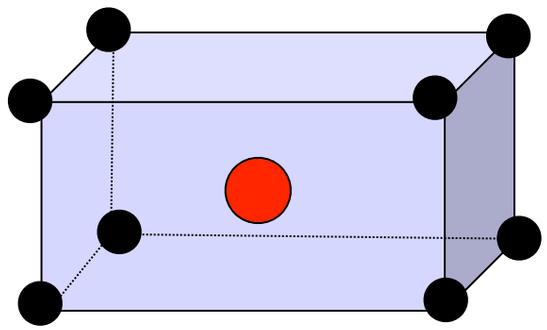


tetrahedral coordination

atom

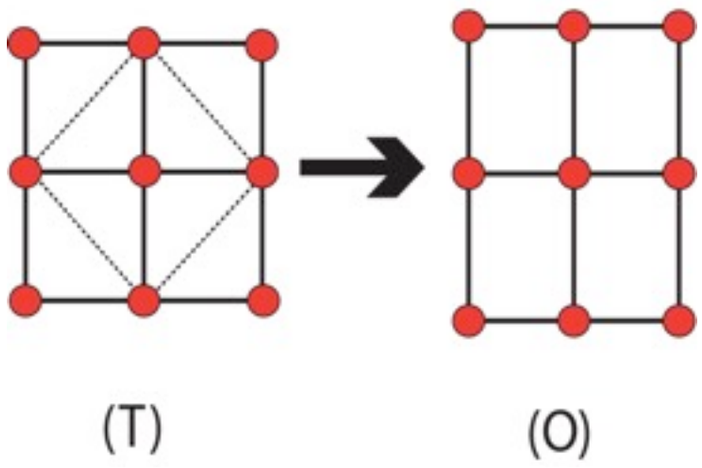


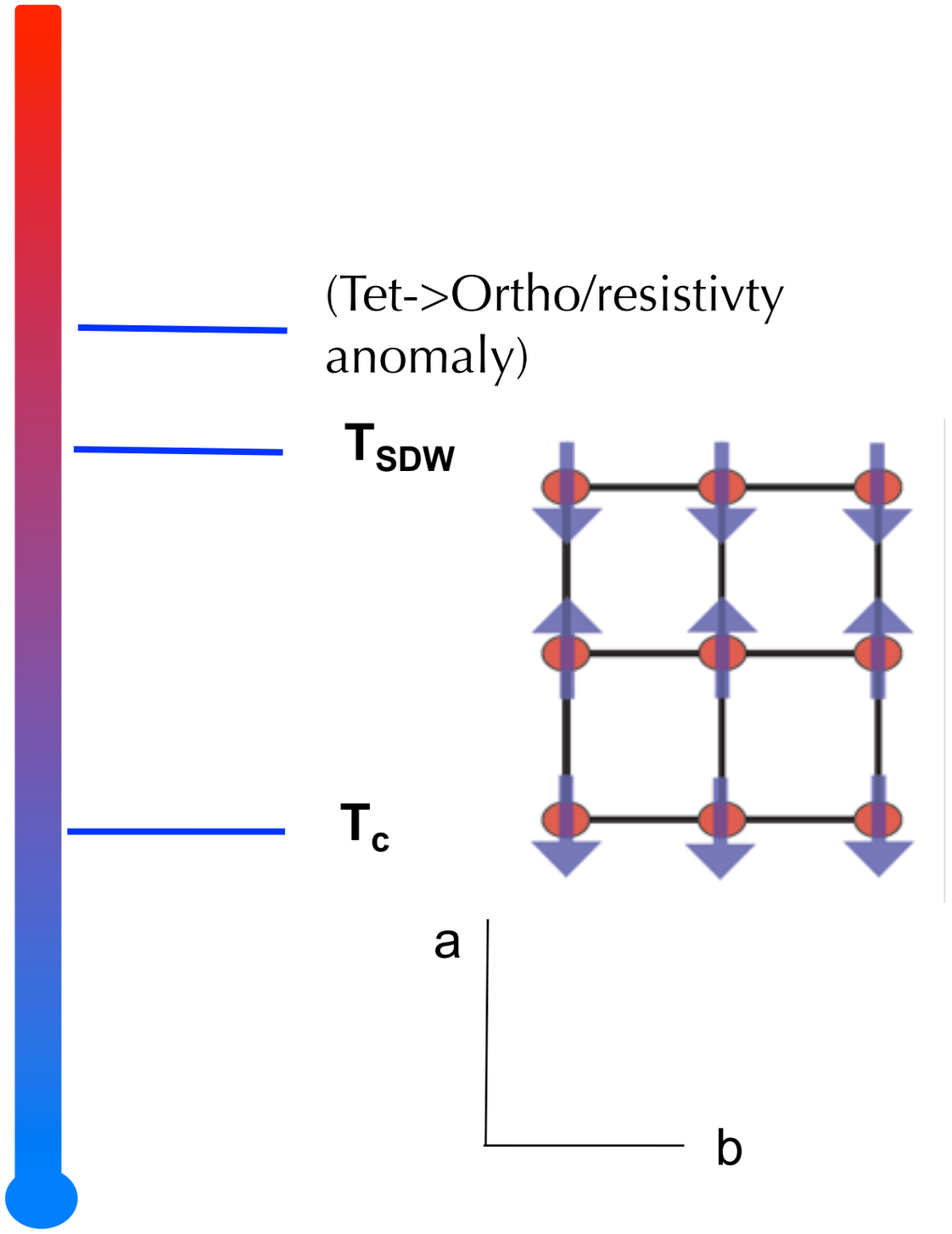
cubic symmetry
(a=b=c)



tetragonal symmetry
(a=b≠c)

Global Features





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

pnictides

d^9

d^6

no orbital
degree of freedom

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

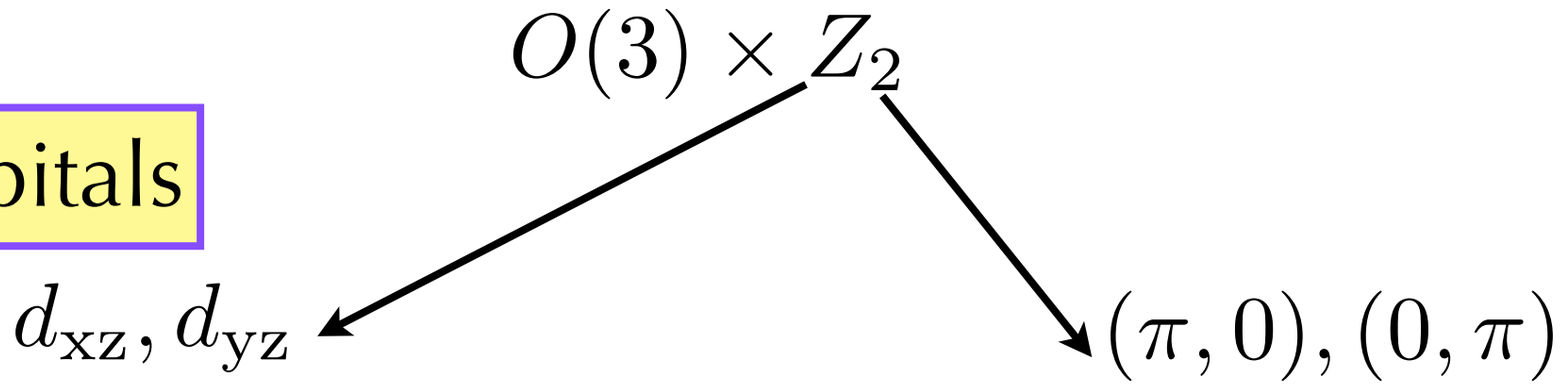
$$O(3) \times Z_2$$

subtle problem

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

subtle problem

orbitals



subtle problem

$O(3) \times Z_2$

orbitals

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

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

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

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

magnetic fluctuations

subtle problem

$O(3) \times Z_2$

orbitals

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

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

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

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

} magnetic fluctuations

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

structural transition

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

} nematic

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

subtle problem

$O(3) \times Z_2$

orbitals

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

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

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

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

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

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

magnetic fluctuations

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

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

structural transition

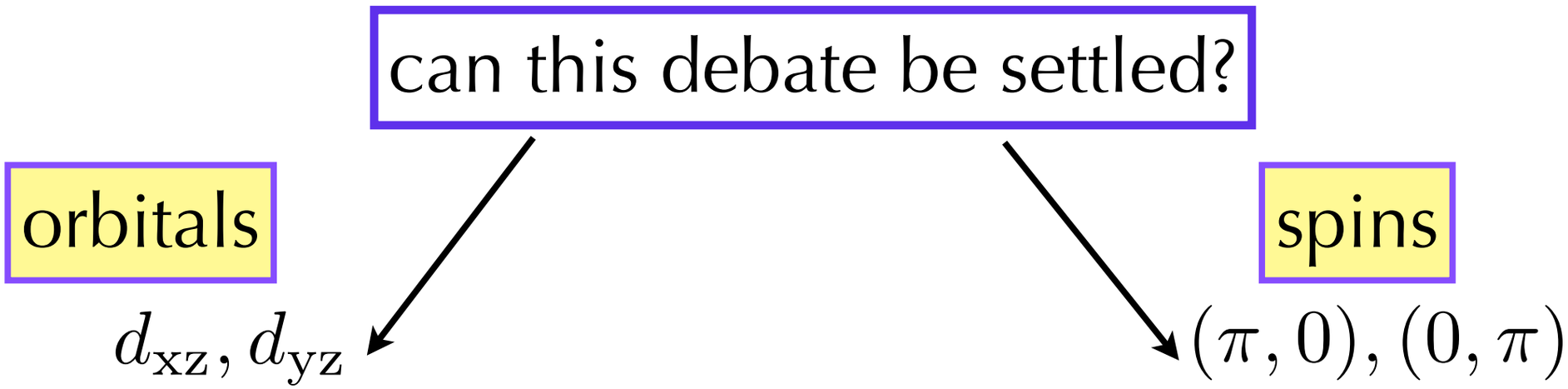
nematic

structural transition

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

magnetism

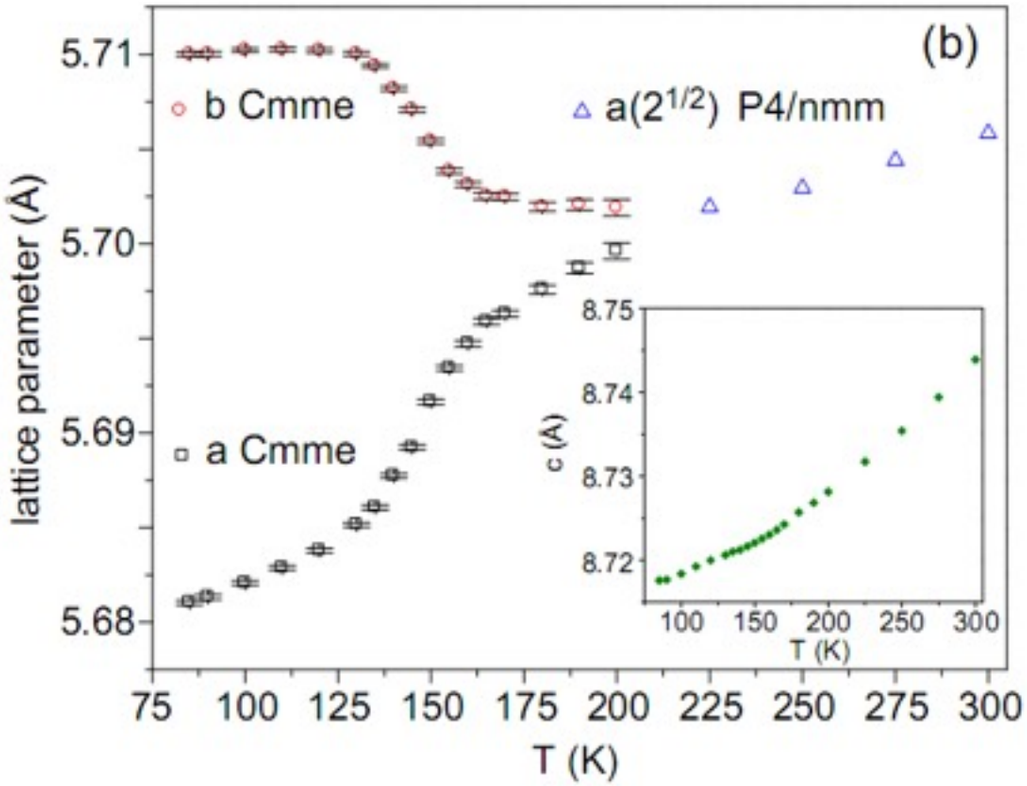
magnetism $\langle \Delta_y \rangle \neq \langle \Delta_x \rangle$

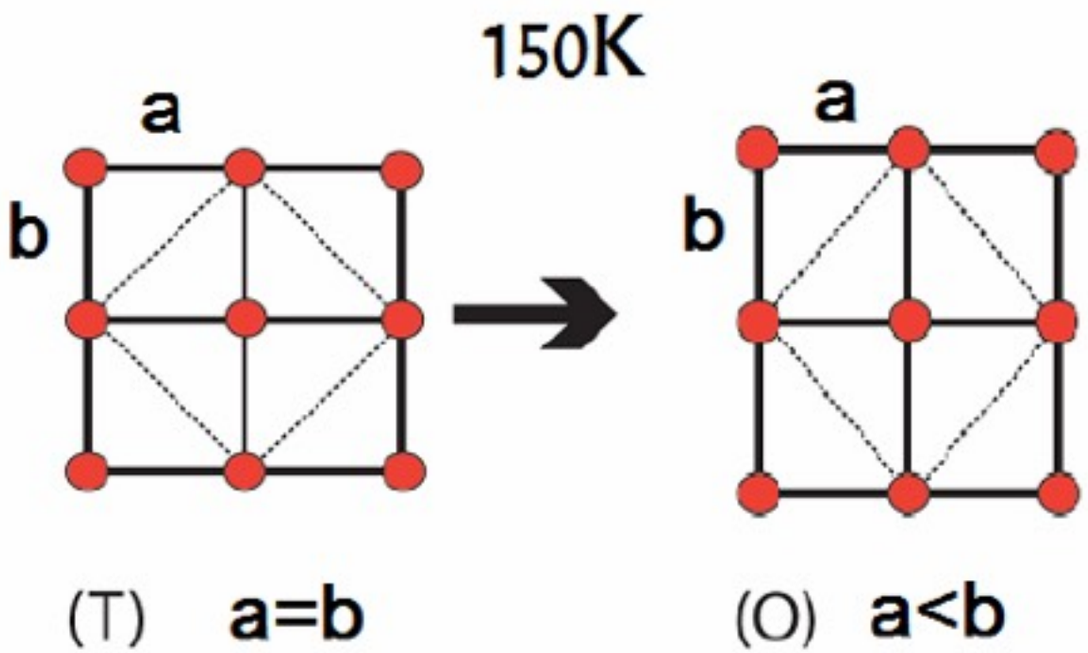

can this debate be settled?
orbitals
spins
d_{xz}, d_{yz}
$(\pi, 0), (0, \pi)$

yes

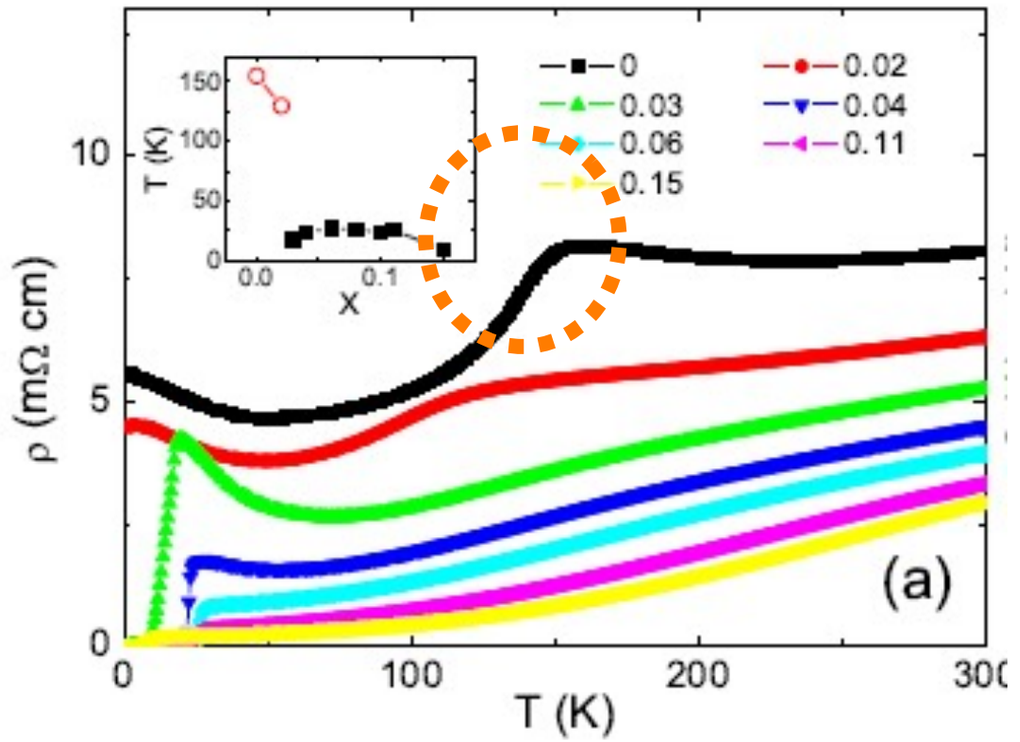
Experimental Puzzle 1?

- **Structural Phase Transition**



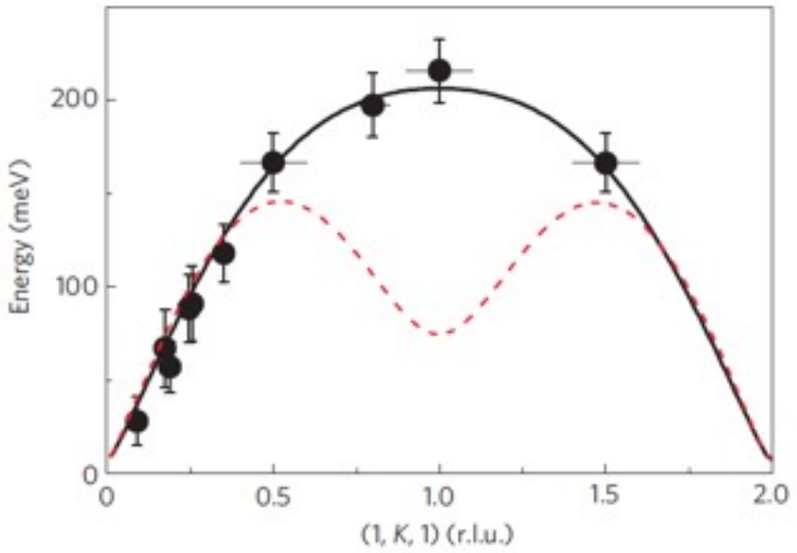


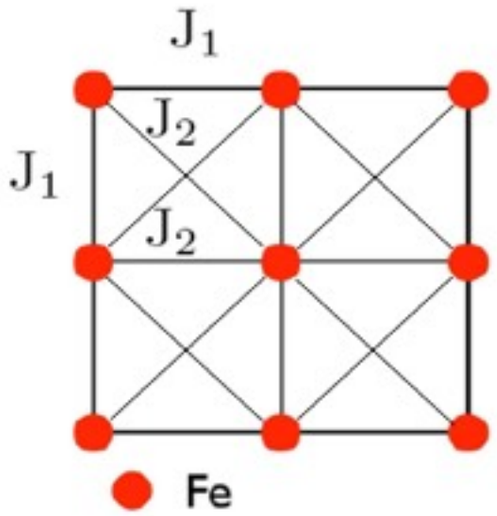
- **Resistivity Anomaly** $T_{\mathrm{RA}} = T_{\mathrm{SPT}}$



Experimental Puzzle 2?

- *Inelastic neutron scattering*





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

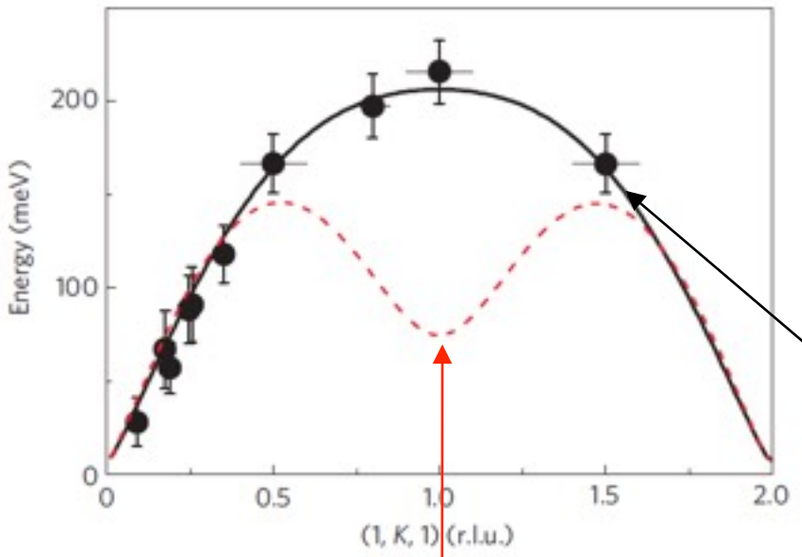
$$
\begin{aligned}
SJ_1^a &= 27\,\text{meV} \\
SJ_1^b &= 25\,\text{meV} \\
SJ_2 &= 36\,\text{meV}
\end{aligned}
$$

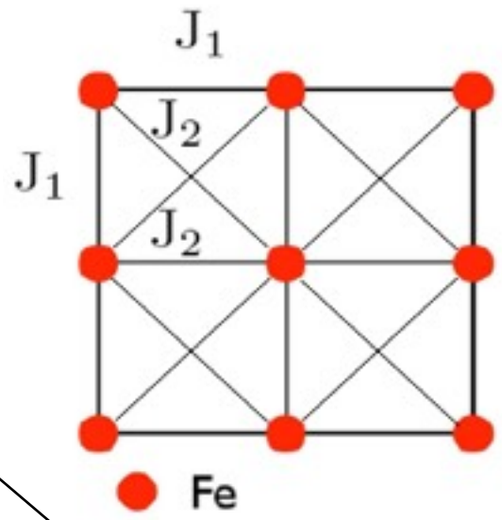
$$
\begin{aligned}
SJ_1^a &= 49.9 \pm 9.9\,\text{meV} \\
SJ_1^b &= -5.7 \pm 4.5\,\text{meV} \\
SJ_2 &= 18.9 \pm 3.4\,\text{meV}
\end{aligned}
$$

Why is the magnetism frustrated?

Experimental Puzzle 2?

- *Inelastic neutron scattering*





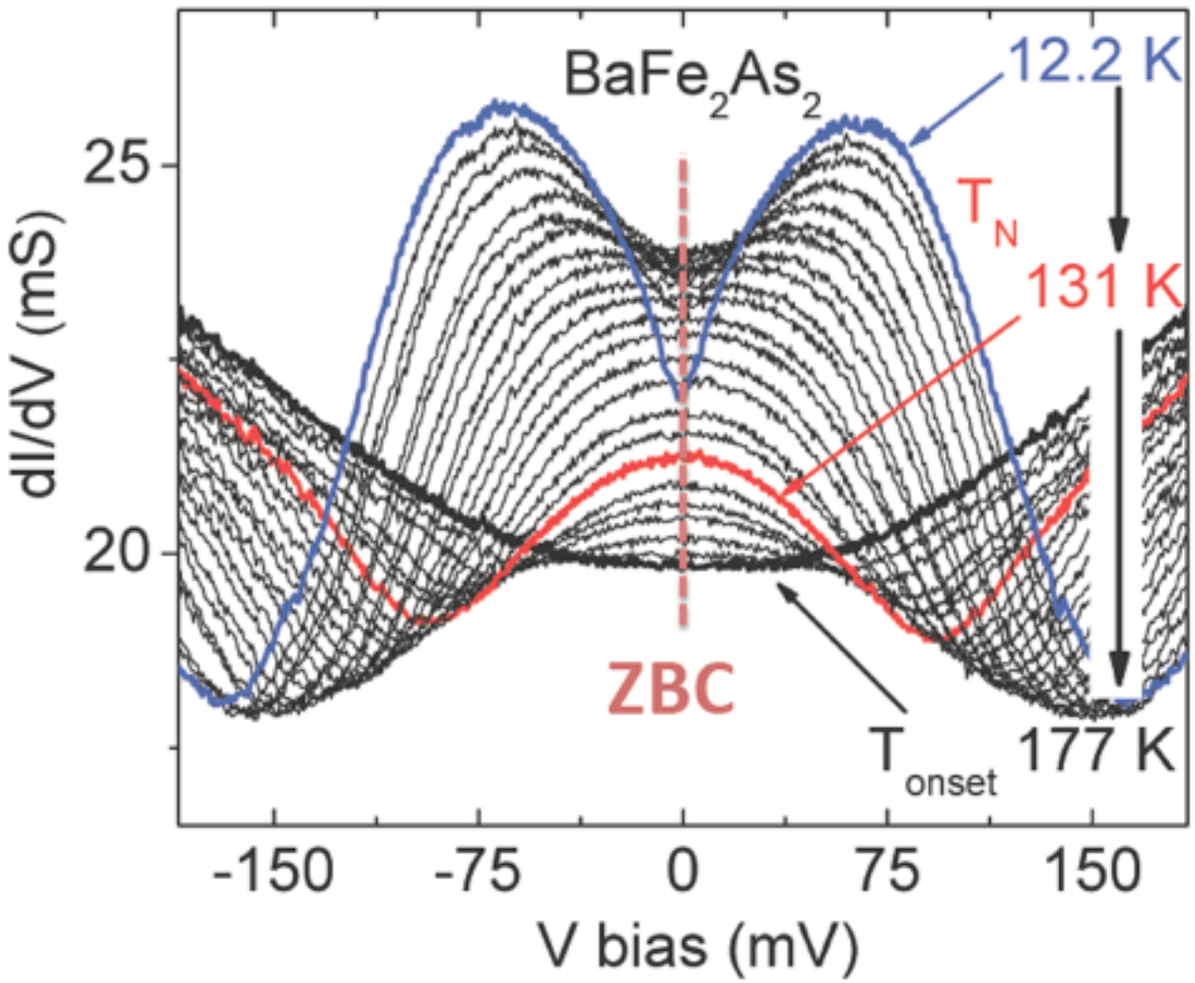
J. Zhao, *et al.* Nature Physics (2009)

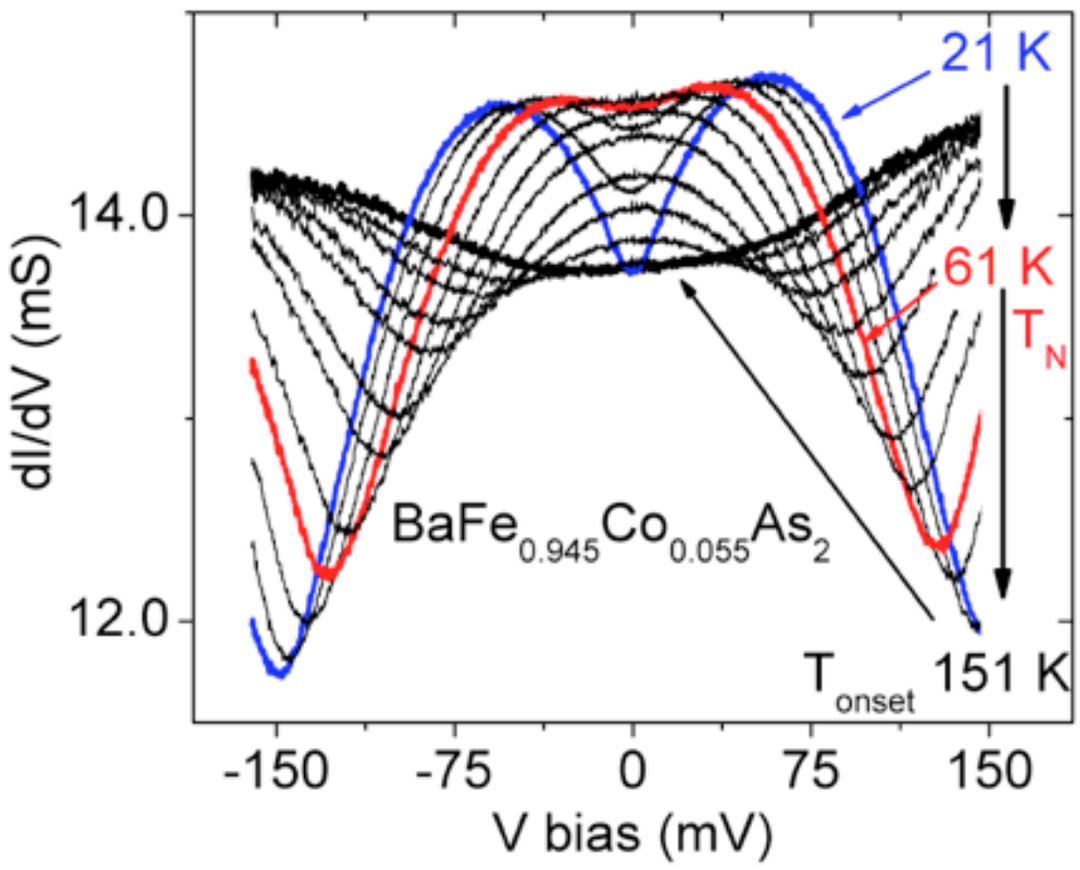
$$
\begin{aligned}
SJ_1^a &= 27\,\text{meV} \\
SJ_1^b &= 25\,\text{meV} \\
SJ_2 &= 36\,\text{meV}
\end{aligned}
$$

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

Why is the magnetism frustrated?

Experimental puzzle 3: What is the origin of the gap-like feature above the structural transition?

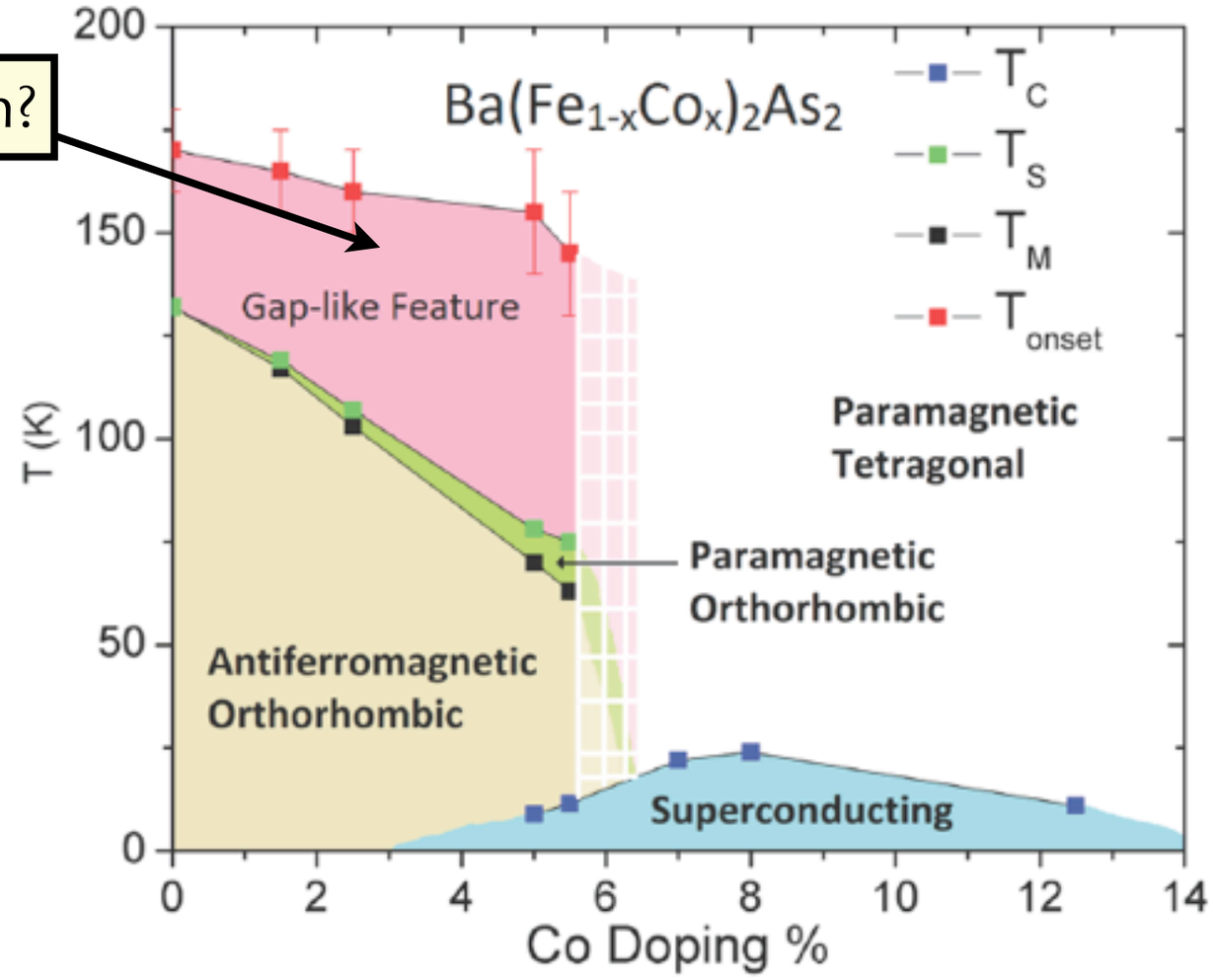




H. Ahram, L. Greene, ... (UIUC)

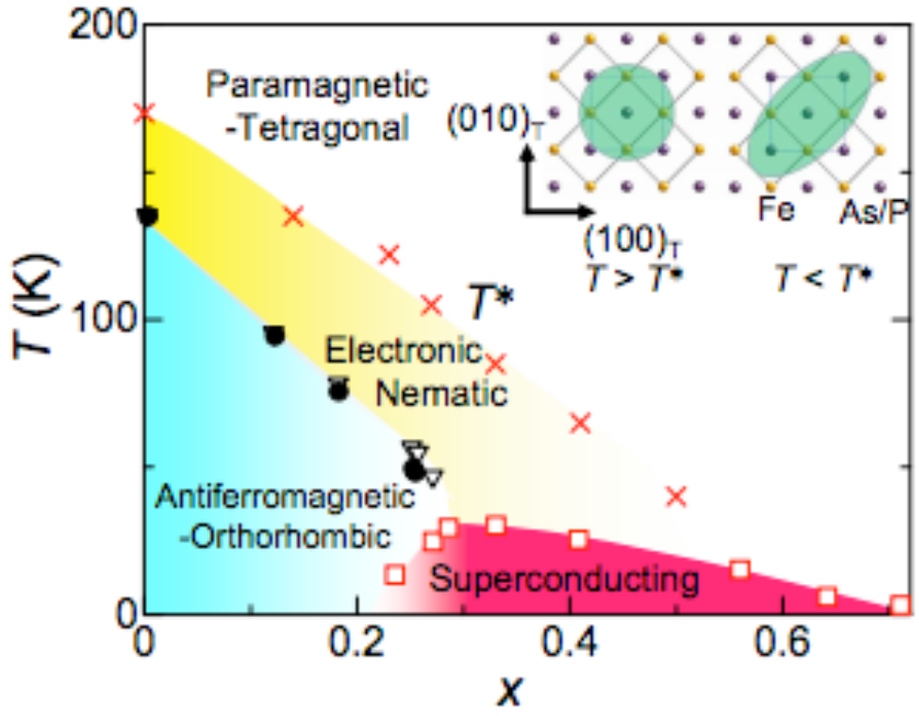
Crossover into a strongly correlated state on the underdoped side of the phase diagram

origin?



Greene, et al.

Nature 486, 382–385 (2012)



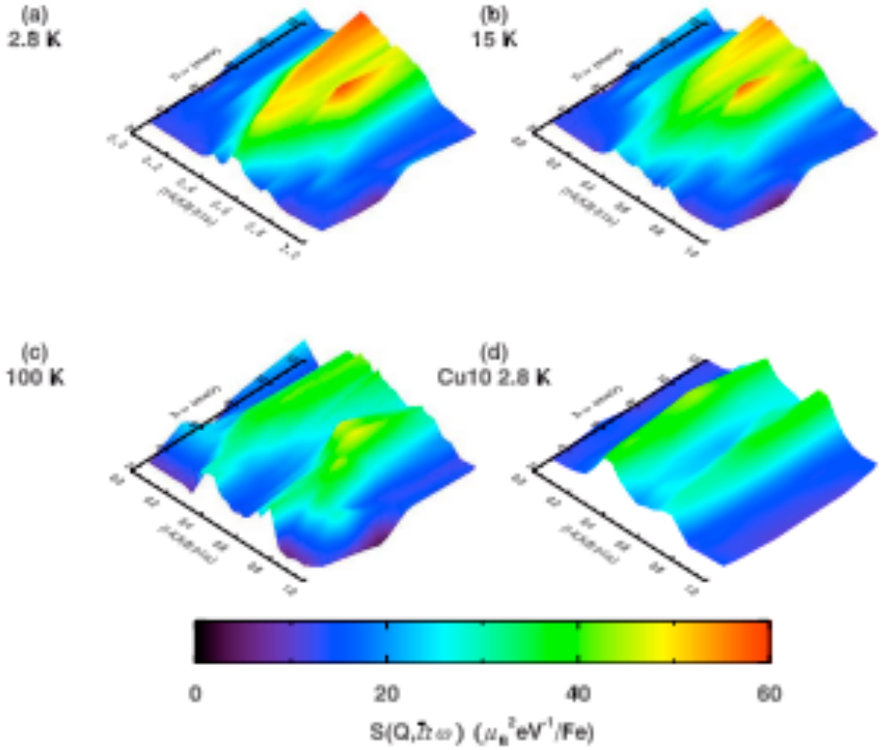
Matsuda, et al.

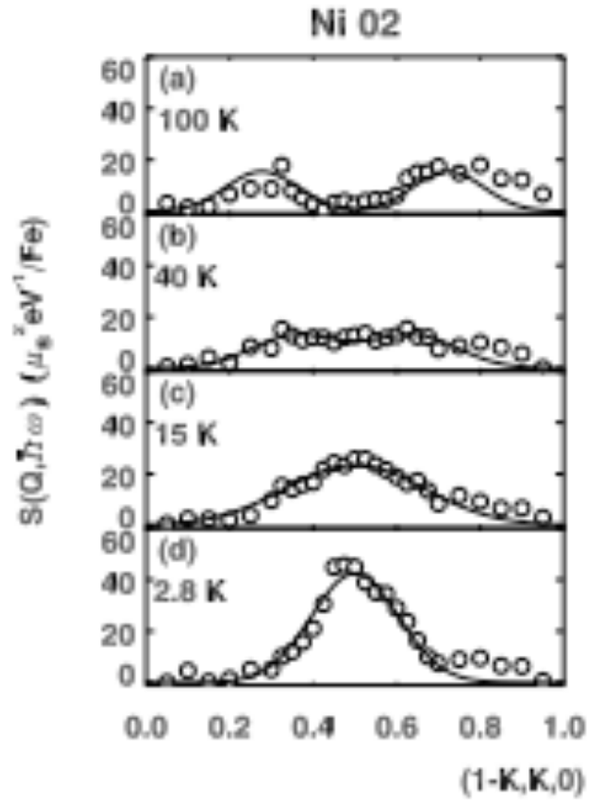
Experimental puzzle 4: What is the origin of the incommensurate-commensurate transition

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,*





incommensurate

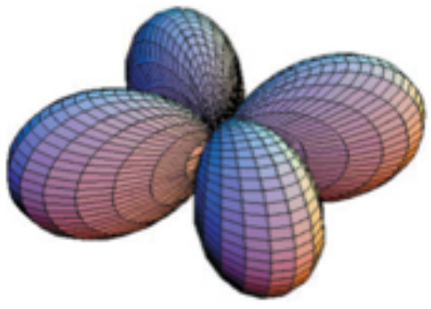
?

commensurate

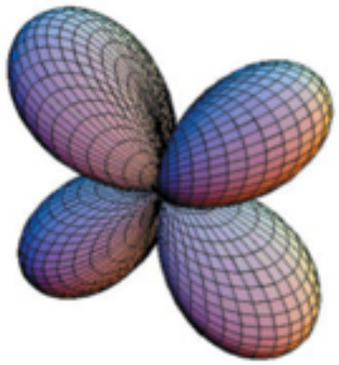
something besides spin degree of freedom

Orbital Ordering

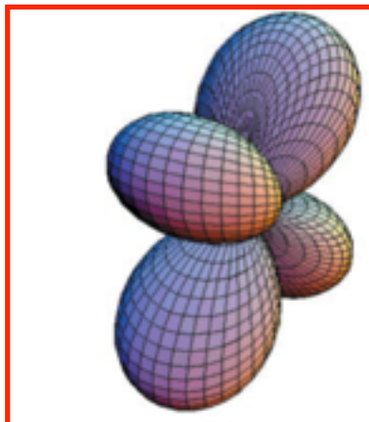
t_{2g}



xy



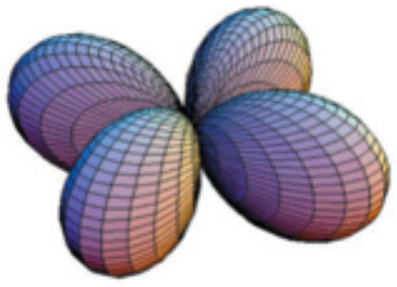
yz



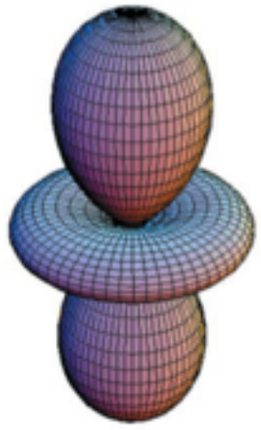
zx

only d_yz and d_xz break rotational symmetry in xy plane.

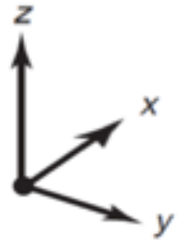
e_g



x^2-y^2



$3z^2-r^2$

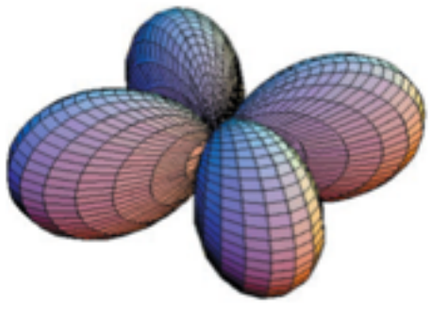


Orbital Ordering

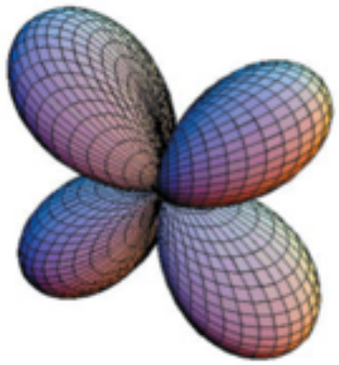
unequal occupancy of d_{xz} and d_{yz}

drive the structural transition, magnetism, ...

