Is there a Common Thread

linking superconductivity in the heavy fermion, actinide, cuprate and Fe superconductors?

D. J. Scalapino
UCSB

Supported by Center for Nanophase Material Science
Oak Ridge National Laboratory, DOE

Is there a Common Thread

linking superconductivity in the heavy fermion, actinide, cuprate and Fe superconductors?

T. Maier ORNL
M. Jarrell LSU
S.R. White UCI
W. Hanke Wurzburg
D. Poilblanc LPL
N. Bulut

P. Hirschfeld UF
S. Graser Univ Augsburg
S. Kivelson Stanford
E. Berg MIT
S. Raguh Stanford
X.-L. Qi Stanford
T. Devereaux Stanford

Acknowledge

I.I. Mazin
D. Singh
A. Chubukov
W. Hanke
Z. Fisk
J. Thompson
F. Steglich

T. Moriya and K. Ueda, Rep Prog. Phys. 66, 1299 (2003)

Is there a Common Thread ?

1. The Materials
2. The neutron scattering resonance in the superconducting state
3. The models
4. The properties of the models
5. Conclusions

1.The Materials

They come in families with:

layered 2D structures

phase diagrams with AF magnetism/ superconductivity

The 115 Heavy Fermion Family

$CeCoIn_5$

$CeIrIn_5$

$CeRhIn_5$

$CeCo(In_{1-x}Cd_x)_5$

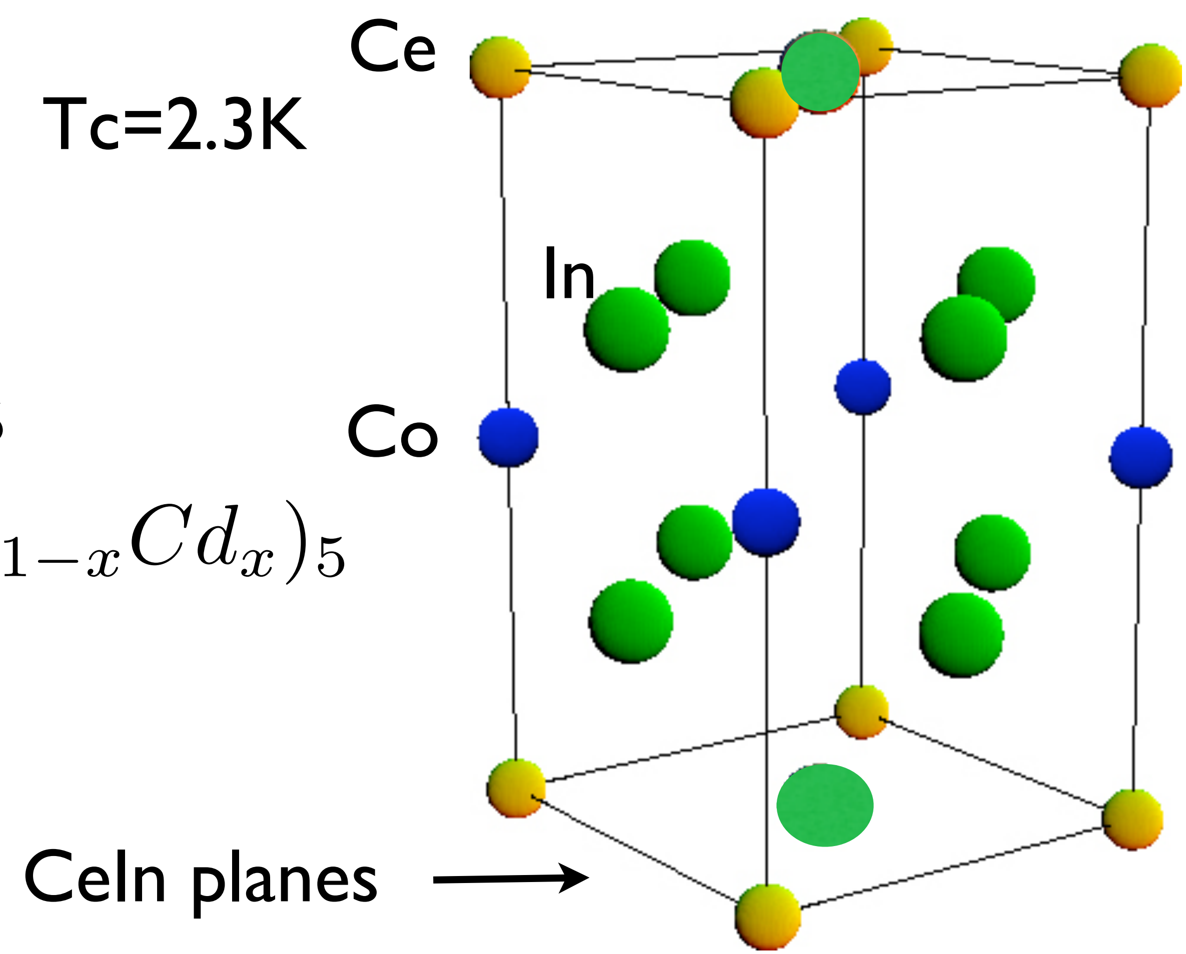
The 115 Heavy Fermion Family

$CeCoIn_5$ Tc=2.3K

$CeIrIn_5$

$CeRhIn_5$

$CeCo(In_{1-x}Cd_x)_5$



N. Curro, Nature (205)

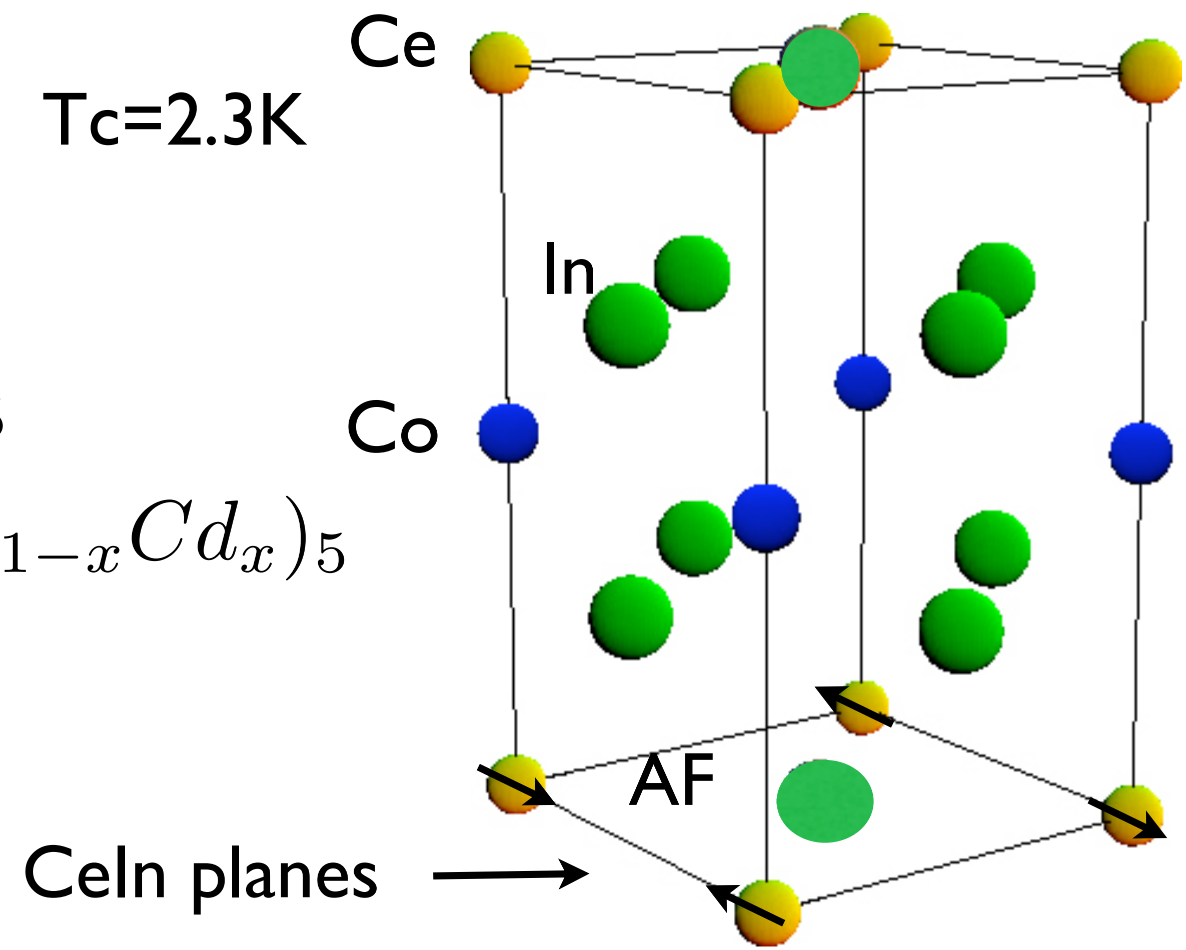
The 115 Heavy Fermion Family

$CeCoIn_5$ Tc=2.3K

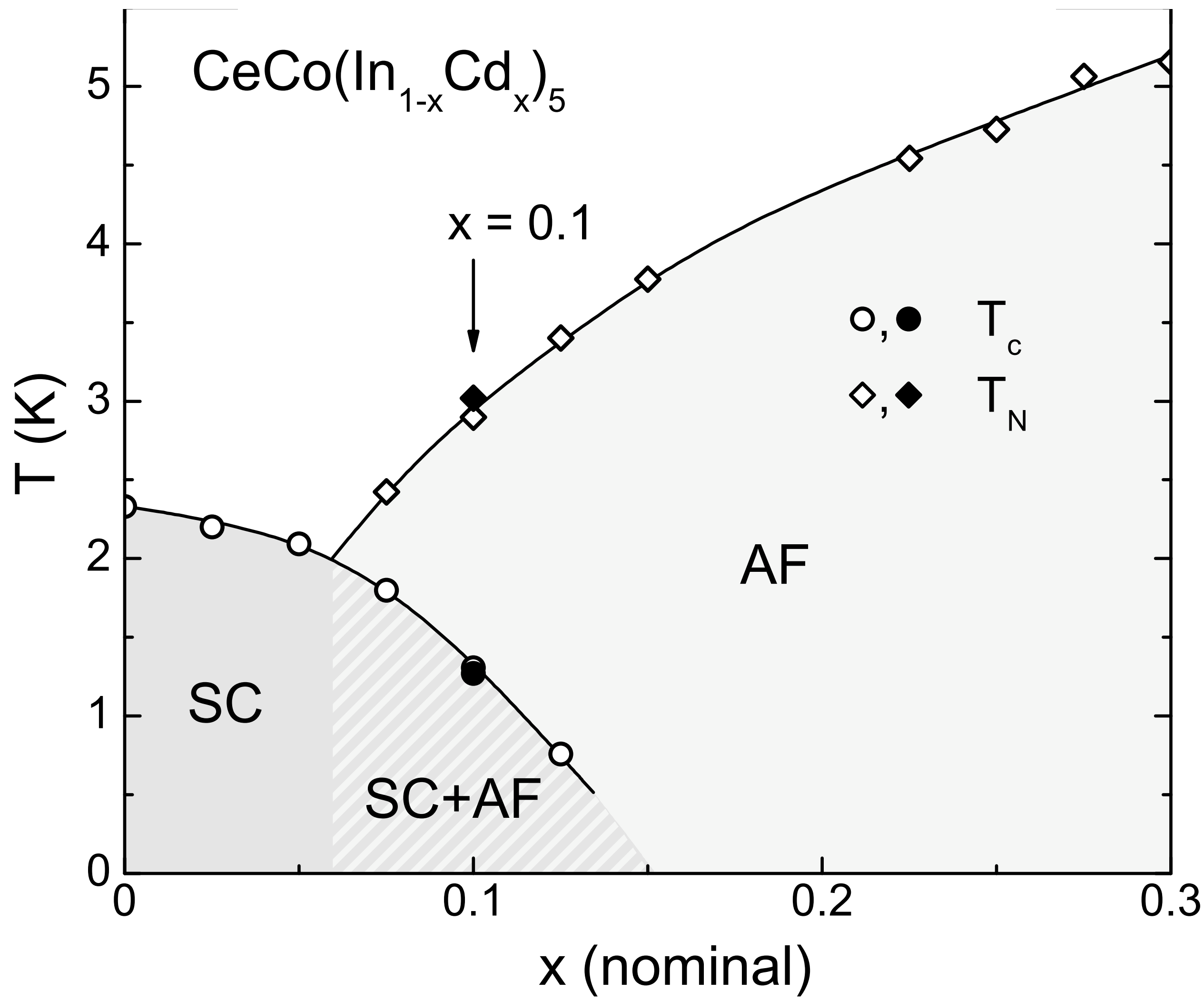
$CeIrIn_5$

$CeRhIn_5$

$CeCo(In_{1-x}Cd_x)_5$

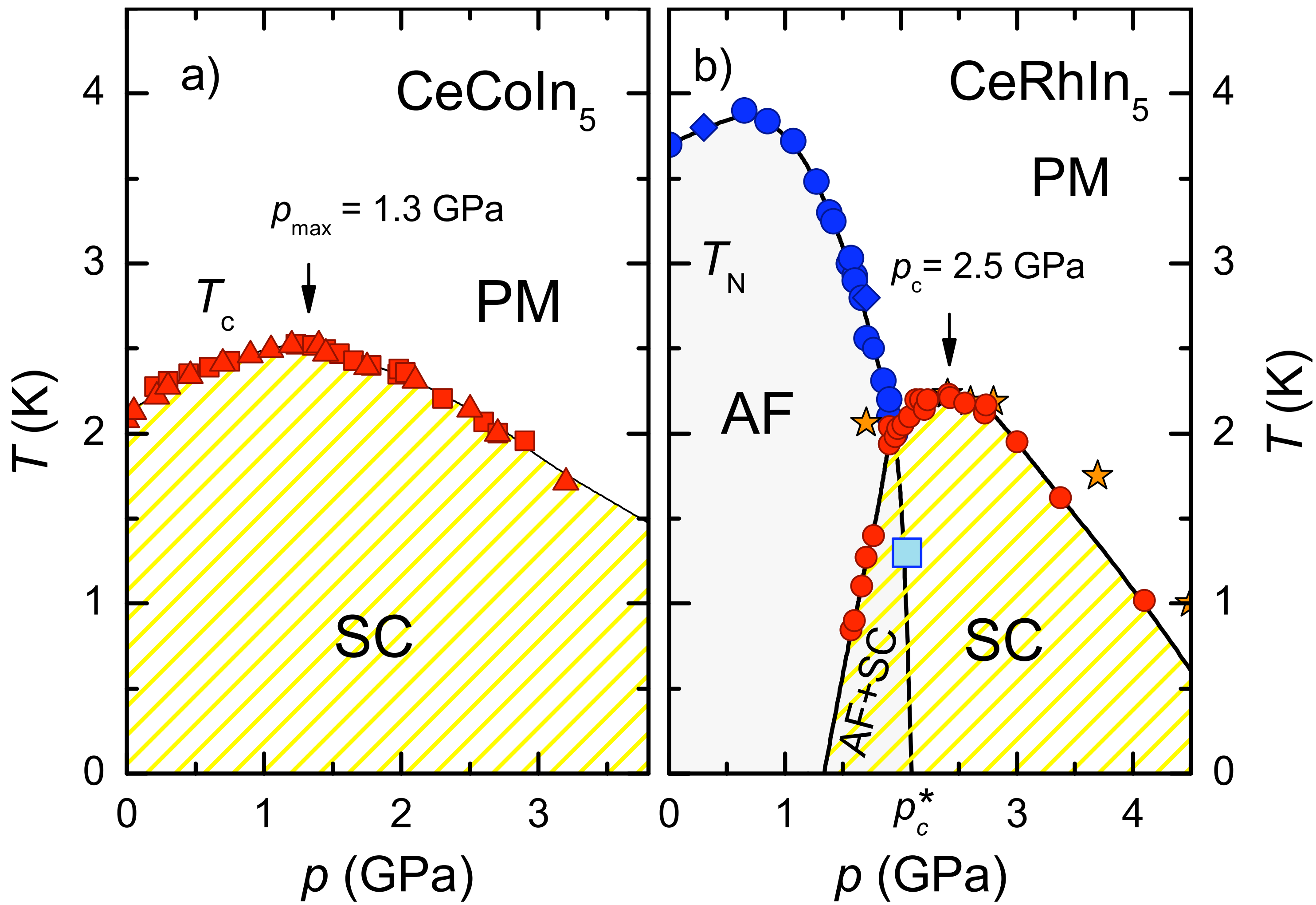


N. Curro, Nature (205)



N. Nicklas et al, PRB 76, 52401

G. Knebel et al, 0908.3980



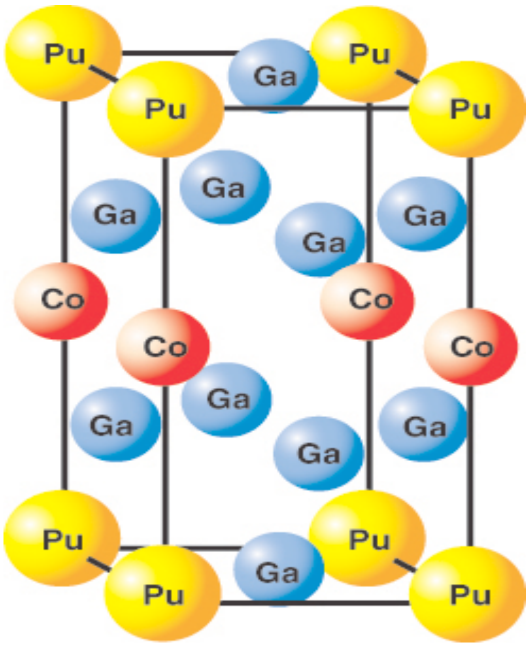
The 115 actinide PuMGa5 family

$PuCoGa_5$ Tc=18.5K

$PuRhGa_5$ Tc~8K

$PuCo_{0.5}Rh_{0.5}Ga_5$

Pu-Ga planes



Cuperate Families

$$HgBa_2Ca_2Cu_3O_8$$