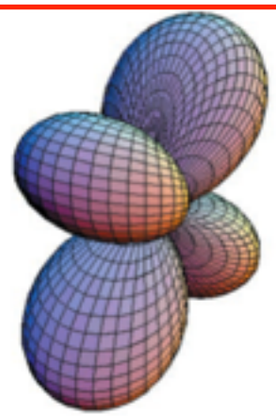
t_{2g}



xy

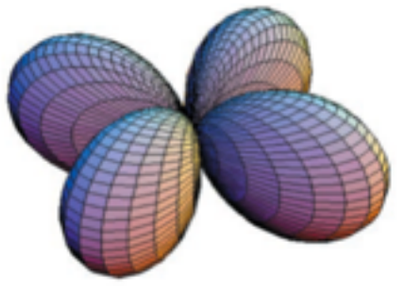


yz

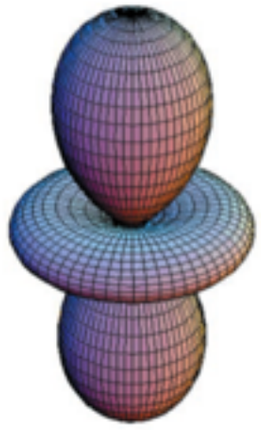


zx

e_g



x^2-y^2



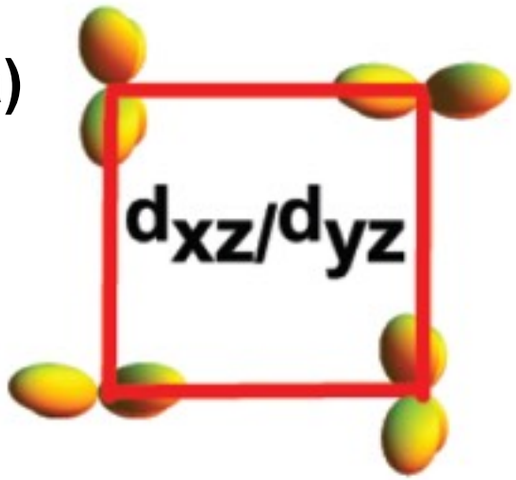
$3z^2$-r^2

only d_yz and d_xz break rotational symmetry in xy plane.

structural transition

$T > T_{SPT}$

a)



b)

$T < T_{SPT}$

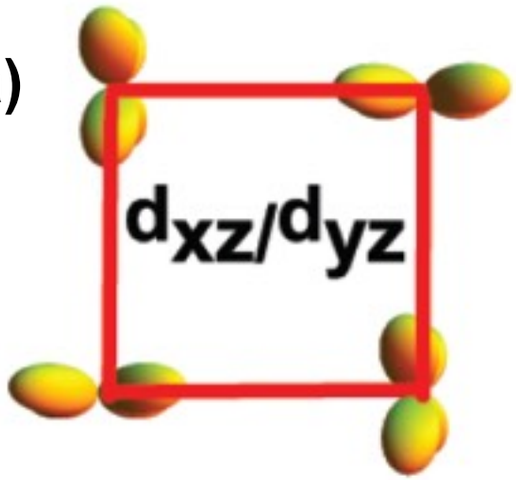
c)

Lv, Wu, PP, 2009

structural transition

$T > T_{SPT}$

a)



b)

$T < T_{SPT}$

c)

Lv, Wu, PP, 2009

Coulomb Repulsion:

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

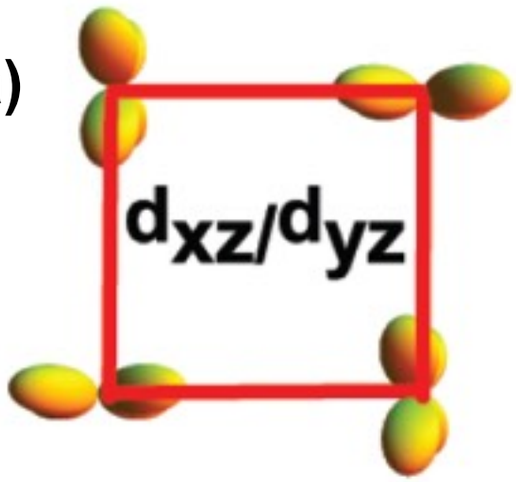
Energy Difference:

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

structural transition

$T > T_{SPT}$

a)



b)

$T < T_{SPT}$

c)

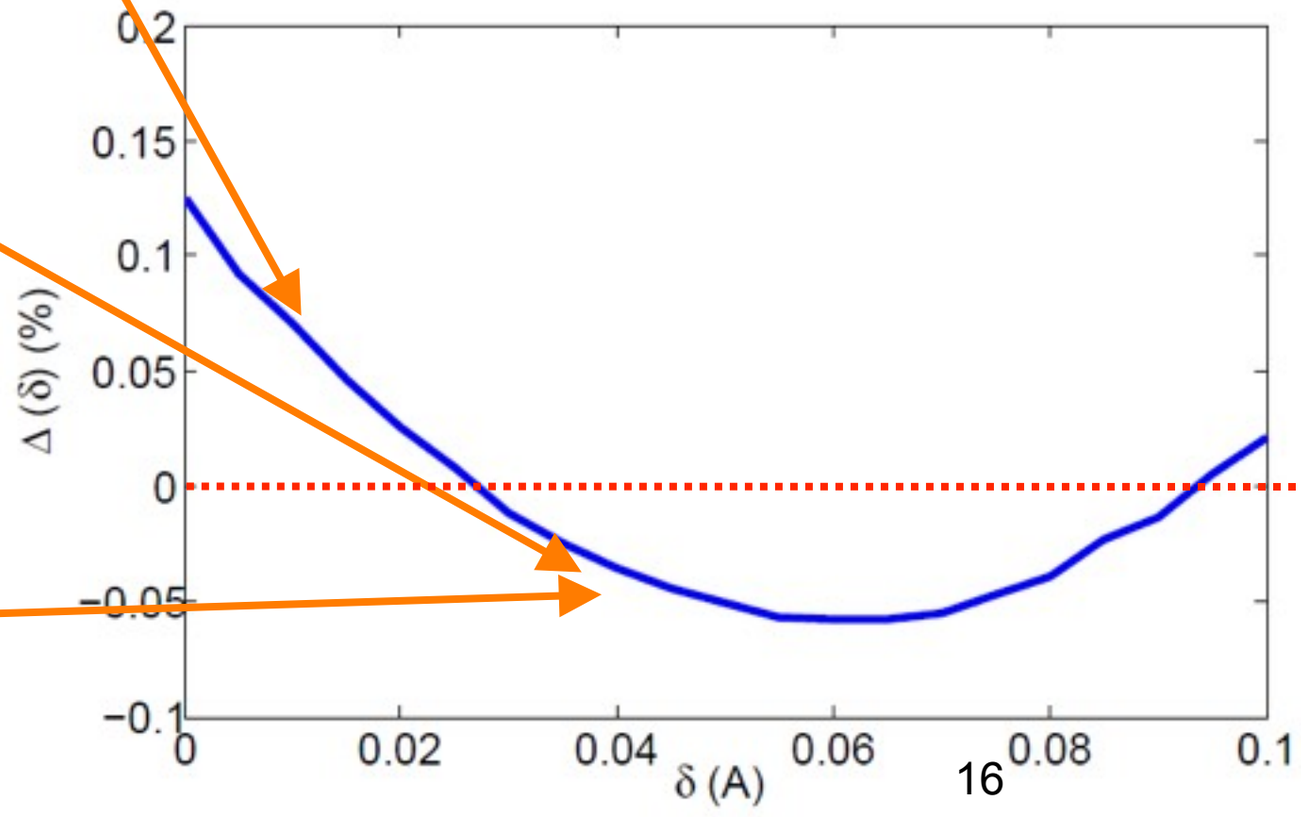
Lv, Wu, PP, 2009

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:

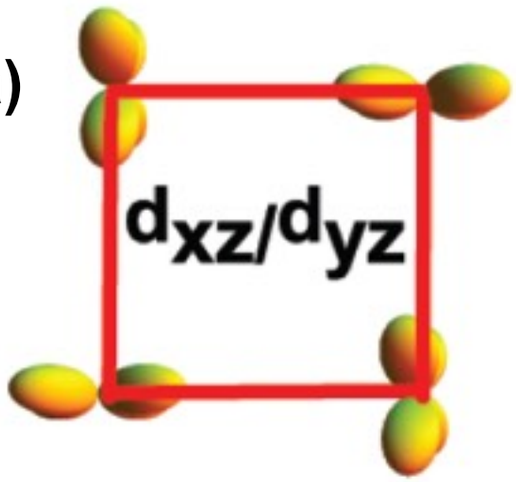
$$\Delta(\delta) = \frac{U_b(\delta) - U_a}{U_a}$$



structural transition

$T > T_{SPT}$

a)



b)

$T < T_{SPT}$

c)

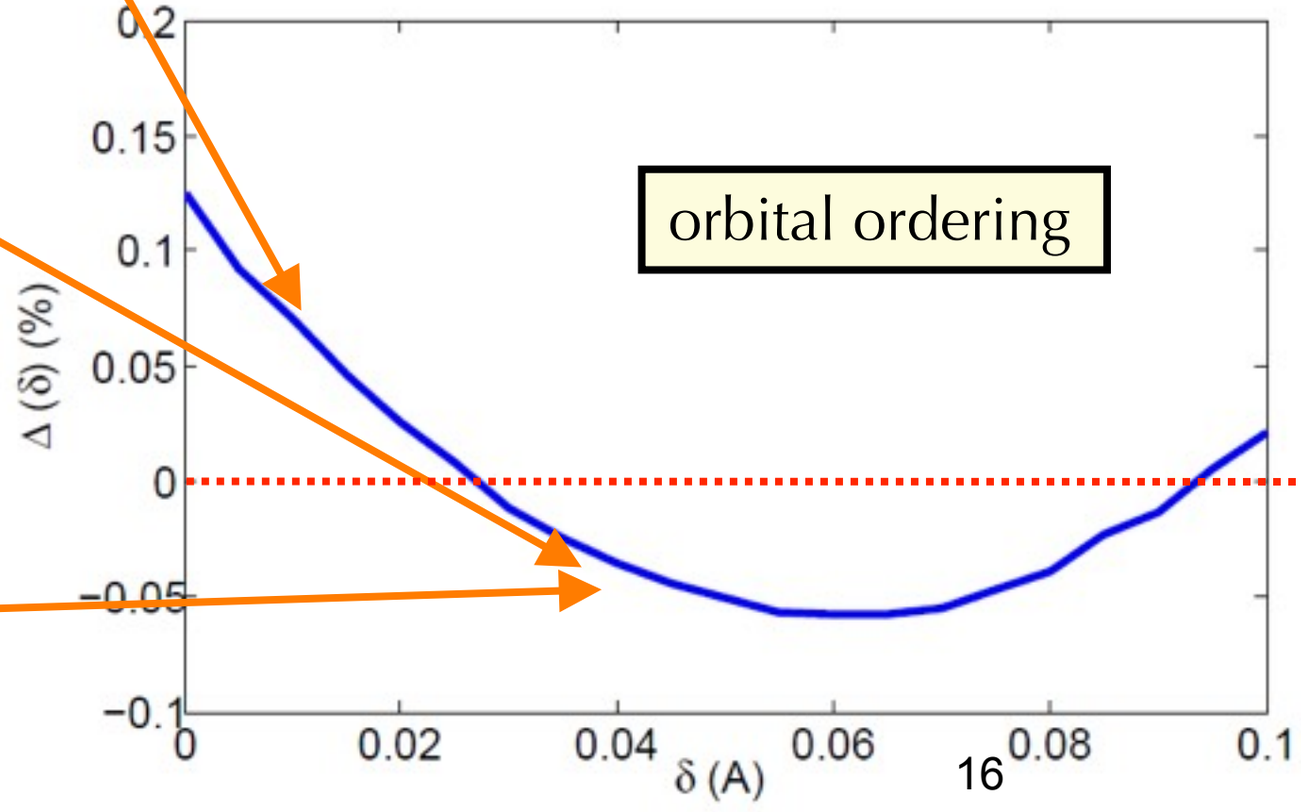
Lv, Wu, PP, 2009

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

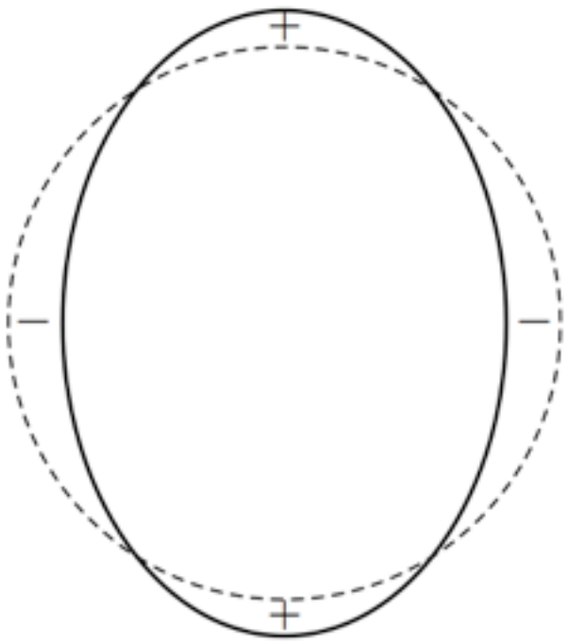
$$H_{\mathrm{SPT}} = -J_{\mathrm{SPT}} \sum_{\langle i,j \rangle} M_i M_j$$

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

structural transition=nematic?

structural transition=nematic?

electron nematic

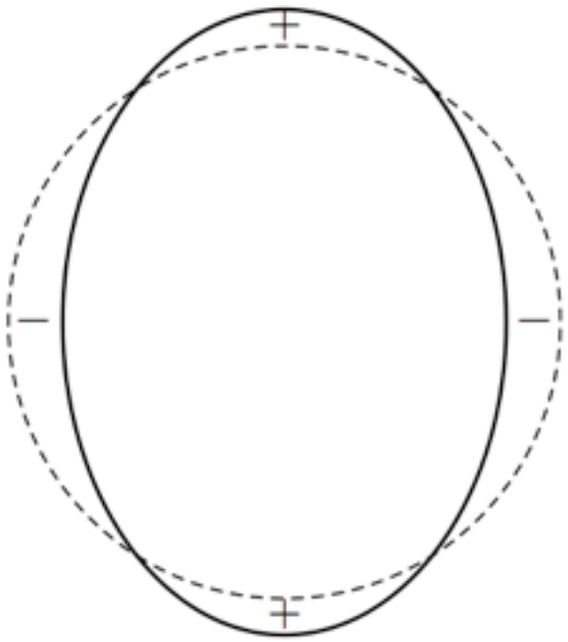


continuous symmetry breaking

goldstone boson

structural transition=nematic?

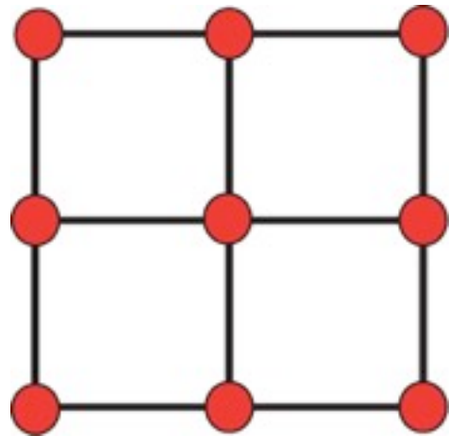
electron nematic



continuous symmetry breaking

goldstone boson

pnictides



C_4

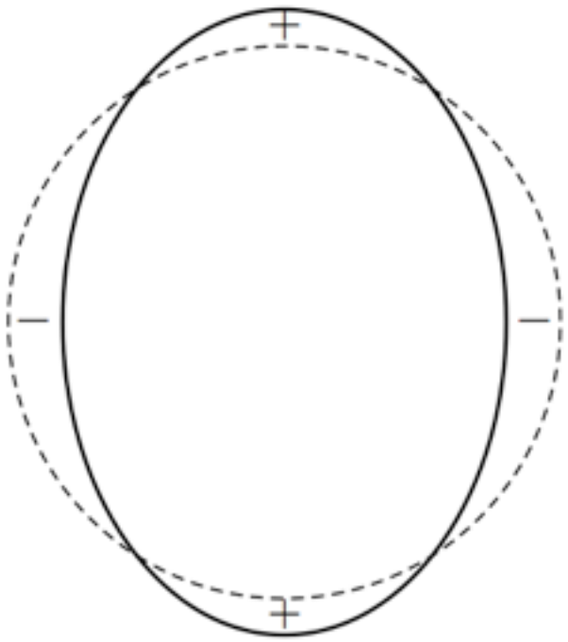
T_s

C_2

no goldstone boson

structural transition=nematic?

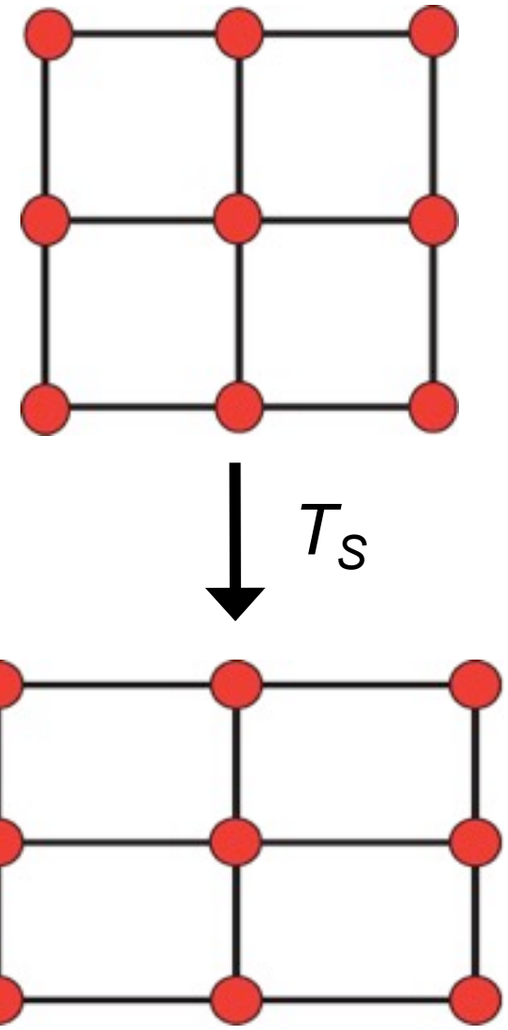
electron nematic



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

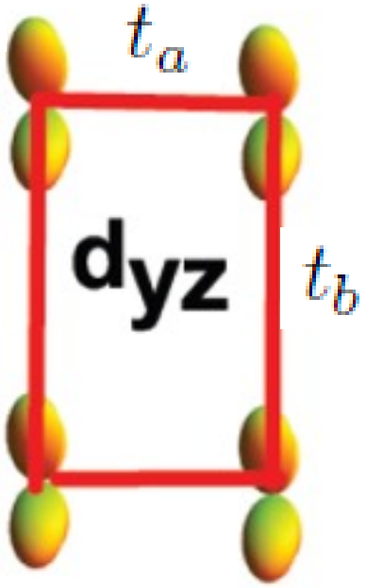
$T > T_{SPT}$

a)

spin disordered

$T < T_{SPT}$

b)



SPT-induced Collinear AF

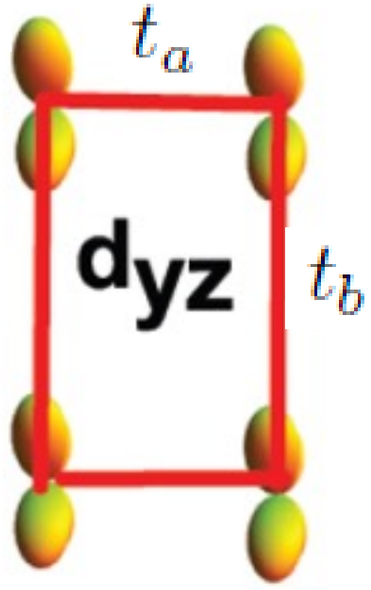
$T > T_{SPT}$

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

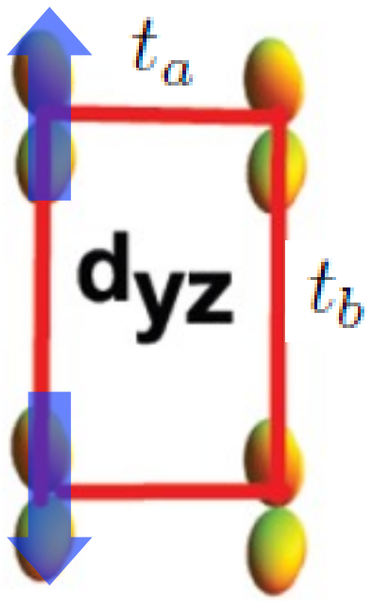
$T > T_{SPT}$

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

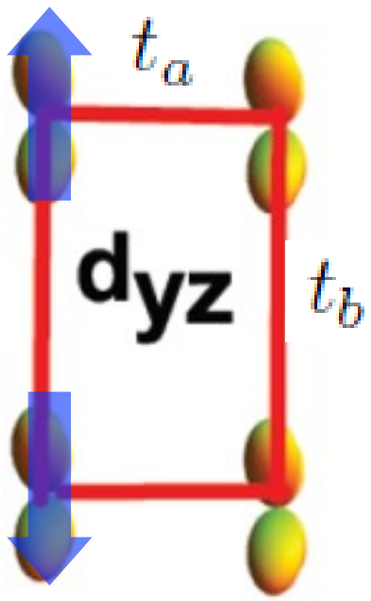
$T > T_{SPT}$

a)

spin disordered

$T < T_{SPT}$

b)

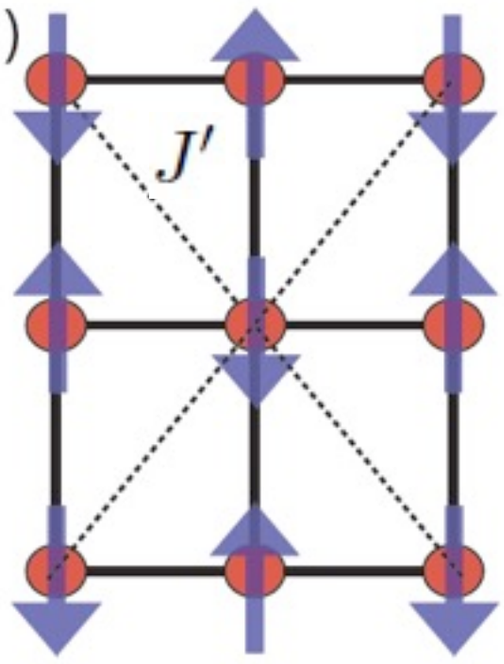


$$t_b > t_a$$

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

$$J_b > J_a$$

AF1)



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

SPT-induced Collinear AF

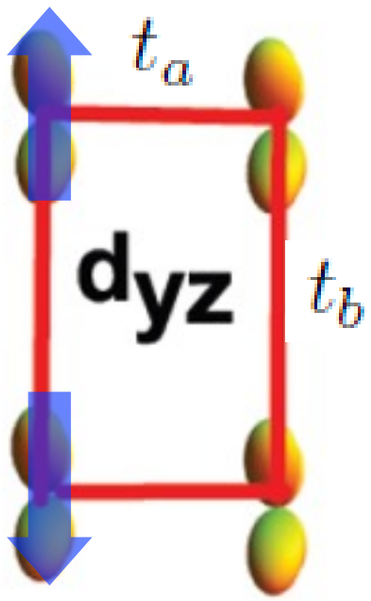
$T > T_{SPT}$

a)

spin disordered

$T < T_{SPT}$

b)

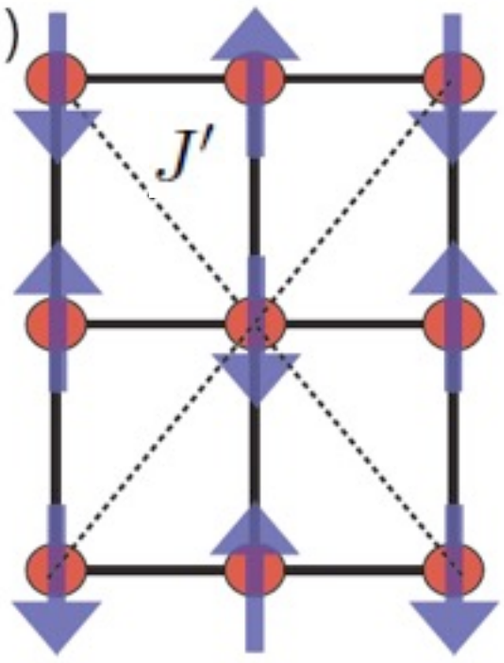


$$t_b > t_a$$

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

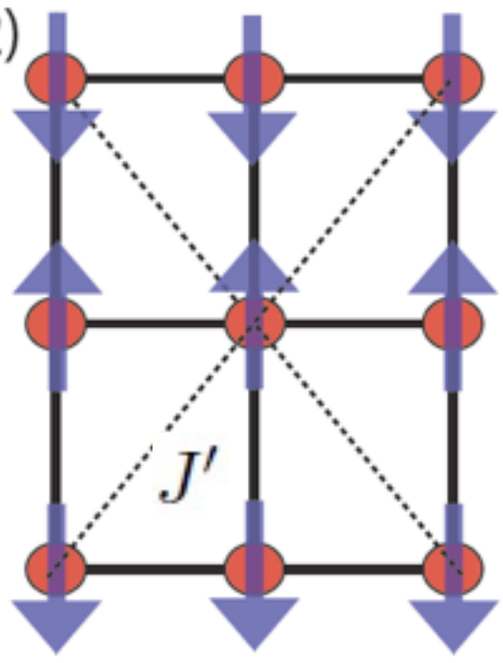
$$J_b > J_a$$

AF1)



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

AF2)



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

SPT-induced Collinear AF

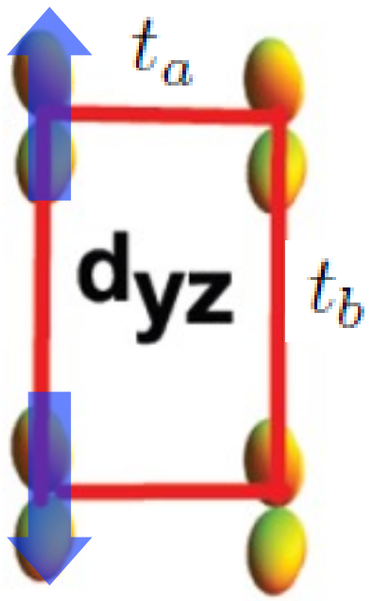
$T > T_{SPT}$

a)

spin disordered

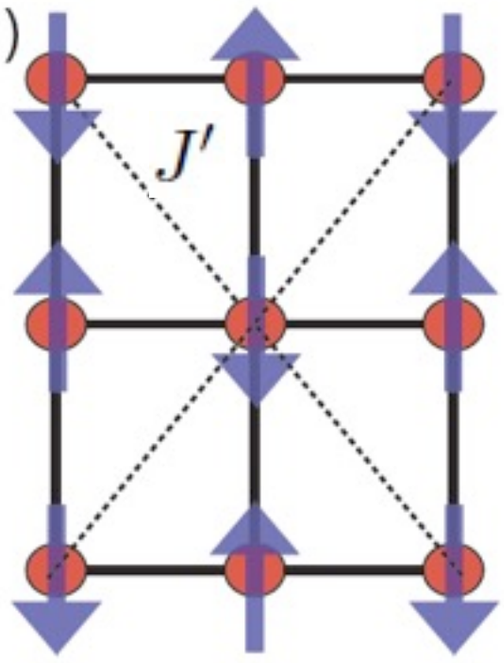
$T < T_{SPT}$

b)



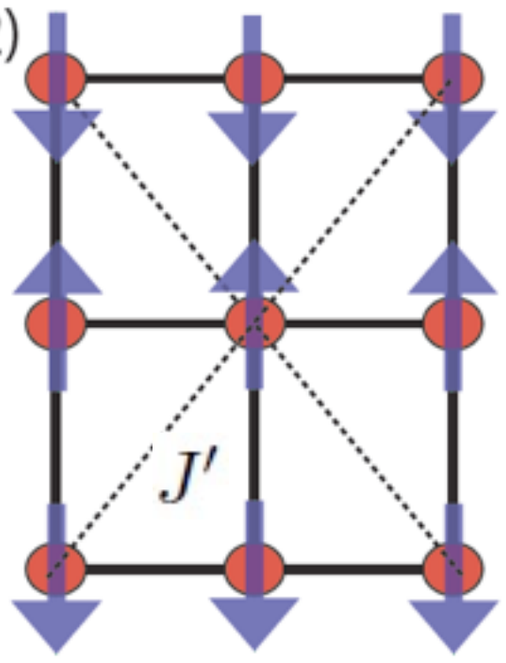
$$t_b > t_a$$
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$

AF1)



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

AF2)



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

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

SPT-induced Collinear AF

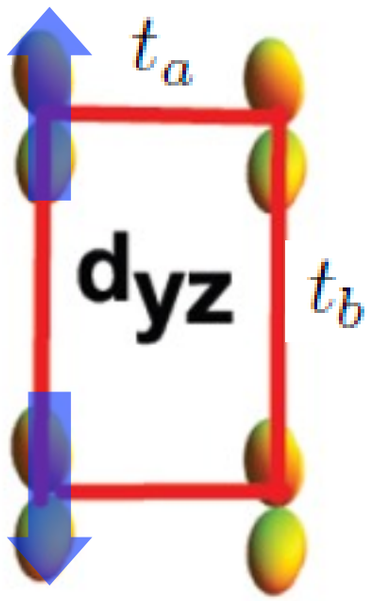
$T > T_{SPT}$

a)

spin disordered

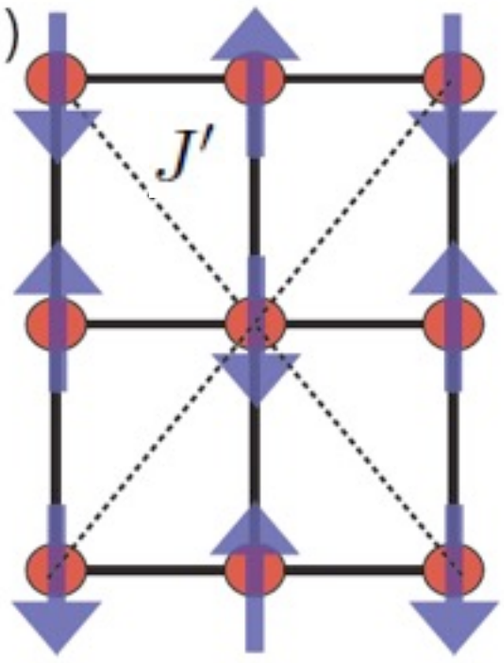
$T < T_{SPT}$

b)



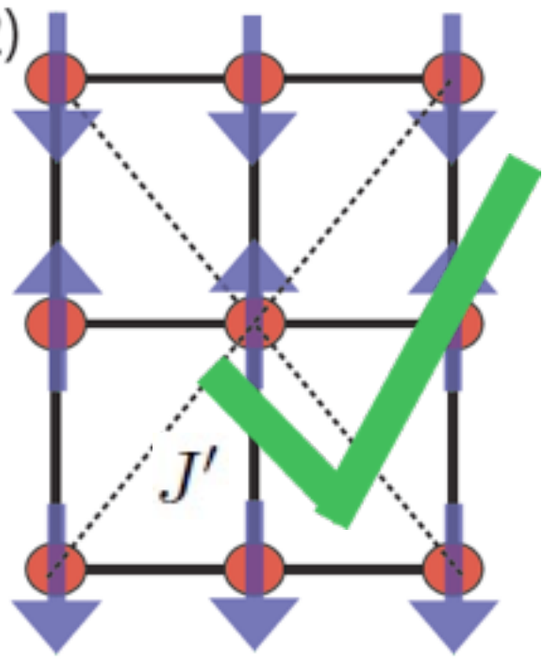
$$t_b > t_a$$
$$J \sim \frac{t^2}{U}$$
$$J_b > J_a$$

AF1)



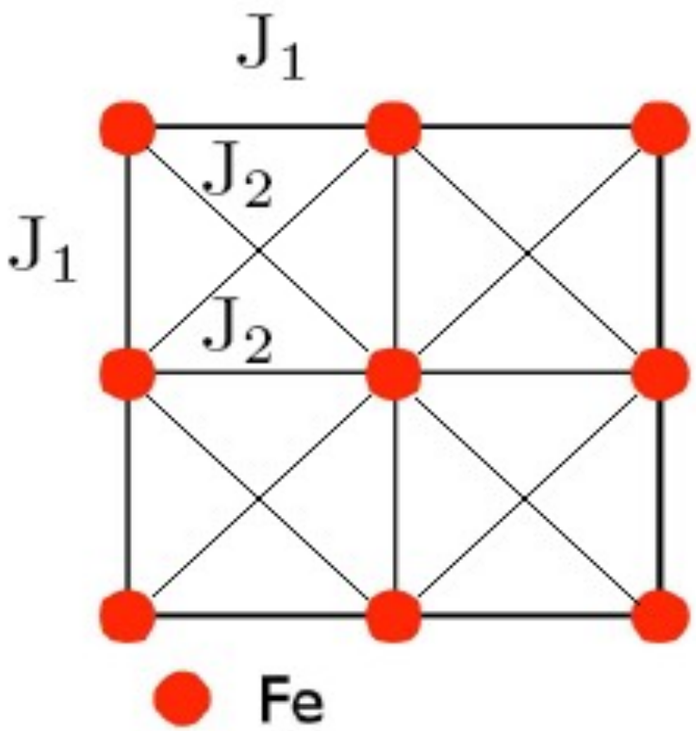
$$E_1 = -2J_a + 4J'$$

AF2)

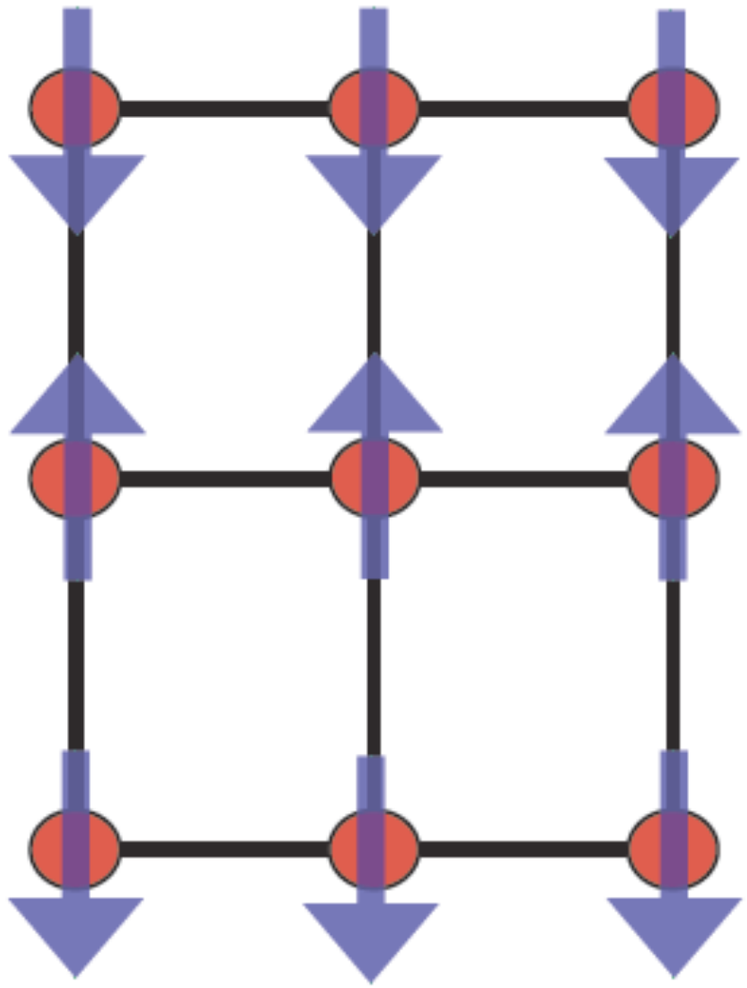


$$E_2 = +2J_a - 4J'$$

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



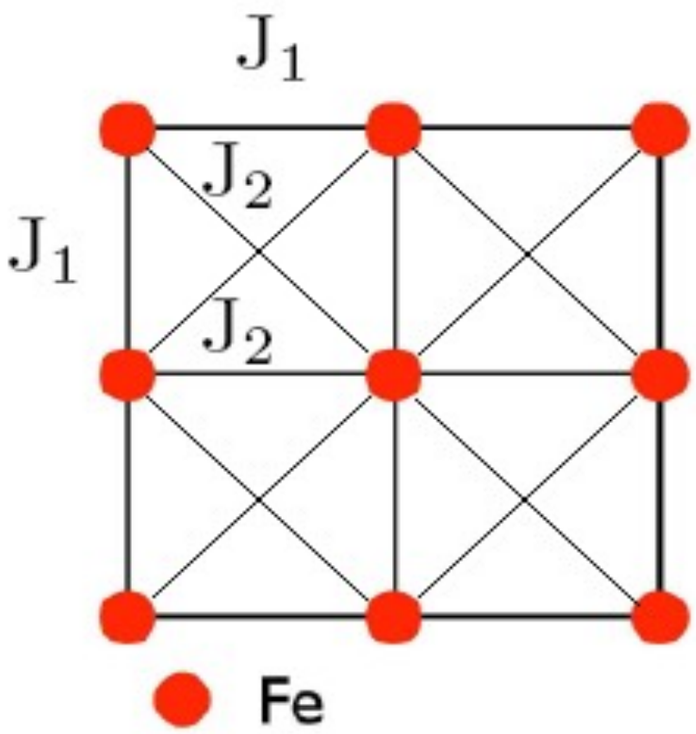
$J_2 > J_1/2$



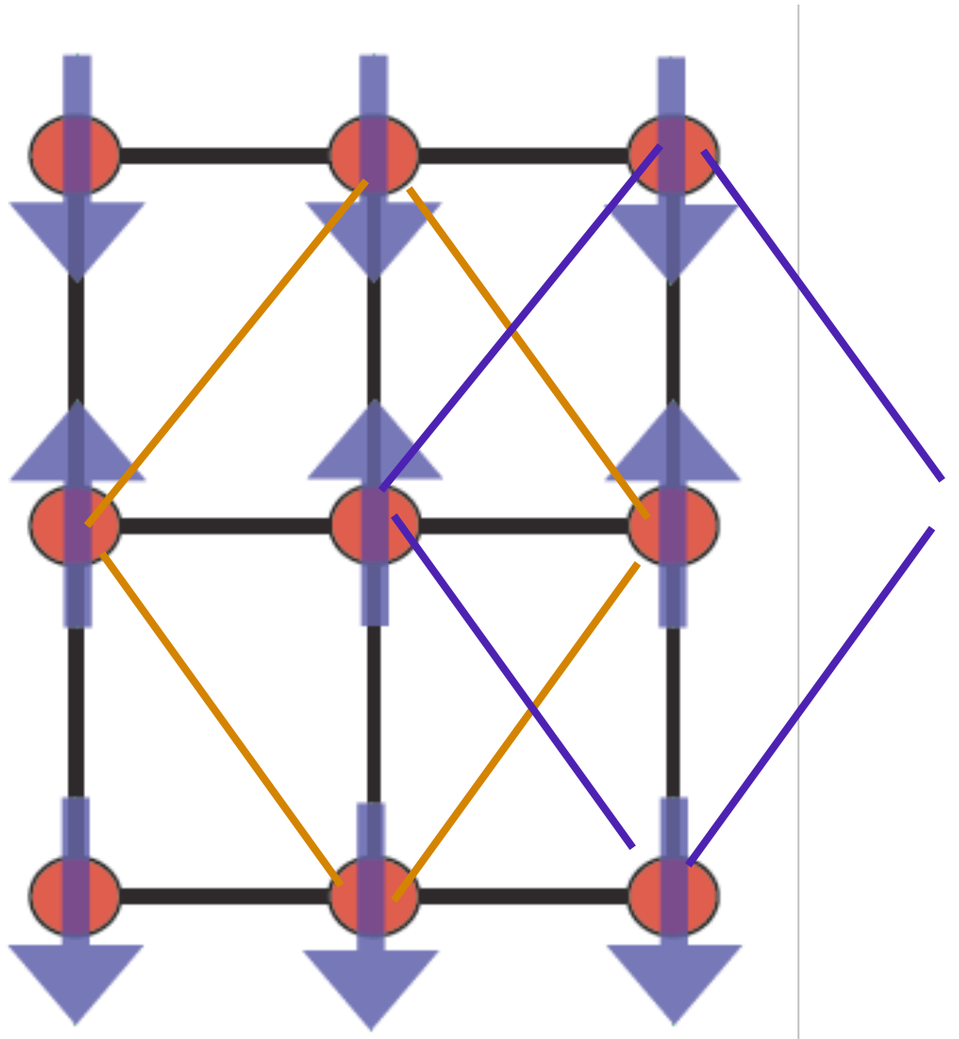
`nematic'

$\langle \varphi \rangle \neq 0$

$\langle n_1 \rangle = \langle n_2 \rangle = 0$



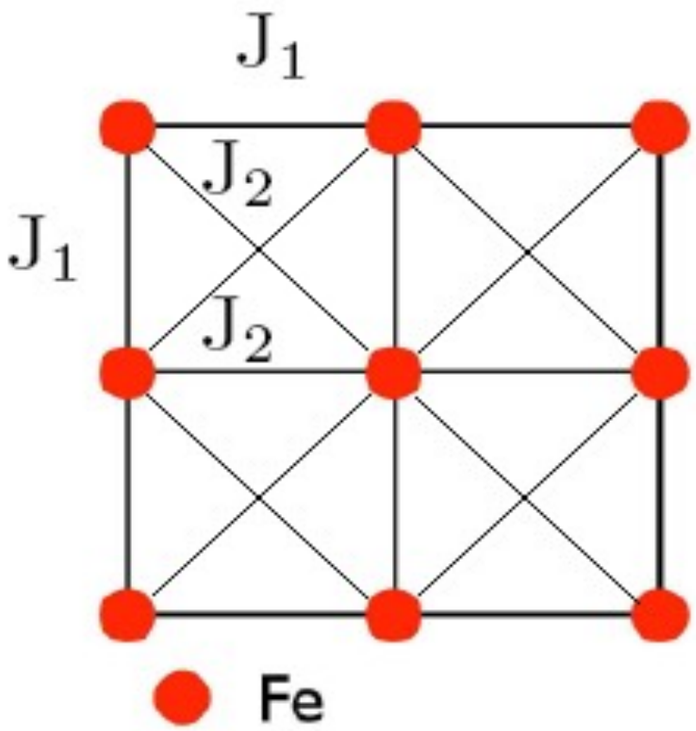
$J_2 > J_1/2$



`nematic' $\langle \varphi \rangle \neq 0$

$\langle n_1 \rangle = \langle n_2 \rangle = 0$

Two interpenetrating AF sublattices



$$J_2 > J_1/2$$

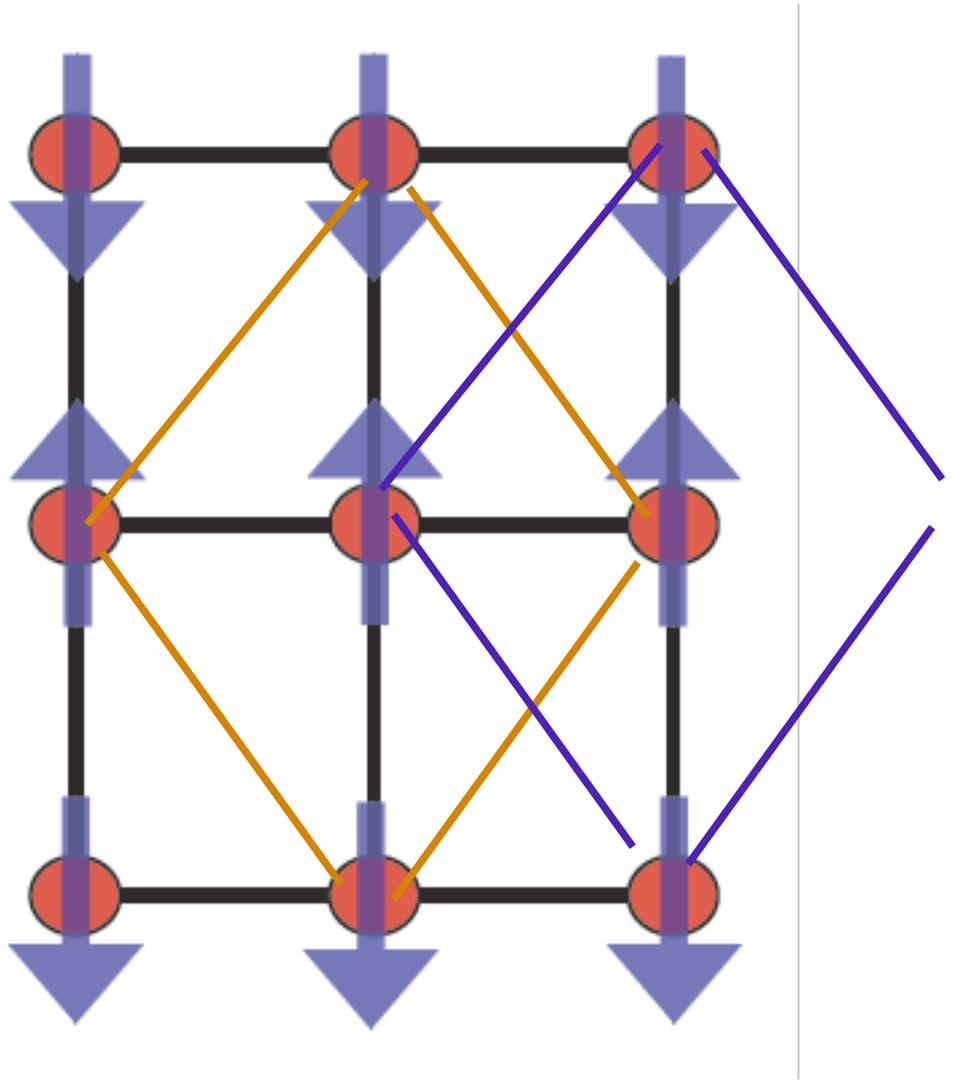
$$\varphi = \hat{n}_1 \cdot \hat{n}_2$$

$$\langle \varphi \rangle \neq 0$$

$$\langle n_1 \rangle = \langle n_2 \rangle \neq 0$$

`nematic' $\langle \varphi \rangle \neq 0$

$$\langle n_1 \rangle = \langle n_2 \rangle = 0$$



Two interpenetrating AF sublattices

SPT-induced magnetism

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

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

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

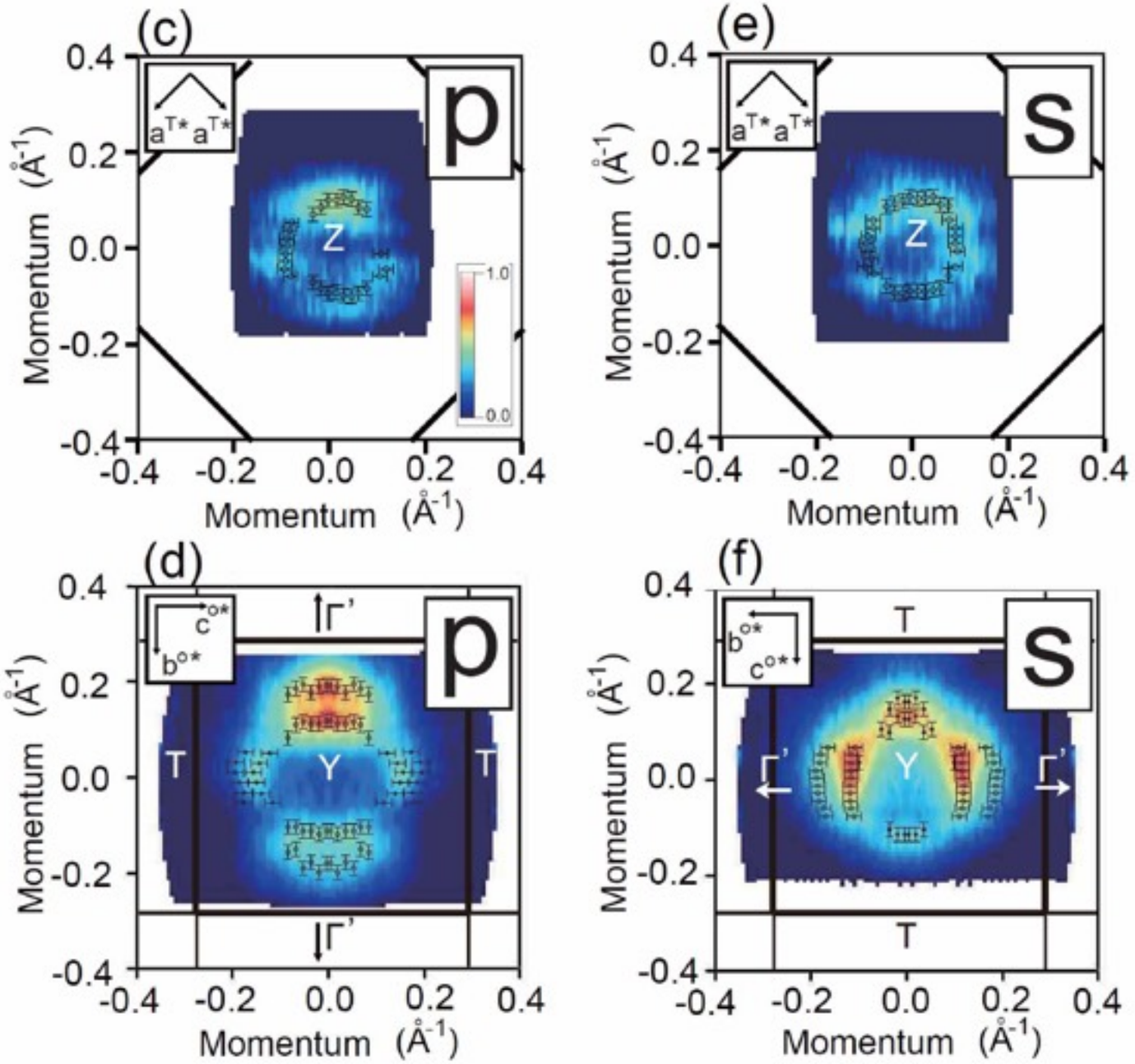
122 Fe-Fe is shorter: J_{1b} is enhanced

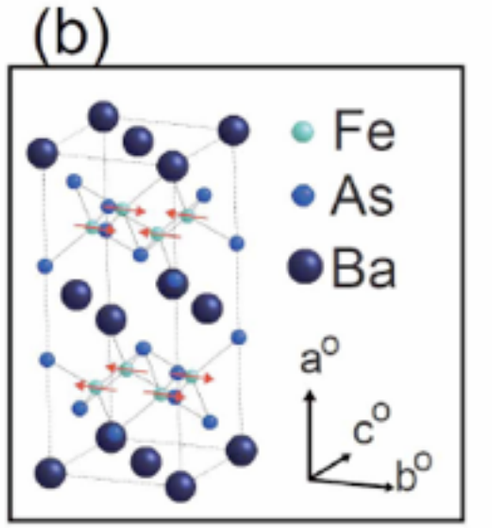
Orbital-polarized Fermi surface in antiferromagnetic state of

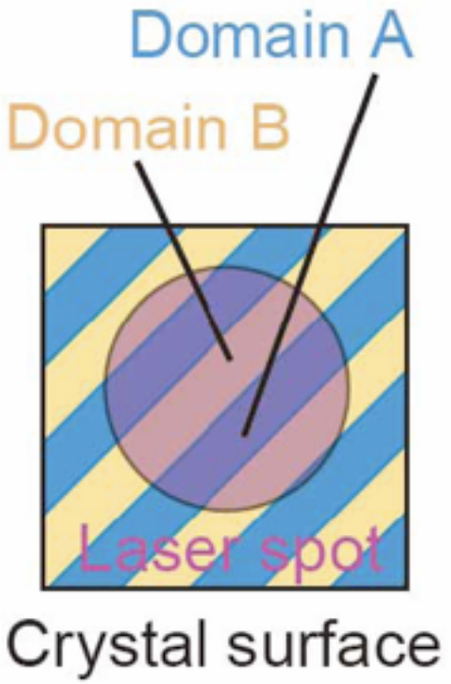
$BaFe_2As_2$

Shimojima, et al.
arXiv:0904.1632

- **Polarized ARPES**





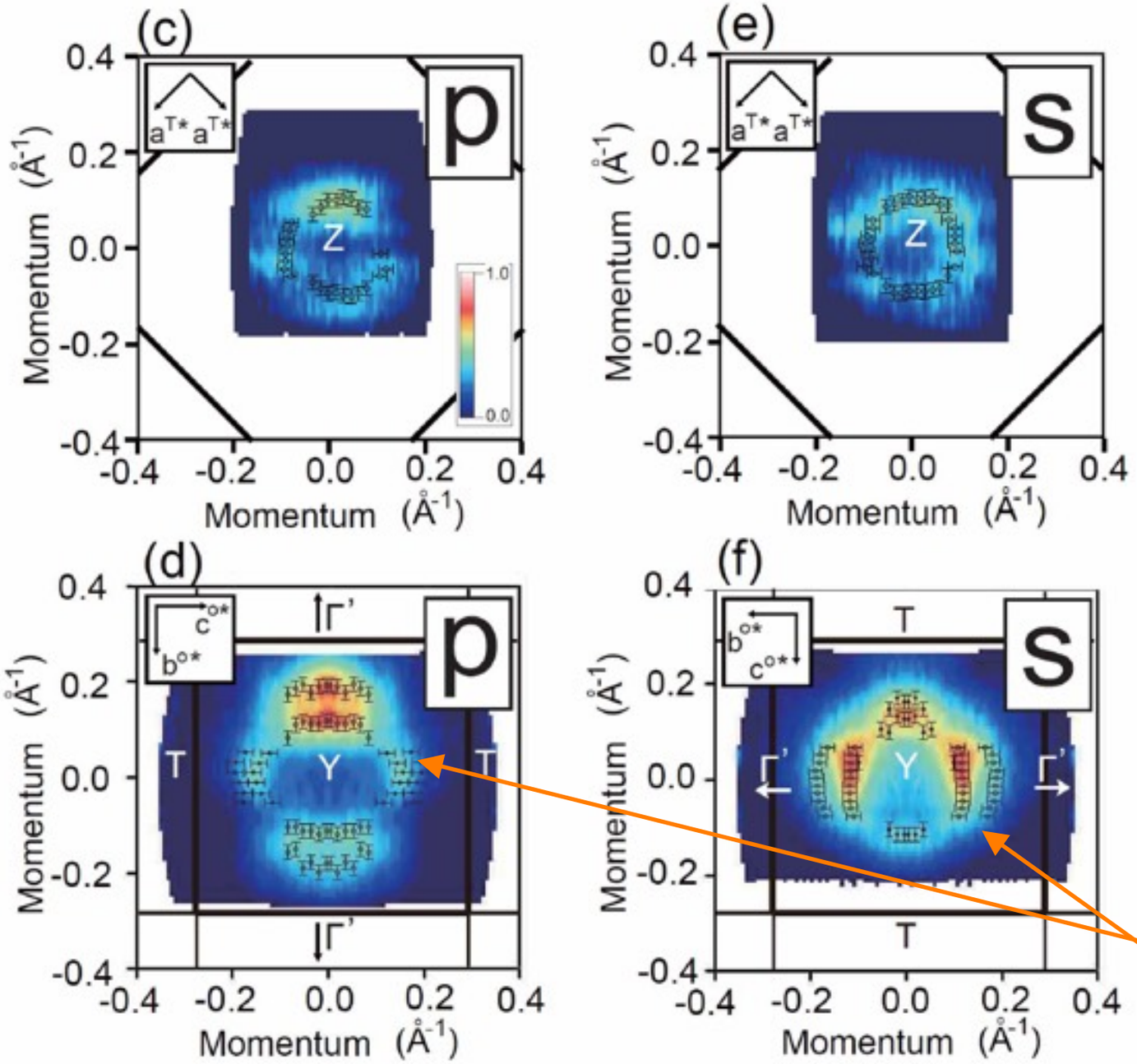


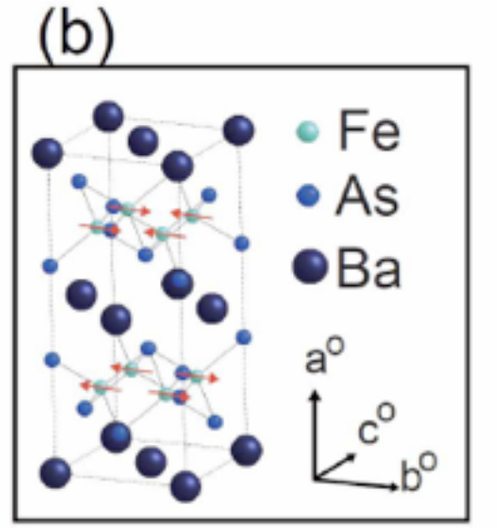
Orbital-polarized Fermi surface in antiferromagnetic state of

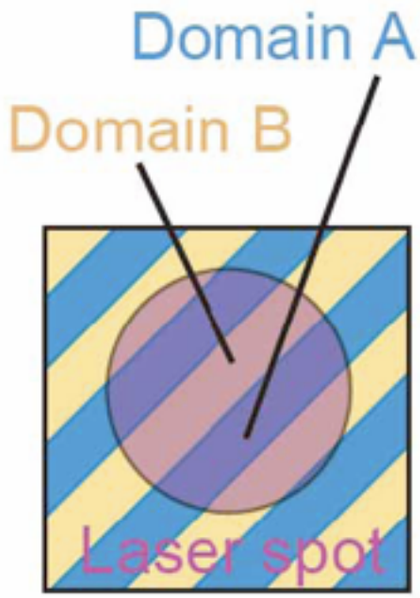
$BaFe_2As_2$

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[6], 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*

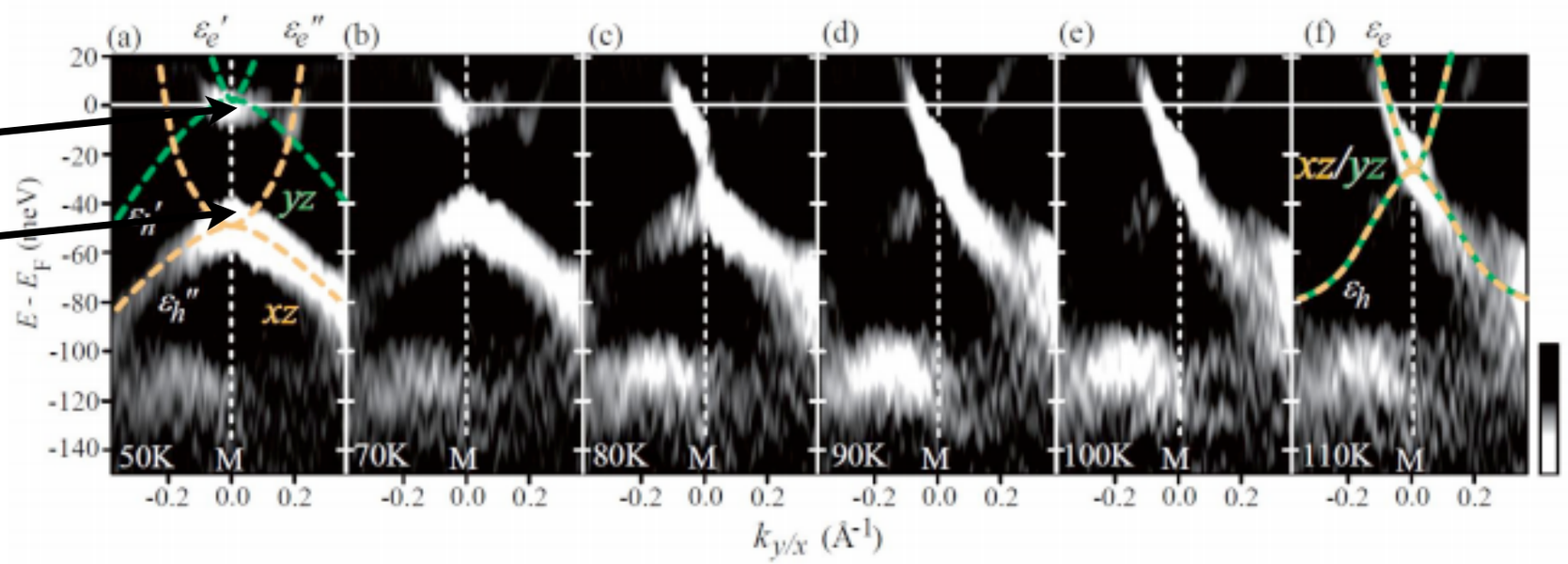
[4]*KEK, Photon Factory, Tsukuba, Ibaraki 305-0801, Japan.*

[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.*

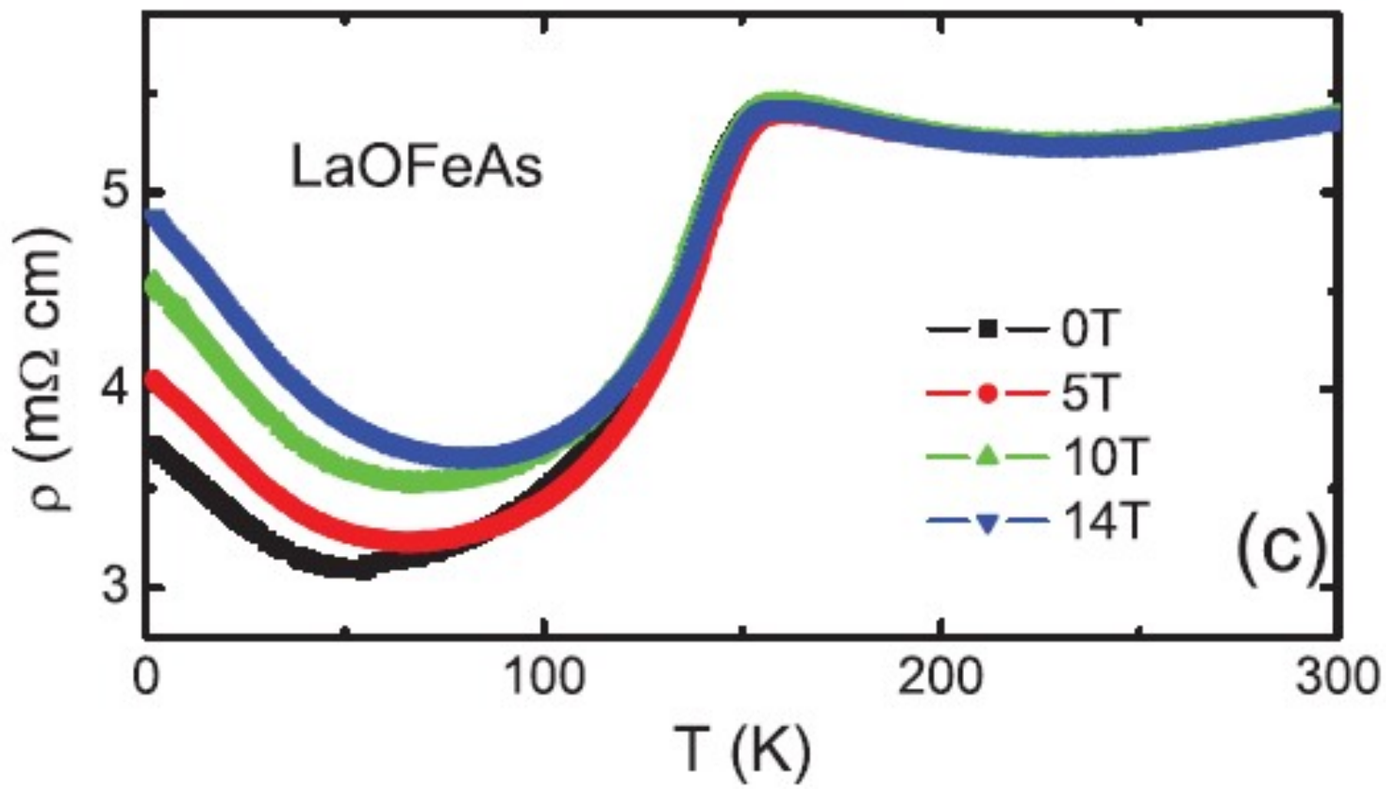
50 meV



as in Na111 and Ba122

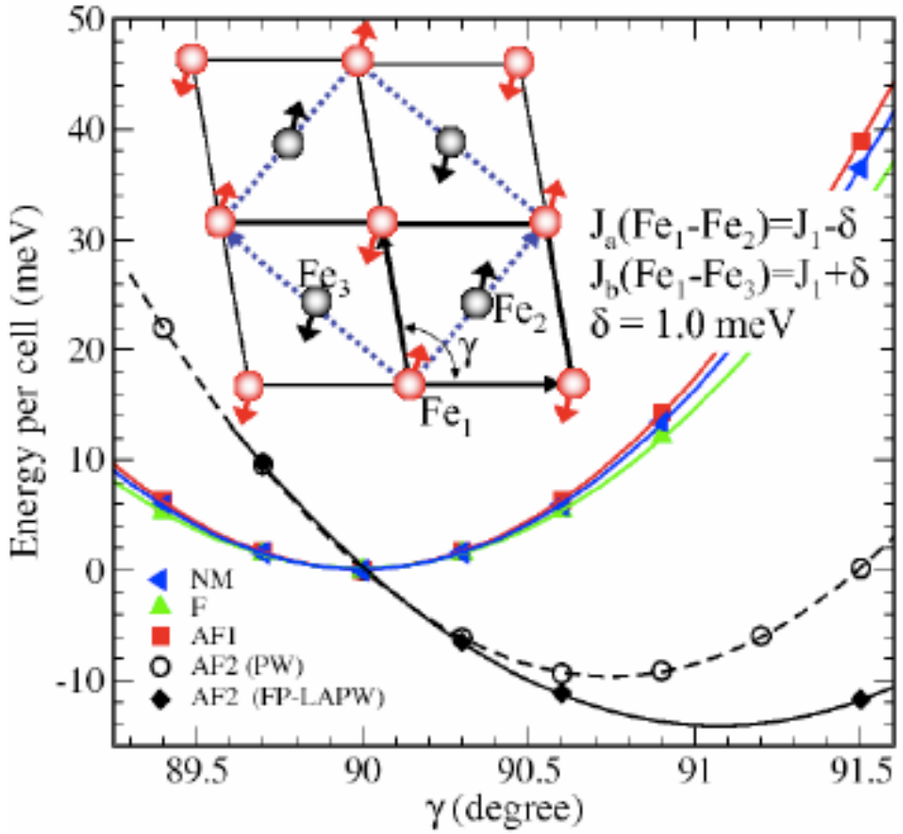
Possible mechanism for SPT?

SPT is insensitive to external magnetic field

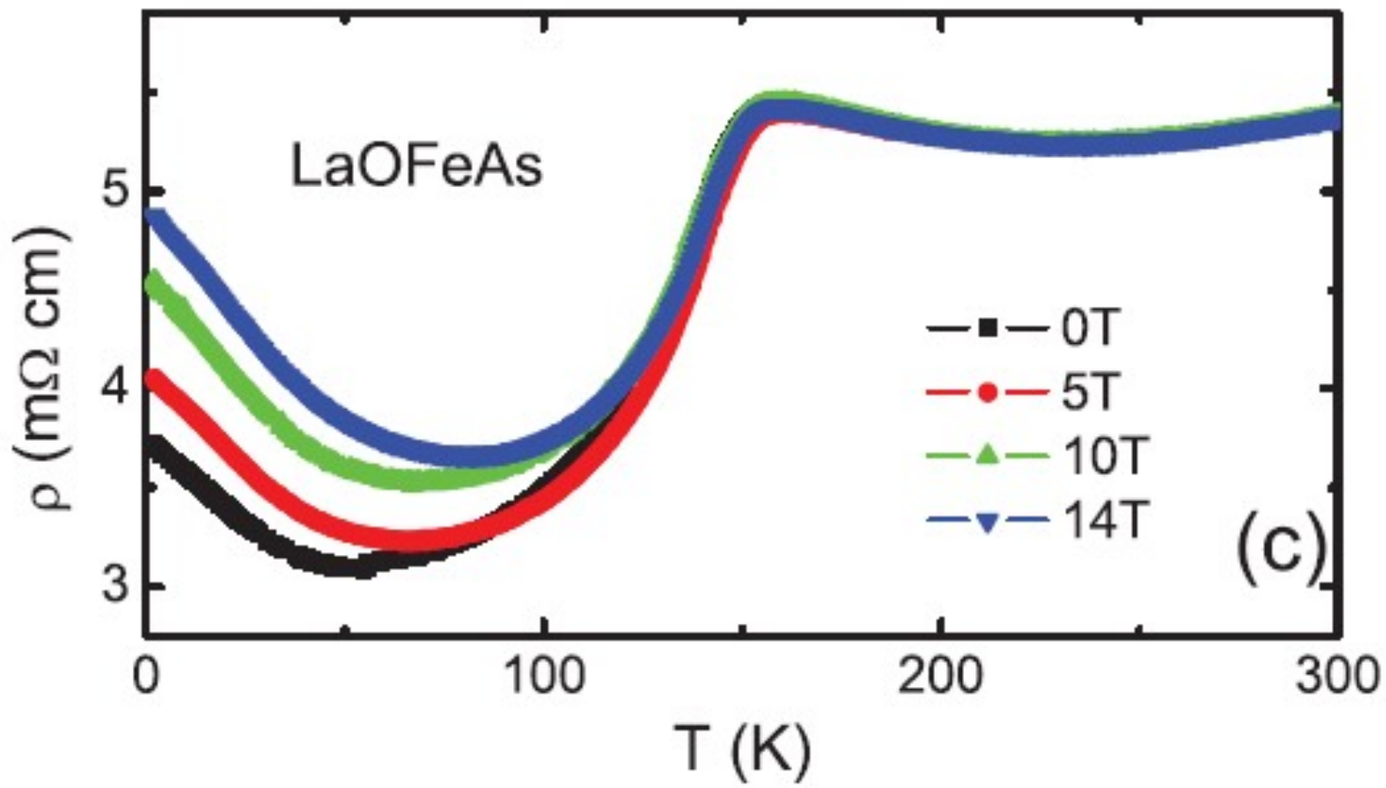


Possible mechanism for SPT?

- Spin-Density wave?



SPT is insensitive to external magnetic field



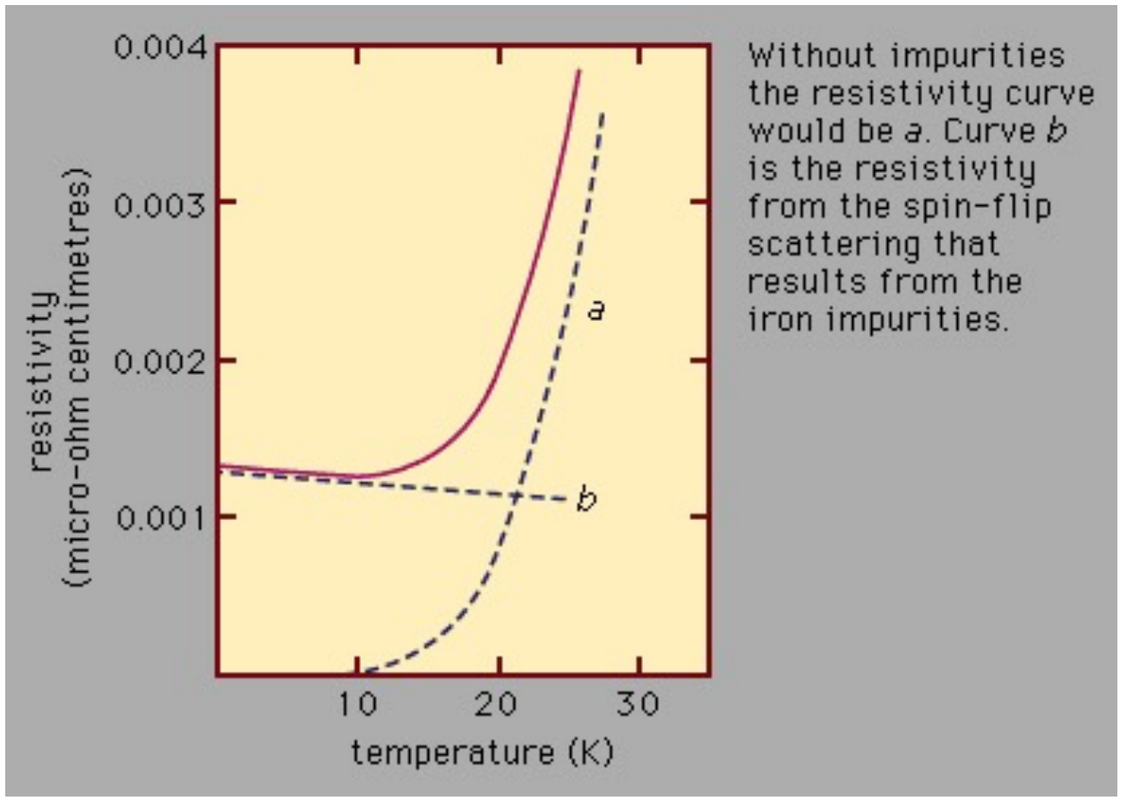
Resistivity Anomaly

$$T > T_{SPT}$$

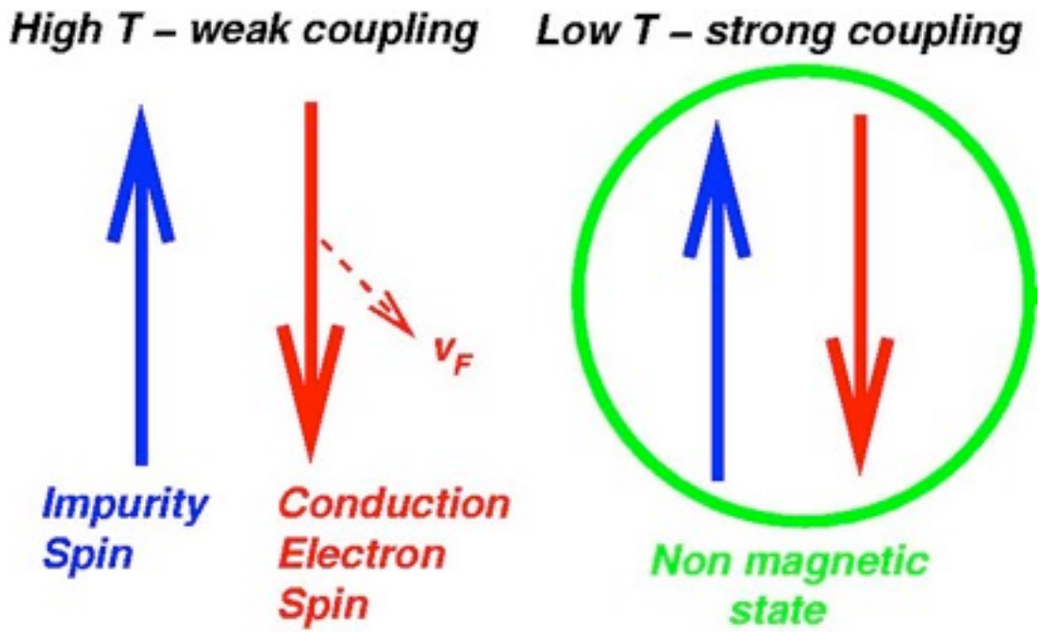
d_{xz}
d_{yz} degenerate

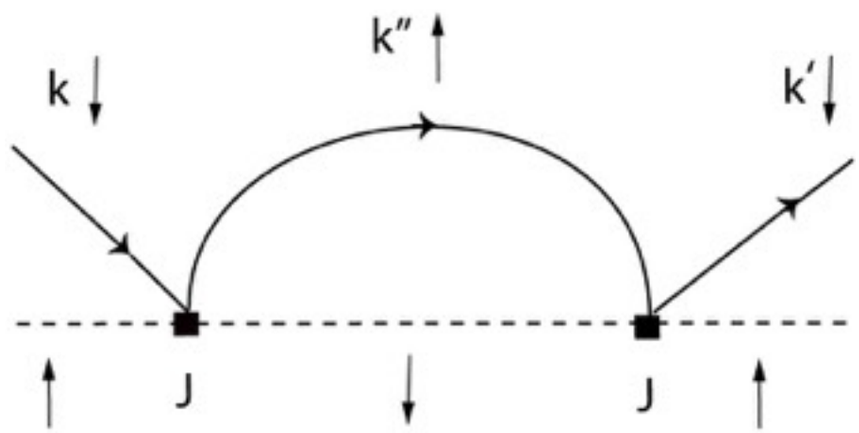
two-level system:
Kondo-like problem

Kondo effect

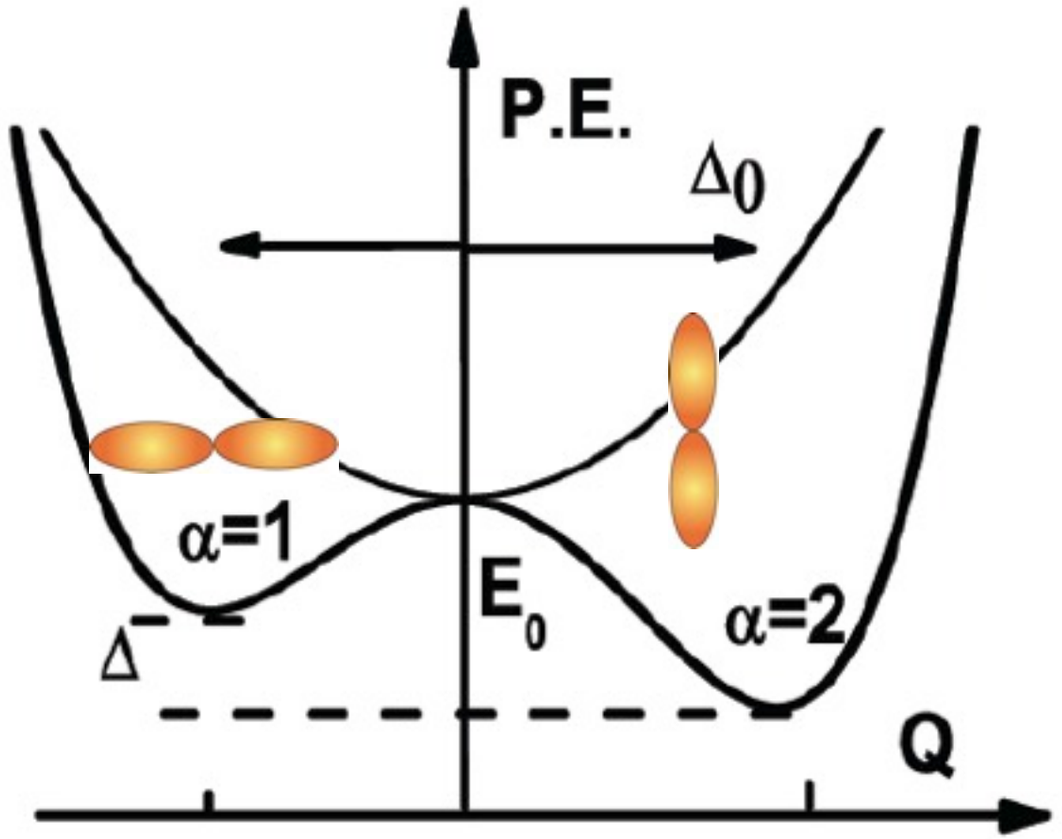


Without impurities the resistivity curve would be *a*. Curve *b* is the resistivity from the spin-flip scattering that results from the iron impurities.





A Two-level System

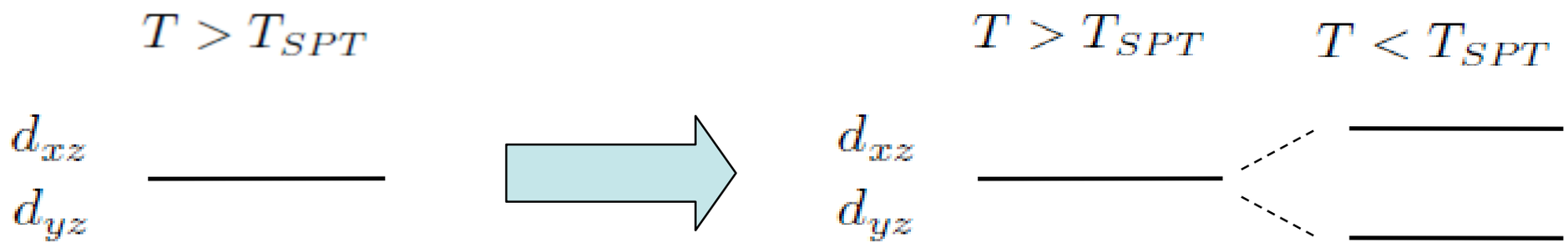


$$H_{\mathrm{TLS}} = \lambda_{ps}\sum_{\alpha} a^{\dagger}_{\alpha}a_{\alpha} + \frac{1}{2}\Delta\sum_{\alpha\beta} a^{\dagger}_{\alpha}\sigma^{z}_{\alpha\beta}a_{\beta} + \frac{1}{2}\Delta_0\sum_{\alpha\beta} a^{\dagger}_{\alpha}\sigma^{x}_{\alpha\beta}a_{\beta}$$

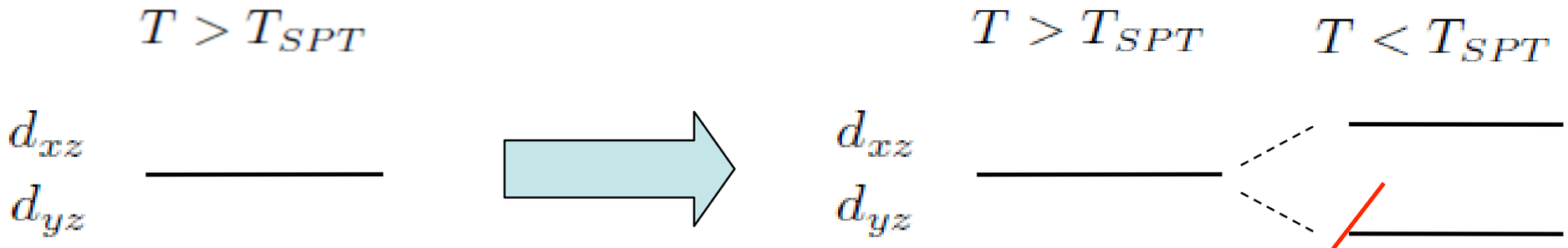
$$E = \sqrt{\Delta_0^2 + \Delta^2}$$

Resistivity anomaly

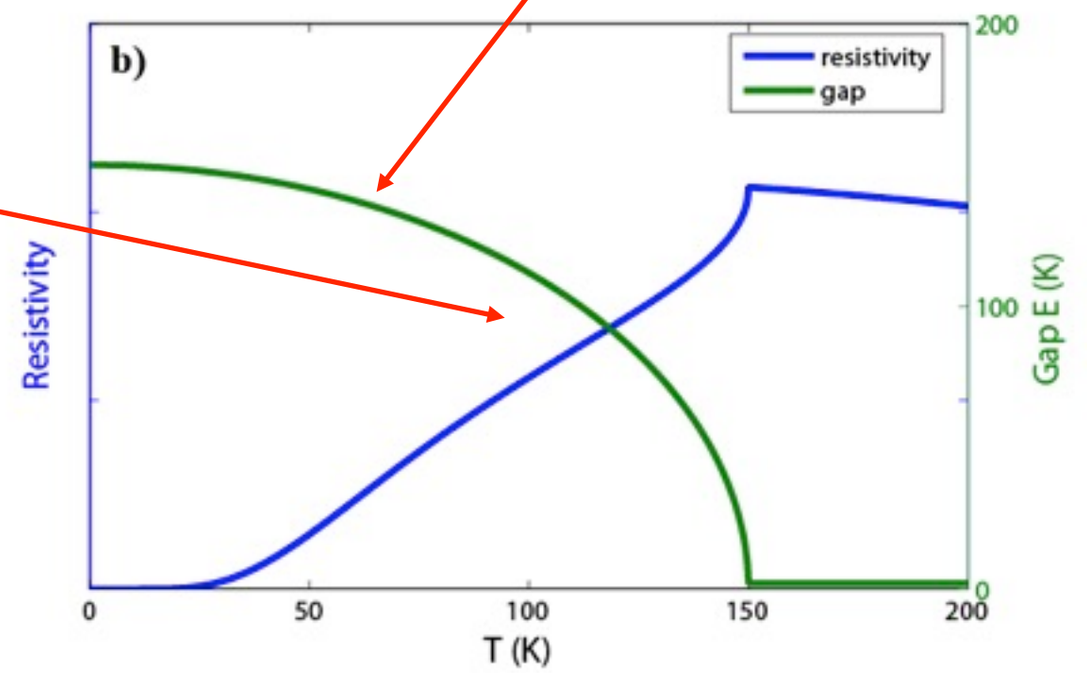
Resistivity anomaly



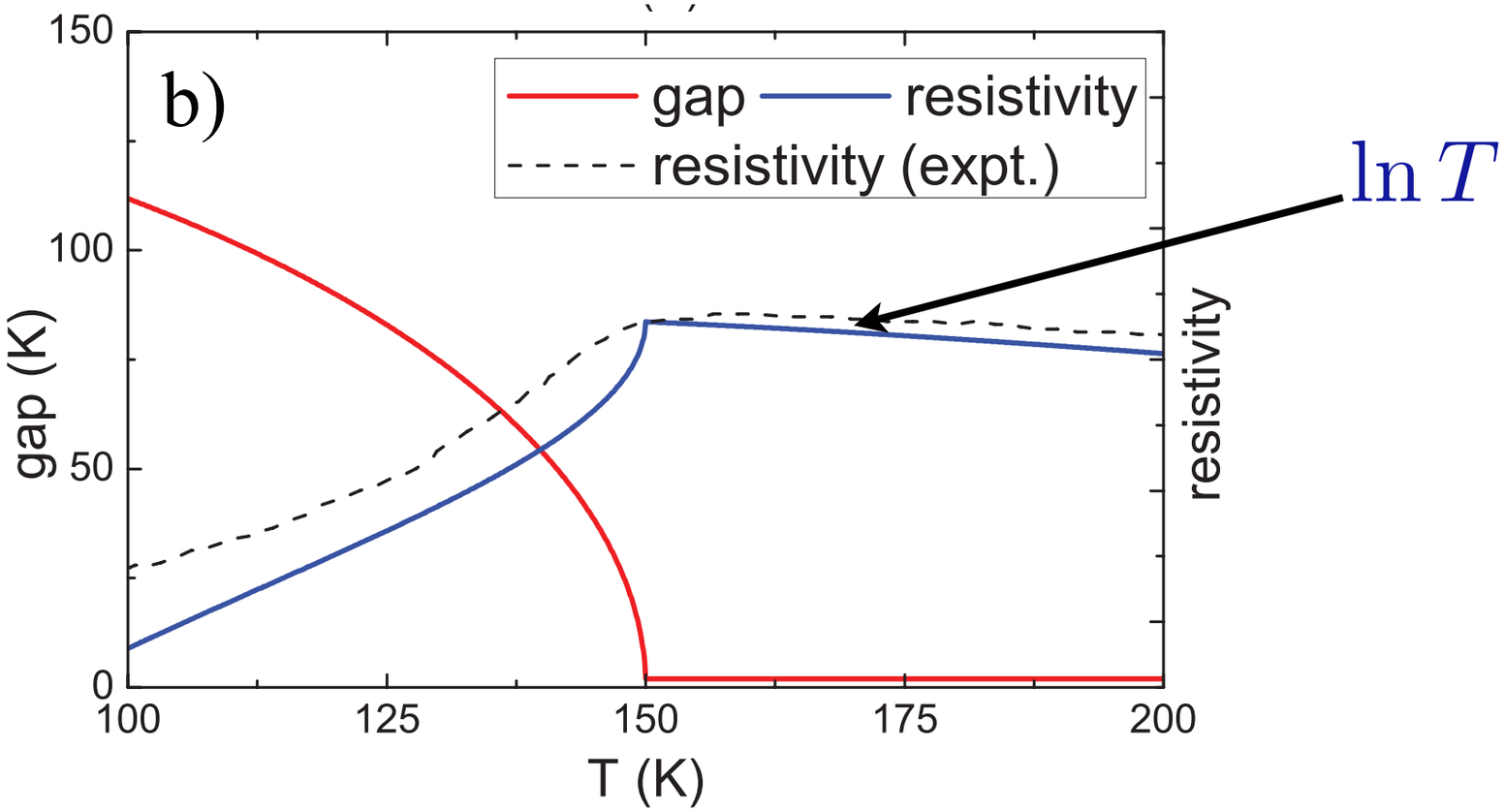
Resistivity anomaly



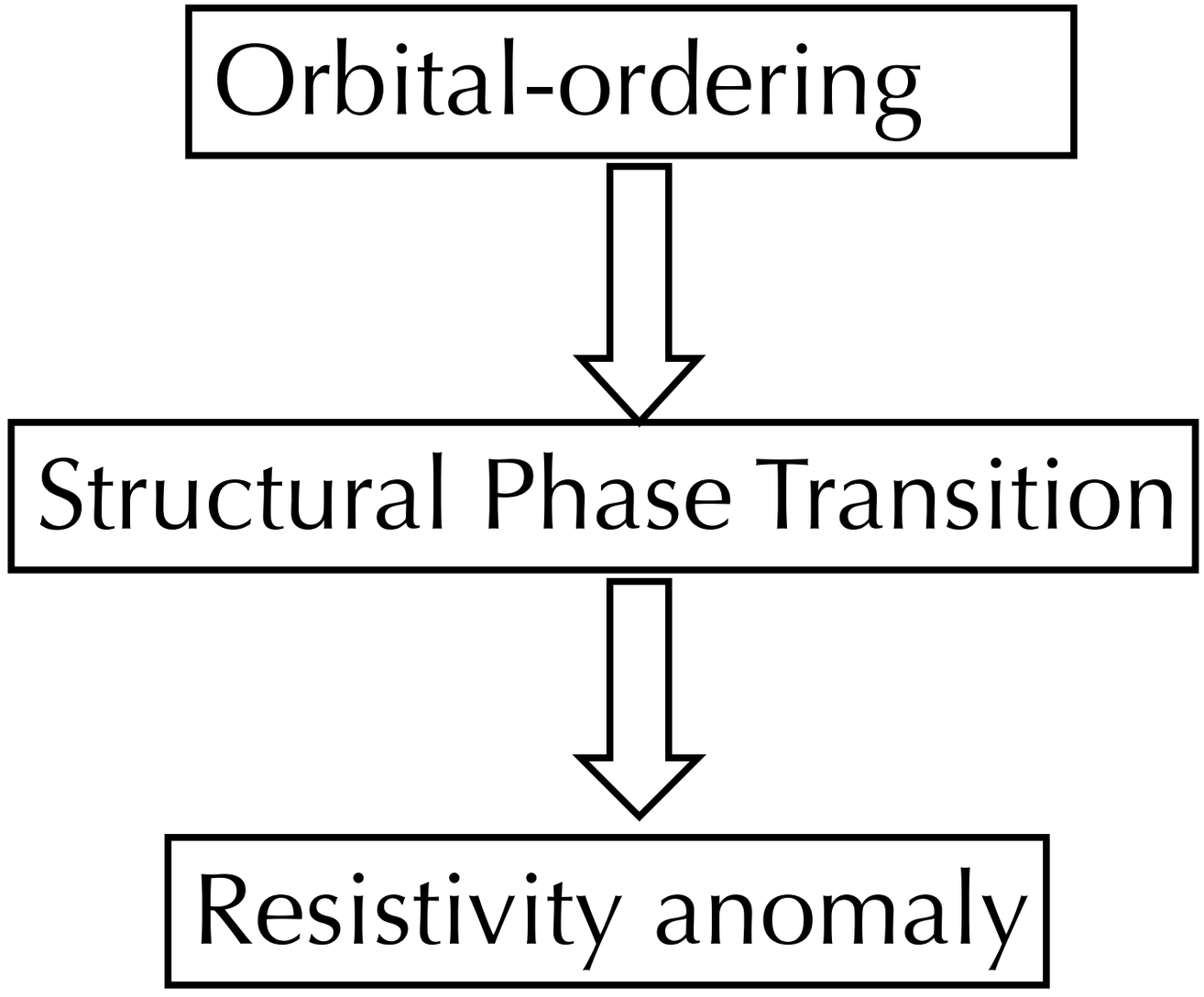
Opening of the gap makes scattering difficult;
Resistivity decreases



Resistivity Anomaly

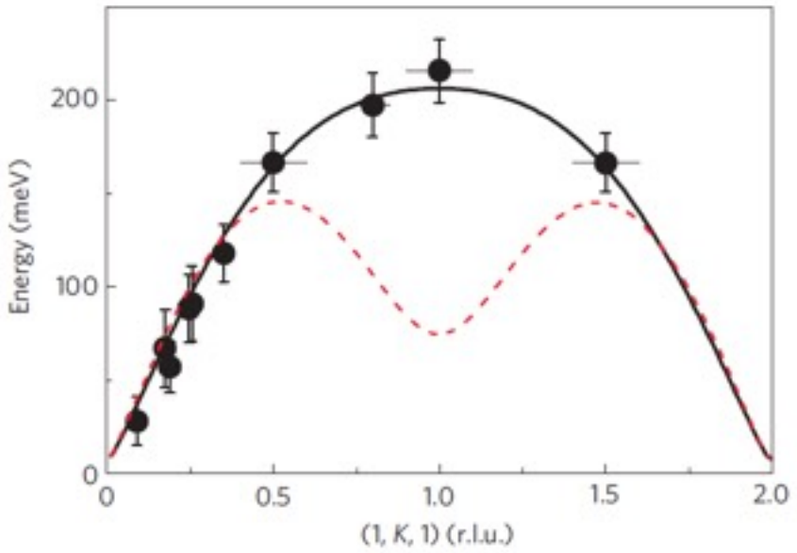


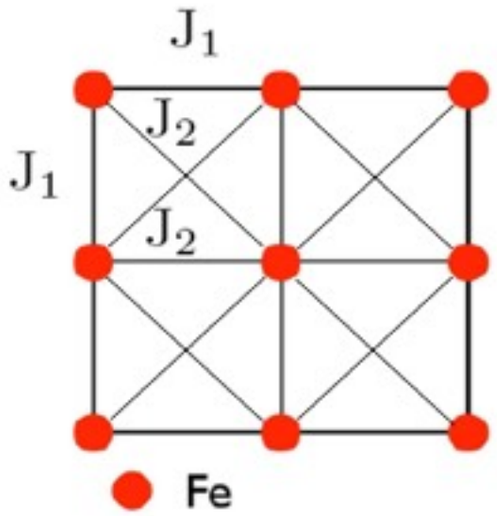
Conclusion I:



- *Inelastic neutron scattering*

Experimental Puzzle 2?