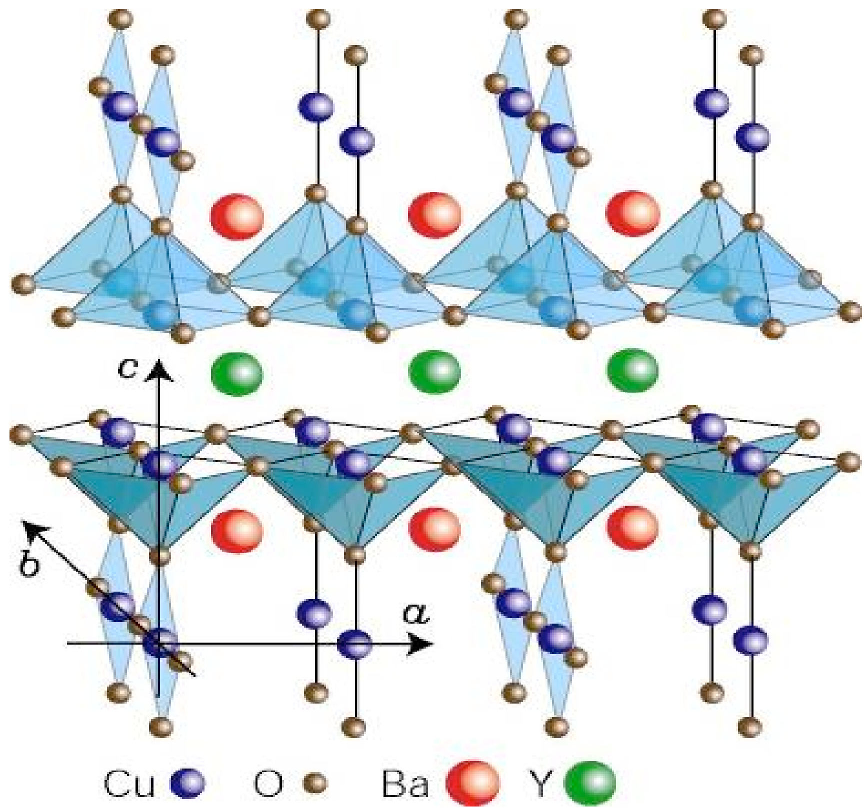
$$HgBa_2CaCu_2O_6$$

$$HgBa_2CuO_4$$

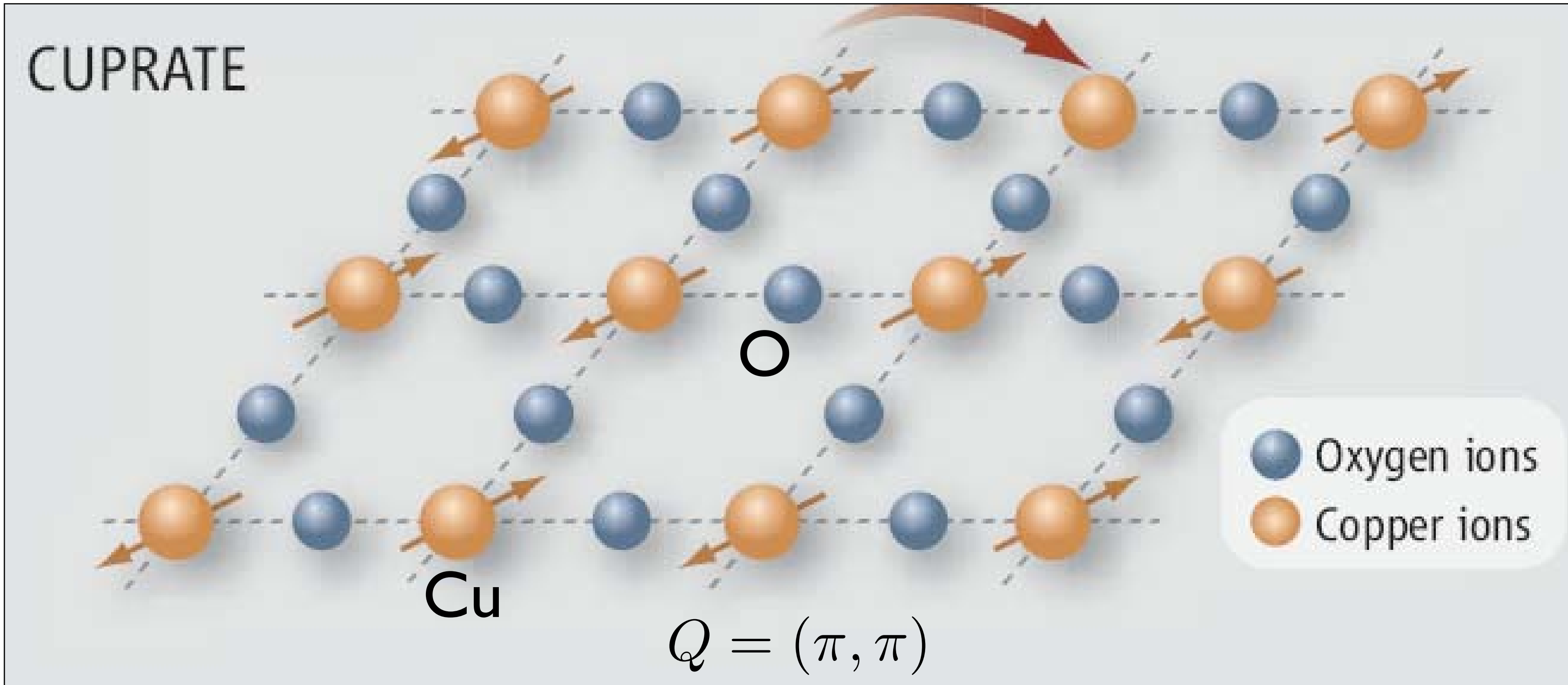
$$Tl_2Ba_2Ca_2Cu_3O_{10}$$

$$Tl_2Ba_2CaCu_2O_8$$

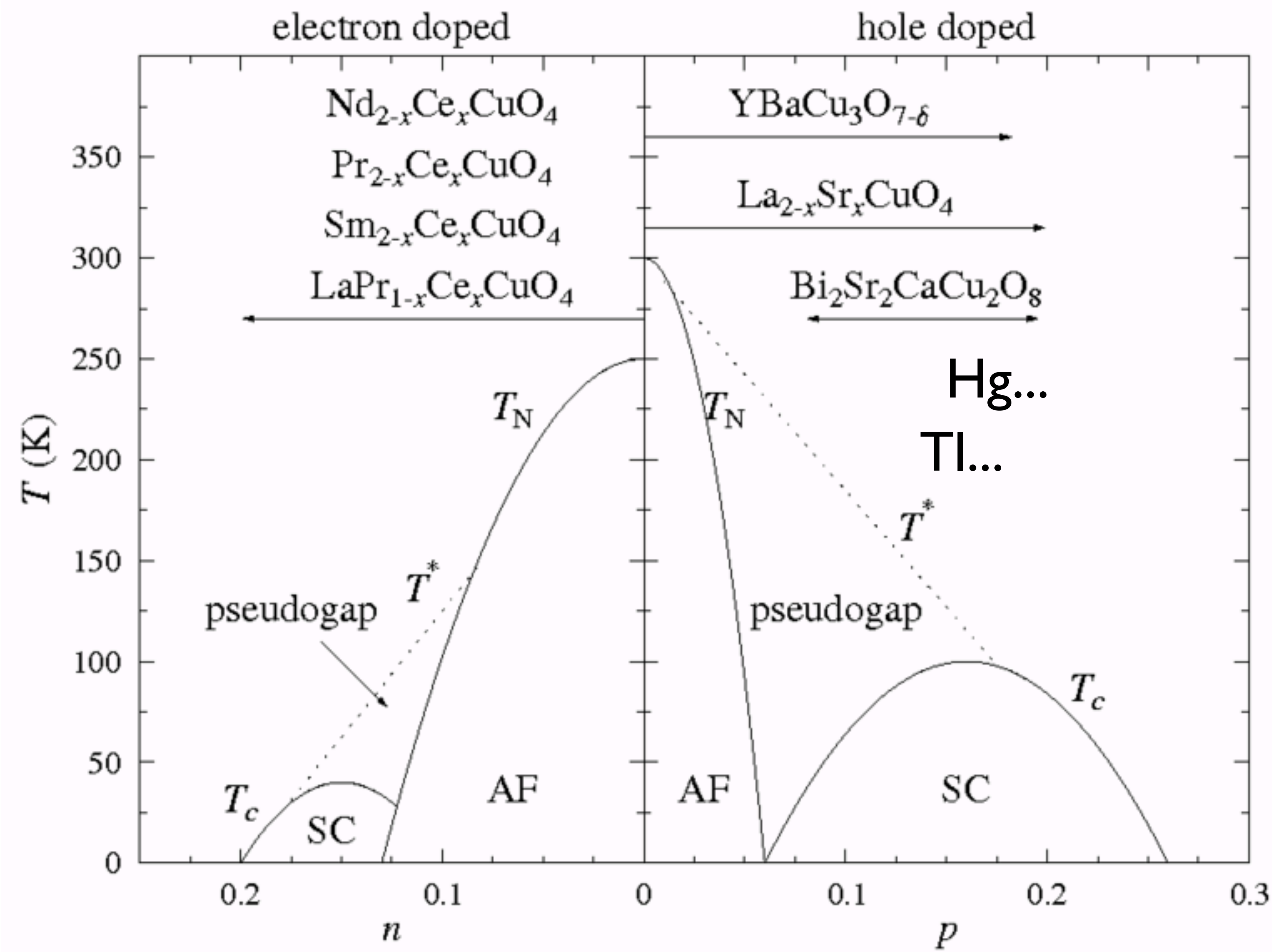
$$Tl_2Ba_2CuO_6$$



YBCO

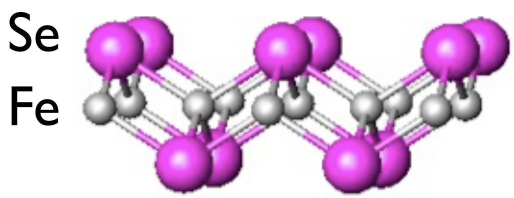

CUPRATE
O
Cu
Oxygen ions
Copper ions
$Q = (\pi, \pi)$

Cuperates



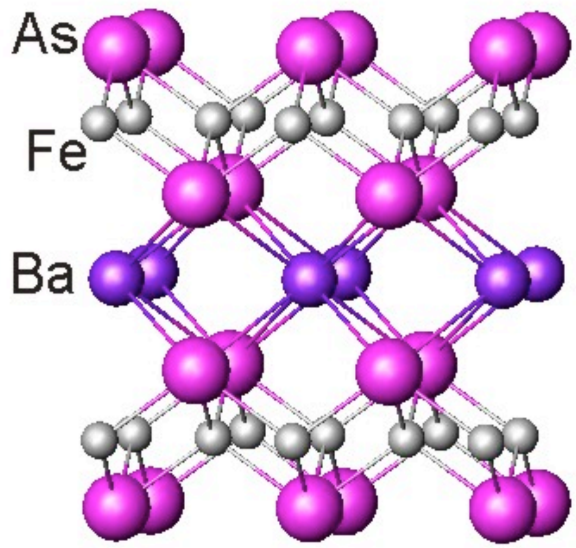
electron doped
hole doped
Nd2-xCexCuO4
Pr2-xCexCuO4
Sm2-xCexCuO4
LaPr1-xCexCuO4
YBaCu3O7-δ
La2-xSrxCuO4
Bi2Sr2CaCu2O8
Hg...
Tl...
T (K)
TN
T*
pseudogap
Tc
SC
AF
n
p
0
50
100
150
200
250
300
350
0.2
0.1
0.3