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

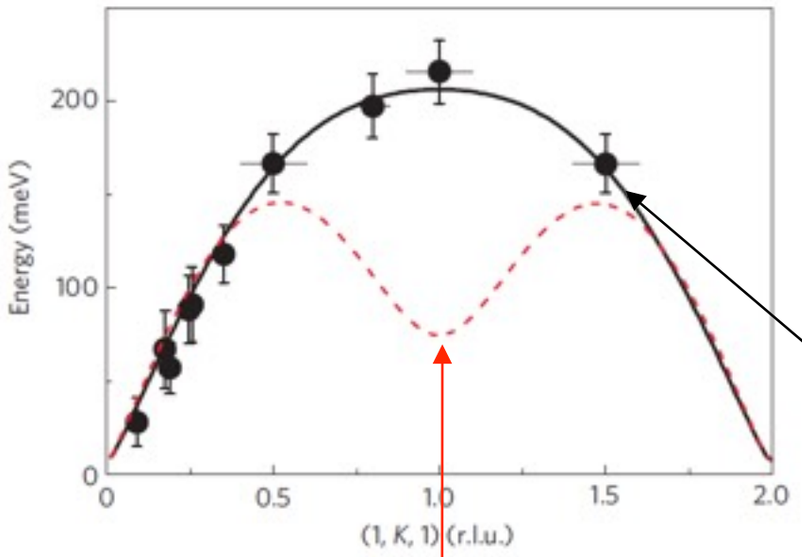
$$
\begin{aligned}
SJ_1^a &= 27\,\text{meV} \\
SJ_1^b &= 25\,\text{meV} \\
SJ_2 &= 36\,\text{meV}
\end{aligned}
$$

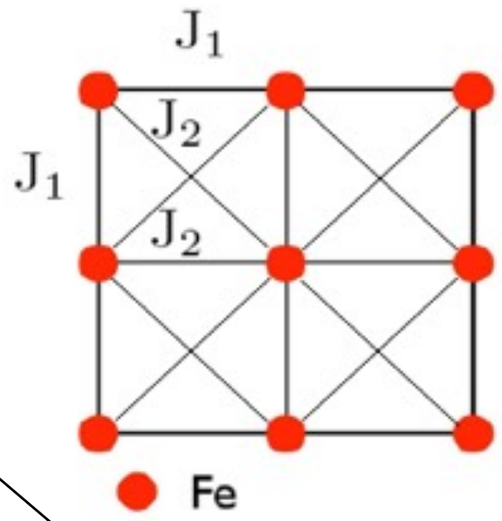
$$
\begin{aligned}
SJ_1^a &= 49.9 \pm 9.9\,\text{meV} \\
SJ_1^b &= -5.7 \pm 4.5\,\text{meV} \\
SJ_2 &= 18.9 \pm 3.4\,\text{meV}
\end{aligned}
$$

Why is the magnetism frustrated?

- *Inelastic neutron scattering*

Experimental Puzzle 2?





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?

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

$$\nu J_H \ll \infty$$

Double-Exchange Model

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

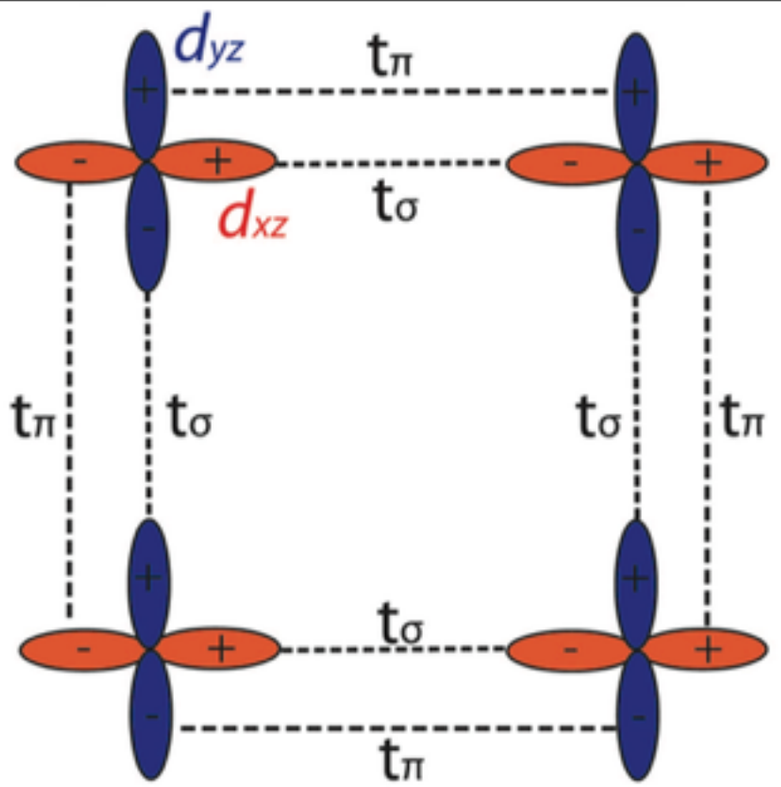
$$\mathcal{H}_{\rm it} = - \sum_{ij,\alpha\beta,\nu} t_{ij}^{\alpha\beta} c_{i\alpha\nu}^{\dagger} c_{j\beta\nu} + \frac{V}{2} \sum_{i,\alpha\neq\beta,\nu\nu'} \hat{n}_{i\alpha\nu} \hat{n}_{i\beta\nu'}$$

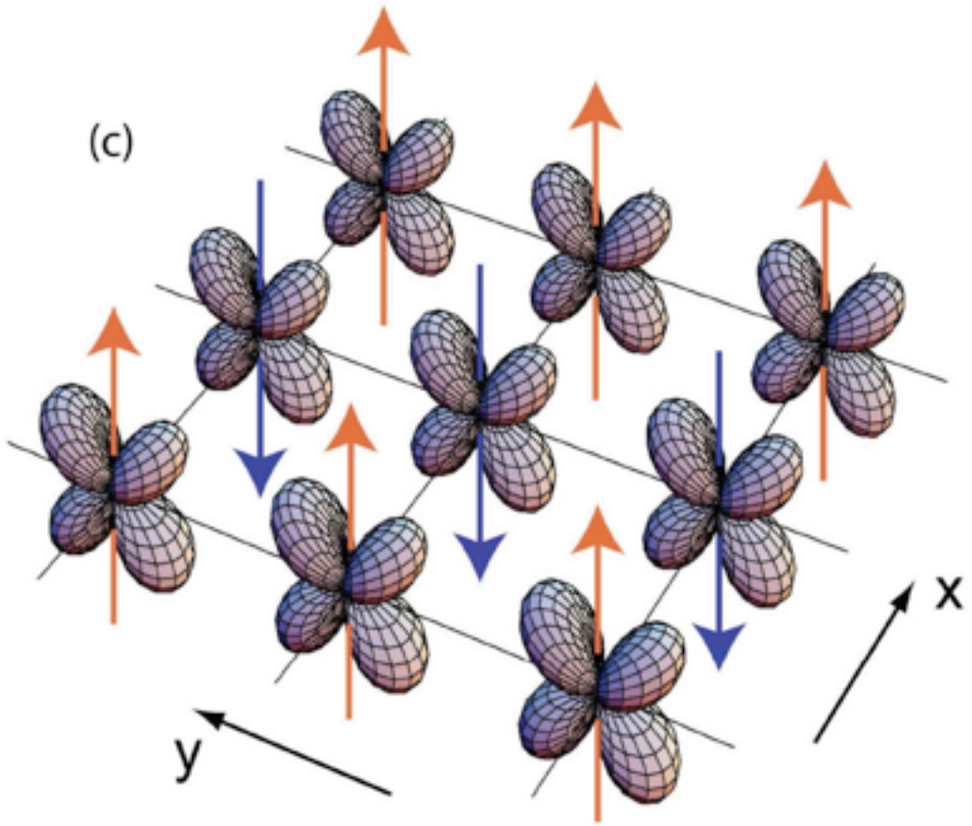
$$\mathcal{H}_{\rm H}^{(0)} = -\frac{J_{\rm H}}{2} \sum_{k,\alpha,\nu} \nu \tilde{c}_{k\alpha\nu}^{\dagger} \tilde{c}_{k\alpha\nu}$$

unlike manganites

$$\nu J_H \ll \infty$$

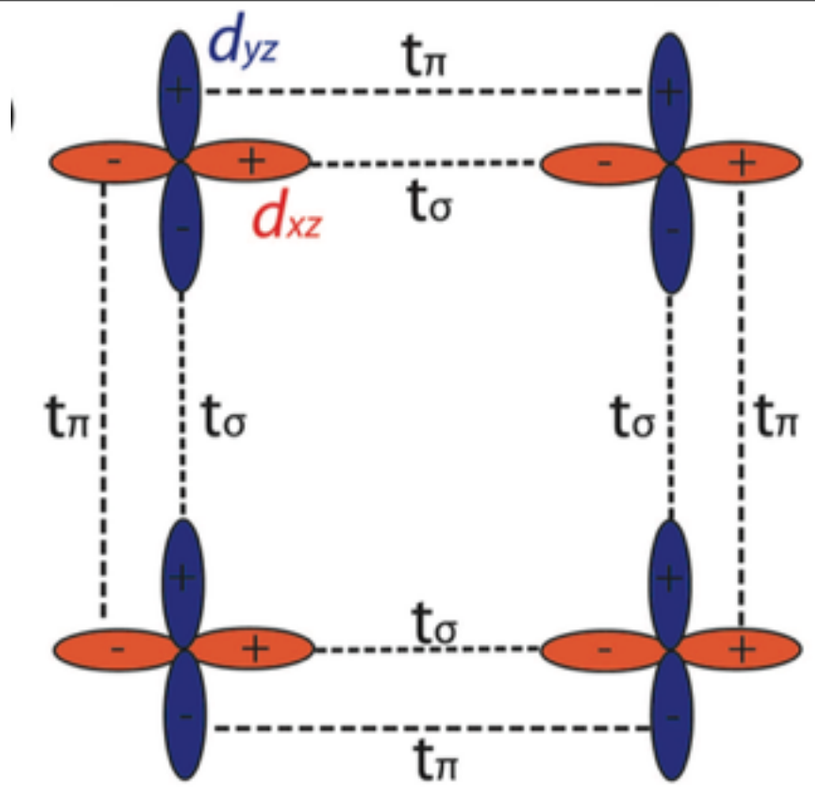
answer: emergent ferro-orbital order from Hund coupling

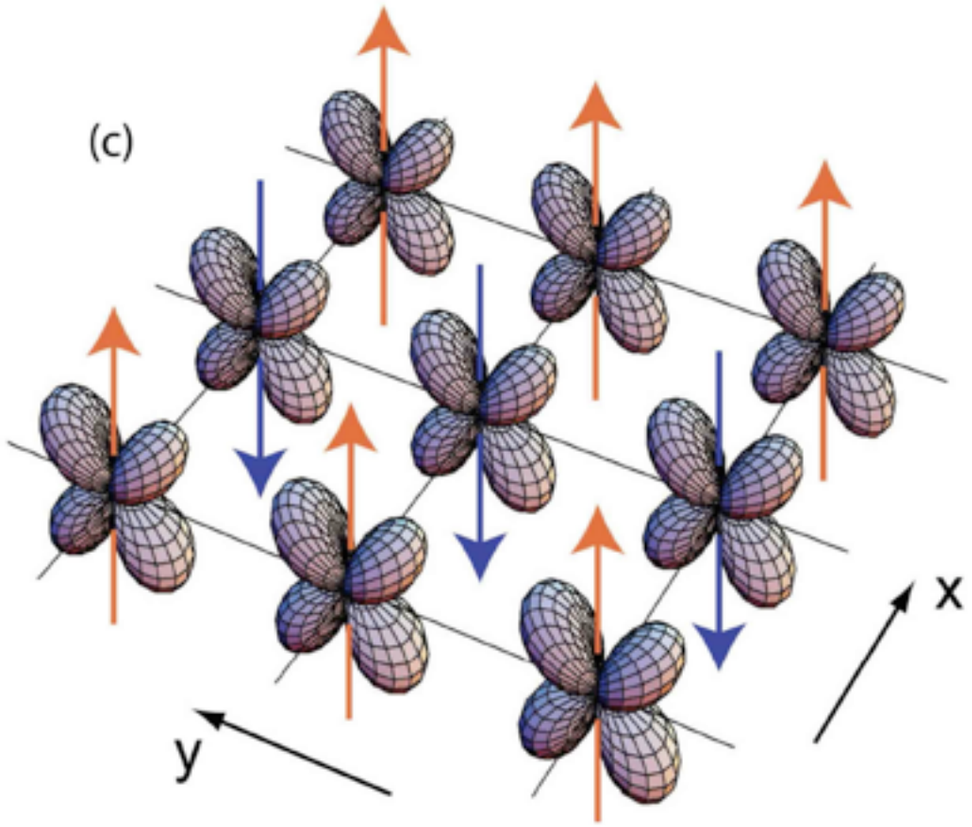


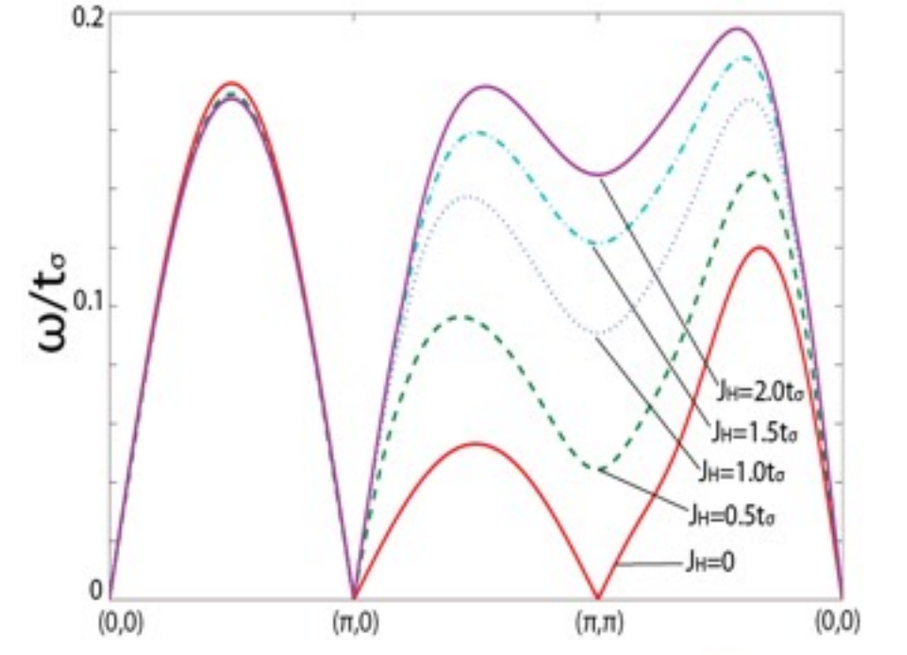


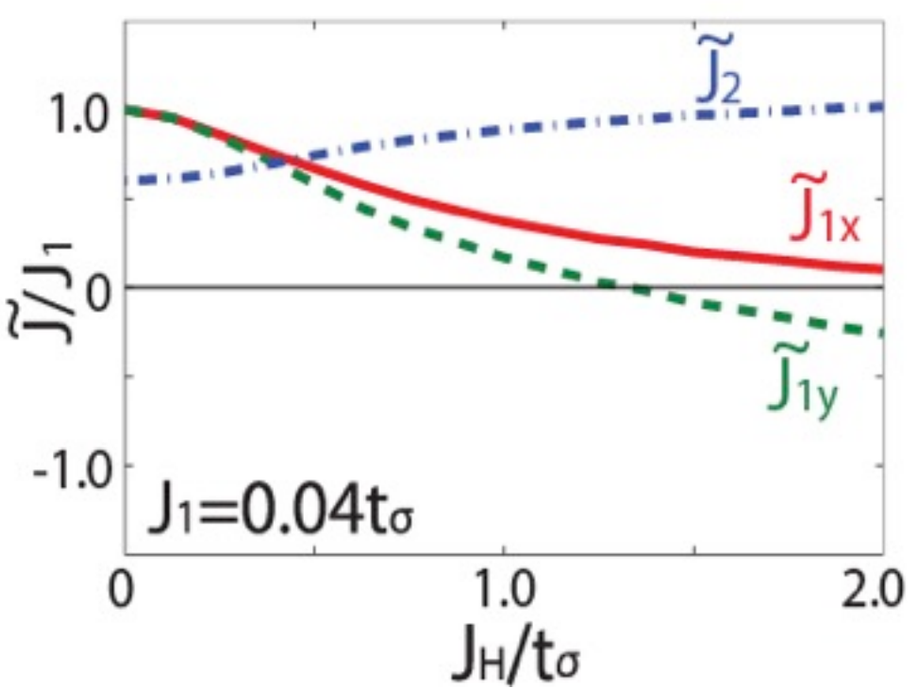
answer: emergent ferro-orbital order from Hund coupling

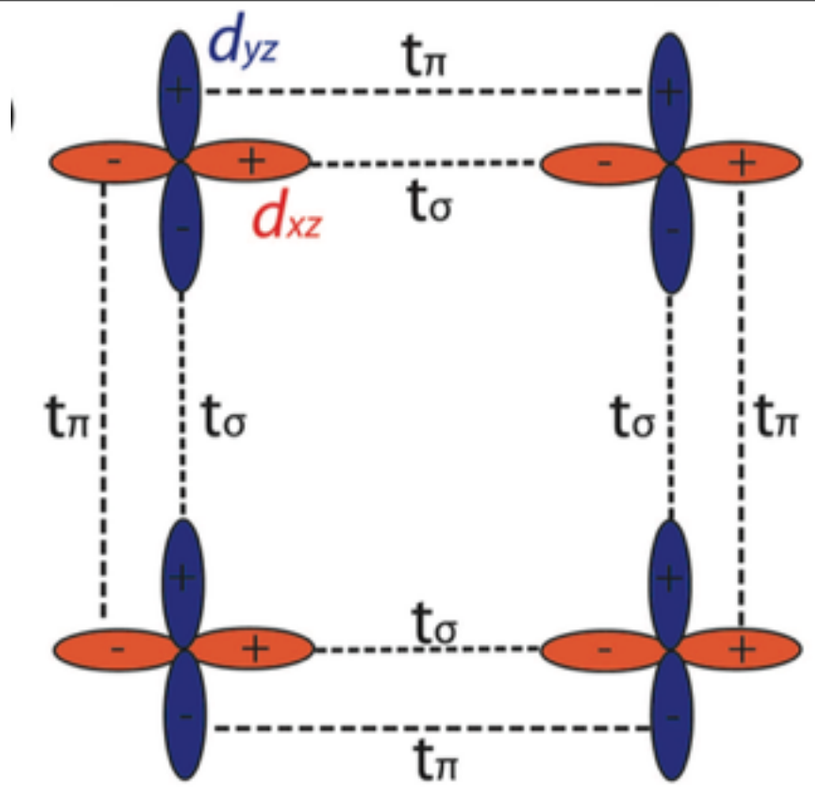
answer: emergent ferro-orbital order from Hund coupling

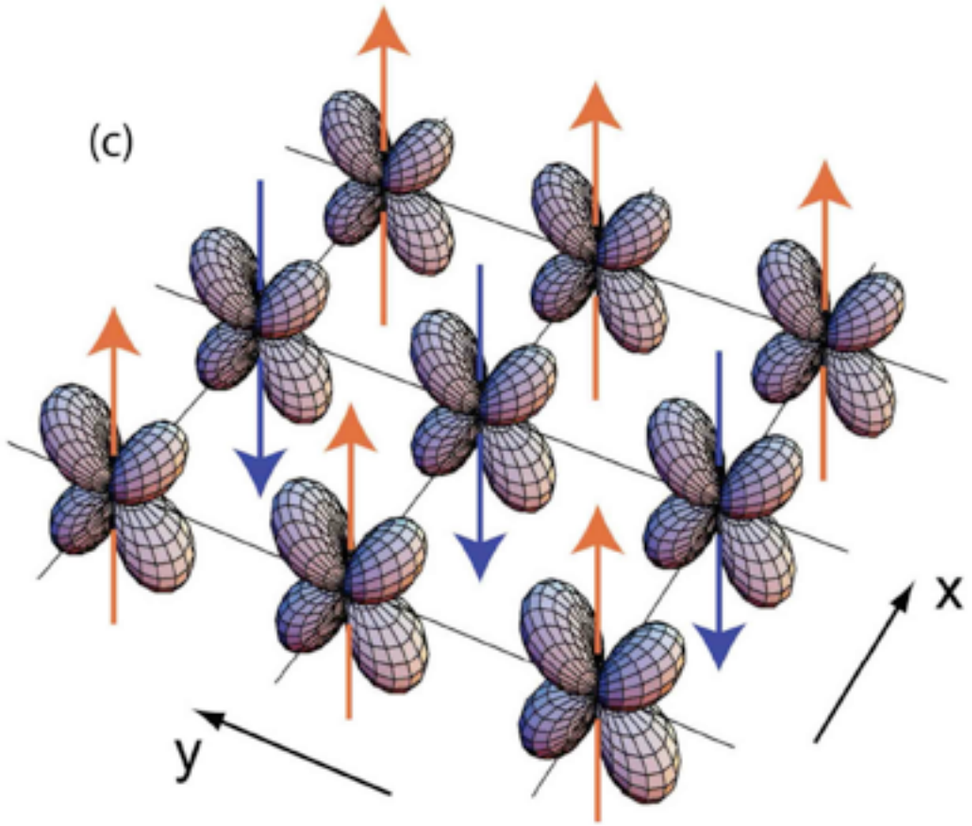




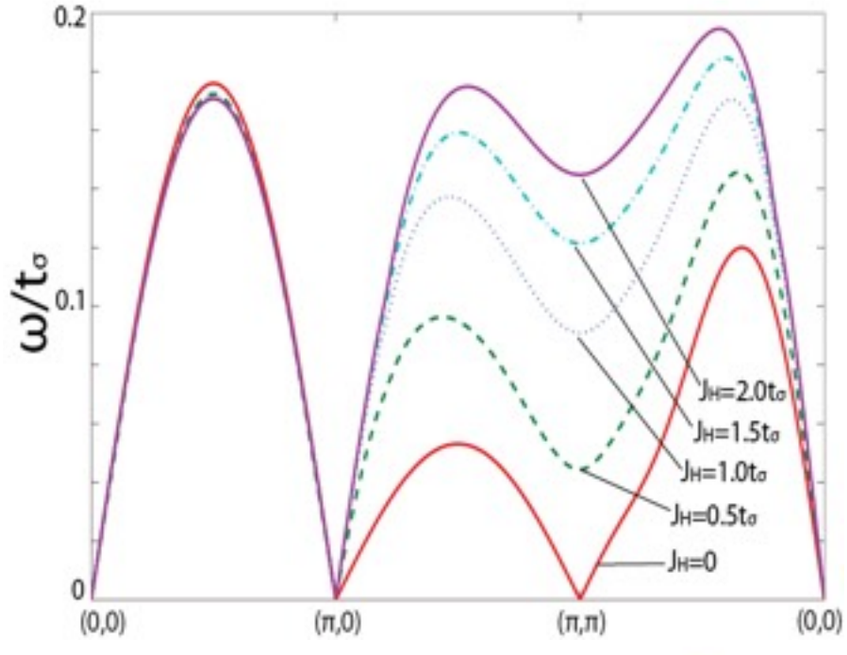


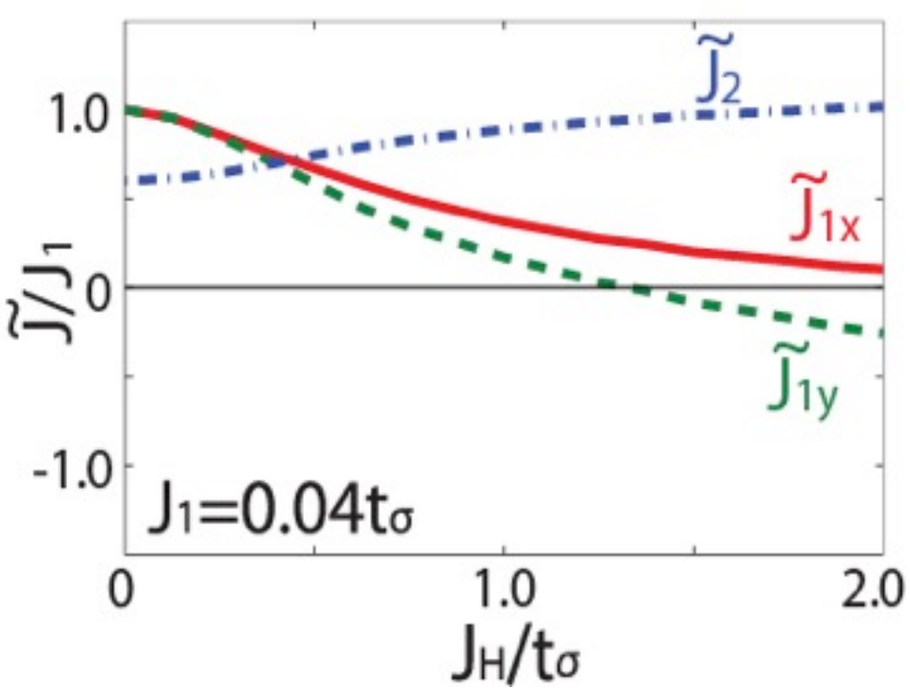






answer: emergent ferro-orbital order from Hund coupling





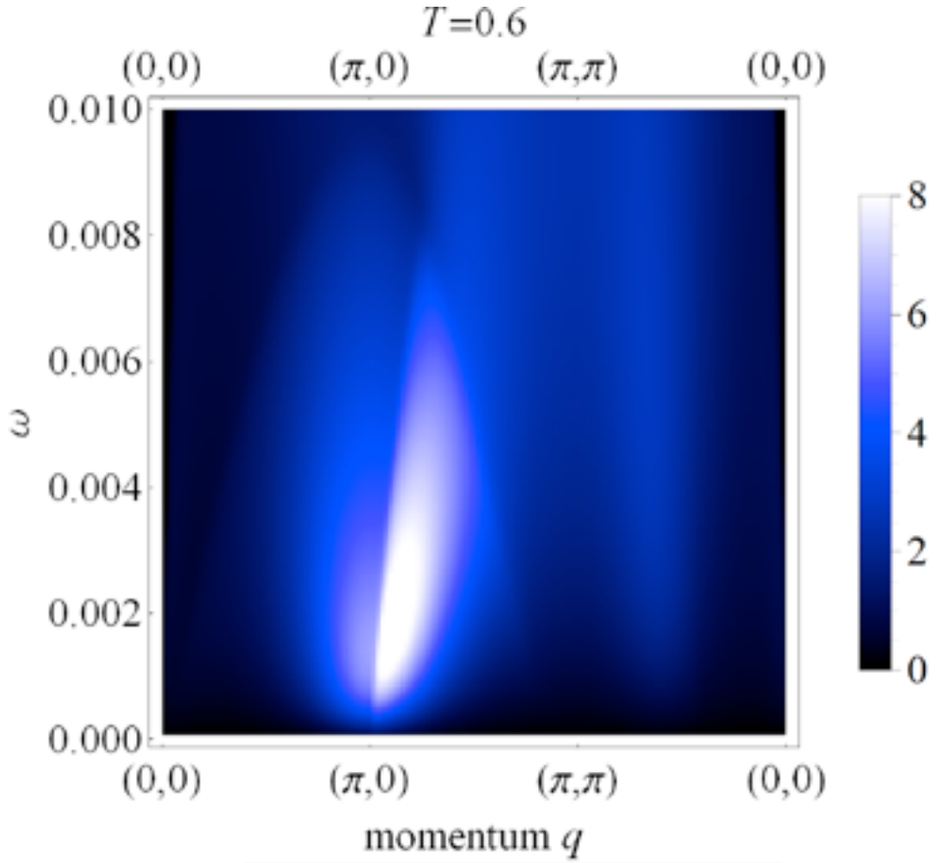
- *Comparison with experiments*:

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

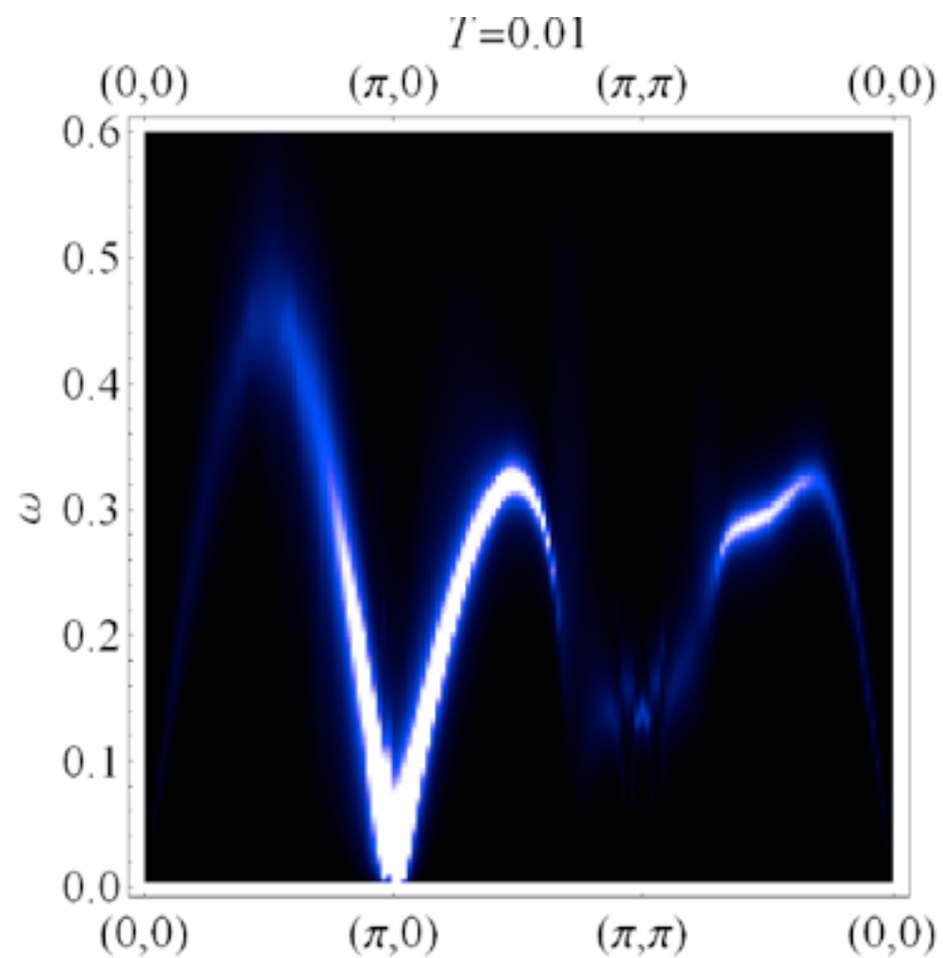
localized/extended electrons+Hund's coupling

orbital ordering

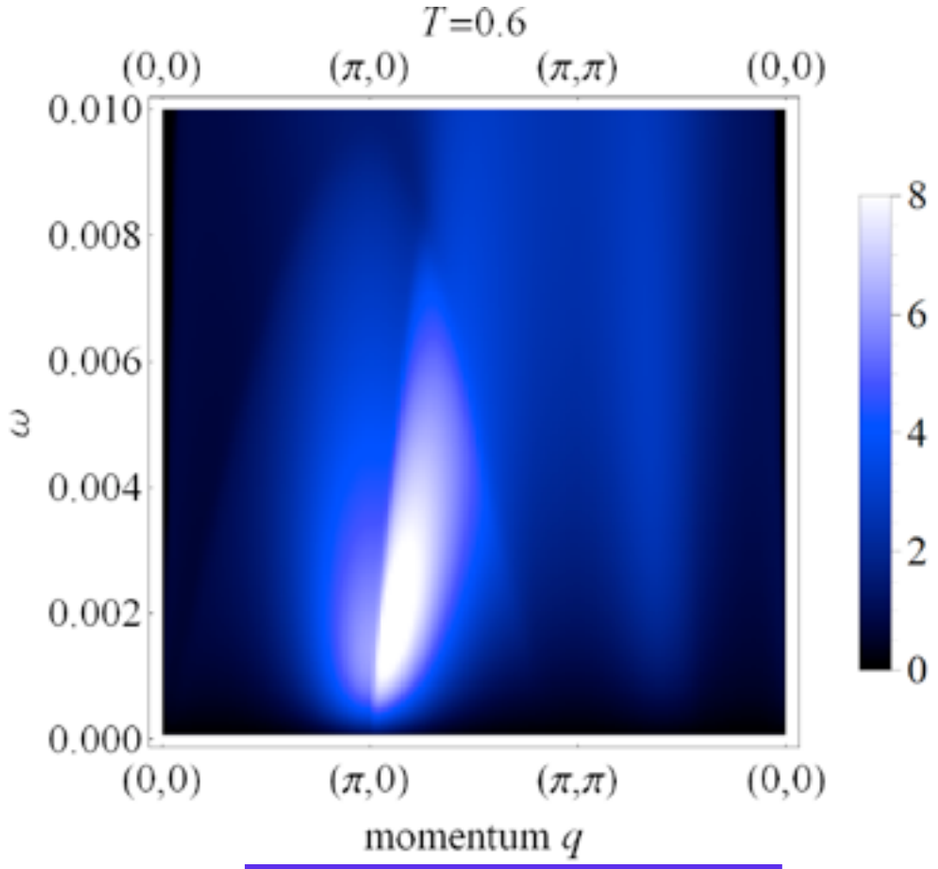
unfrustrated magnetism, SPT, RA



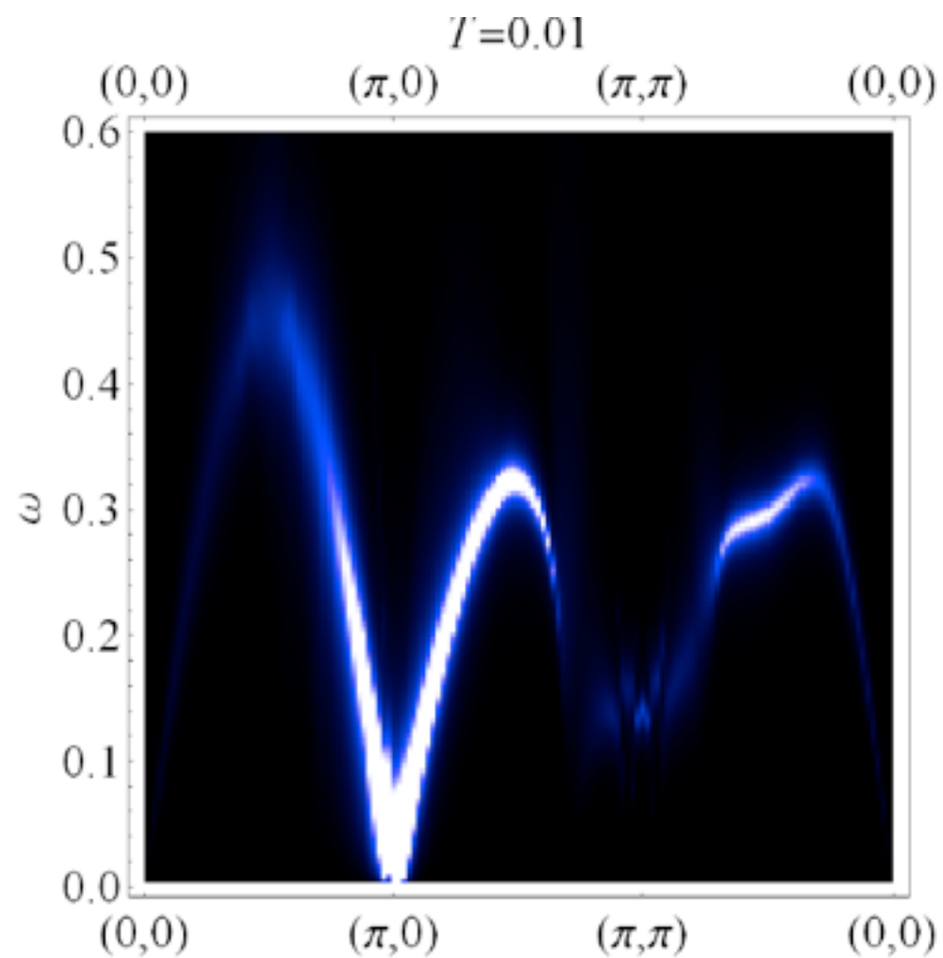
high T
paramagnetic state



low T
ordered state

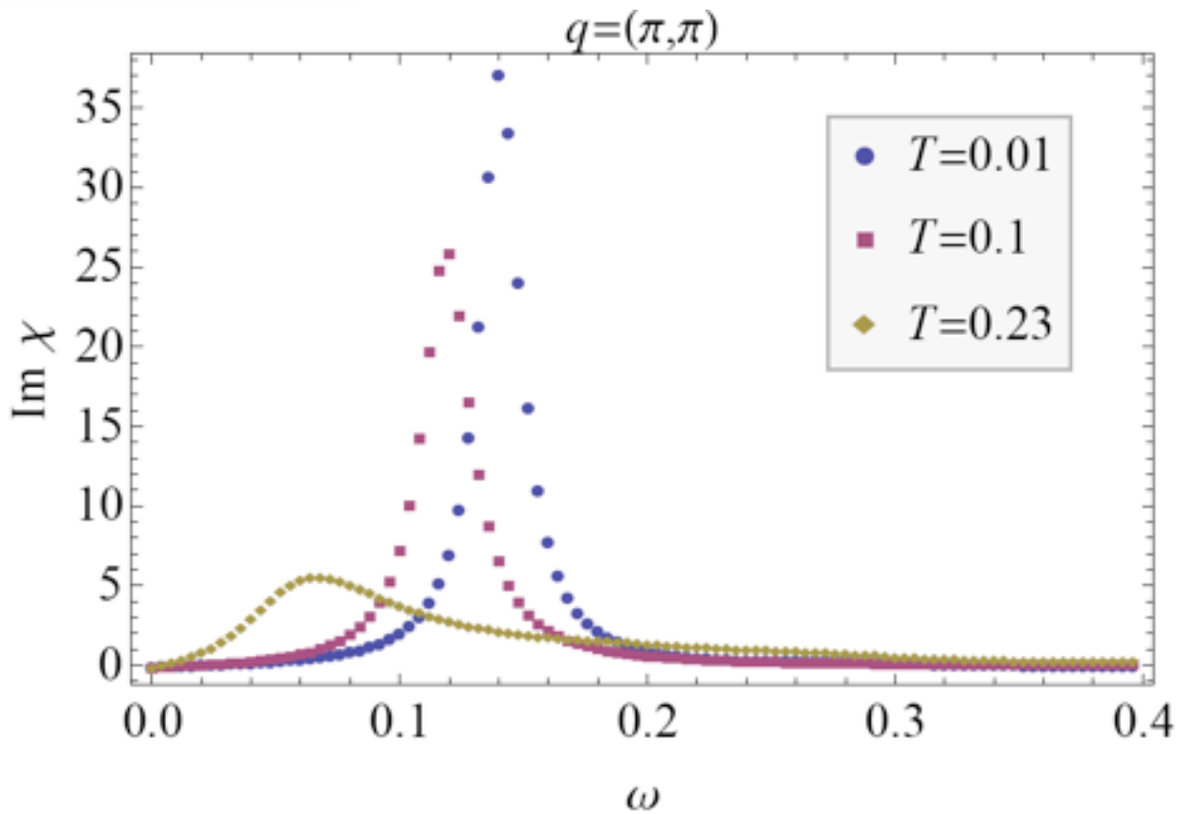


high T
paramagnetic state



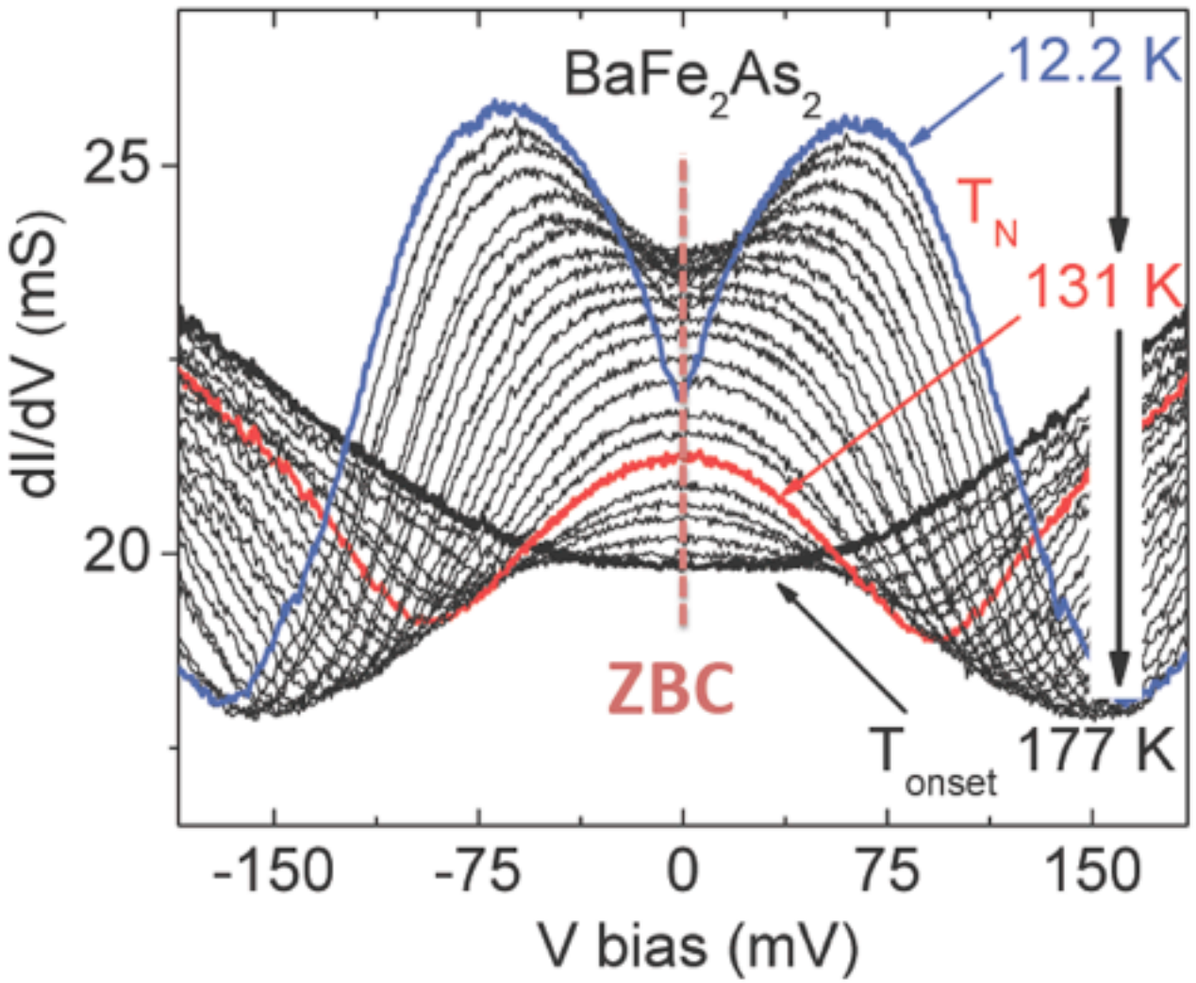
low T
ordered state

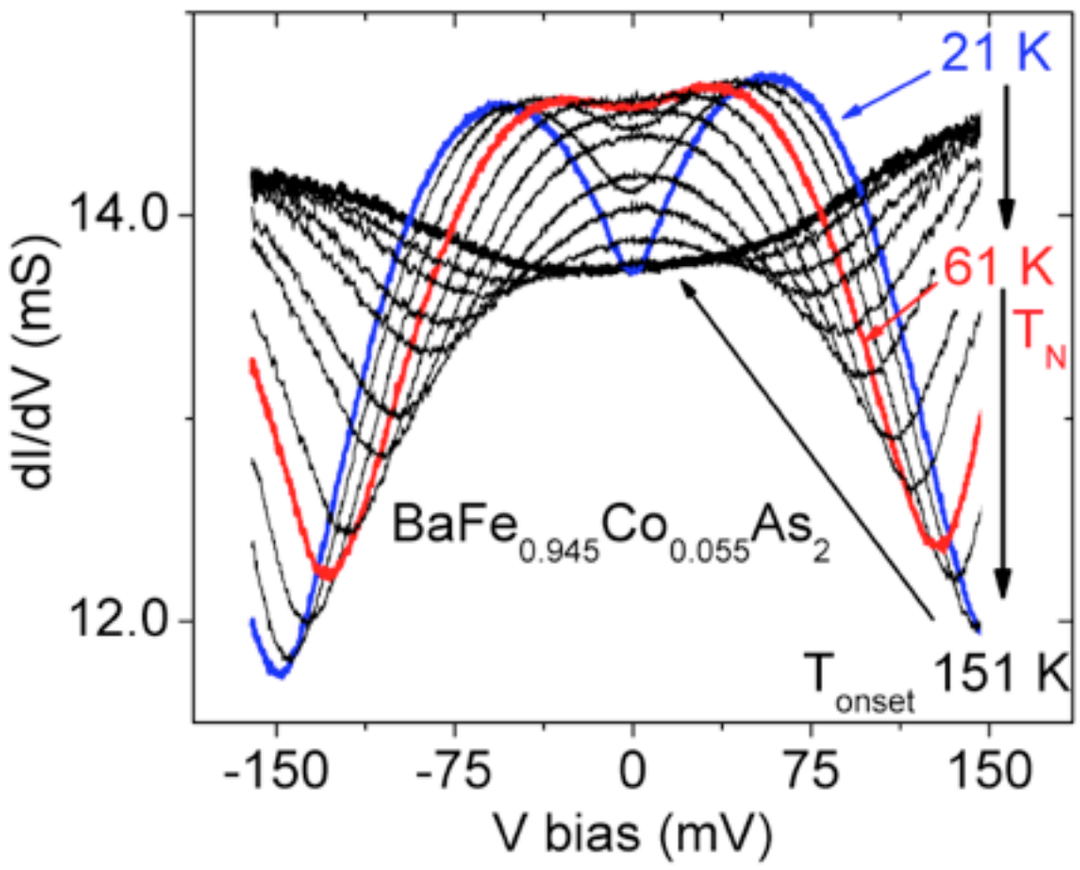
prediction:
Landau damping
increases
as T increases



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

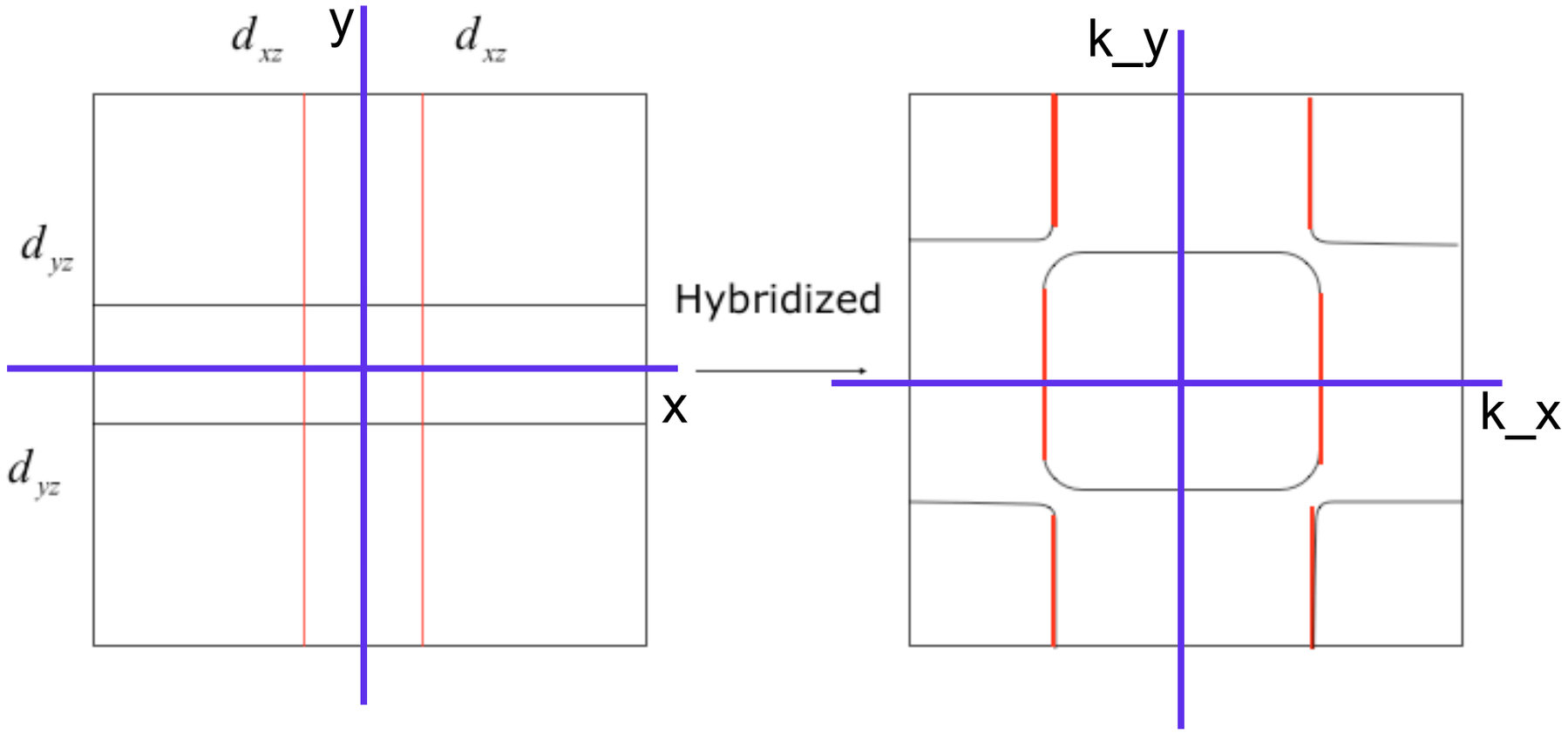
Experimental puzzle 3: What is the origin of the excess conductance above the structural transition?



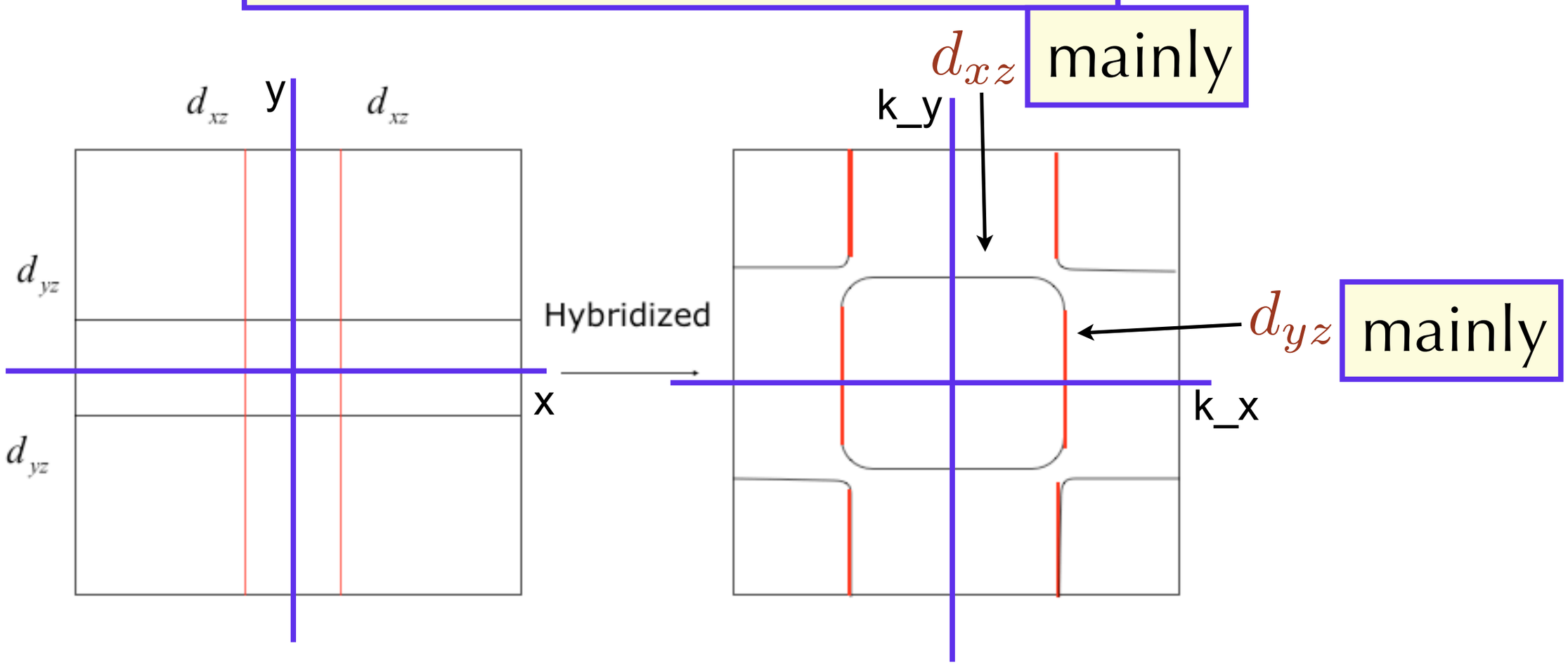


H. Ahram, L. Greene, ... (UIUC)

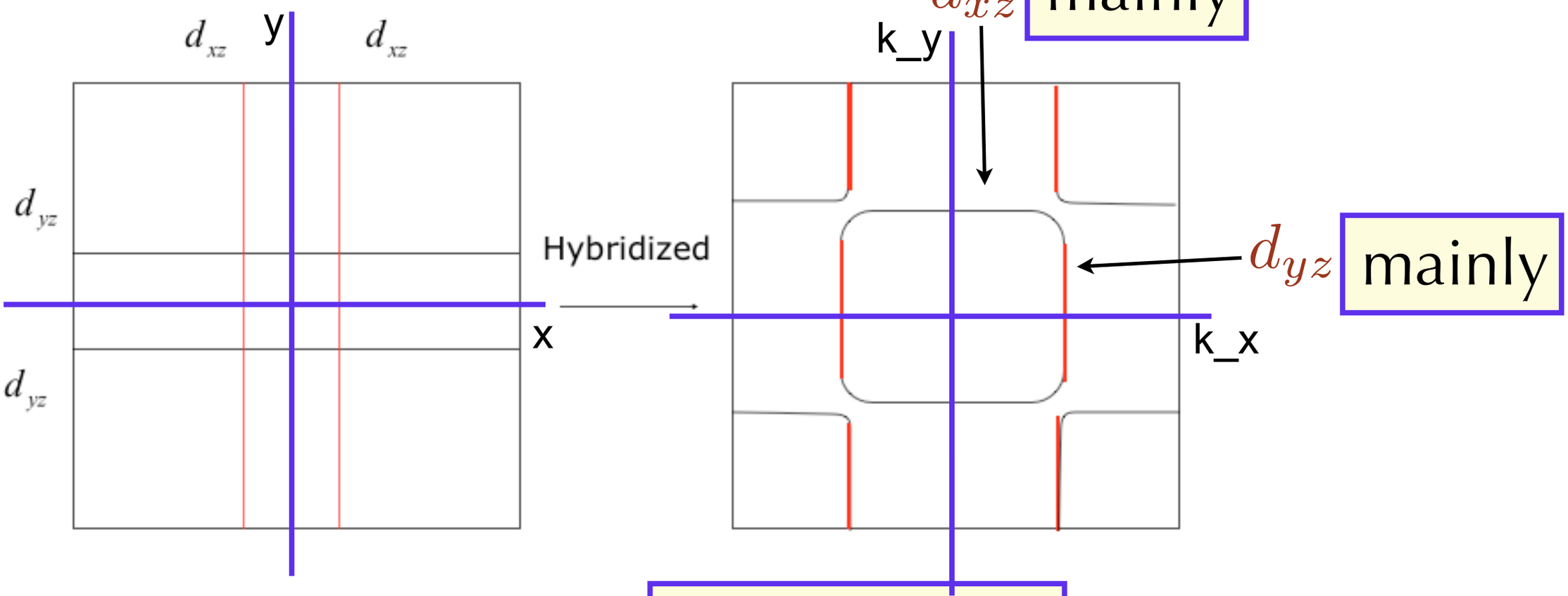
Fermi surface in Brillouin zone



Fermi surface in Brillouin zone



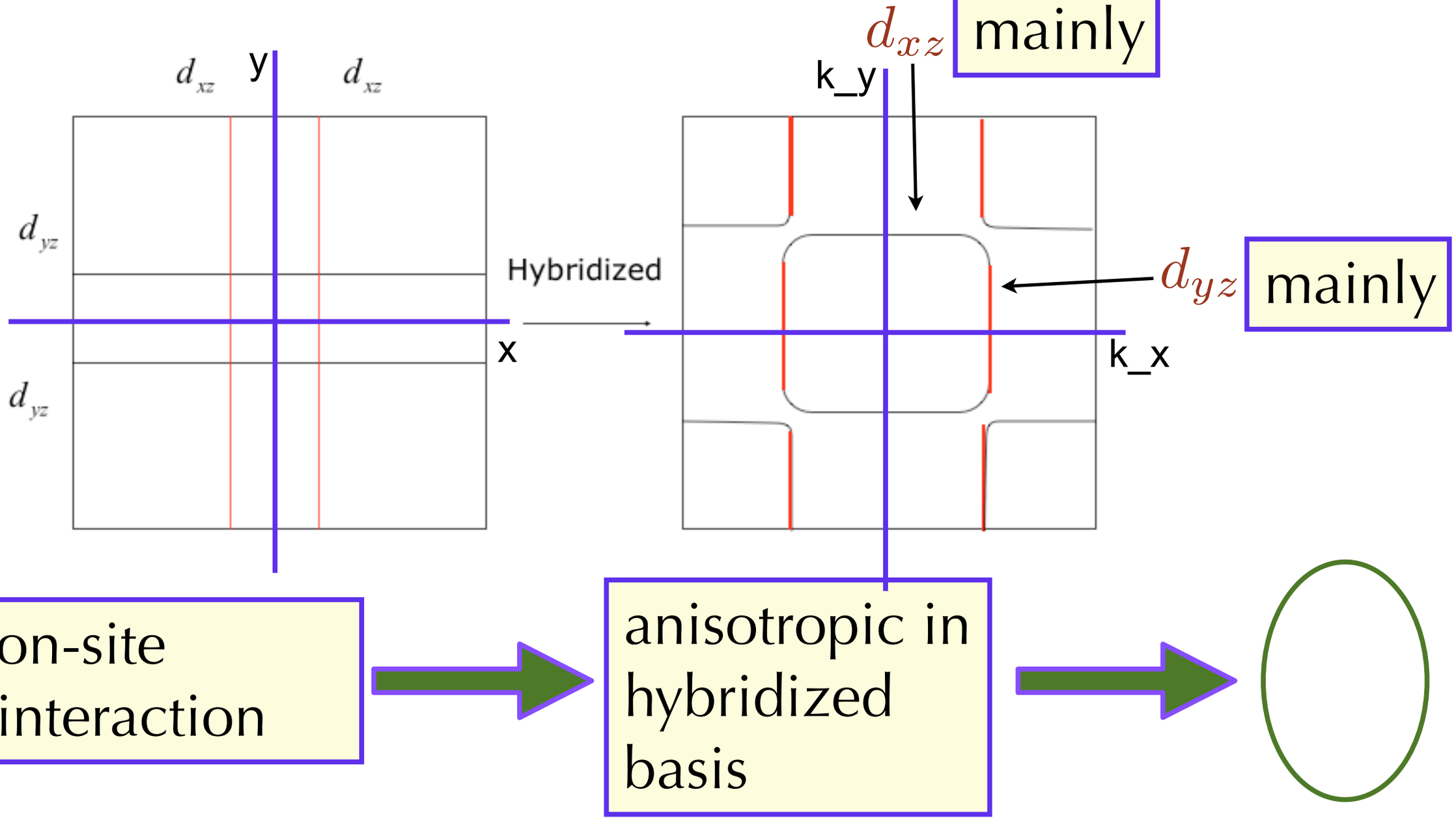
Fermi surface in Brillouin zone



on-site interaction

anisotropic in hybridized basis

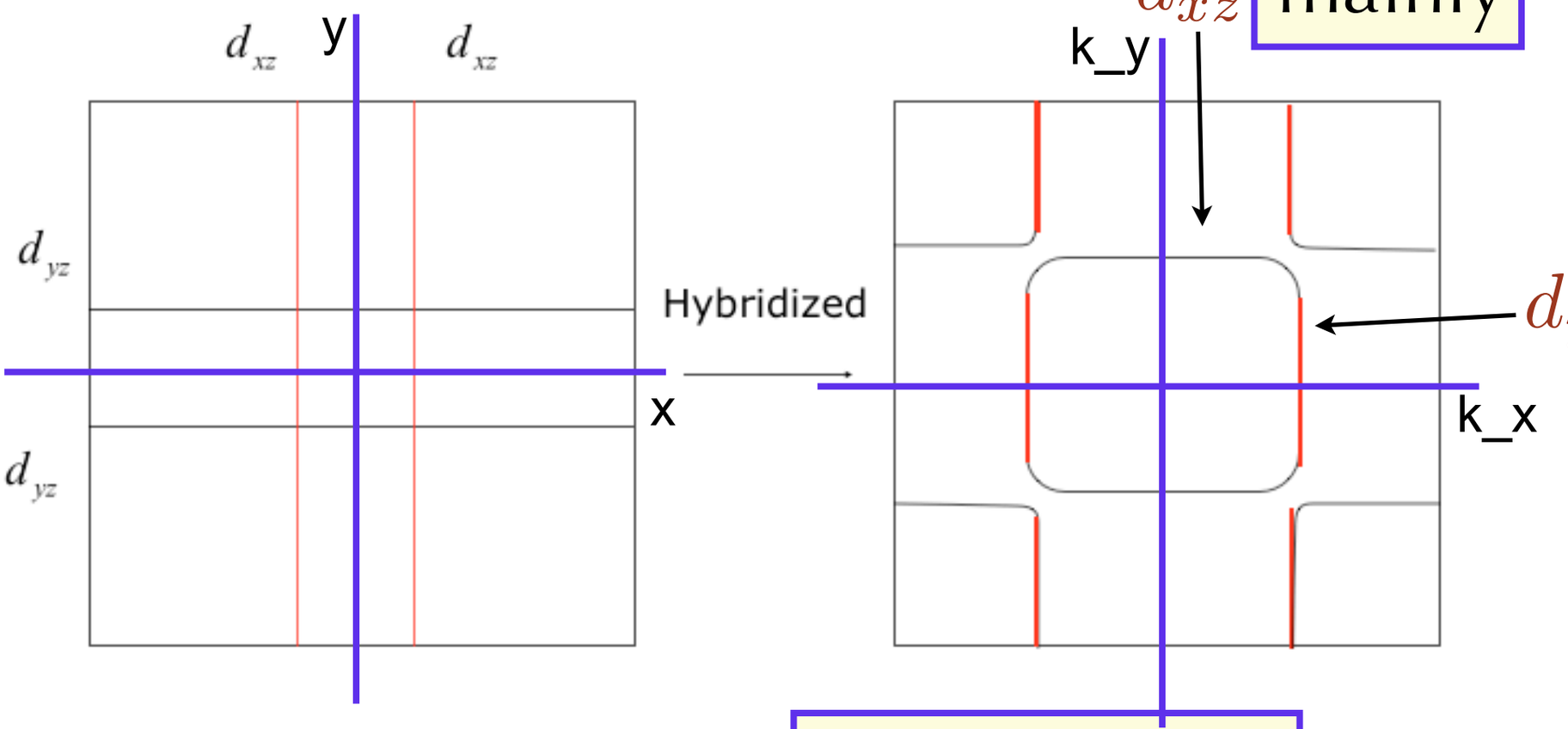
Fermi surface in Brillouin zone



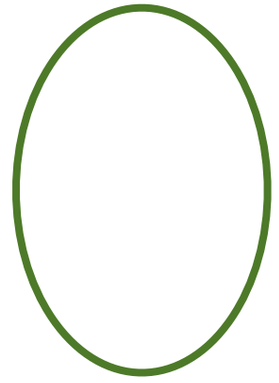
on-site interaction

anisotropic in hybridized basis

Fermi surface in Brillouin zone



on-site interaction → anisotropic in hybridized basis →



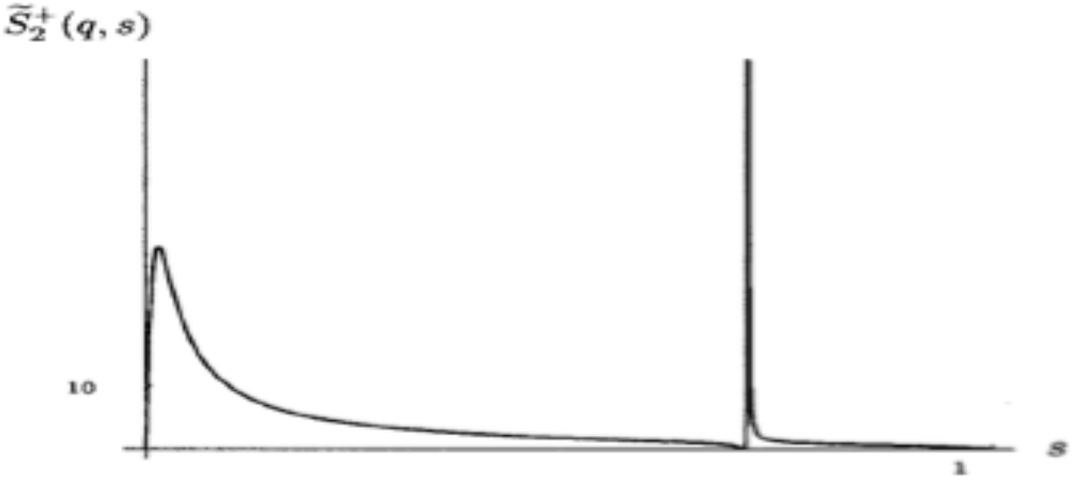
orbital ordering in multi-orbital system = nematic order

nematic ordering of a Fermi surface

- The interaction can be written as:

$$F_2 = \iiint dk dk' dq \; f_2(q) \cos 2(\theta_k - \theta_{k'}) c^+_{k+q/2,\sigma} c^+_{k'-q/2,\sigma'} c_{k'+q/2,\sigma'} c_{k-q/2,\sigma}$$

- Overdamped collective mode induced by this interaction:



- Non-Fermi liquid behavior is caused because these overdamped modes dominate low-energy physics near the critical point and also inside the nematic phase.

Multiorbital Hubbard Model

$$H = H_t + H_I$$

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

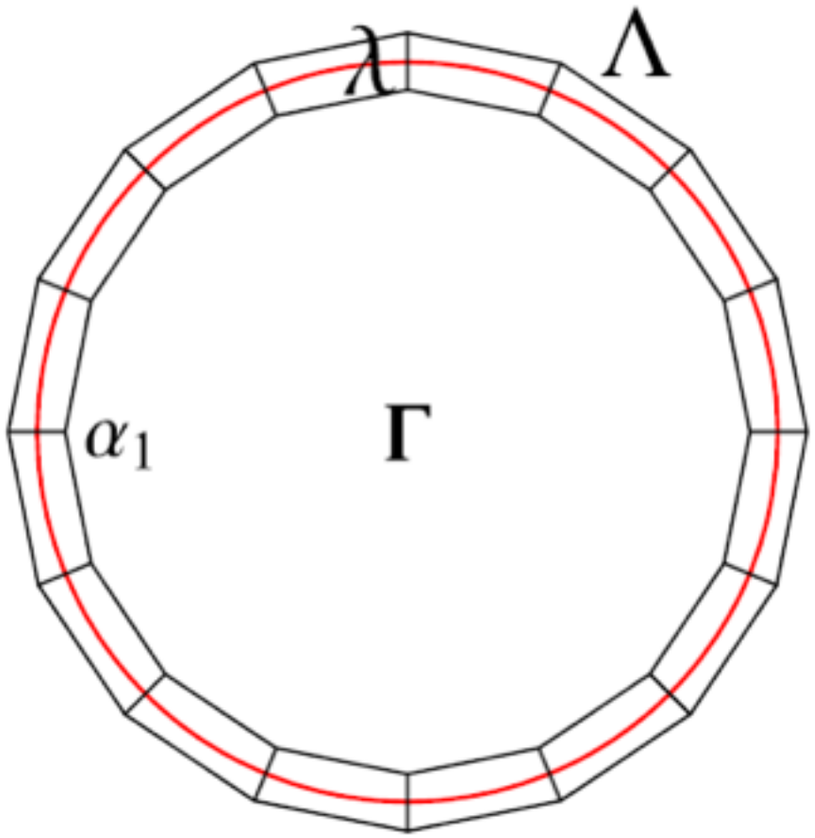
$$H_I = \sum_{ia} U n_{ia\uparrow} n_{ia\downarrow} + \sum_{i,b>a}\left(U' - \frac{J}{2}\right) n_{ia} n_{ib} - 2J\vec{S}_{ia}\times\vec{S}_{ib} + J\left(c_{ia\uparrow} c_{ia\downarrow} c_{ib\downarrow}^{+} c_{ib\uparrow}^{+} + h.c.\right)$$

$$U' = U - 2J$$

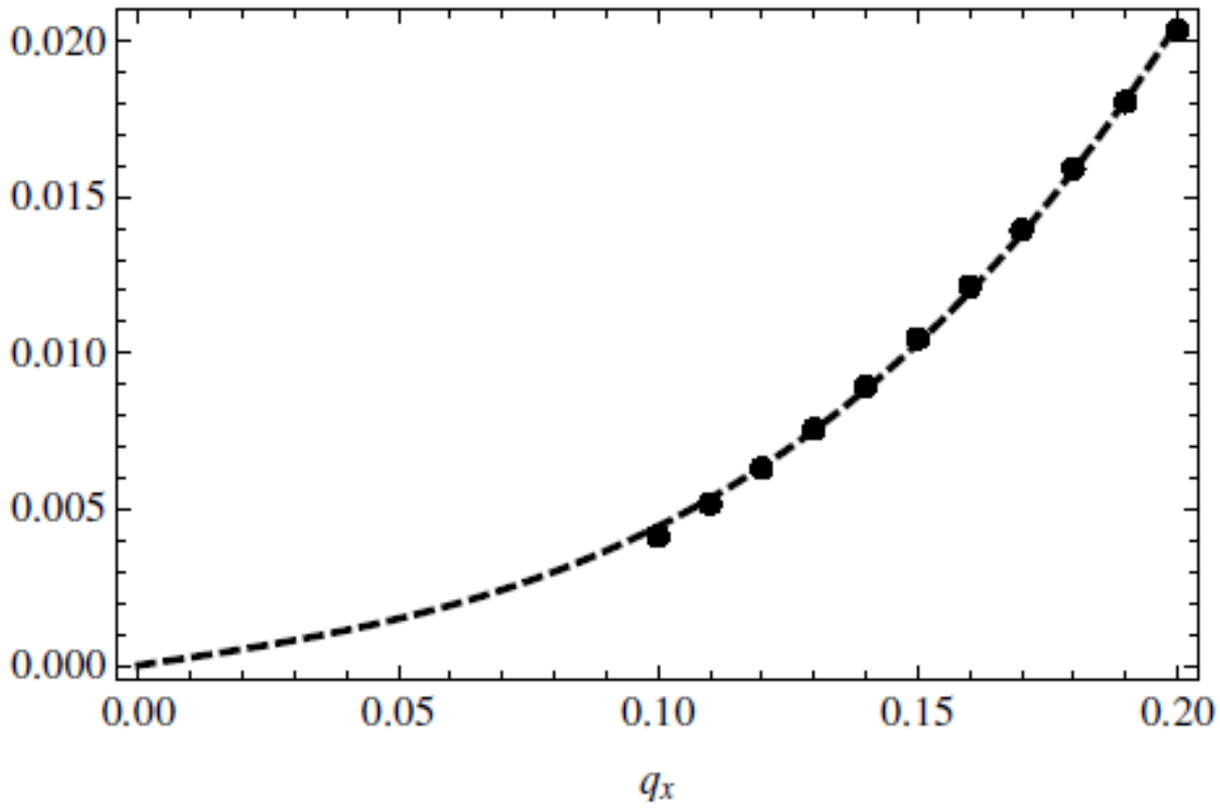
Theoretical approaches:

- 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



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

RPA Study of a Five-Orbital Model

RPA Study of a Five-Orbital Model

- Two-particle correlation function

RPA Study of a Five-Orbital Model

- Two-particle correlation function

RPA Study of a Five-Orbital Model

- Two-particle correlation function

RPA Study of a Five-Orbital Model

- Two-particle correlation function

RPA Study of a Five-Orbital Model

- Two-particle correlation function

RPA Study of a Five-Orbital Model

- Two-particle correlation function

RPA Study of a Five-Orbital Model

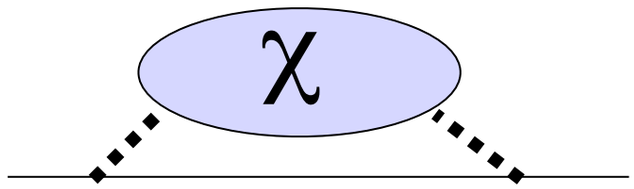
- Two-particle correlation function

$$\chi(q,\omega) = \int dt\, e^{-i\omega t} \left\langle \left[\hat{O}^{+}(q,t), \hat{O}(q,0) \right] \right\rangle \quad , \quad \hat{O}(q,t) = n(q,t), S(q,t)$$

$$H_{\text{int}} = \sum_{q} V_q \hat{O}(q)\hat{O}(-q)$$

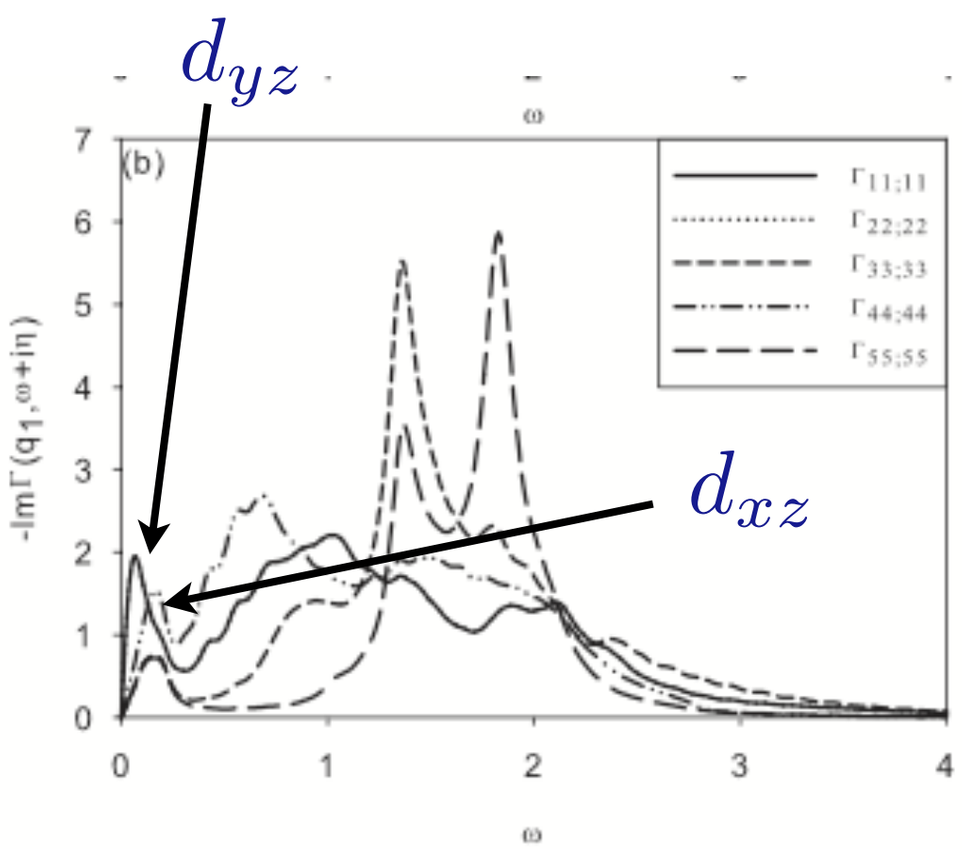
- Correction to electron self energy

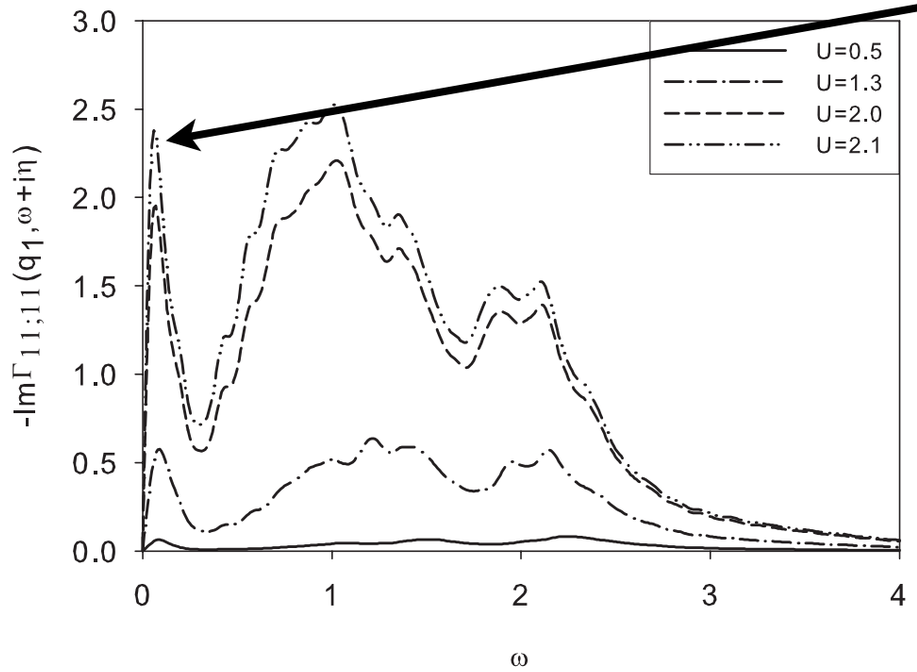
$$\Sigma(k,\nu_n) =$$



$$= \frac{1}{\beta N} \sum_{q,\omega_n} V_q^2 \chi(q,\omega_n) G^0(k-q,\nu_n - \omega_n)$$

is the ZBC incipient orbital ordering: quantum fluctuations

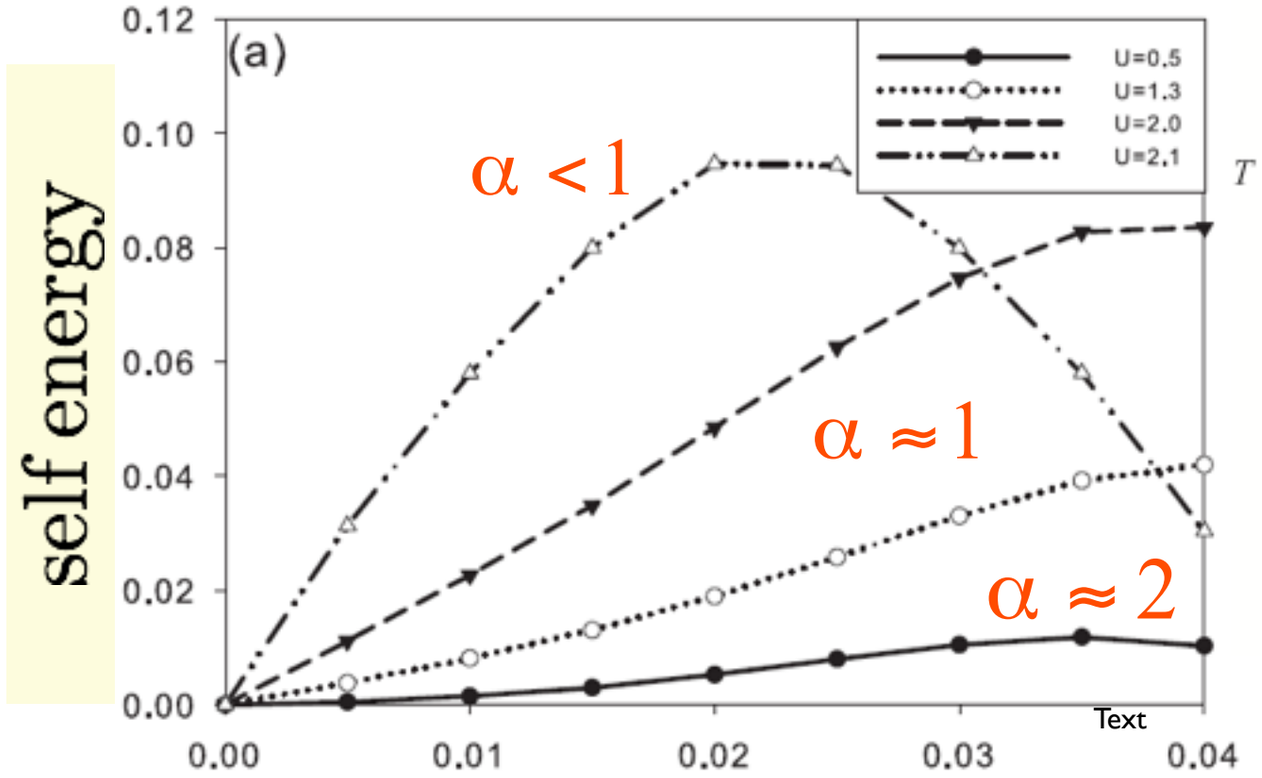


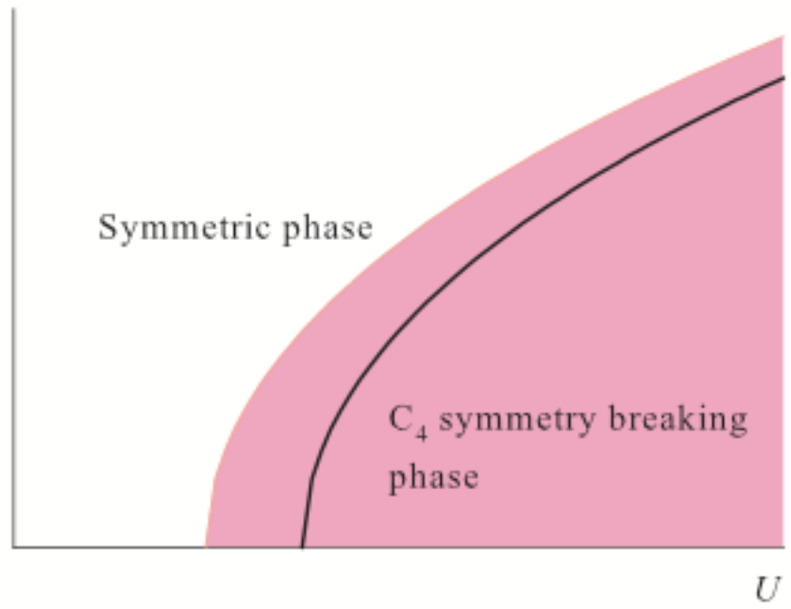


overdamped collective mode

Lee, PP, arXiv:1110.5917

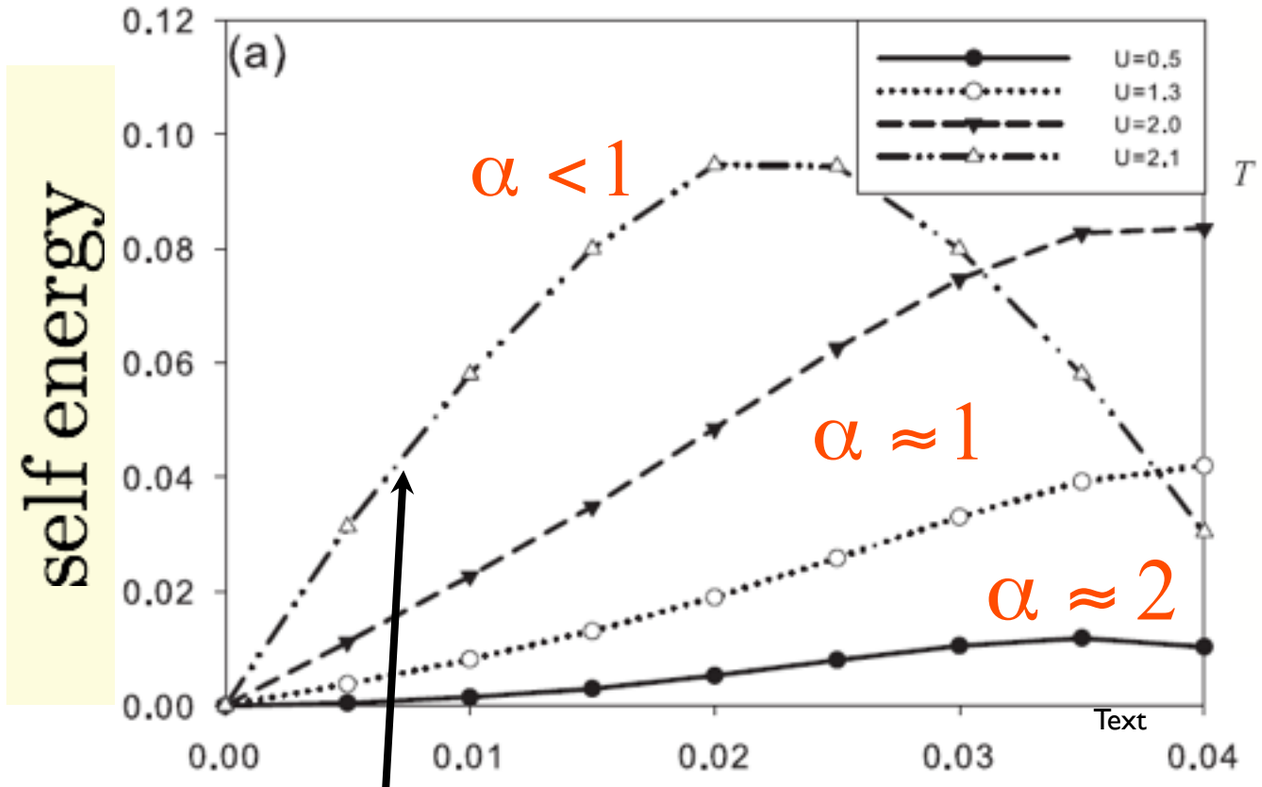
Self-Energy with One Loop Corrections (2-band model)

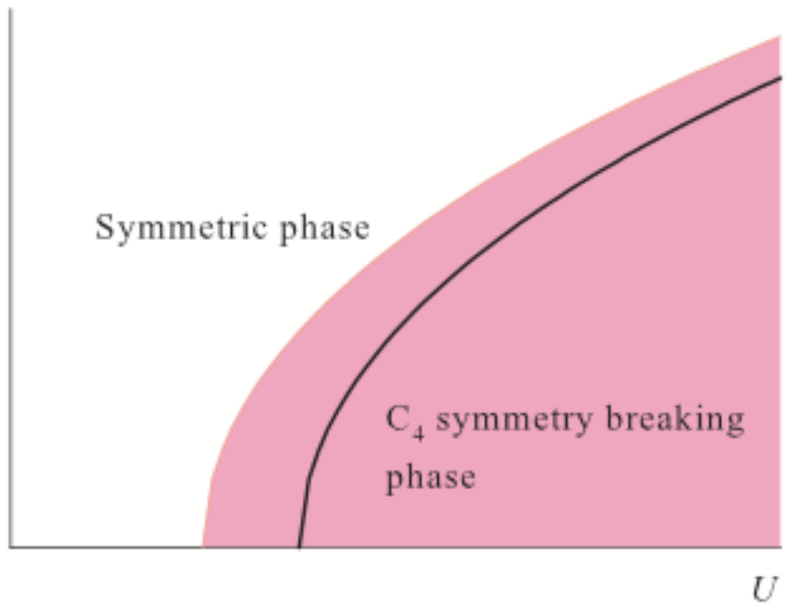




Wei-Cheng Lee, and Philip W. Phillips, Phys. Rev. B **86**, 245113 (2012)