The Fe Superconductors



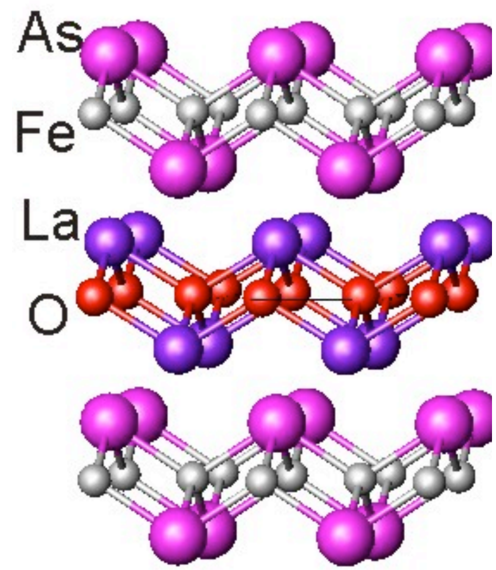
FeSe

[11]



$BaFe_2As_2$

[122]



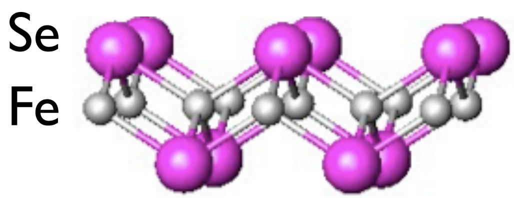
LaFeAsO

[1111]

FeAsLi

[111]