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

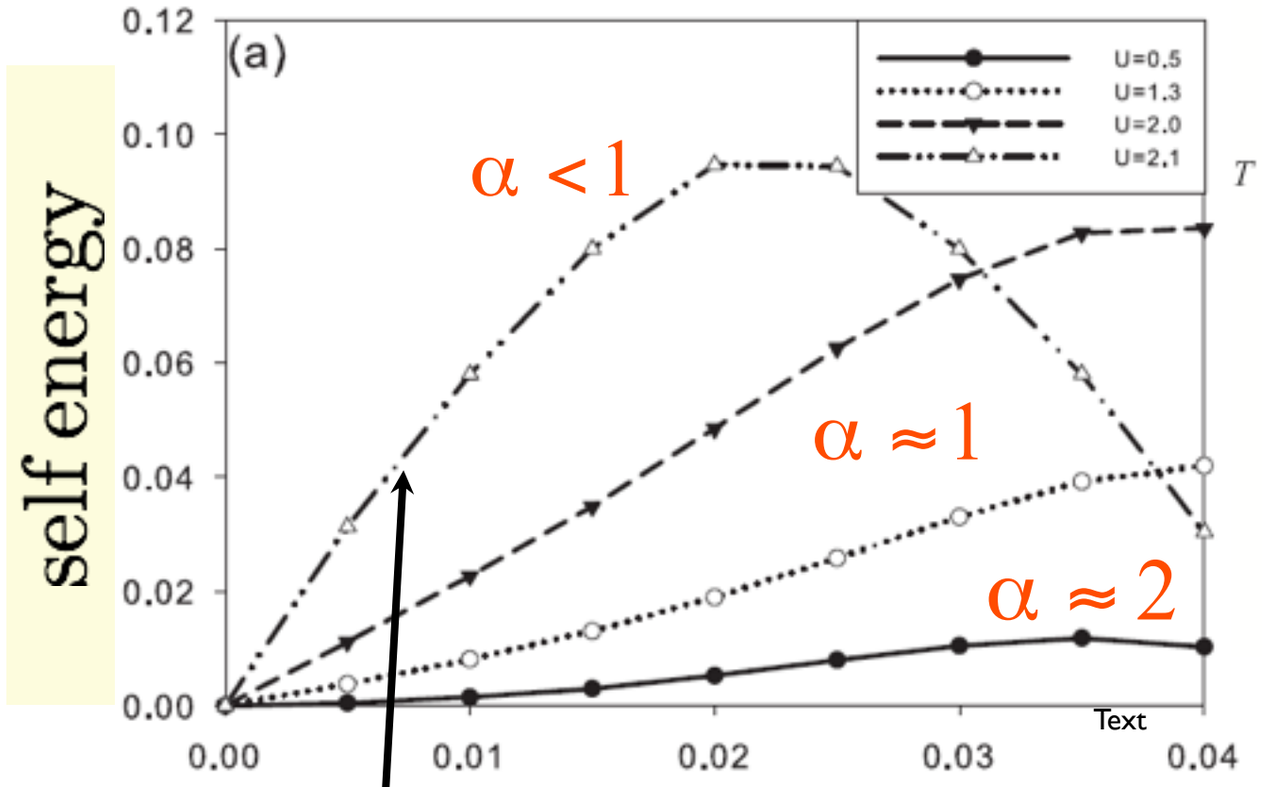


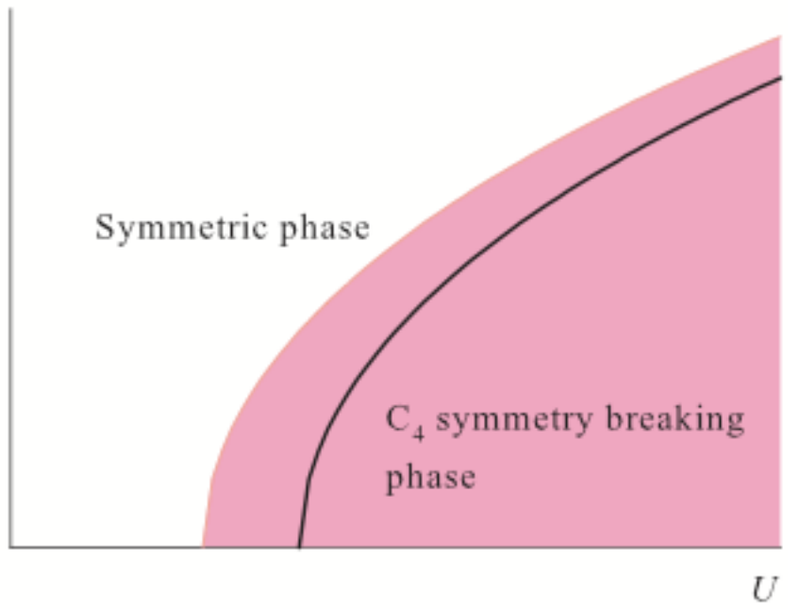


possible ARPES experiment

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

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





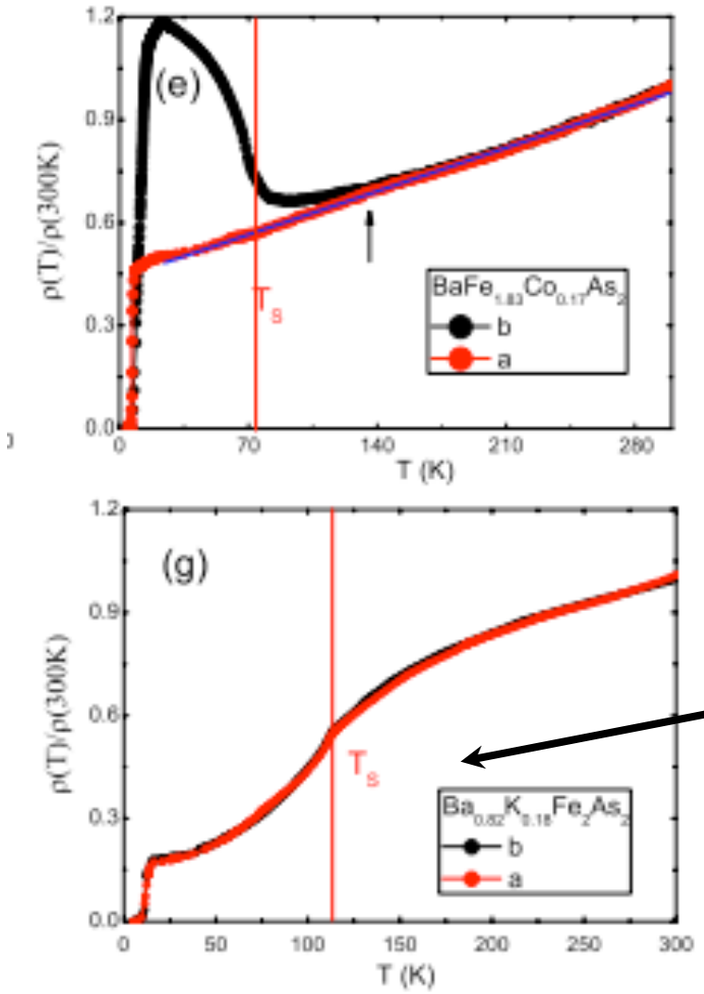
possible ARPES experiment

$$N^*(\omega) = N^*(0) + B\omega^{2/3}\ln\omega + \ldots$$ Lawler, et al., Phys. Rev. B **73**, 085101 (2006)

zero-bias anomaly

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*

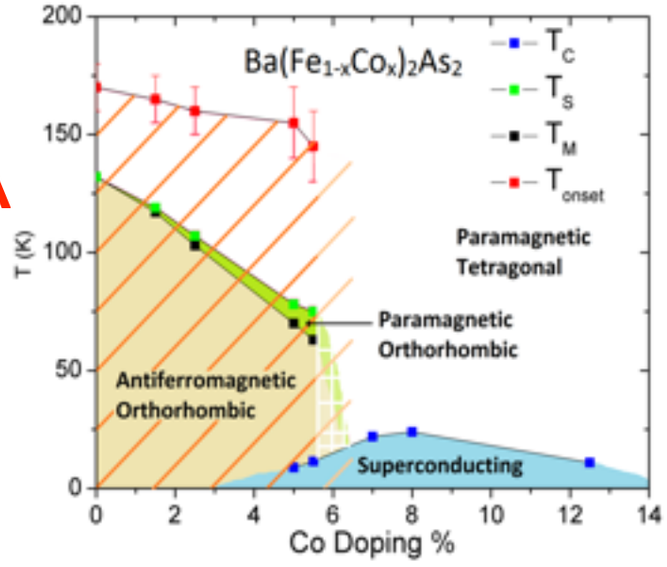
(Received 13 December 2010; published 2 August 2011)

PCS on Fe pnictides and chalcogenides

Greene group has studied these materials:

Column A

1. $Ba(Fe_{1-x}Co_x)_2A$
2. $SrFe_2As_2$
3. Fe_xTe_y
4. Co: NaFeAs
5. $BaFe_2(As_{2-x}P_x)$



EXCESS conductance around zero observed bias in the "normal" state (above the phase transition): Correlated with observed

Electronic `Nematicity'.

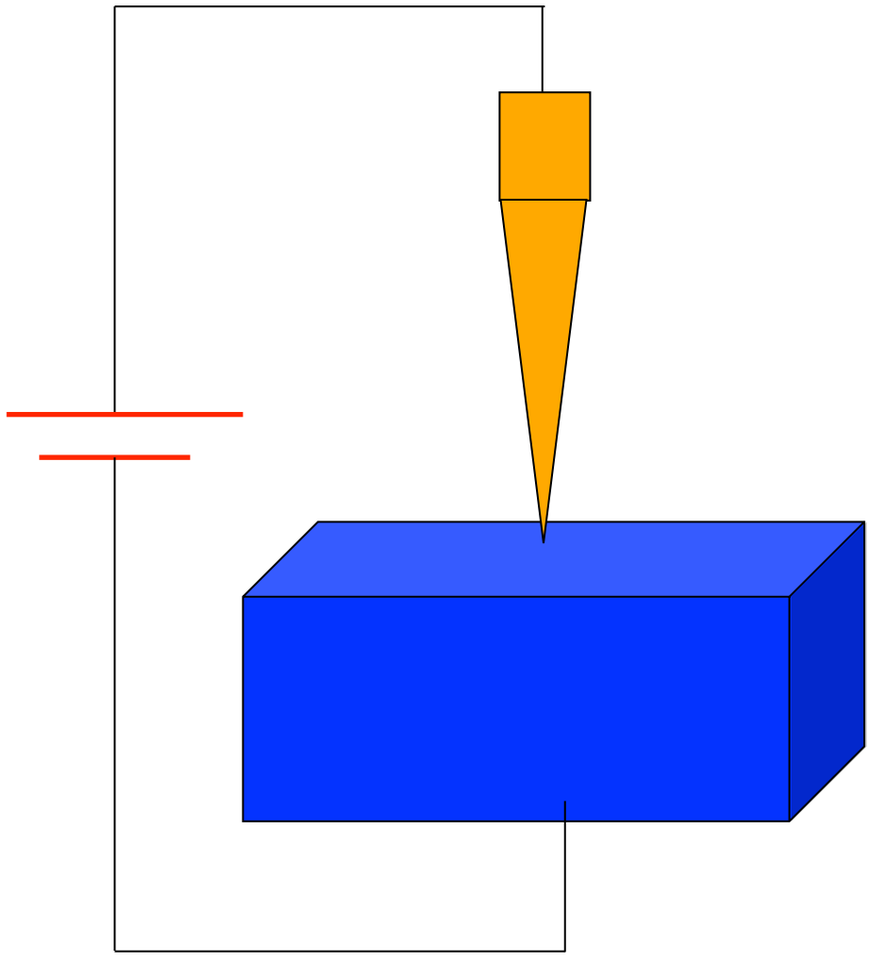
Column B

1. $CaFe_2As_2$
2. $Ba_{0.8}K_{0.2}Fe_2As_2$ *

NO such EXCESS conductance observed:

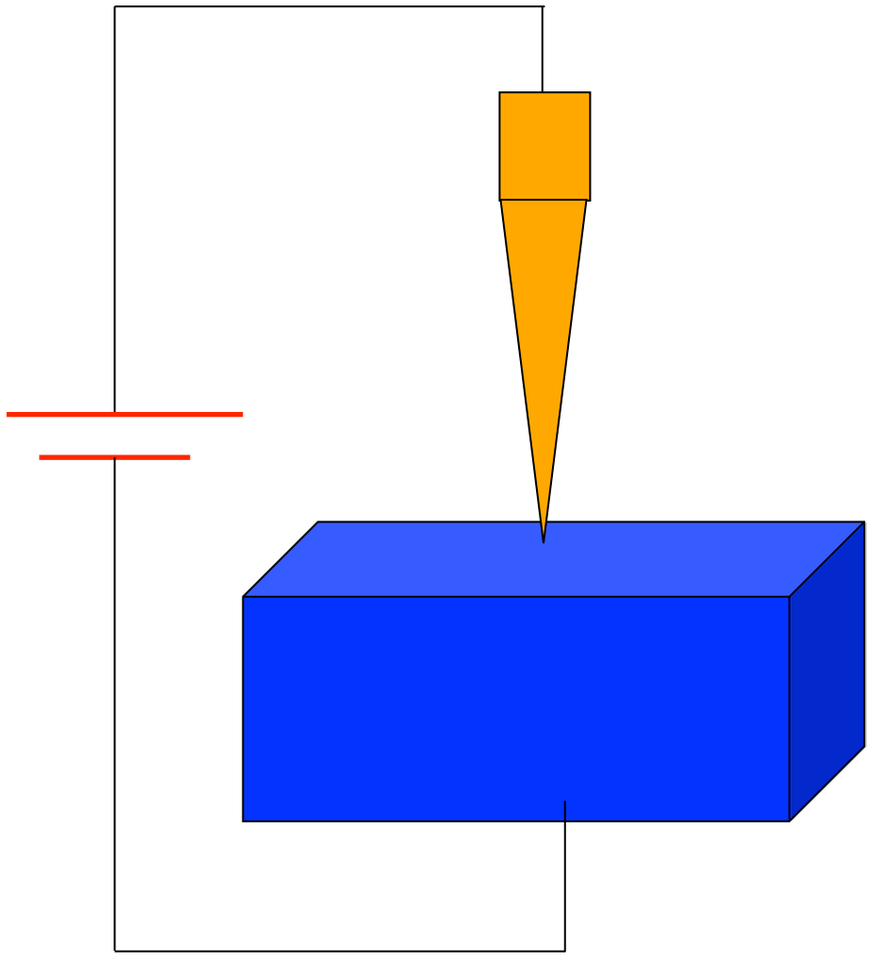
Resistivity anisotropy not seen (*or over a smaller T-range**)** in these compounds. (PRL 107, 067001 (2011))

Point Contact Spectroscopy



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

Point Contact Spectroscopy

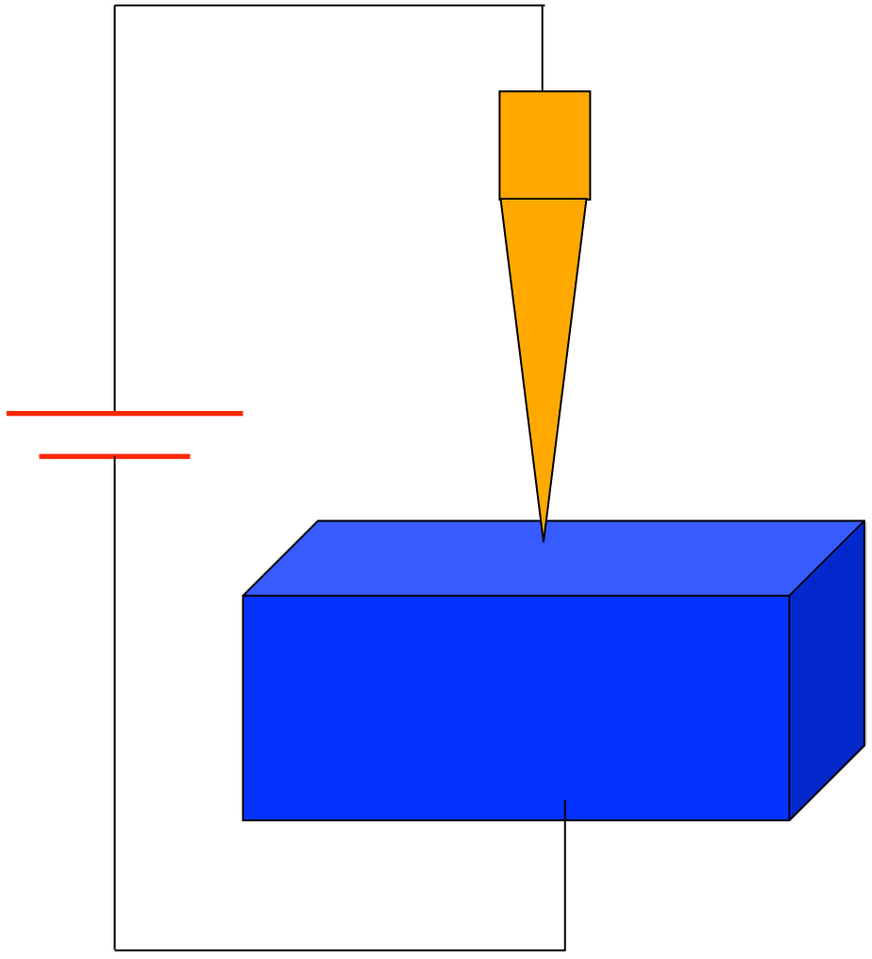


Using Keldysh formalism, for small voltage bias,

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

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

Point Contact Spectroscopy



Using Keldysh formalism, for small voltage bias,

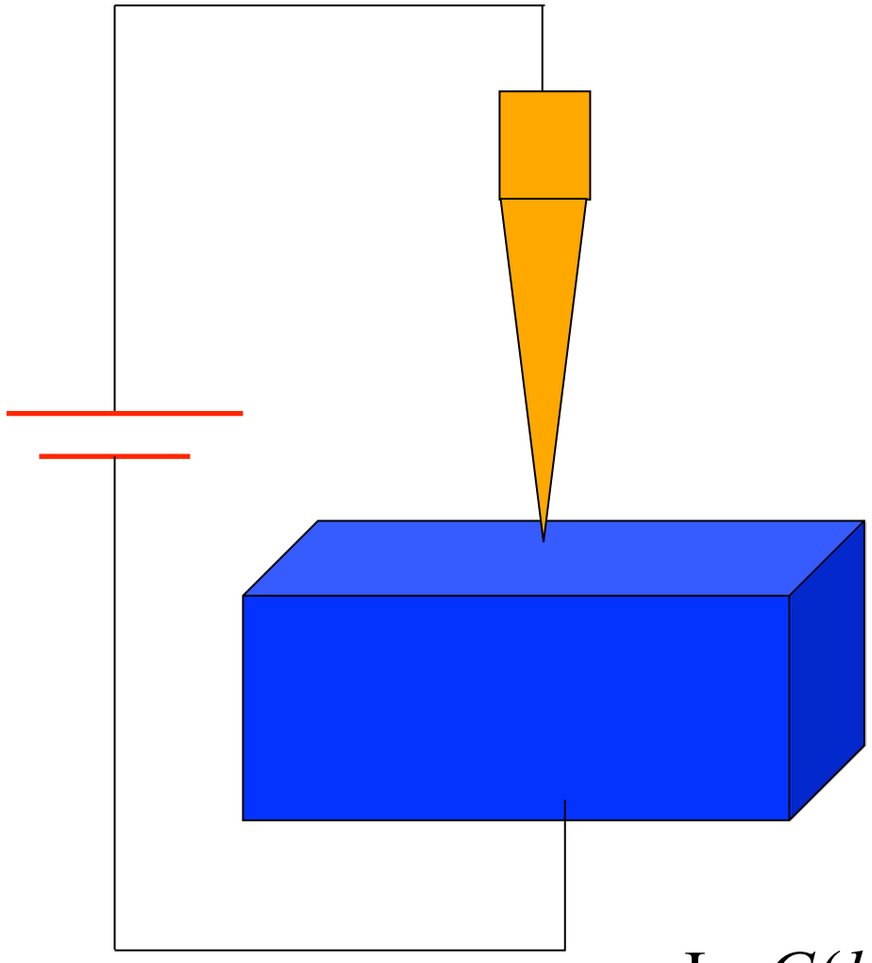
$$\frac{dI}{dV} \propto \int dk\, T(k, eV)\, \mathrm{Im}\, G(k, eV)$$

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.,* 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

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

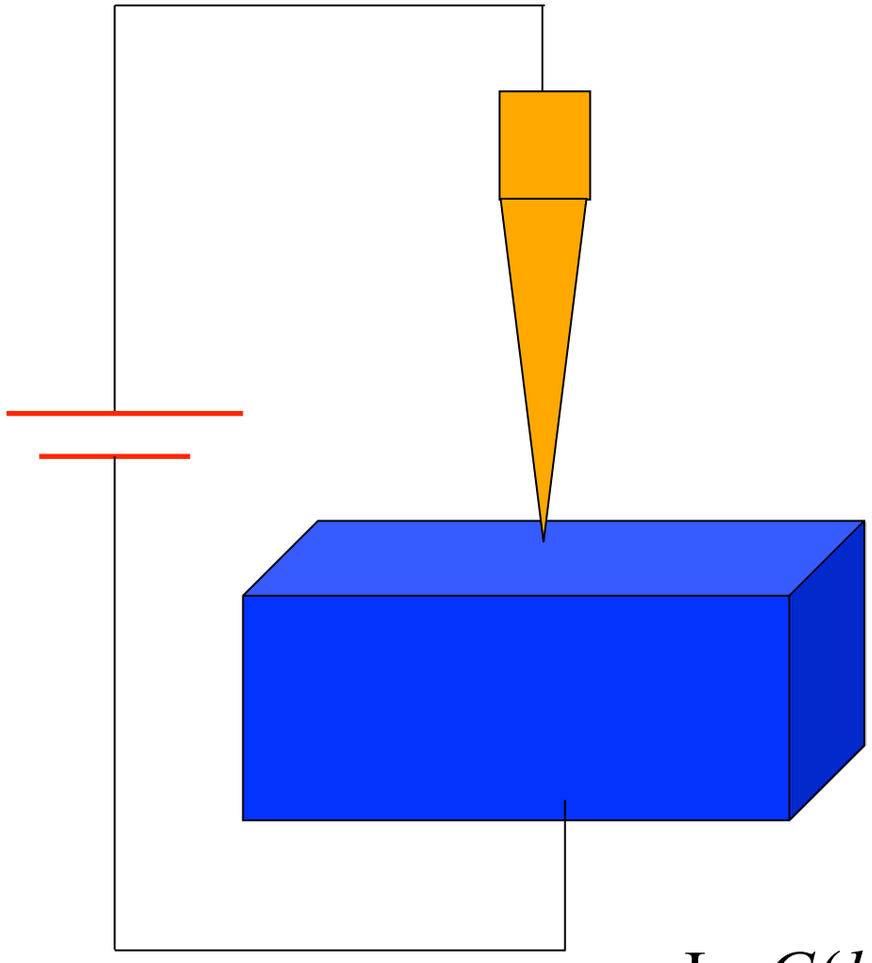
For non-Fermi liquid due to nematic QCP,

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

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

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

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

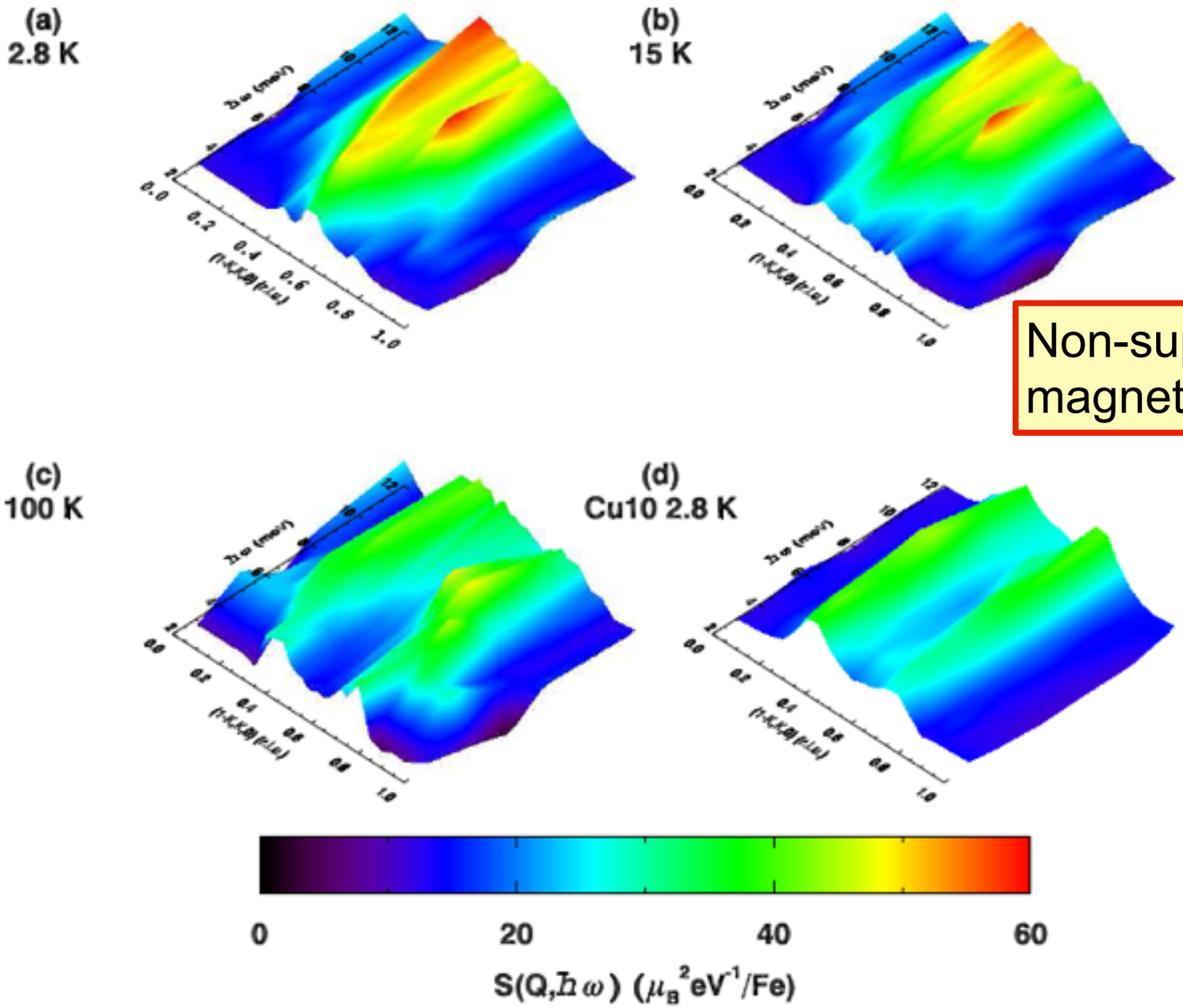
$$\frac{dI}{dV} \propto \int d\vec{k}\, \mathrm{Im}\, G(k, eV) = const. + A(eV / E_F)^{2/3} \ln(eV / E_F)$$

a peak at eV=0!!!

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

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

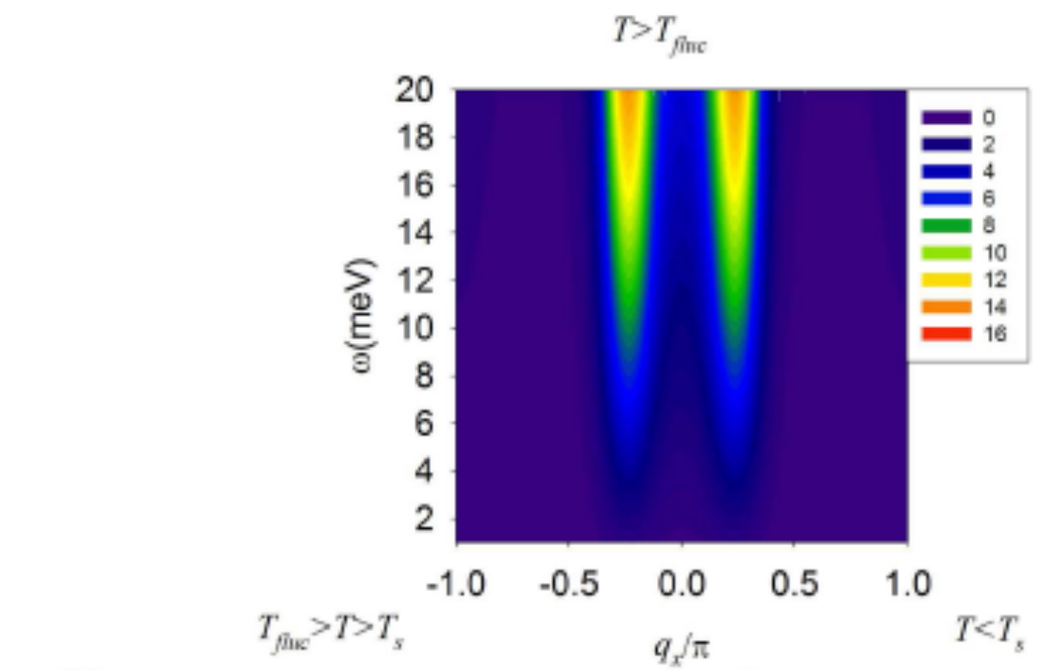
Incommensurate-to-Commensurate Transformation in $Fe_{1-x}Ni_xTe_{0.5}Se_{0.5}$



Non-superconducting - Incommensurate magnetic excitation all the time

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

RPA + Gaussian Fluctuations



normal state without orbital fluctuations

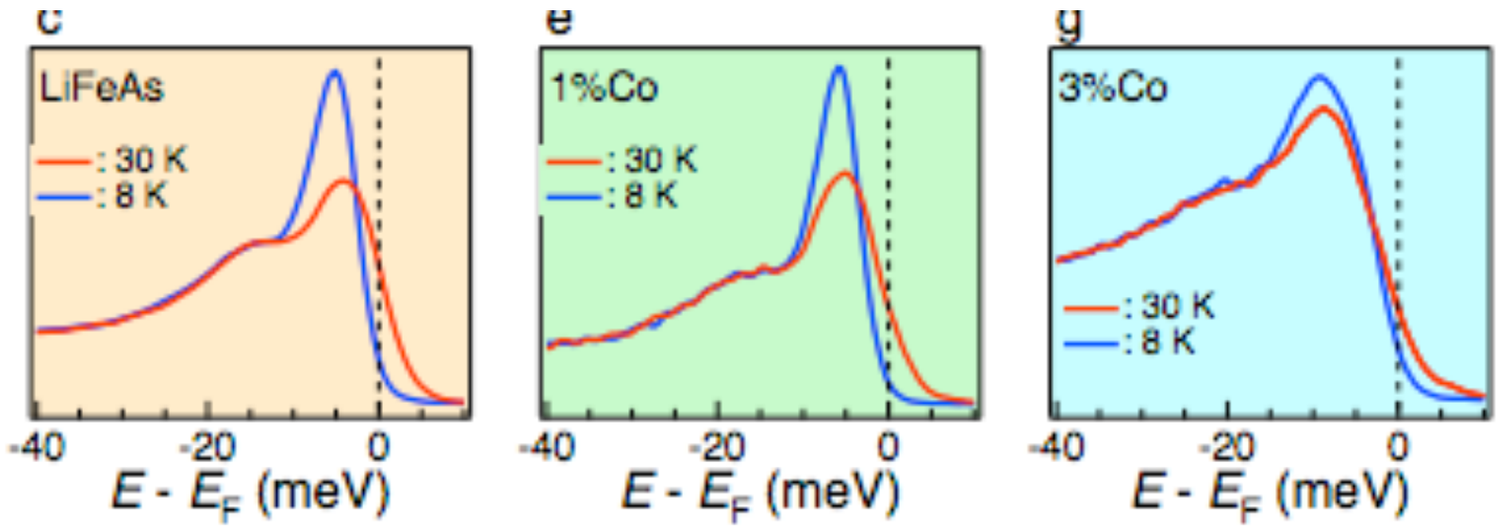
Fluctuating orbital order (modeled by Gaussian fluctuation model)

Orbital ordered state

orbital ordering
not spin physics (nematicity)

Observation of strong electron pairing on bands without Fermi surfaces in $LiFe_{1-x}Co_xAs$

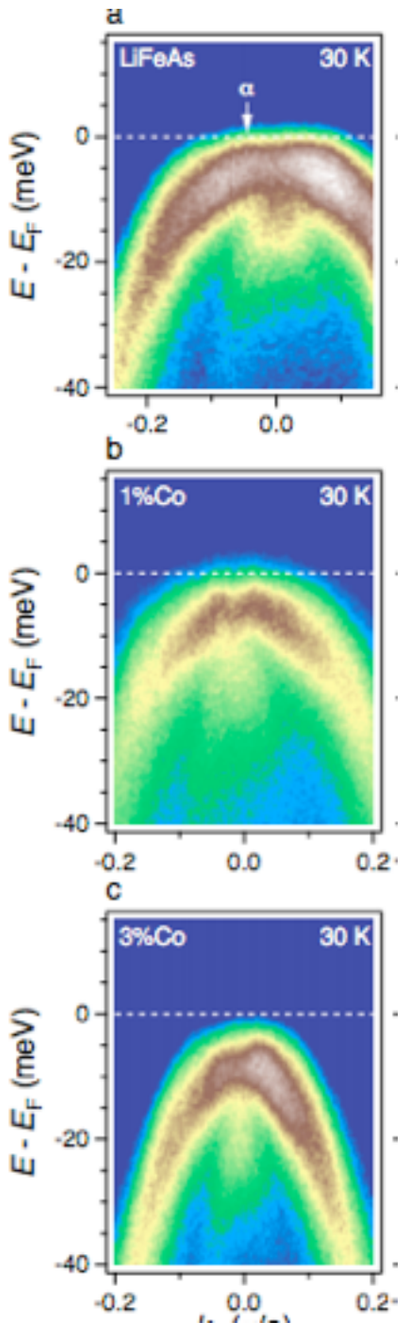
H. Miao[1], T. Qian[1,*], X. Shi[1], P. Richard[1,2], T. K. Kim[3], M. Hoesch[3], L. Y. Xing[1], X. –C. Wang[1], C. –Q. Jin[1,2], J. –P. Hu[1,2,4] and H. Ding[1,2,*]



gapped degrees of freedom=> beyond particles (BCS)

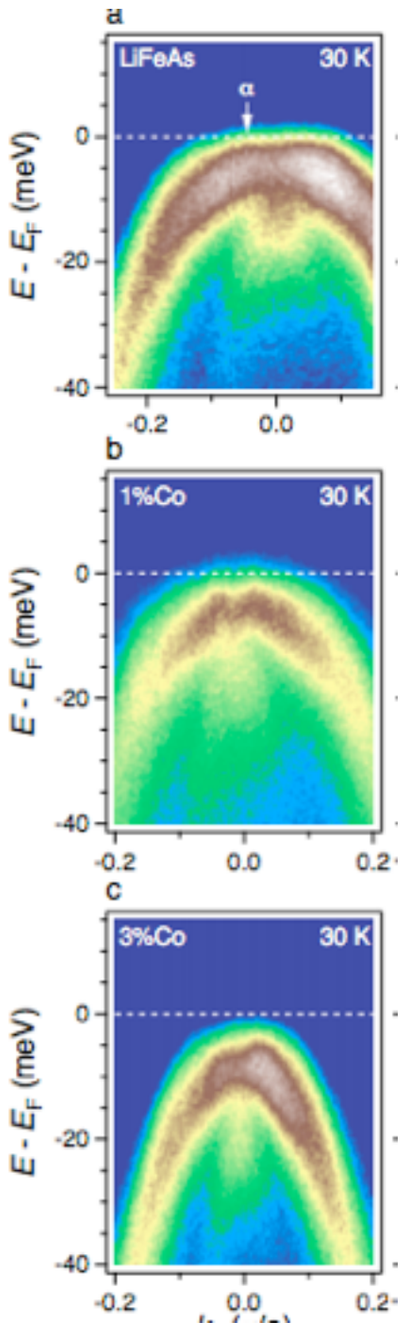
$LiFe_{1-x}Co_xAs$

H. Ding
1406.0983



$LiFe_{1-x}Co_xAs$

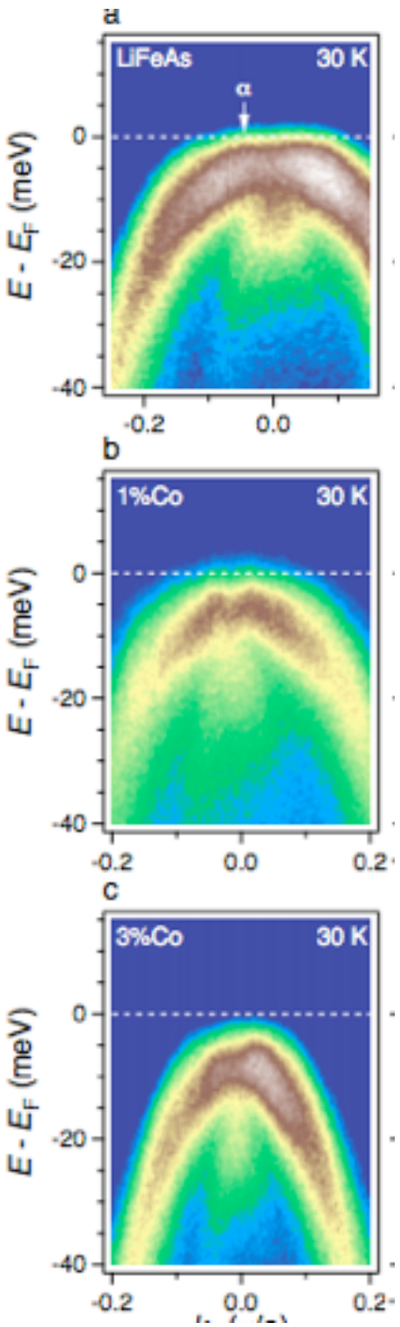
H. Ding
1406.0983



$> \Delta_{SC}$

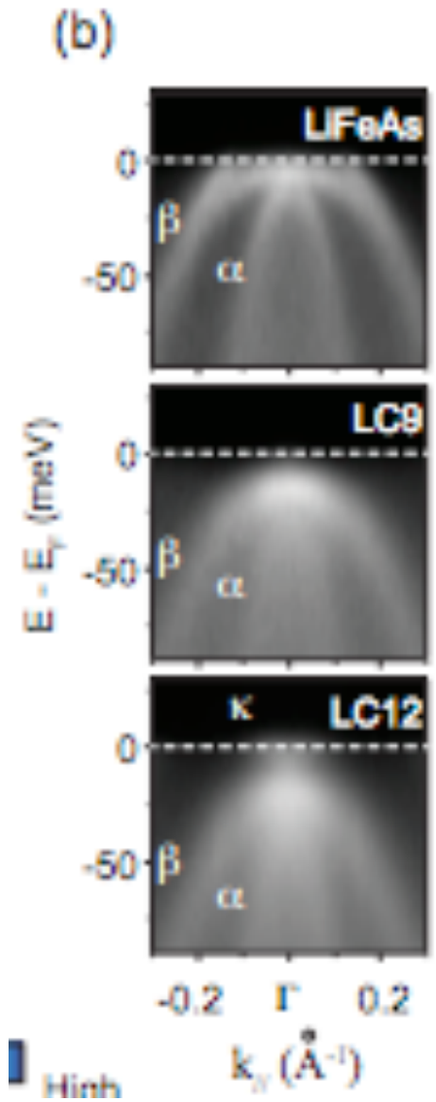
$LiFe_{1-x}Co_xAs$

H. Ding
1406.0983



$> \Delta_{SC}$

Z. R. Ye



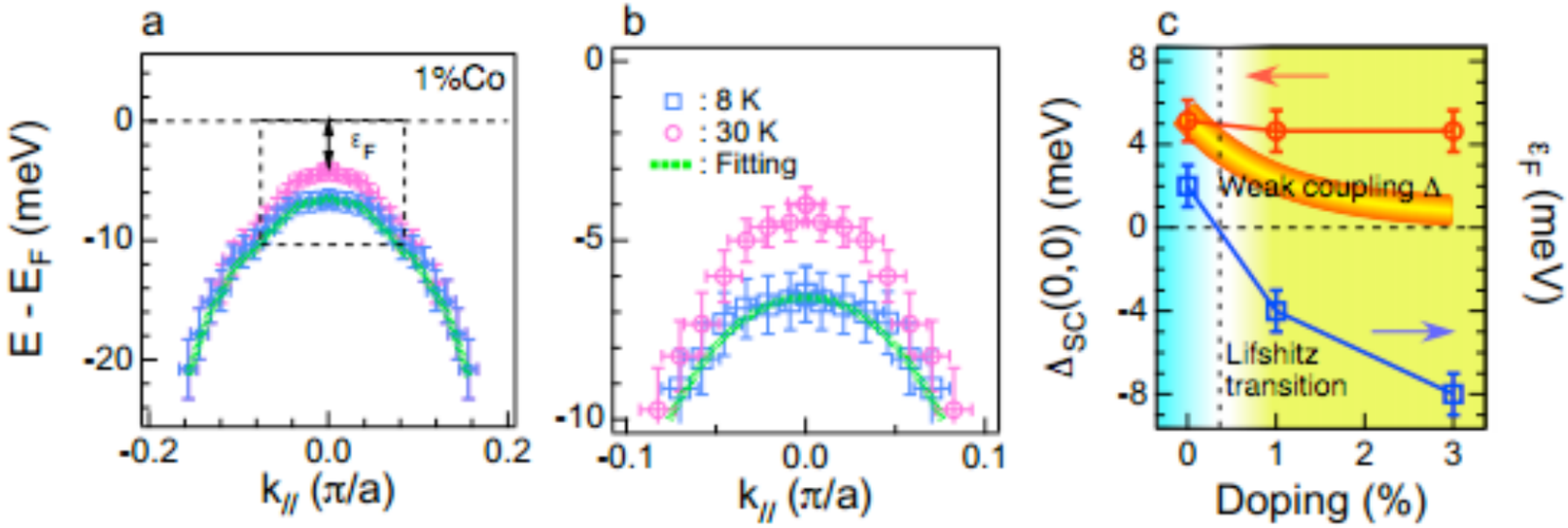
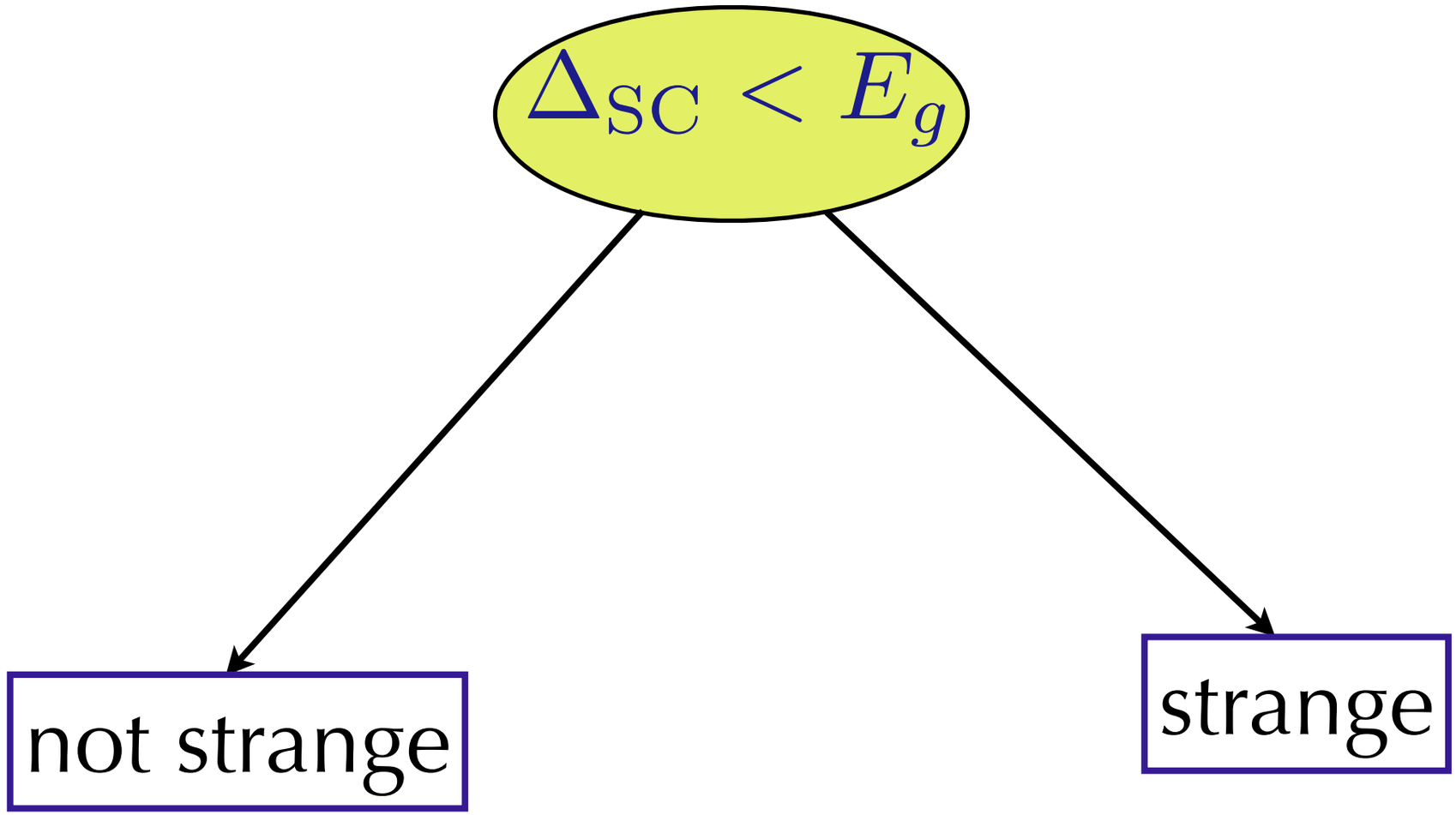

a
1%Co
E - E_F (meV)
0
-10
-20
ε_F
-0.2
0.0
0.2
k_// (π/a)
b
: 8 K
: 30 K
: Fitting
0
-5
-10
-0.1
0.0
0.1
k_// (π/a)
c
Δ_SC(0,0) (meV)
8
4
0
-4
-8
Weak coupling Δ
Lifshitz
transition
0
1
2
3
Doping (%)
ε_F (meV)