The Fe Superconductors

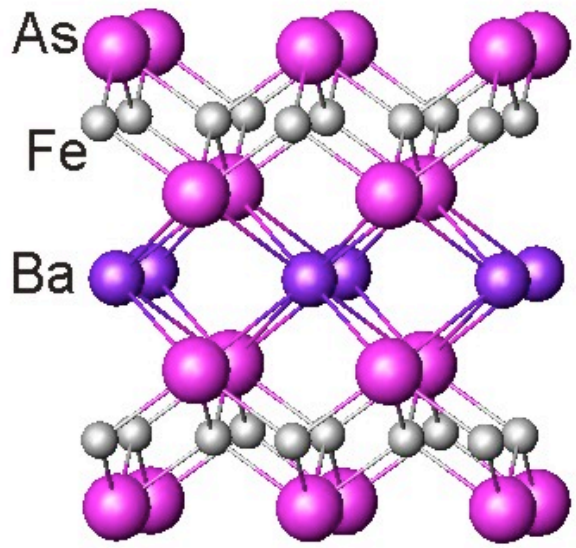


FeSe

$$T_c = 9K - 37K$$

FeAsLi

$$T_c = 14K$$



$BaFe_2As_2$

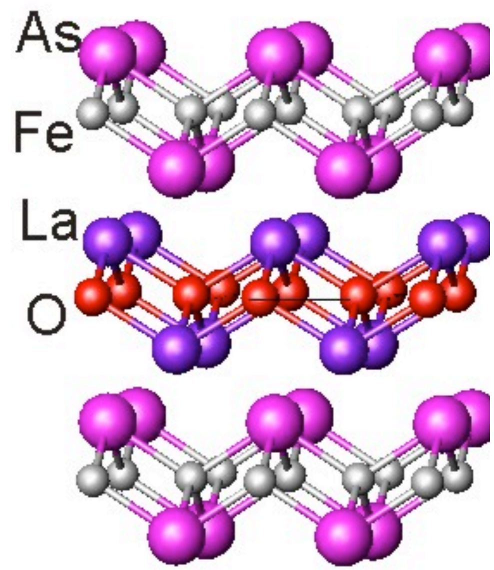
$$Ba_{1-x}K_xFe_2As_2$$

$$T_c = 38K$$

h

$$Ba(Fe_{1-x}Co_x)_2As_2$$

$$T_c = 22K$$



LaFeAsO

$$LaFeAsO_{0.9}F_{0.1}$$

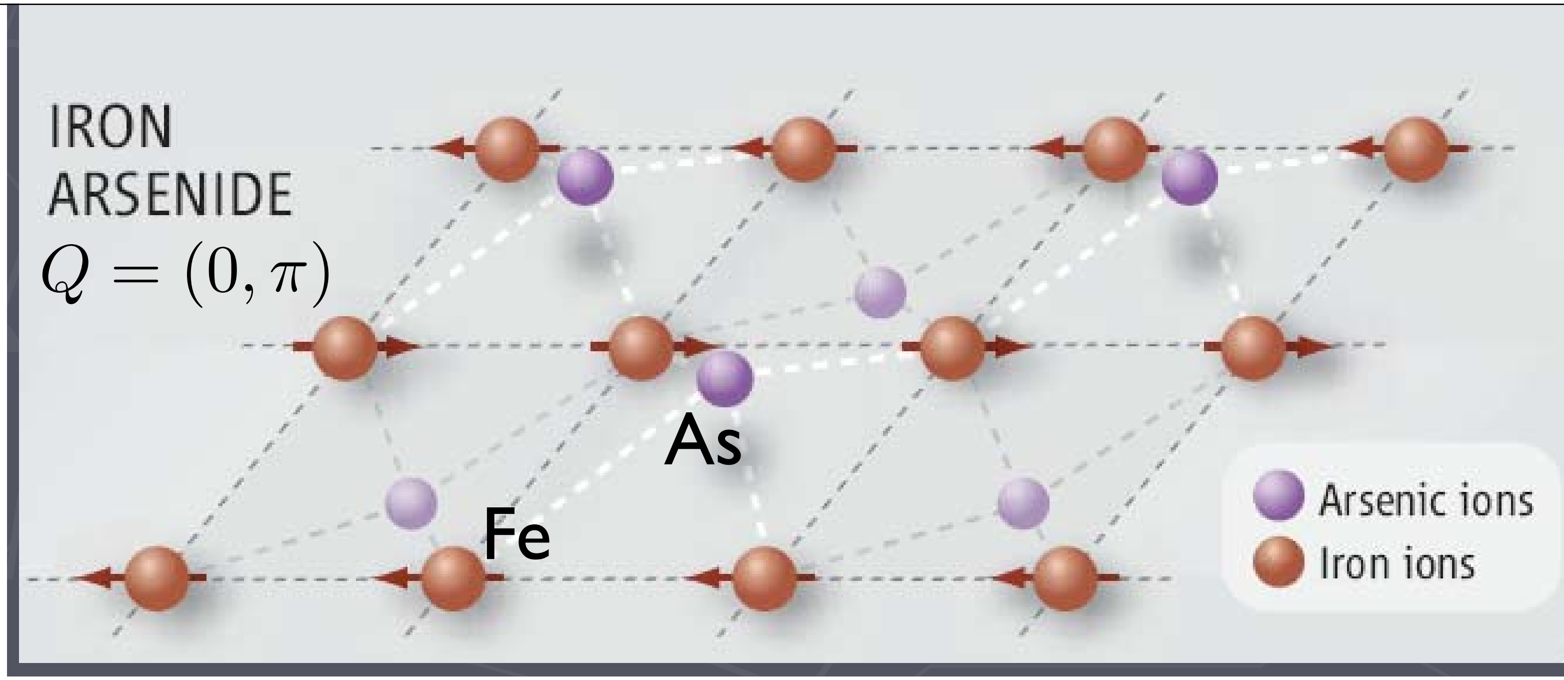
$$T_c = 28K$$

$$SmFeAsO_{0.8}F_{0.2}$$

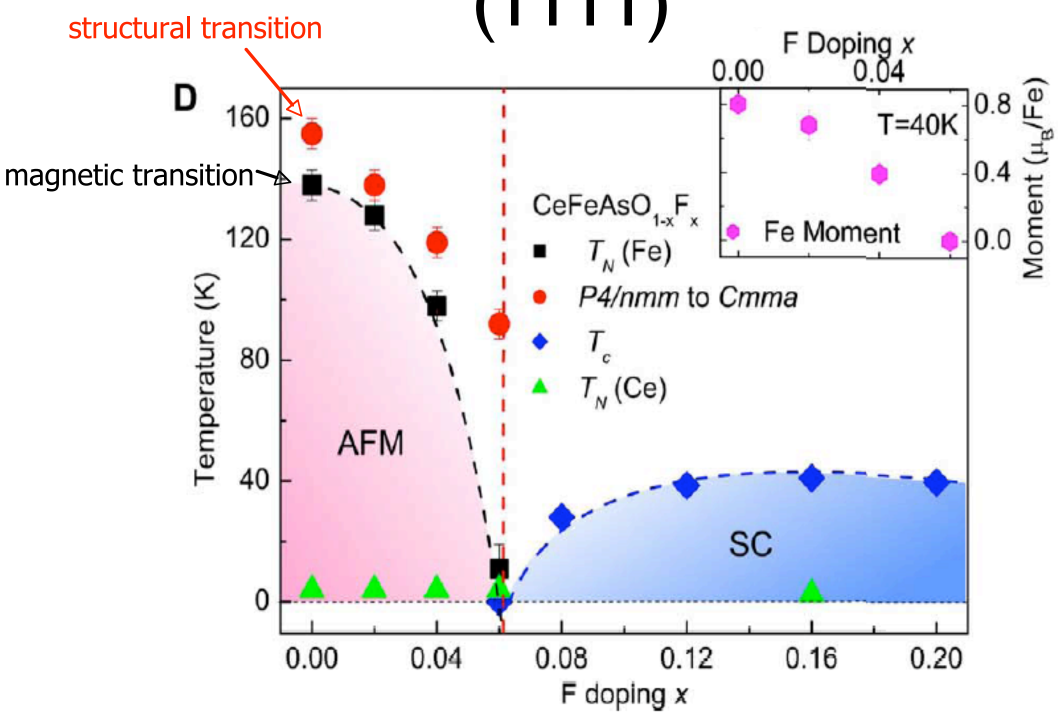
$$T_c = 55K$$

$$LaFePO$$

$$T_c = 6K$$

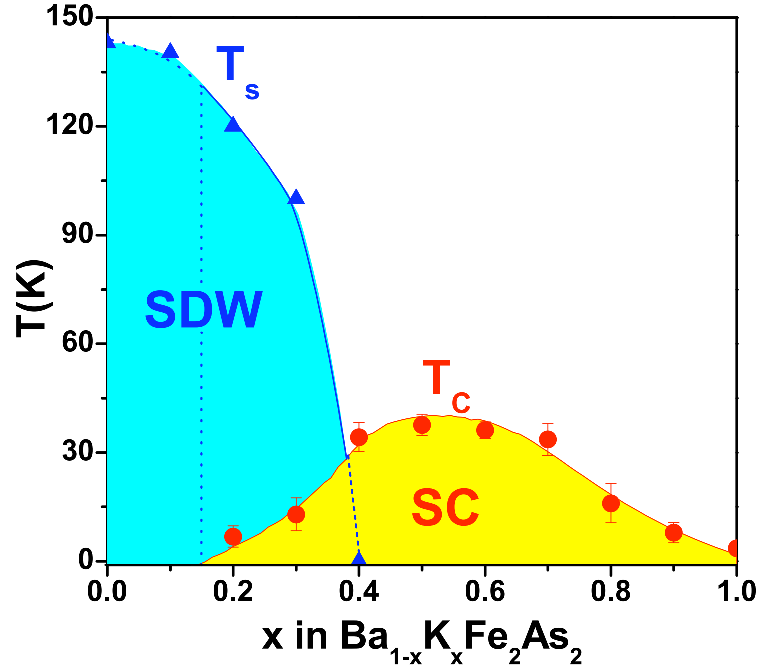

IRON
ARSENIDE
$Q = (0, \pi)$
As
Fe
Arsenic ions
Iron ions

(1111)