Figure 4

pairing without a Fermi surface?



not strange

5-band model

not strange

5-band model

e-repulsion

$$Z_i(2n+1)\Delta_i(2n+1) = \pi k_B T \sum_m \sum_j \frac{\Delta_j(2m+1)}{\sqrt{k_m^2 + \delta_j^2(2m+1)}} \left[V_{ij}^{\rm ph}(n-m) - V_{ij}^{\rm ee} \right]$$

not strange

5-band model

e-repulsion

$$Z_i(2n+1)\Delta_i(2n+1) = \pi k_B T \sum_m \sum_j \frac{\Delta_j(2m+1)}{\sqrt{k_m^2 + \delta_j^2(2m+1)}} \left[V_{ij}^{\rm ph}(n-m) - V_{ij}^{\rm ee} \right]$$

$$\Delta_1 > 0$$

not strange

5-band model

e-repulsion

$$Z_i(2n+1)\Delta_i(2n+1) = \pi k_B T \sum_m \sum_j \frac{\Delta_j(2m+1)}{\sqrt{k_m^2 + \delta_j^2(2m+1)}} \left[V_{ij}^{\mathrm{ph}}(n-m) - V_{ij}^{\mathrm{ee}} \right]$$

$V_{ij}^{\mathrm{ph}} = 0$

$\Delta_1 > 0$

$\Delta_2 < 0$

not strange

5-band model

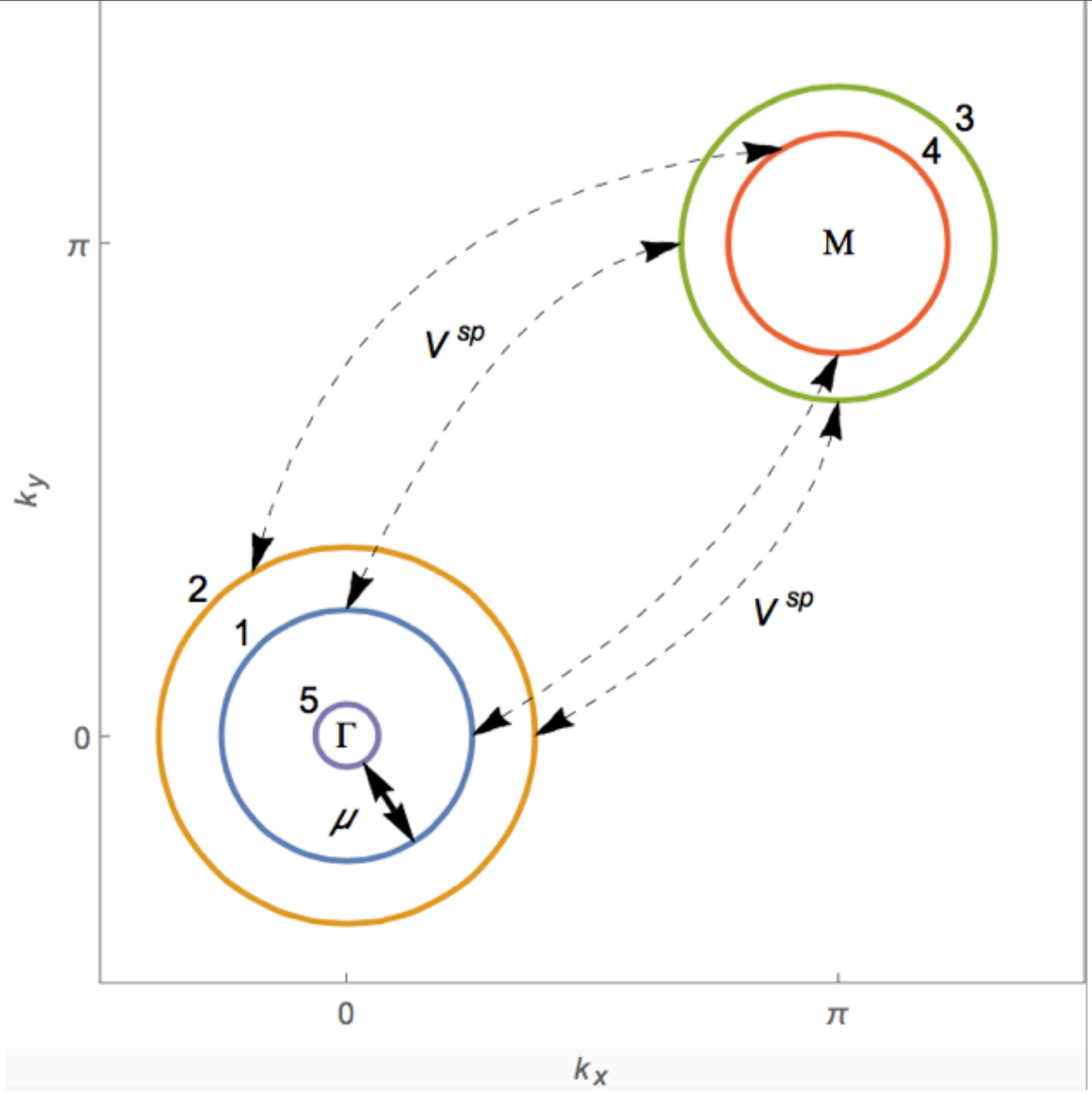
e-repulsion

$$Z_i(2n+1)\Delta_i(2n+1) = \pi k_B T \sum_m \sum_j \frac{\Delta_j(2m+1)}{\sqrt{k_m^2 + \delta_j^2(2m+1)}} \left[V_{ij}^{\mathrm{ph}}(n-m) - V_{ij}^{\mathrm{ee}} \right]$$

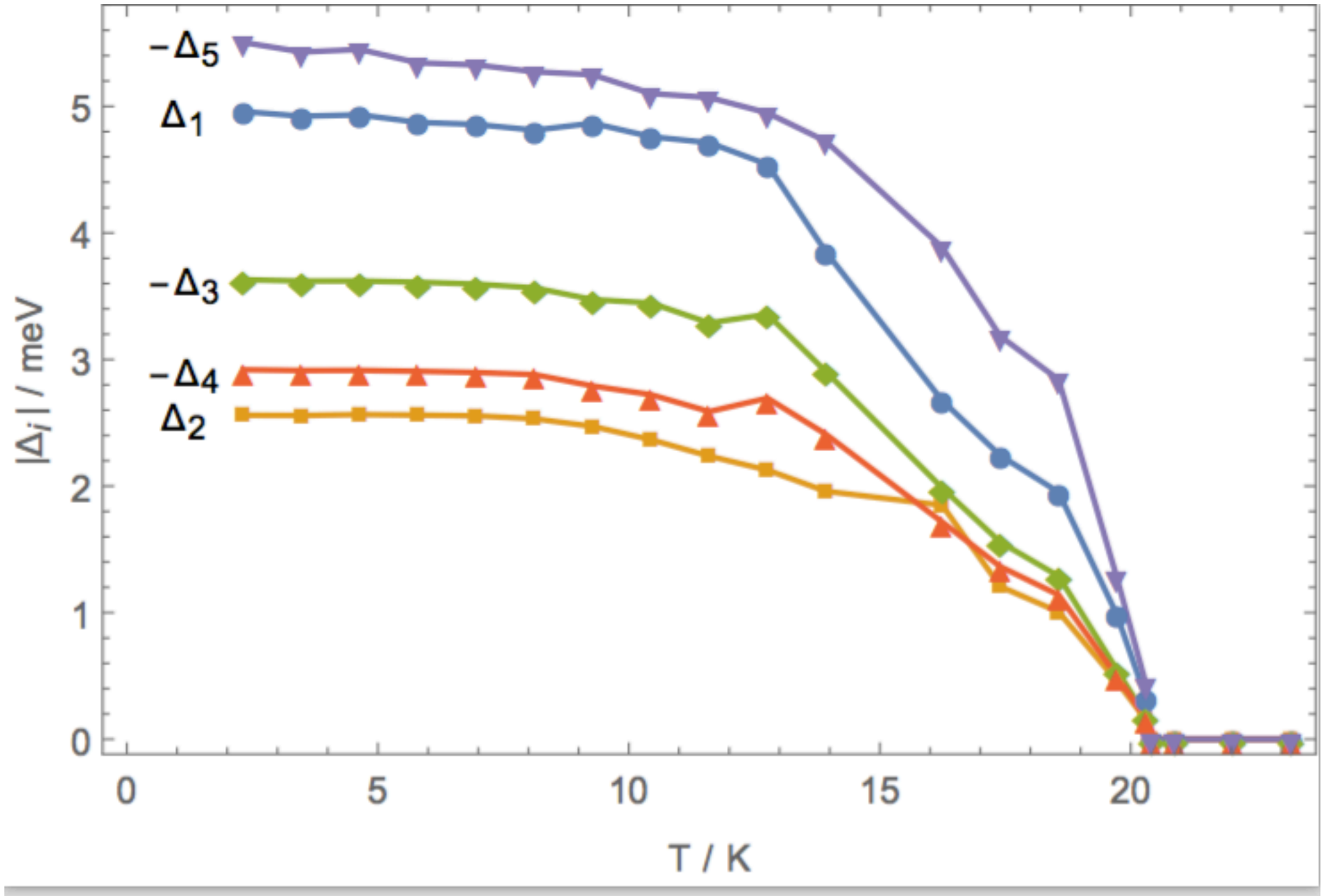
$$V_{ij}^{\mathrm{ph}} = 0$$

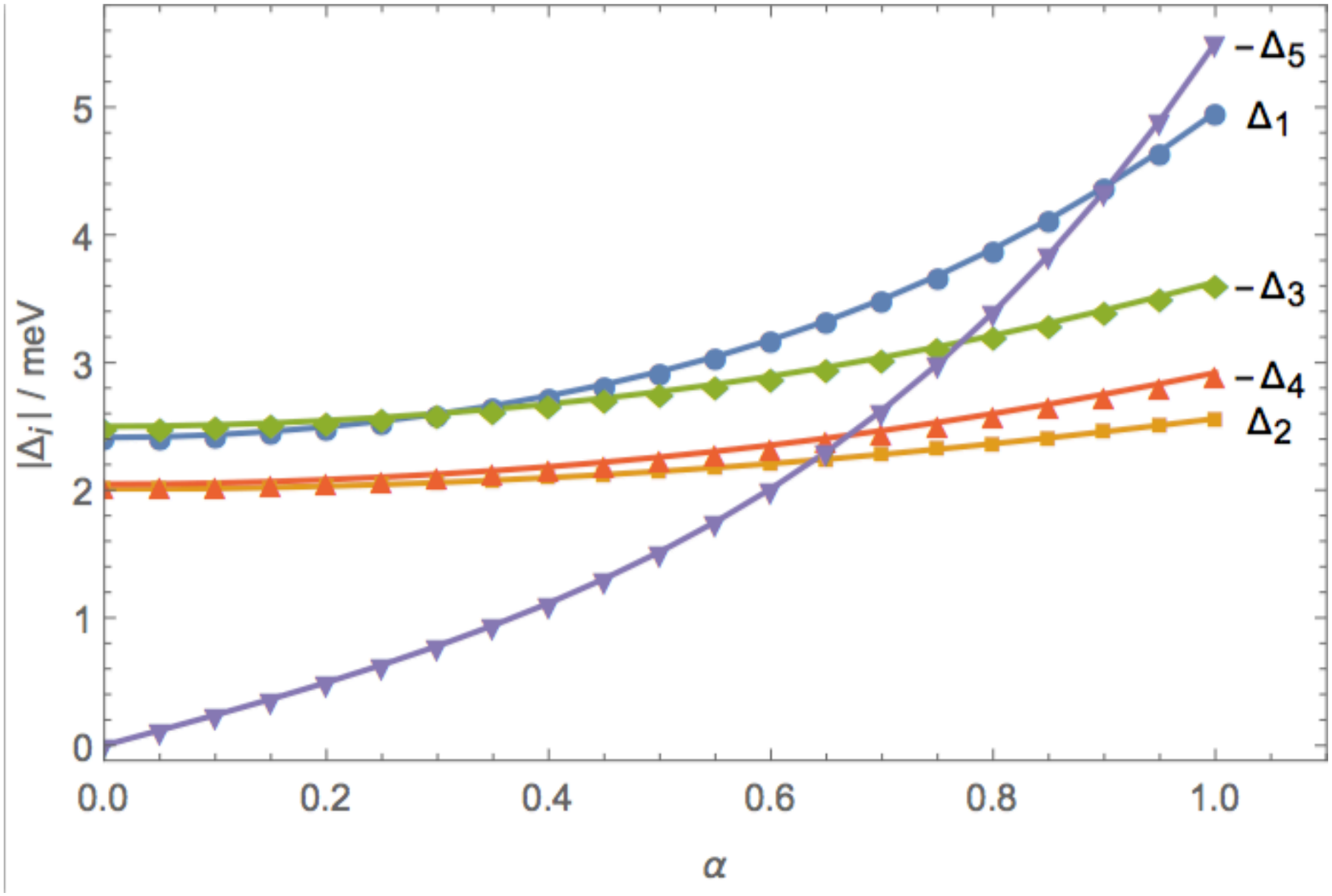
$$\Delta_1 > 0 \qquad \Delta_2 < 0$$

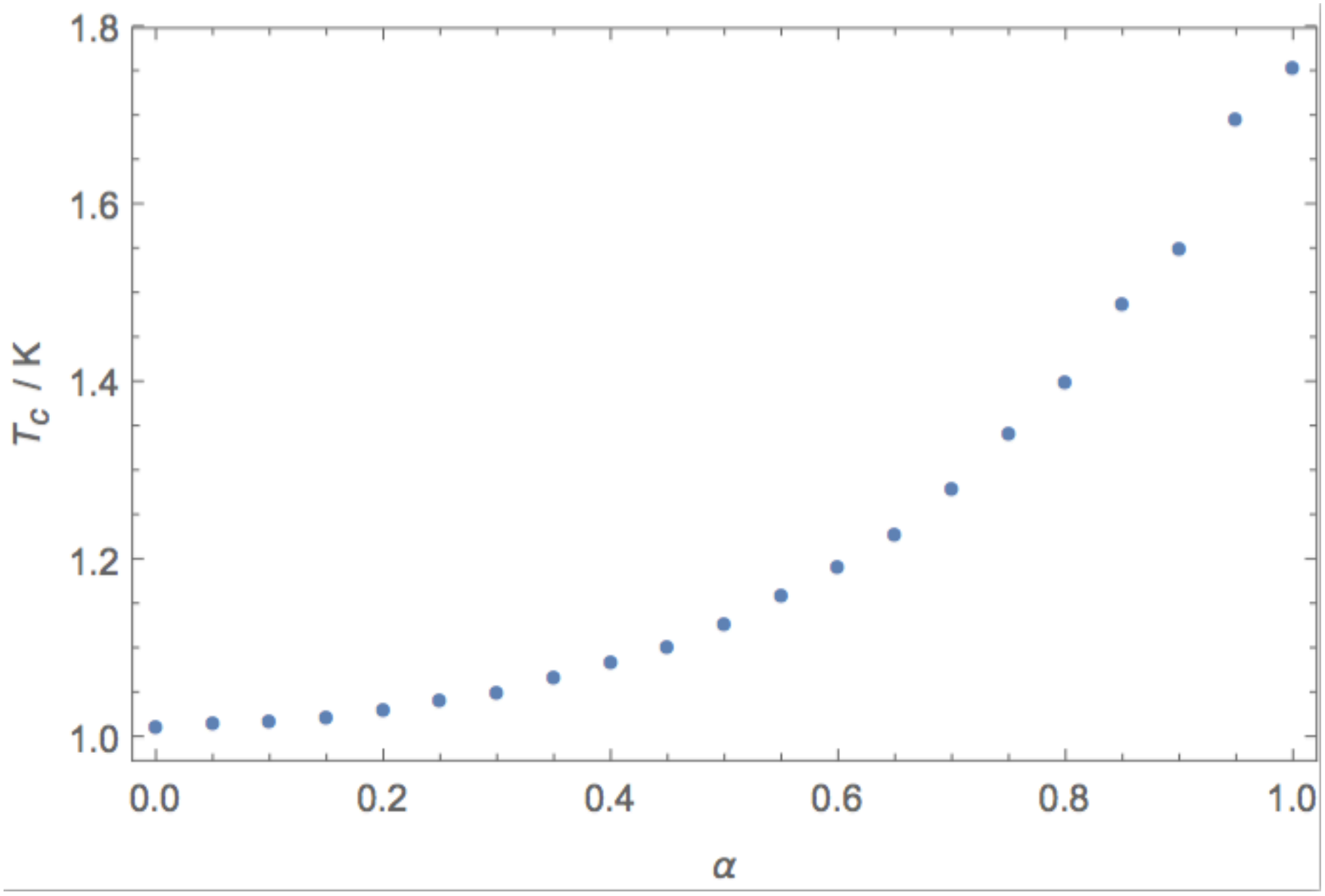
$s^{\pm}$ superconductivity


3
4
M
V^{sp}
V^{sp}
2
1
5
Γ
μ
π
0
k_y
0
π
k_x

Solve Eliashberg Equations

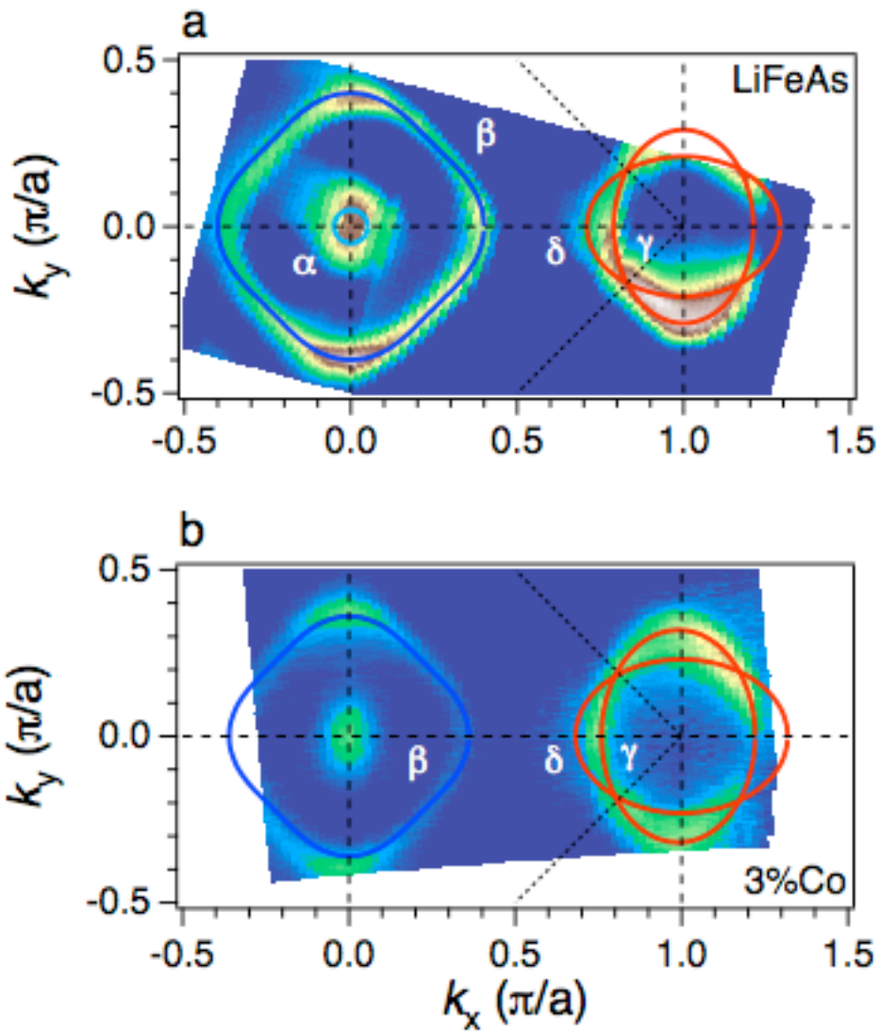

−Δ5
Δ1
−Δ3
−Δ4
Δ2
|Δi| / meV
0
1
2
3
4
5
0
5
10
15
20
T / K


$-\Delta_5$
Δ_1
$-\Delta_3$
$-\Delta_4$
Δ_2
$|\Delta_i|$ / meV
0
1
2
3
4
5
0.0
0.2
0.4
0.6
0.8
1.0
α

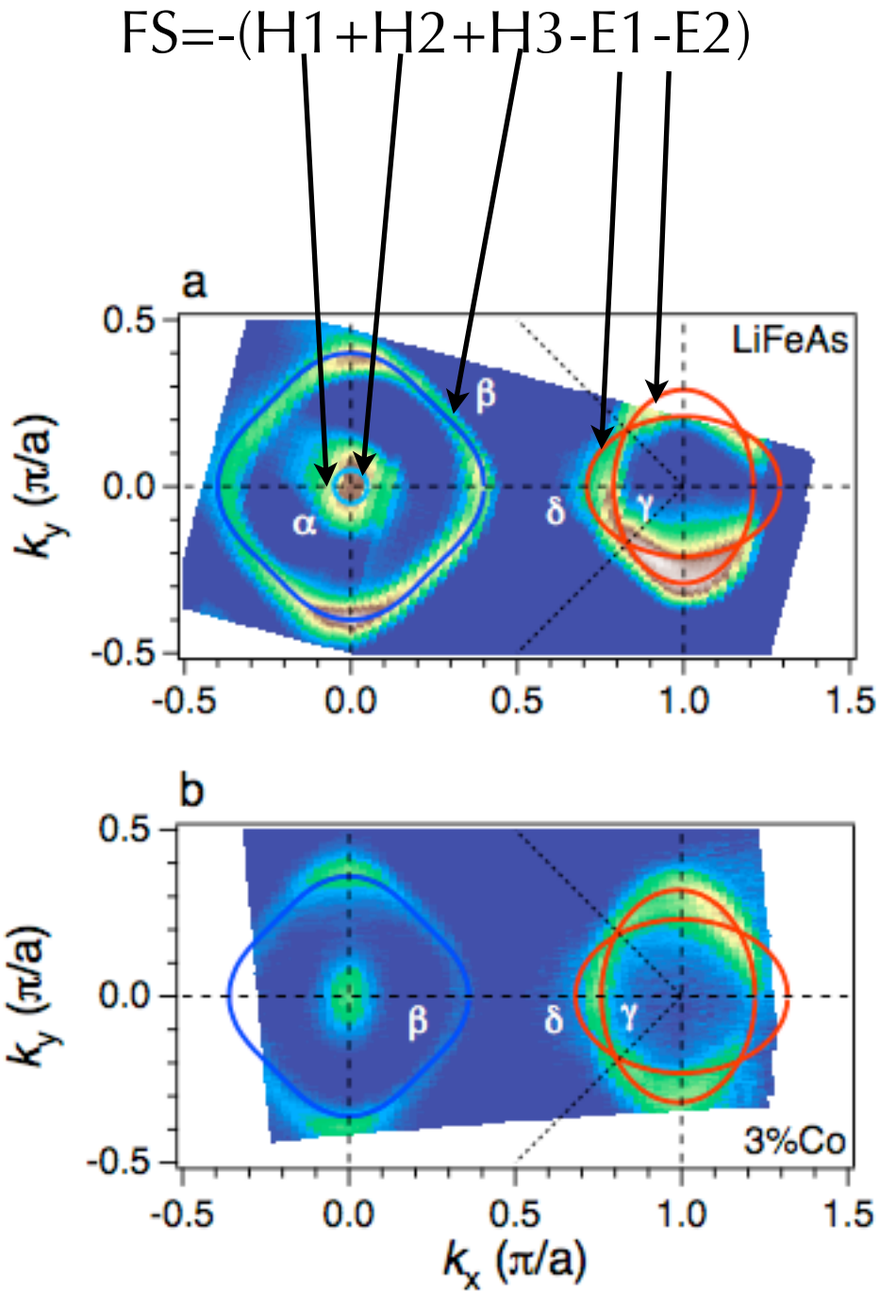

1.8
1.6
1.4
1.2
1.0
T_c / K
0.0
0.2
0.4
0.6
0.8
1.0
α

strange

compute FS volume

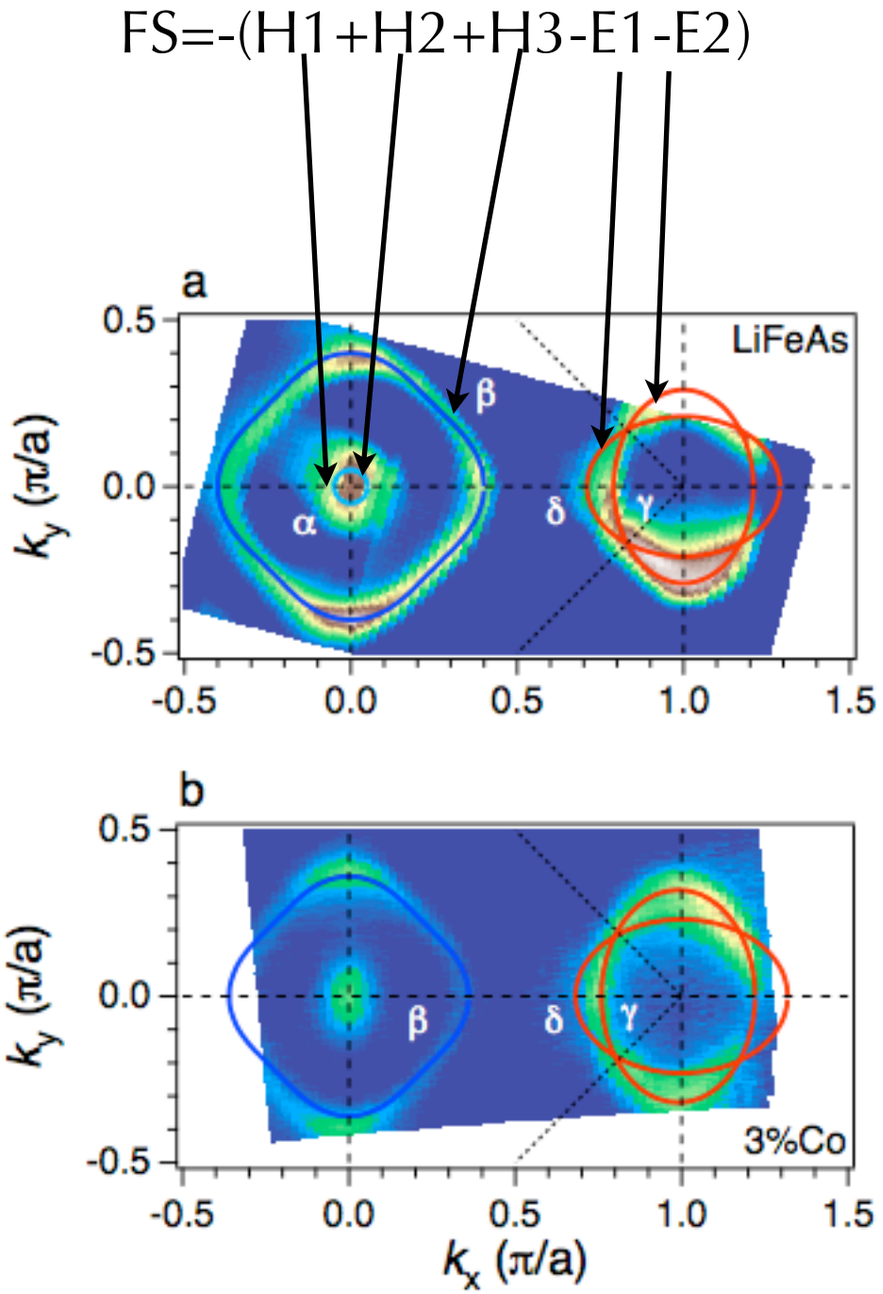


compute FS volume



compute FS volume

FS=-(H1+H2+H3-E1-E2)

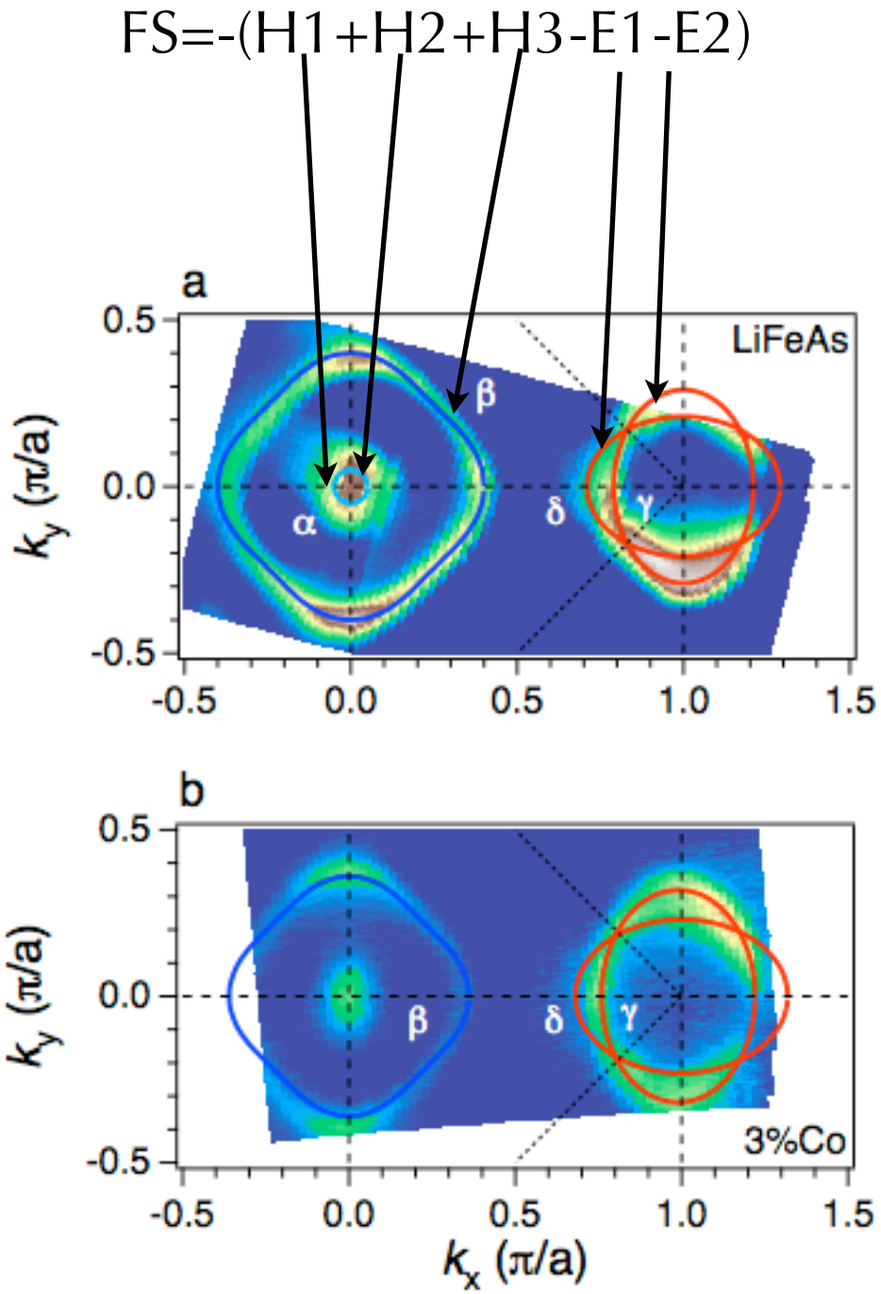


Undoped LiFeAs:
H1=0.00336
H2=0.00336
H3=0.219
E1=0.0948
E2=0.0944

3% Co-doped LiFeAs:
H1=0
H2=0
H3=0.177
E1=0.115
E2=0.115

compute FS volume

FS=-(H1+H2+H3-E1-E2)



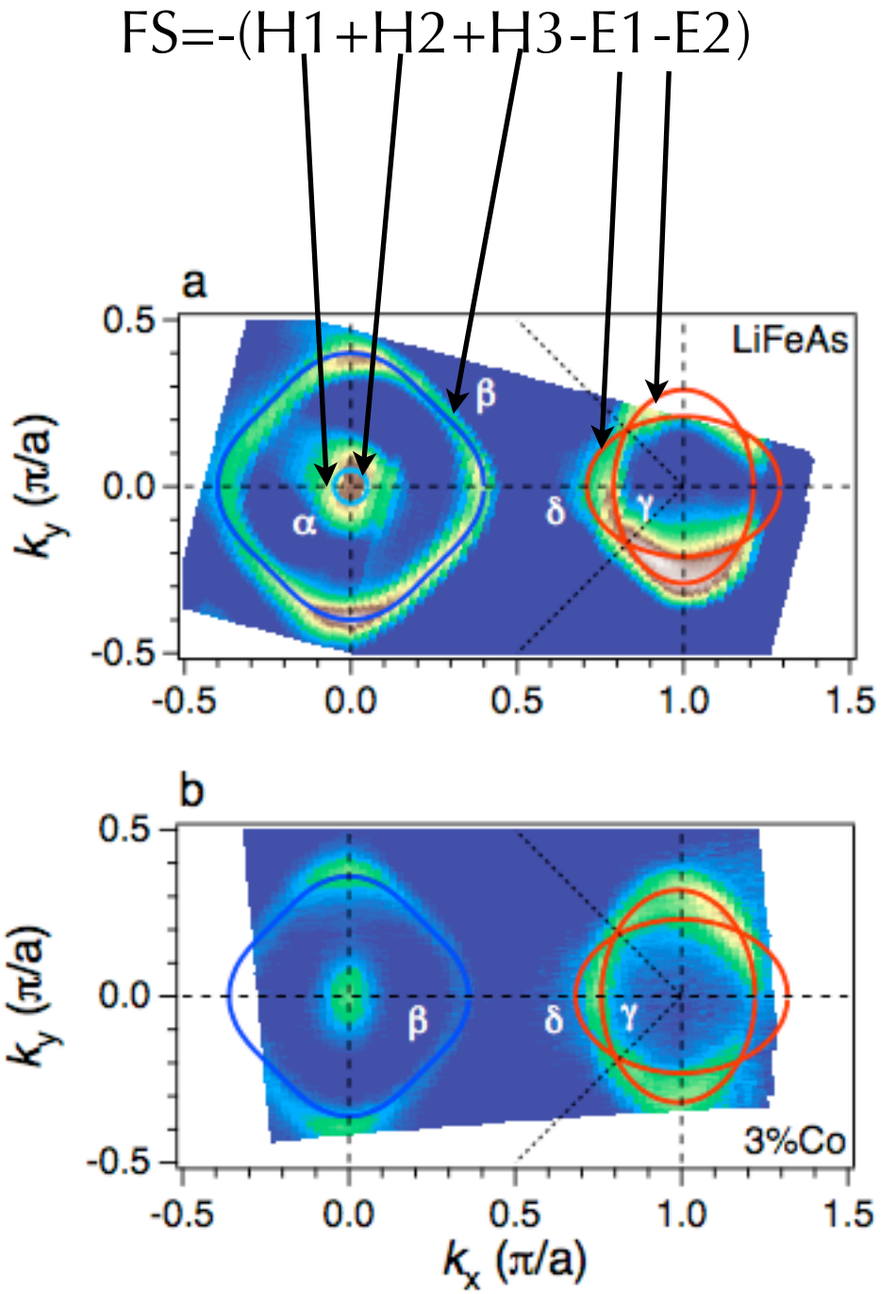
Undoped LiFeAs:
H1=0.00336
H2=0.00336
H3=0.219
E1=0.0948
E2=0.0944

3% Co-doped LiFeAs:
H1=0
H2=0
H3=0.177
E1=0.115
E2=0.115

FS(b)-FS(a)=0.09

compute FS volume

FS=-(H1+H2+H3-E1-E2)



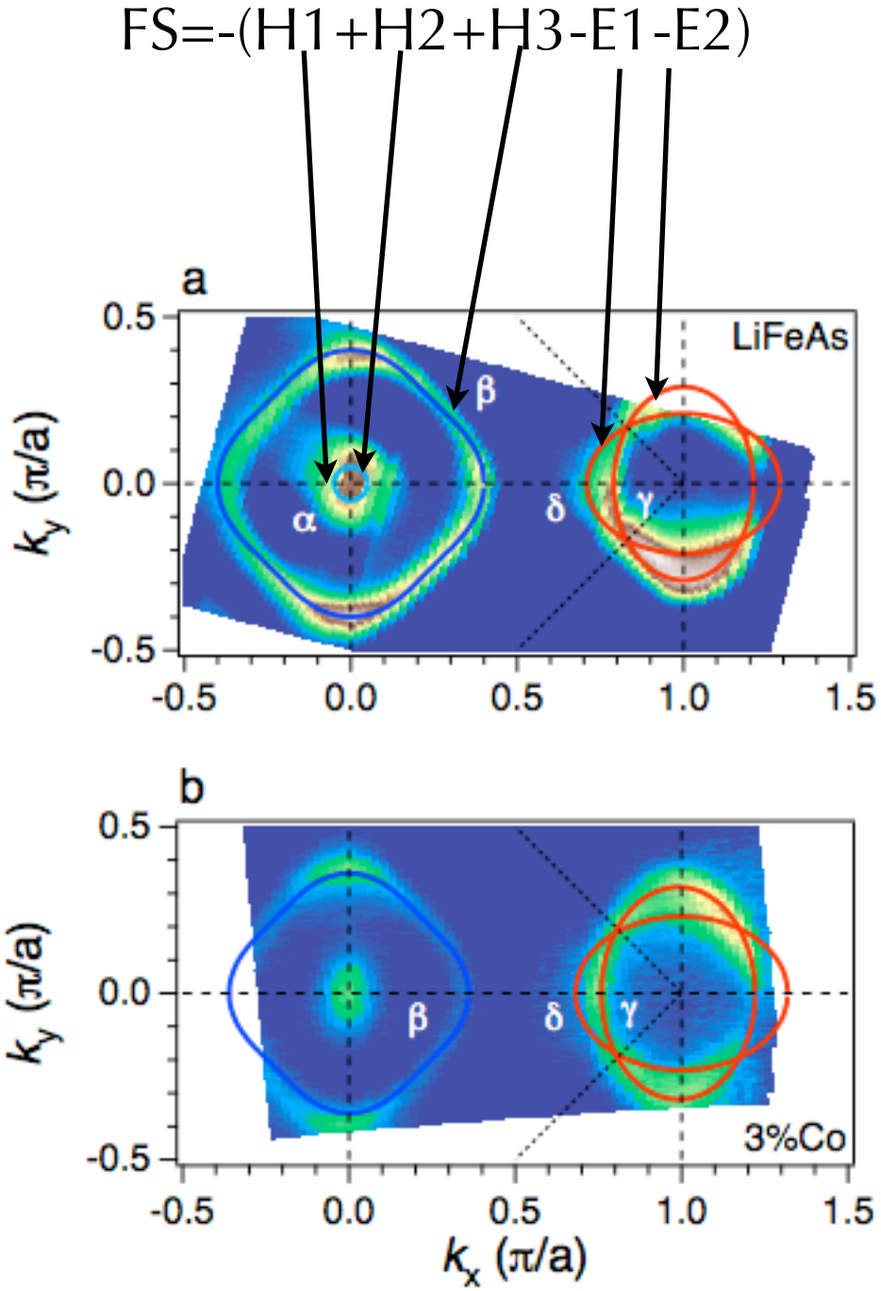
Undoped LiFeAs:
H1=0.00336
H2=0.00336
H3=0.219
E1=0.0948
E2=0.0944

3% Co-doped LiFeAs:
H1=0
H2=0
H3=0.177
E1=0.115
E2=0.115

FS(b)-FS(a)=0.09 ≈ 0.03

compute FS volume

FS=-(H1+H2+H3-E1-E2)



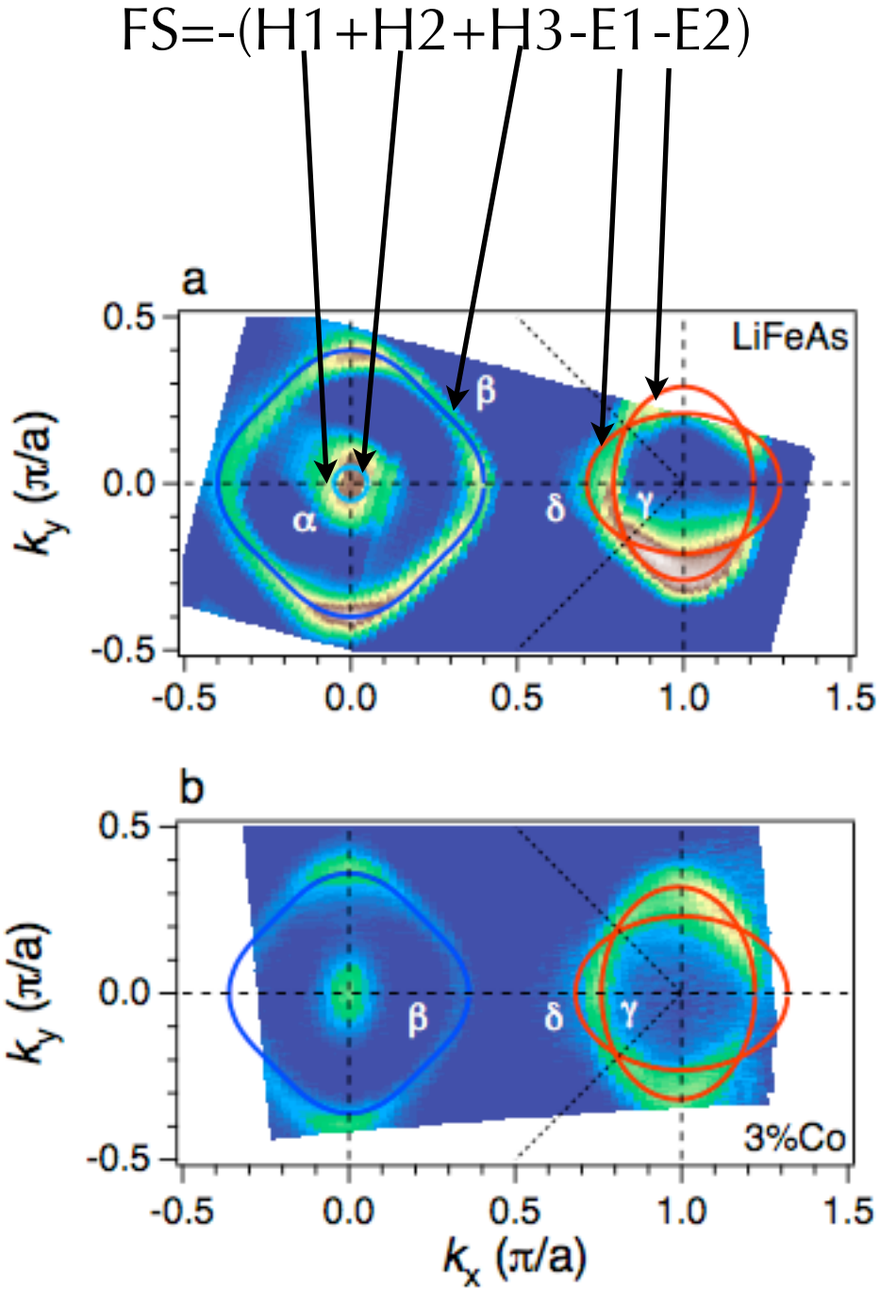
Undoped LiFeAs:
H1=0.00336
H2=0.00336
H3=0.219
E1=0.0948
E2=0.0944

3% Co-doped LiFeAs:
H1=0
H2=0
H3=0.177
E1=0.115
E2=0.115

FS(b)-FS(a)=0.0 ≈ 0.03

compute FS volume

FS=-(H1+H2+H3-E1-E2)



Undoped LiFeAs:
H1=0.00336
H2=0.00336
H3=0.219
E1=0.0948
E2=0.0944

3% Co-doped LiFeAs:
H1=0
H2=0
H3=0.177
E1=0.115
E2=0.115

FS(b)-FS(a)=0.0 ≈ 0.03

off by a factor of 3

What happens when Luttinger's theorem Fails?

What happens when Luttinger's theorem Fails?

unparticles

What happens when Luttinger's theorem Fails?

$$n = 2 \sum_{\mathbf{k}} \Theta(\Re G(\mathbf{k}, \omega = \mathbf{0}))$$

unparticles

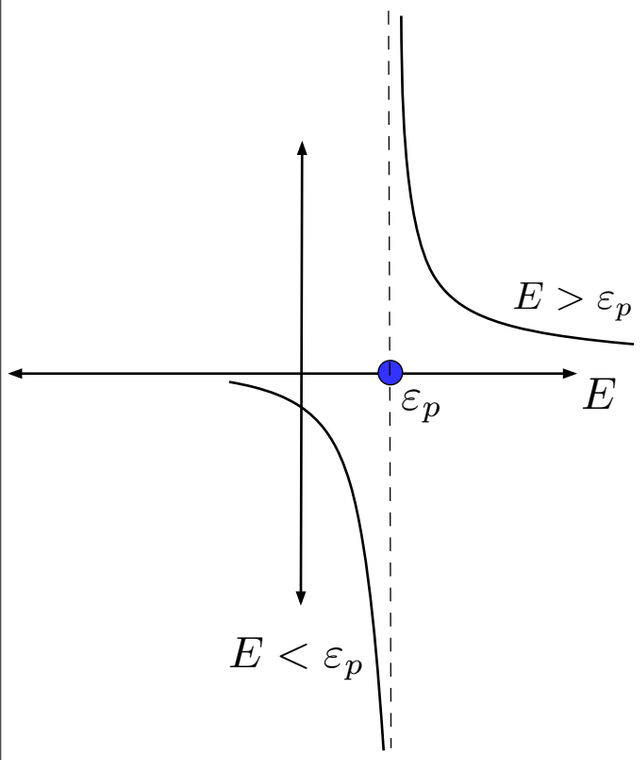
Luttinger theorem: singularities of $\ln G$

$$n = 2 \sum_{\mathbf{k}} \Theta(\Re G(\mathbf{k}, \omega = \mathbf{0}))$$

?

particles

Luttinger theorem: singularities of $\ln G$

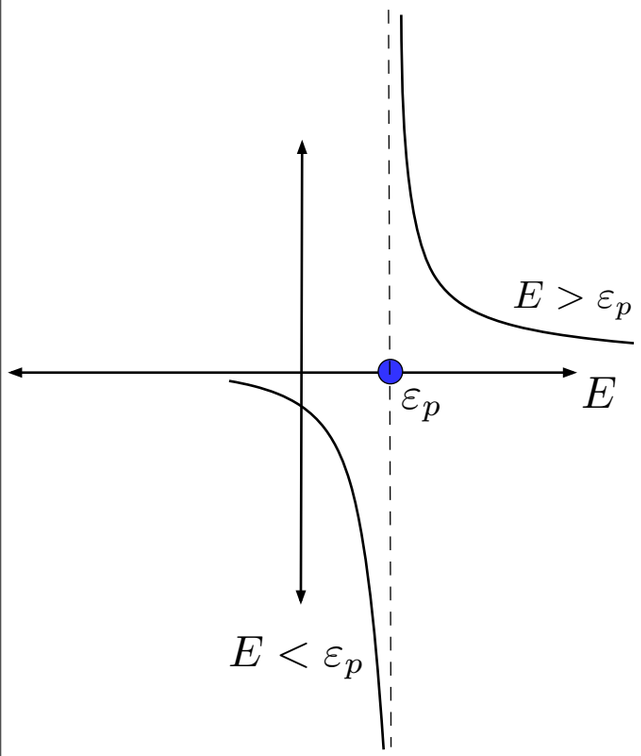


particles

$$n = 2\sum_{\mathbf{k}} \Theta(\Re G(\mathbf{k}, \omega = \mathbf{0}))$$

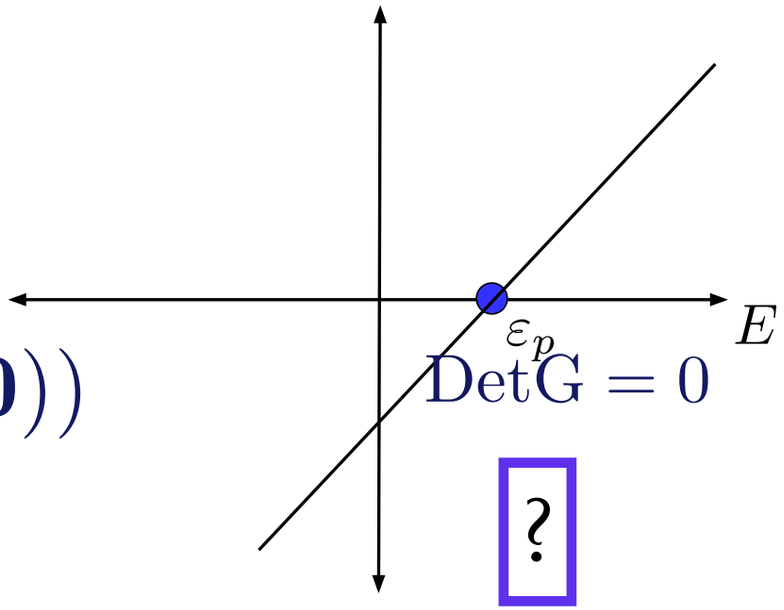
?

Luttinger theorem: singularities of $\ln G$

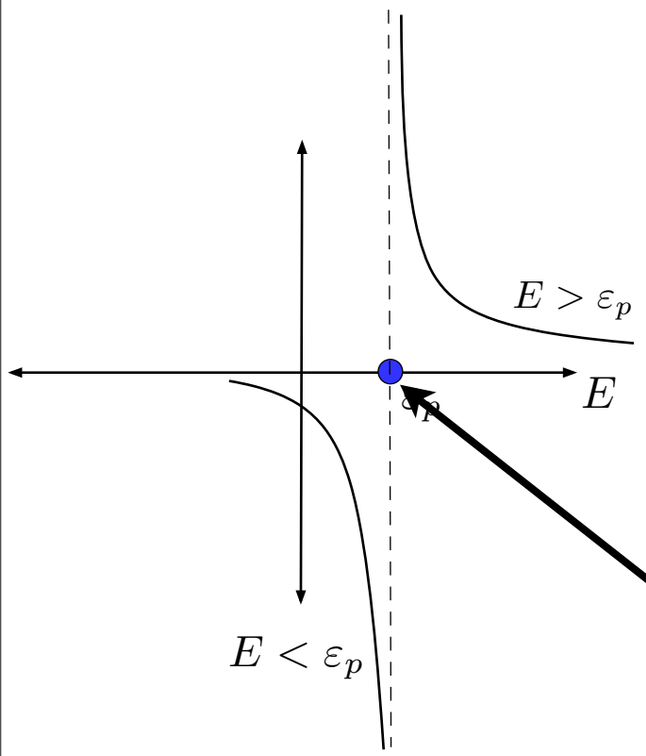


particles

$$n = 2\sum_{\mathbf{k}} \Theta(\Re G(\mathbf{k}, \omega = \mathbf{0}))$$

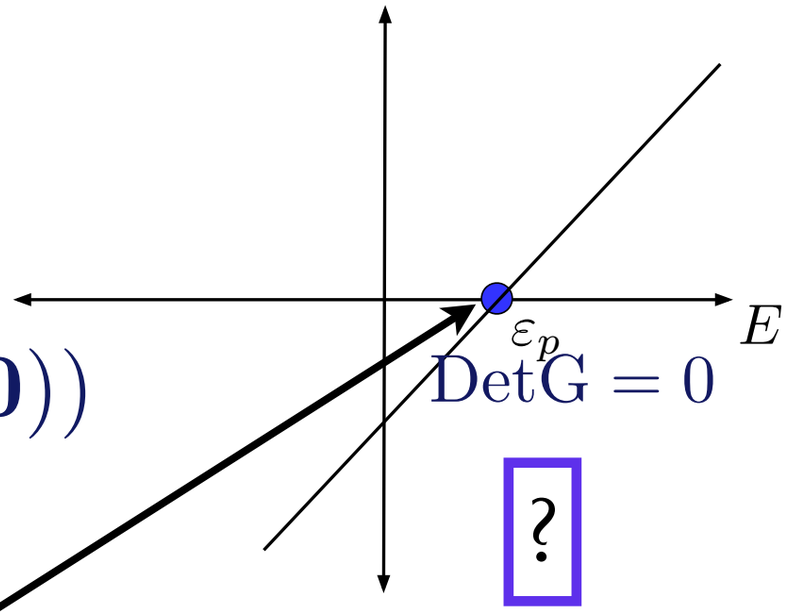


Luttinger theorem: singularities of $\ln G$



particles

$$n = 2\sum_{\mathbf{k}} \Theta\left(\Re G(\mathbf{k}, \omega = \mathbf{0})\right)$$



poles+zeros
(all sign changes)

Problem

G=0

Problem

G=0

$$G = \frac{1}{E - \varepsilon_p - \Sigma} \rightarrow \infty$$

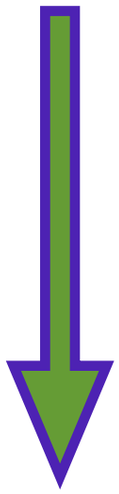
inherent problem

inherent problem

$$\delta I[G] = \int d\omega \Sigma \delta G$$

inherent problem

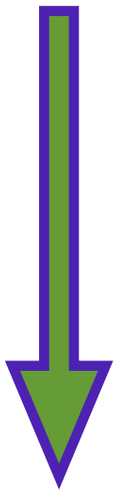
$$\delta I[G] = \int d\omega \Sigma \delta G$$



$$\text{if } \Sigma \to \infty$$

inherent problem

$$\delta I[G] = \int d\omega \Sigma \delta G$$



if $\Sigma \to \infty$

integral does not exist

inherent problem

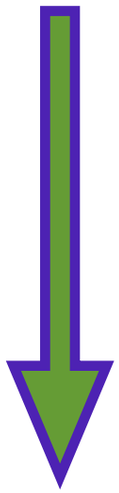
$$\delta I[G] = \int d\omega \Sigma \delta G$$

if $\Sigma \to \infty$

integral does not exist

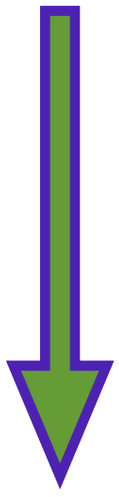
inherent problem

$$\delta I[G] = \int d\omega \Sigma \delta G$$



if $\Sigma \to \infty$

integral does not exist



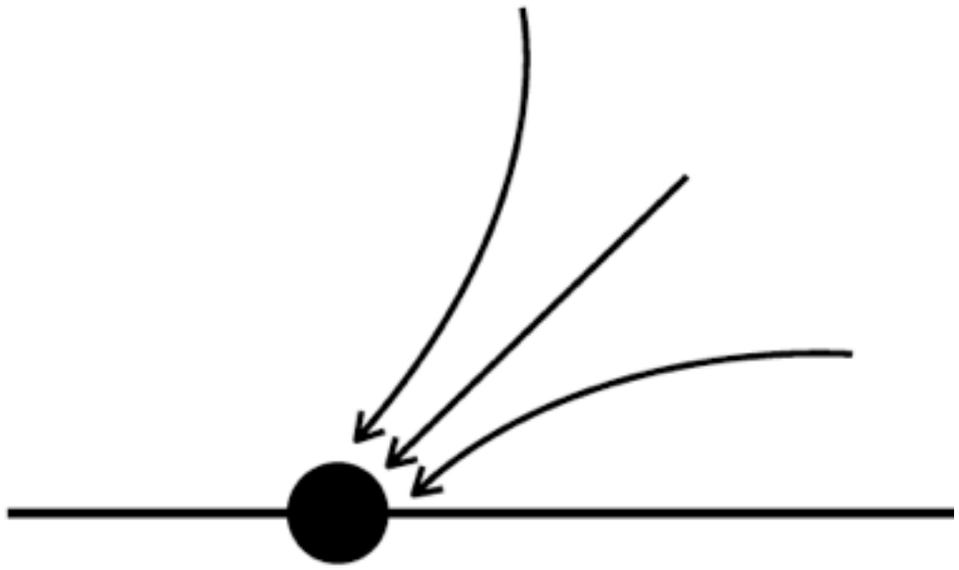
Luttinger's Theorem

inherent problem

$$\delta I[G] = \int d\omega \Sigma \delta G$$

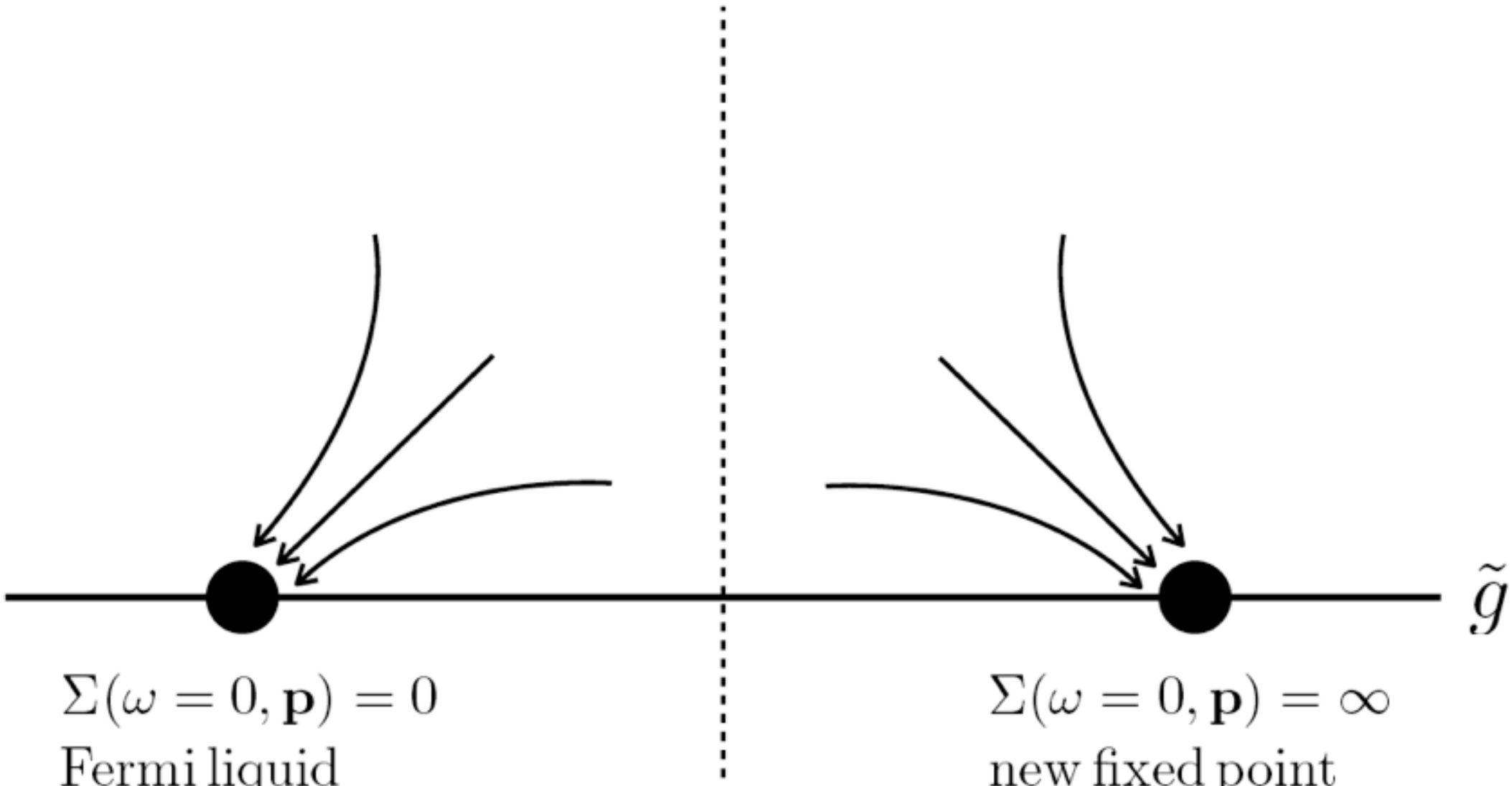
if $\Sigma \to \infty$

integral does not exist



$\Sigma(\omega = 0, \mathbf{p}) = 0$

Fermi liquid

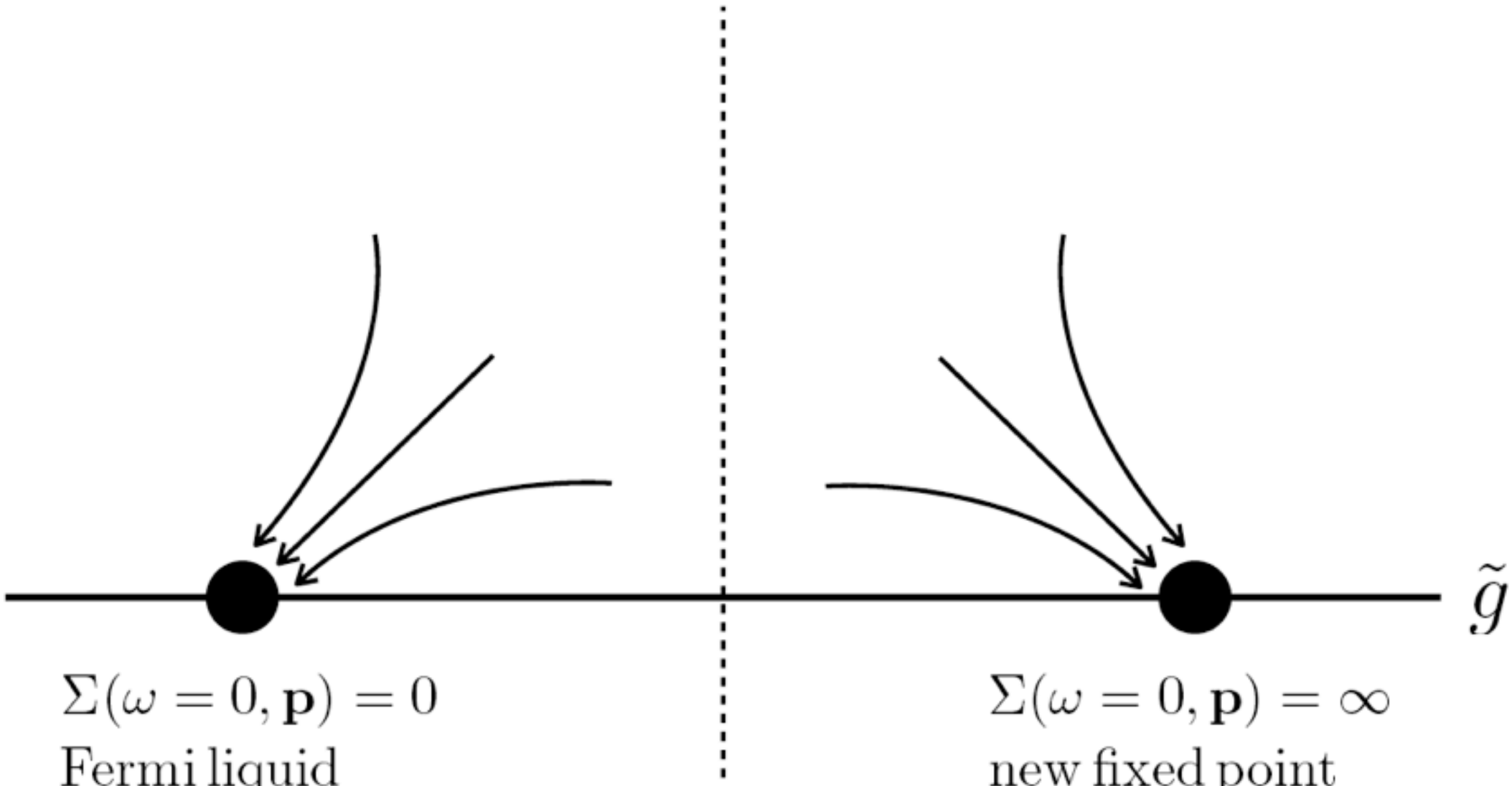


$\Sigma(\omega = 0, \mathbf{p}) = 0$

Fermi liquid

$\Sigma(\omega = 0, \mathbf{p}) = \infty$

new fixed point



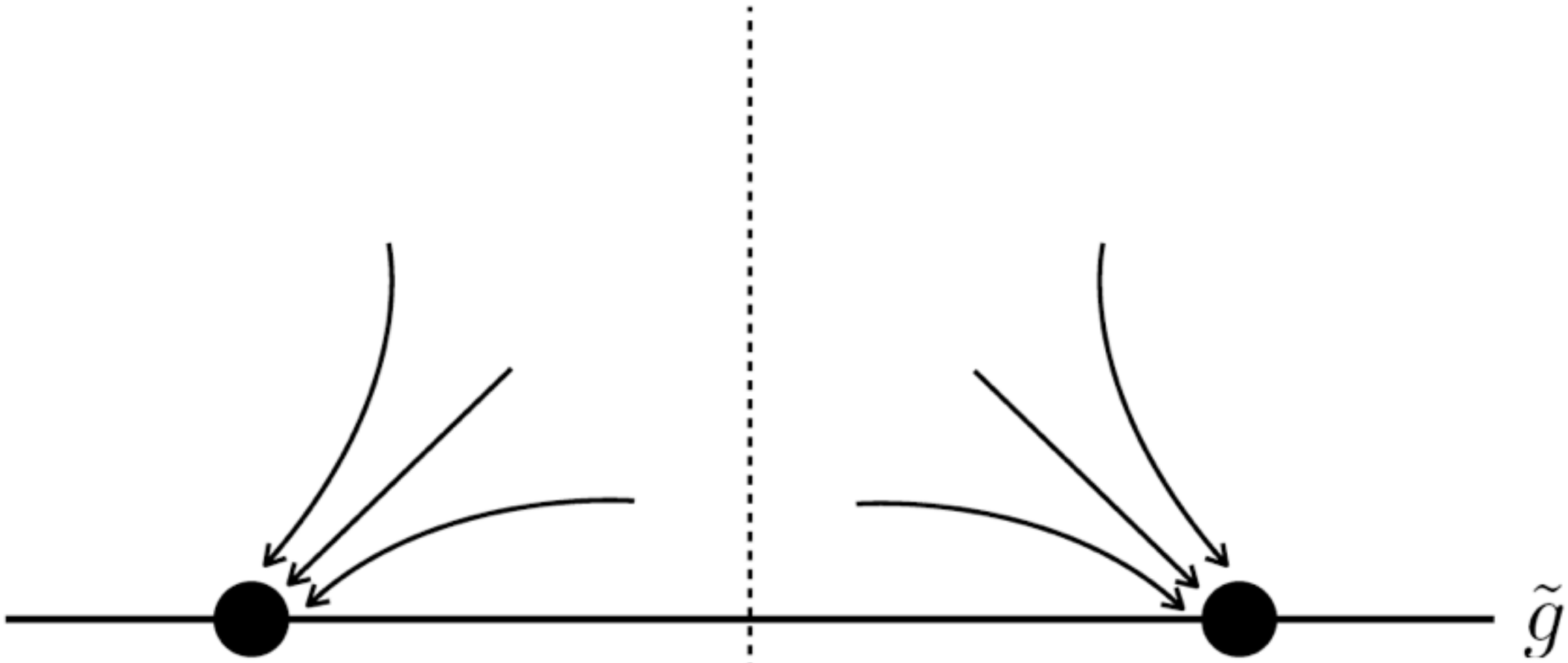
$\Sigma(\omega = 0, \mathbf{p}) = 0$

Fermi liquid

$\Sigma(\omega = 0, \mathbf{p}) = \infty$

new fixed point

scale invariance



$\Sigma(\omega = 0, \mathbf{p}) = 0$

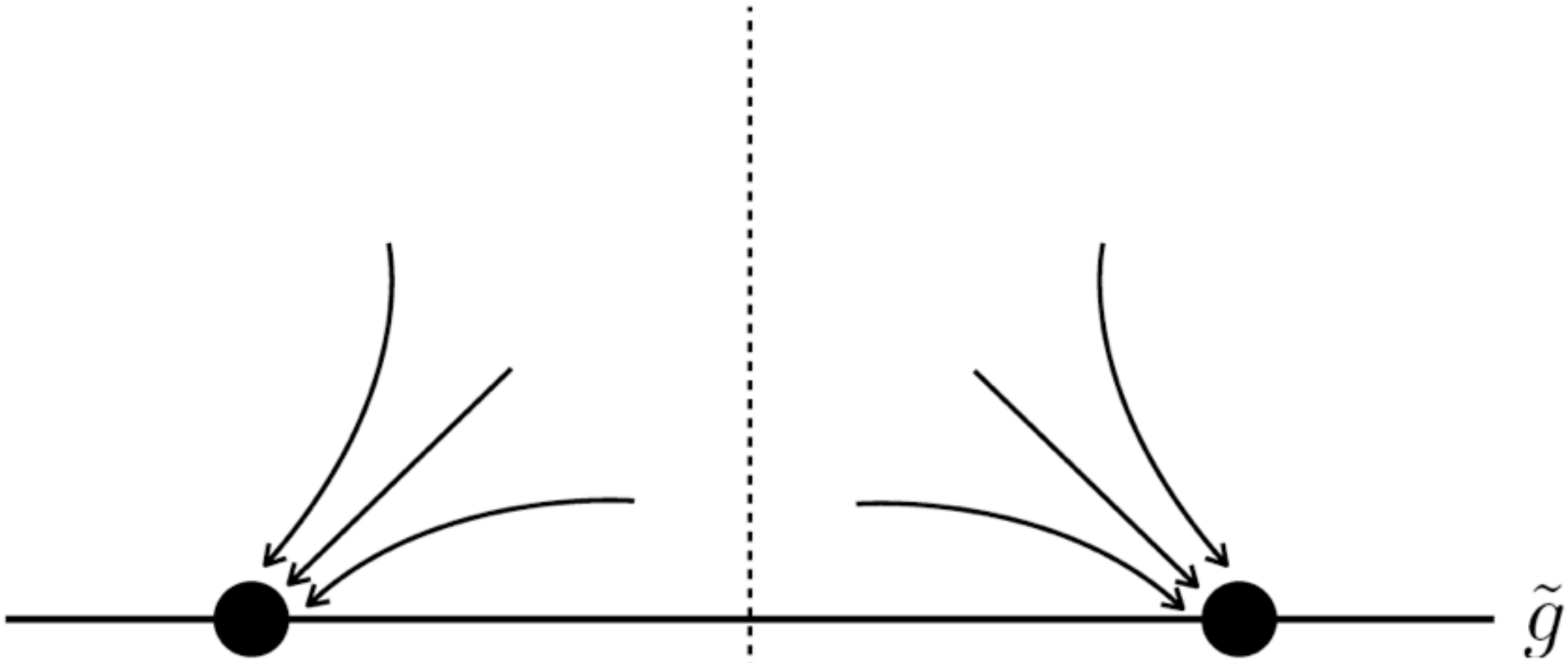
Fermi liquid

$\Sigma(\omega = 0, \mathbf{p}) = \infty$

new fixed point

$$G_U \propto \left(p^2\right)^{d_U - d/2}$$

scale invariance



$\Sigma(\omega = 0, \mathbf{p}) = 0$

Fermi liquid

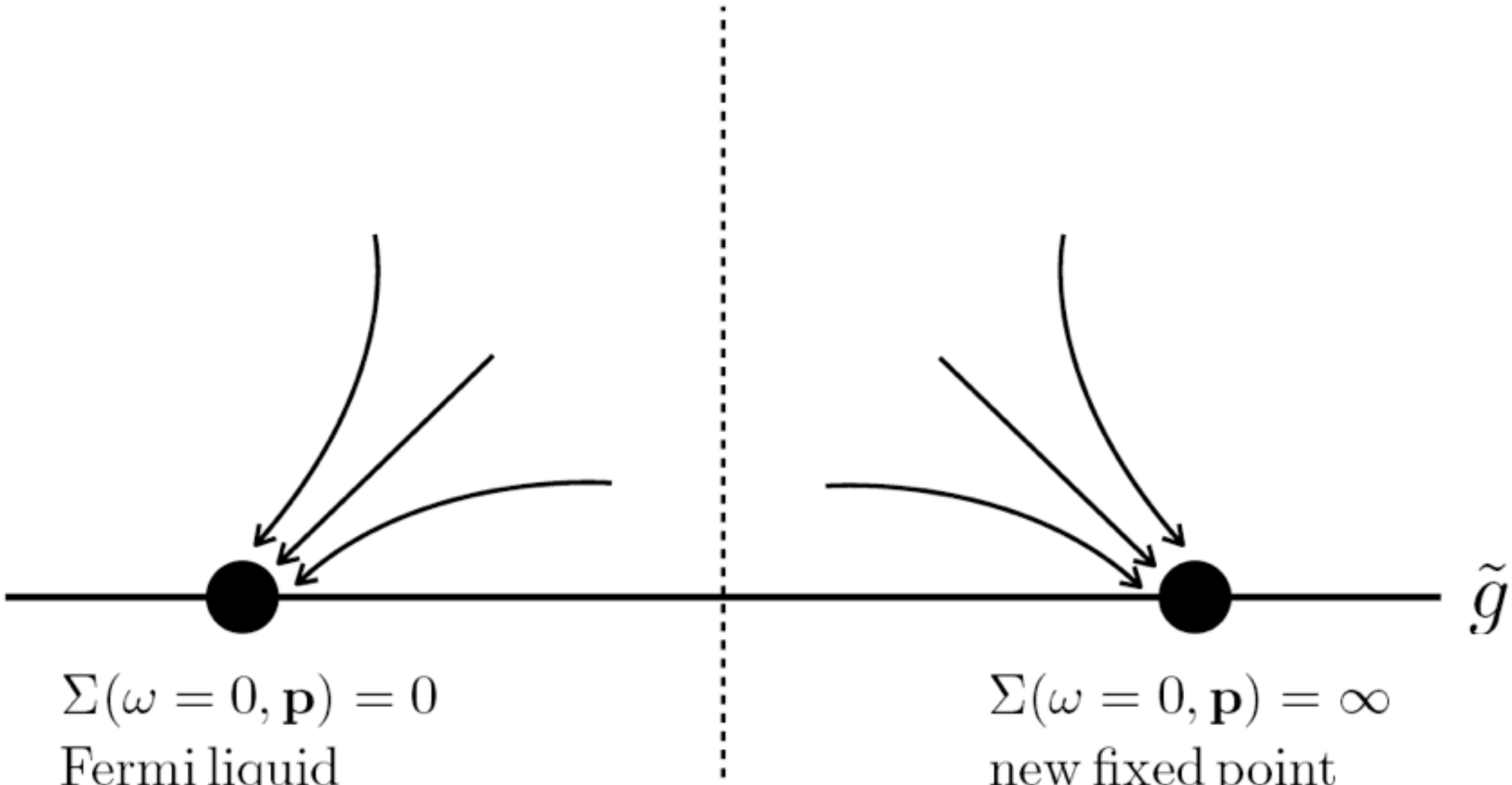
$\Sigma(\omega = 0, \mathbf{p}) = \infty$

new fixed point

$G_U \propto \left(p^2\right)^{d_U - d/2}$

scale invariance

$d_U > d/2$



$\Sigma(\omega = 0, \mathbf{p}) = 0$

Fermi liquid

$\Sigma(\omega = 0, \mathbf{p}) = \infty$

new fixed point

$G_U \propto (p^2)^{d_U - d/2}$

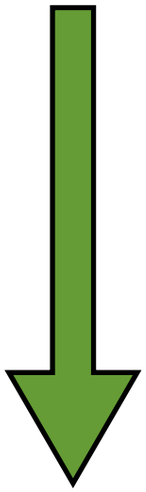
unparticles

scale invariance

$d_U > d/2$

unparticles

unparticles



no well-defined mass
(all possible mass, energy
incoherent stuff)

unparticles

no well-defined mass
(all possible mass, energy
incoherent stuff)

$$\mathcal{L}_{\rm eff} = \int_0^\infty \mathcal{L}(x, m^2) dm^2$$

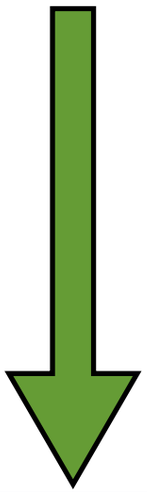
unparticles

no well-defined mass
(all possible mass, energy
incoherent stuff)

$$\mathcal{L}_{\text{eff}} = \int_0^\infty \mathcal{L}(x, m^2) dm^2$$

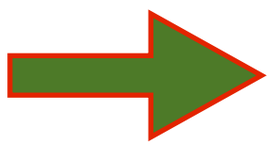
but $m \propto 1/L$

unparticles



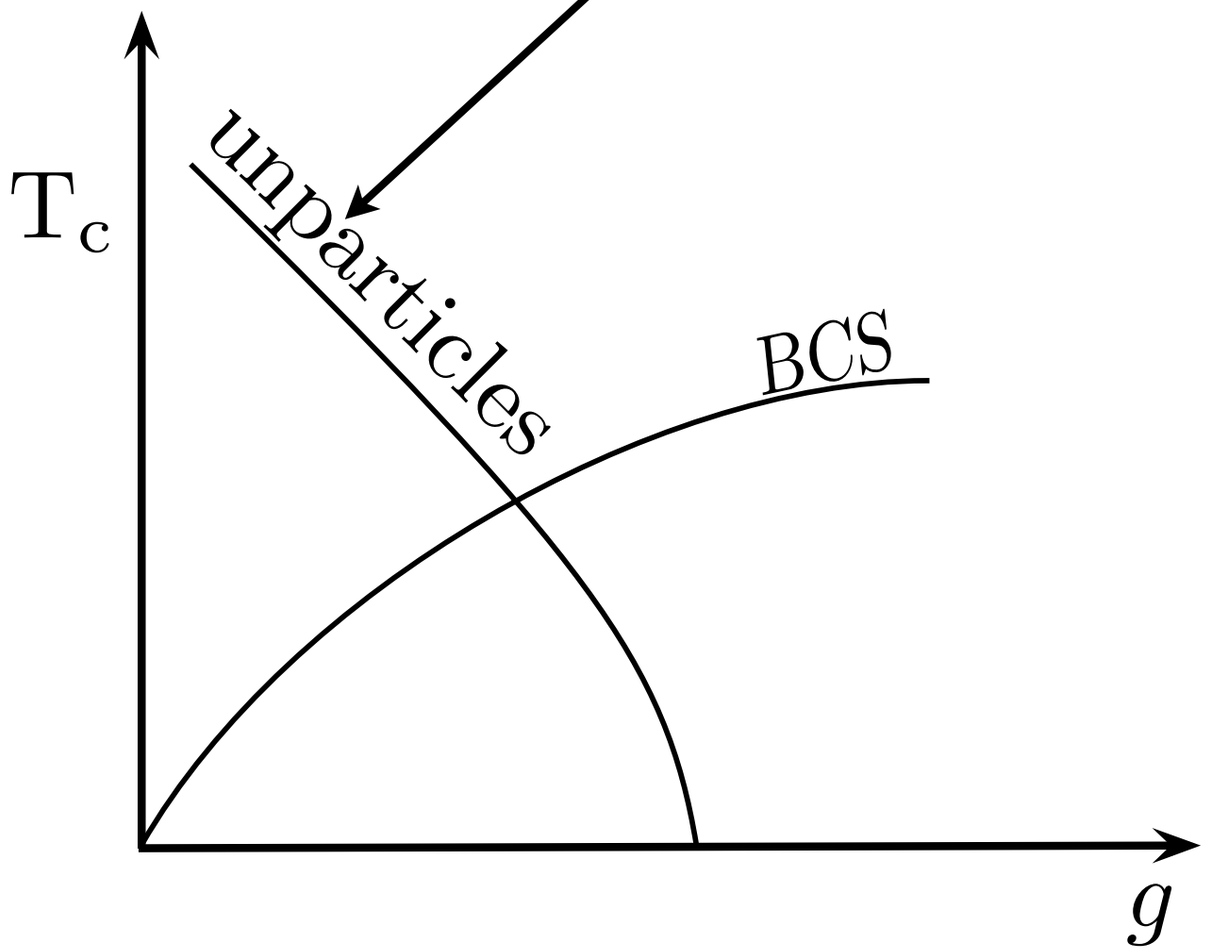
no well-defined mass
(all possible mass, energy
incoherent stuff)

$$\mathcal{L}_{\text{eff}} = \int_0^\infty \mathcal{L}(x, m^2) dm^2$$

but $m \propto 1/L$ 

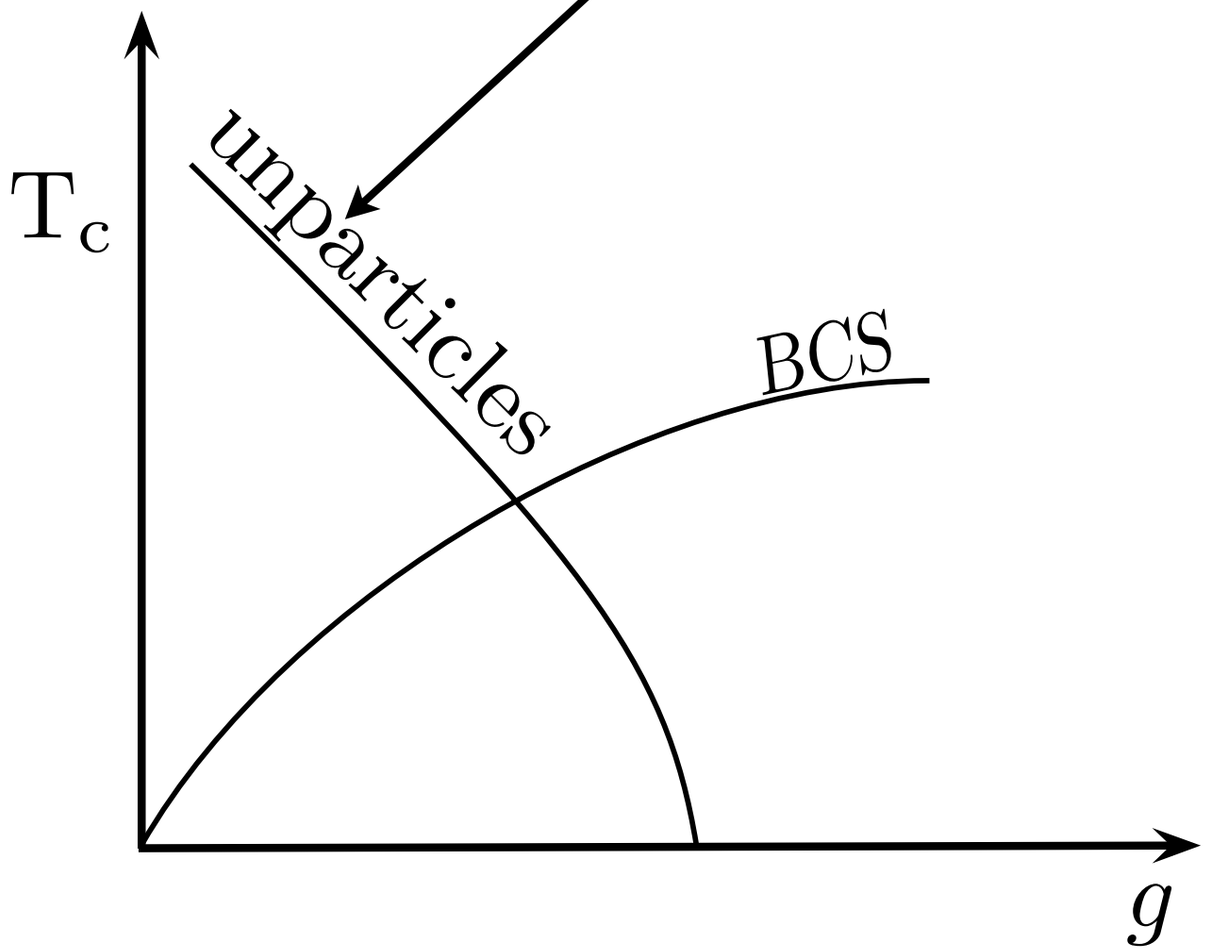
hidden extra
dimension

$$\frac{d\ln g}{d\ln \beta} \quad = \quad 4d_U - d > 0$$



tendency towards pairing (any instability which establishes a gap)

$$\frac{d\ln g}{d\ln \beta} = 4d_U - d > 0$$



tendency towards pairing (any instability which establishes a gap)

see also, dresden group, 1407.8492

prediction: algebraic pairing susceptibility

$$G\left(\Lambda k, i\Lambda\omega_n\right) \quad = \quad \Lambda^{2d_U - D} G\left(k, i\omega_n\right).$$

$$\chi\left(0, i\Omega\right) \quad = \quad \frac{T}{N} \sum_{n,k} G\left(-k, -i\omega_n\right) G\left(k, i\omega_n + i\Omega\right)$$

prediction: algebraic pairing susceptibility

$$G\left(\Lambda k, i\Lambda\omega_n\right) \quad = \quad \Lambda^{2d_U - D} G\left(k, i\omega_n\right).$$

$$\chi\left(0, i\Omega\right) \quad = \quad \frac{T}{N}\sum_{n,k} G\left(-k, -i\omega_n\right) G\left(k, i\omega_n + i\Omega\right)$$

$$\chi\left(0, i\Omega\right) \quad \propto \quad \Omega^{4d_U - D}.$$

$$d_U > D/2$$

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

$La_2Co_2Se_2O_3$

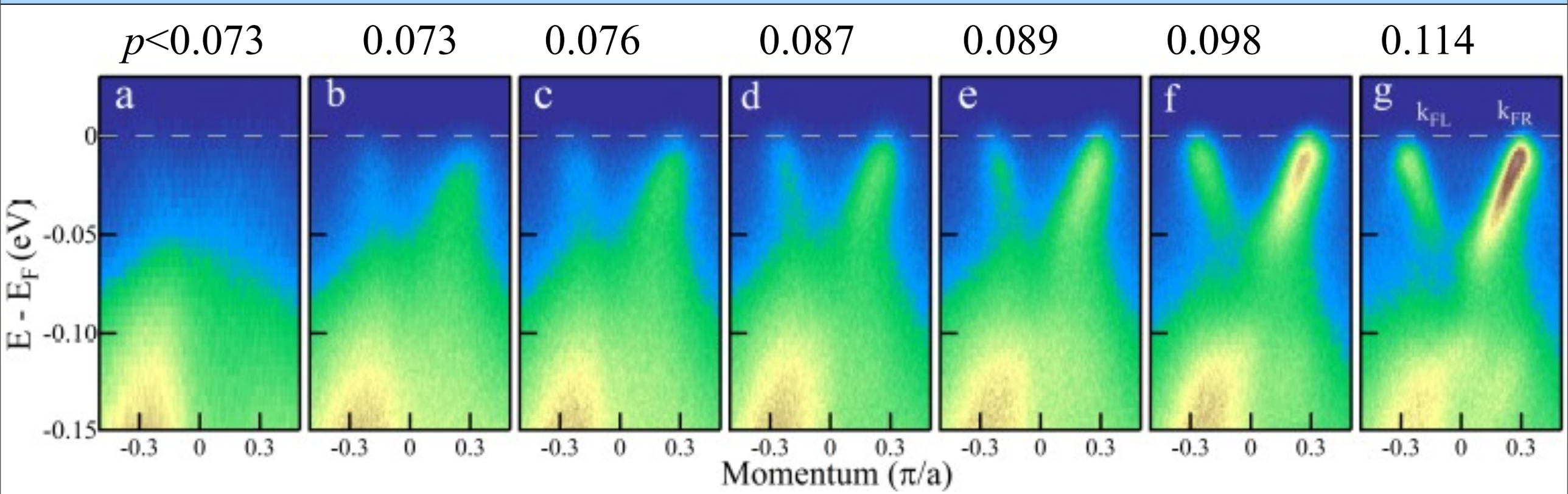
$Na_2OCu_4OSe_2$

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]

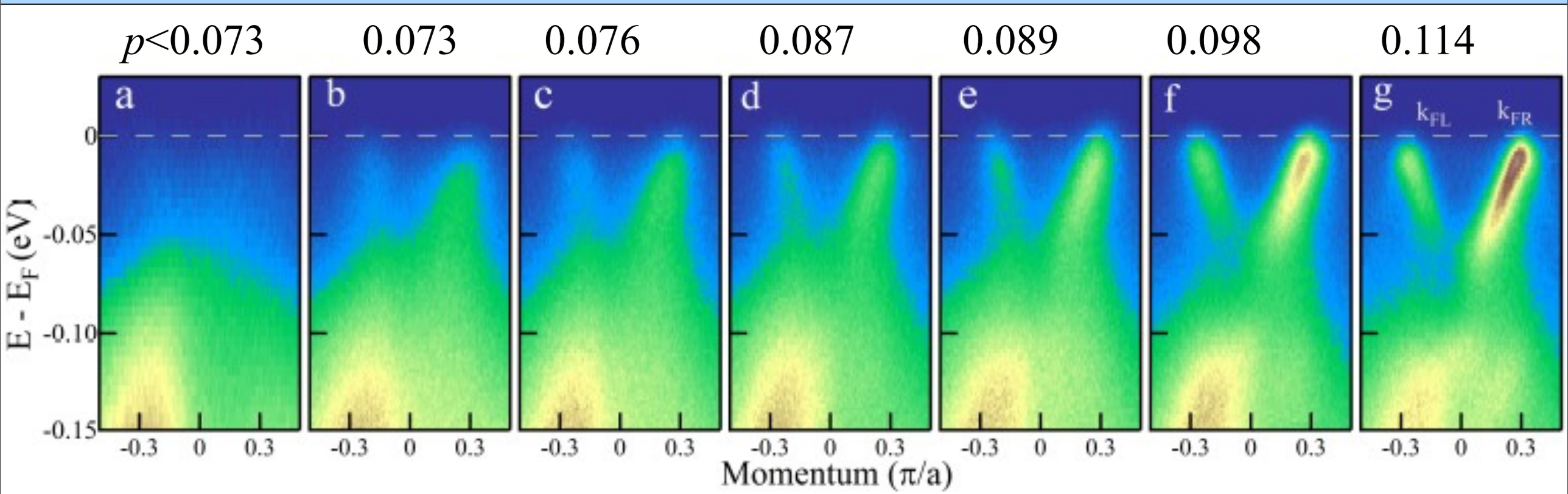
[1] *Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2] *Department of Physics & Astronomy, Rice University, Houston, Texas 77005, USA*
[3] *Department of Physics, Zhejiang University, Hangzhou 310027, P. R. China*
[4] *University at Buffalo, SUNY, Buffalo, New York 14260, USA*
[5] *Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08855, USA**

Insulator-Superconductor Transition in S-Phase of Single-Layer FeSe/$SrTiO_3$



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

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.

Is this what is going on in FeSe?