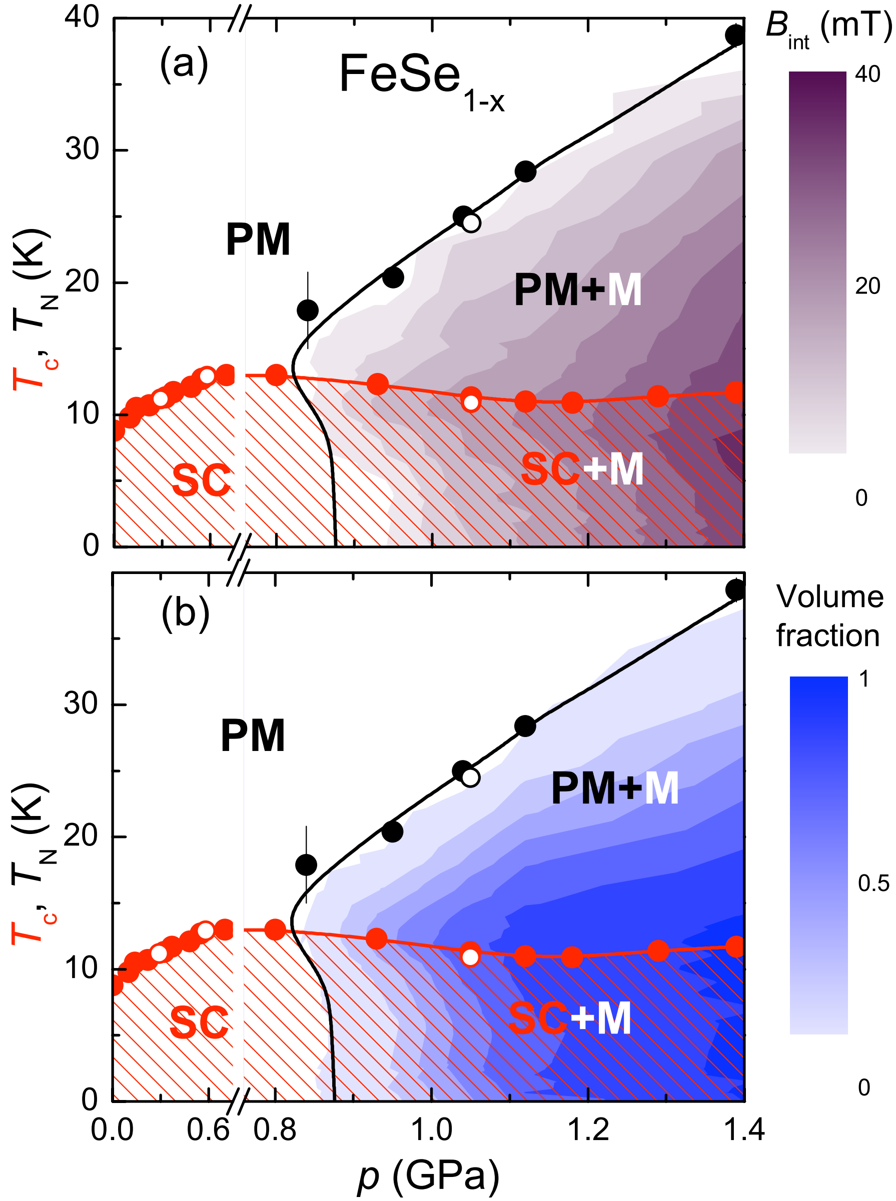


Zhao et al arXiv:0806.2528

(122)



H. Chen et al



R. Khasanov et al, 0908.2734

Heavy fermions : f-electrons hybridize with conduction spd electrons. Parent is a low T coherent, heavy mass paramagnetic metal (pressure or doping AF/SC).

Heavy fermions : f-electrons hybridize with conduction spd electrons. Parent is a low T coherent, heavy mass paramagnetic metal (pressure or doping AF/SC).

Actinides: Pu f-electrons hybridize with spd electrons along with direct f-f hopping. Parent is itinerant heavy 5f electron material.

Heavy fermions : f-electrons hybridize with conduction spd electrons. Parent is a low T coherent, heavy mass paramagnetic metal (pressure or doping AF/SC).

Actinides: Pu f-electrons hybridize with spd electrons along with direct f-f hopping. Parent is itinerant heavy 5f electron material.

Cuperates : Cu 3d electrons hybridize with O p-orbitals and the parent compound is a charge-transfer AF Mott insulator. (doping leads to SC)

Heavy fermions : f-electrons hybridize with conduction spd electrons. Parent is a low T coherent, heavy mass paramagnetic metal (pressure or doping AF/SC).

Actinides: Pu f-electrons hybridize with spd electrons along with direct f-f hopping. Parent is itinerant heavy 5f electron material.

Cuperates : Cu 3d electrons hybridize with O p-orbitals and the parent compound is a charge-transfer AF Mott insulator. (doping leads to SC)

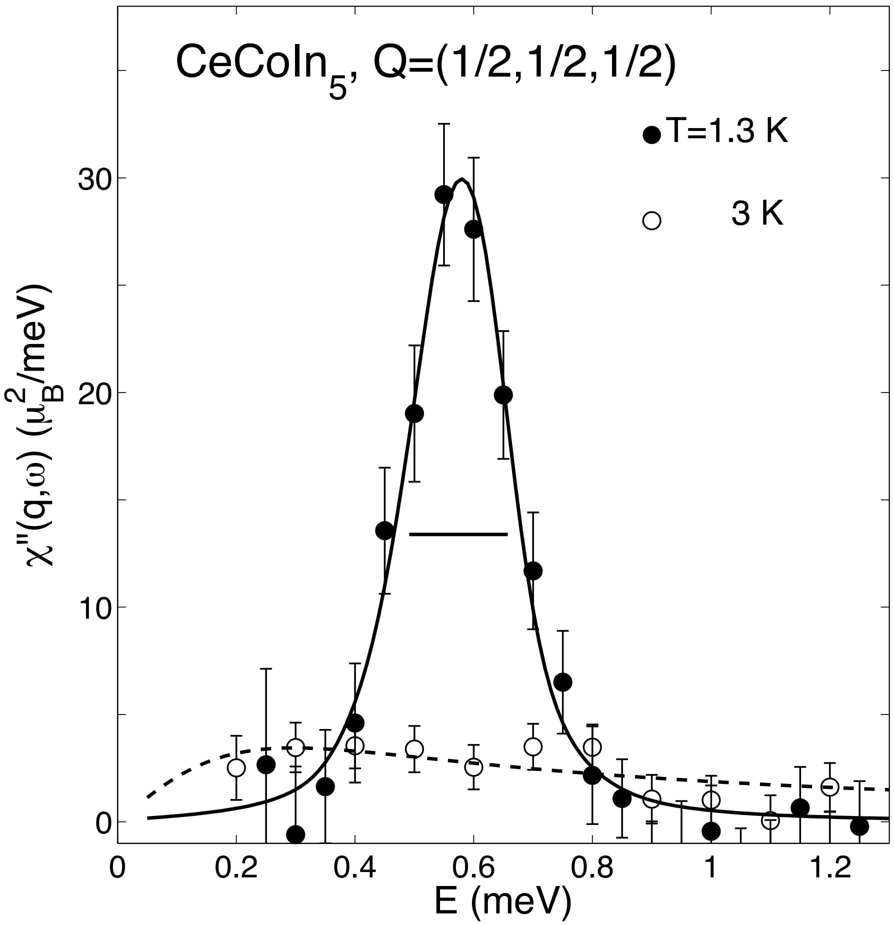
Fe-pnictides and chalcogens : Fe 3d orbitals hybridize through As or Se 4p . Parent compound is a semi-metallic AF (pressure or doping can lead to SC).

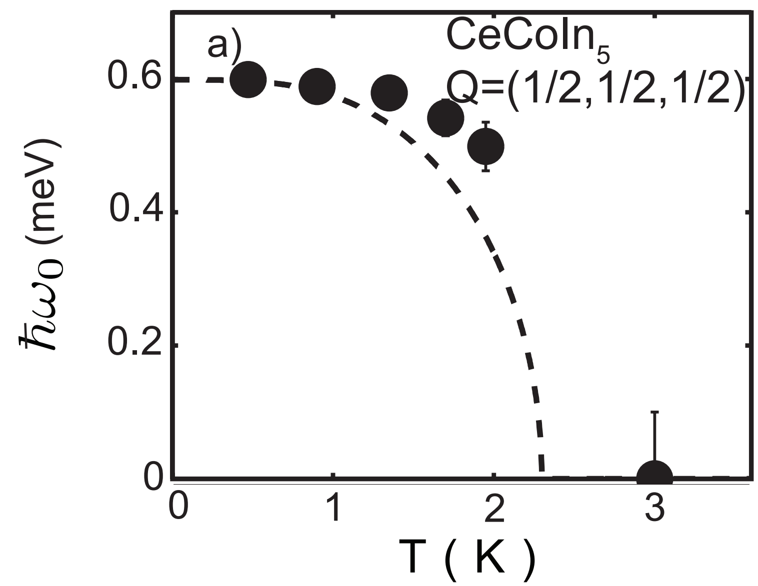
2. The neutron scattering resonance in the superconducting state

This can occur because the BCS coherence factor

$$\frac{1}{2}\left(1 - \frac{\Delta(k+Q)\Delta(k)}{E(k+Q)E(k)}\right) \longrightarrow 1$$

when $\Delta(k+Q) = -\Delta(k)$



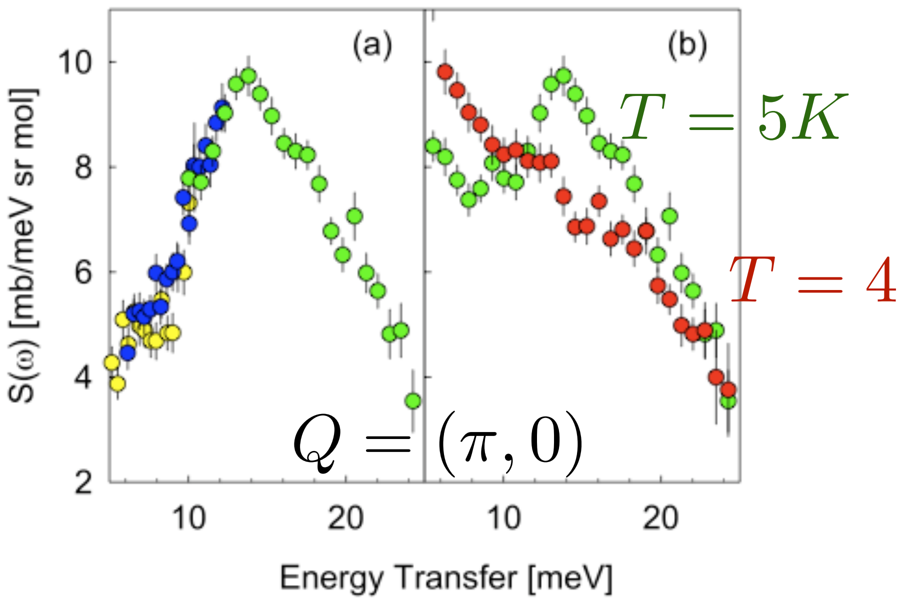


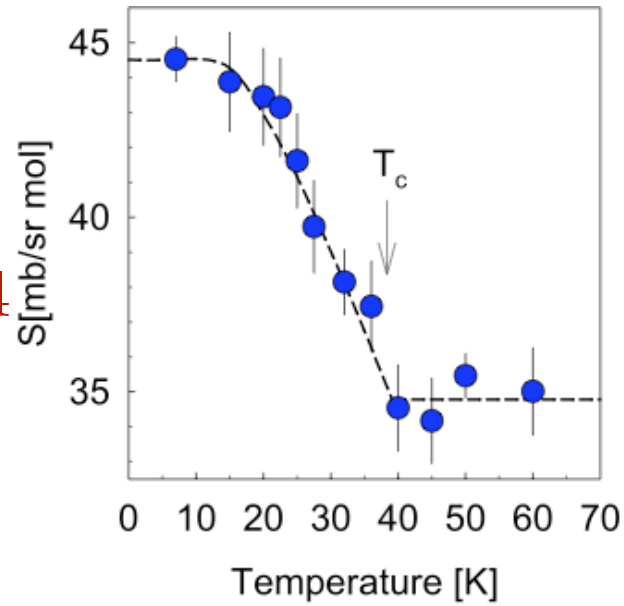
$$\frac{\hbar\omega_{res}}{2\Delta_0} = 0.65$$

C. Stock, C. Broholm, J. Hudis, H. J. Kang, C. Petrovic

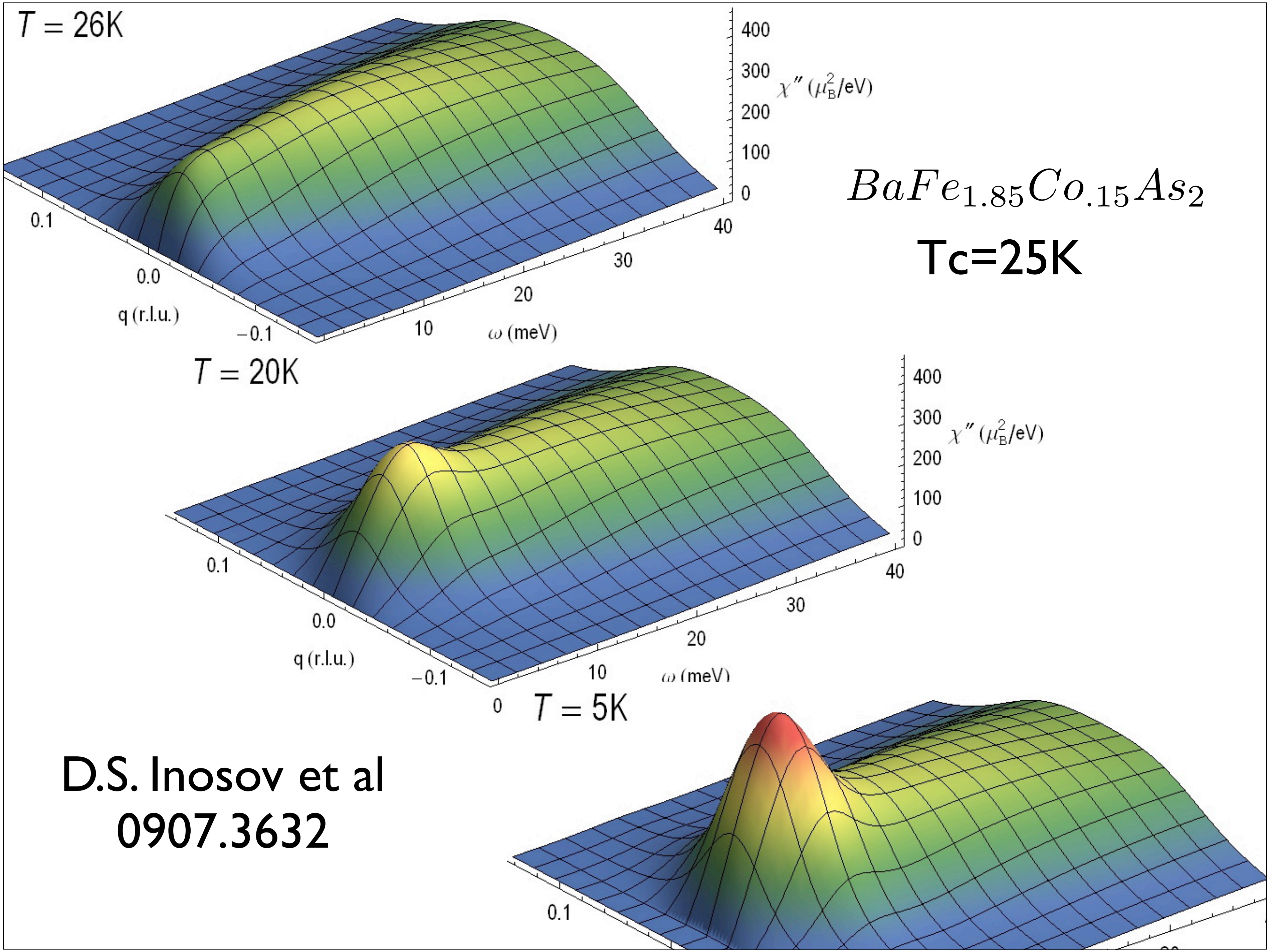
PRL 100, 87001 (2008)

$Ba_{0.6}K_{0.4}Fe_2As_2$ A.D.Christianson et al 0807.3932





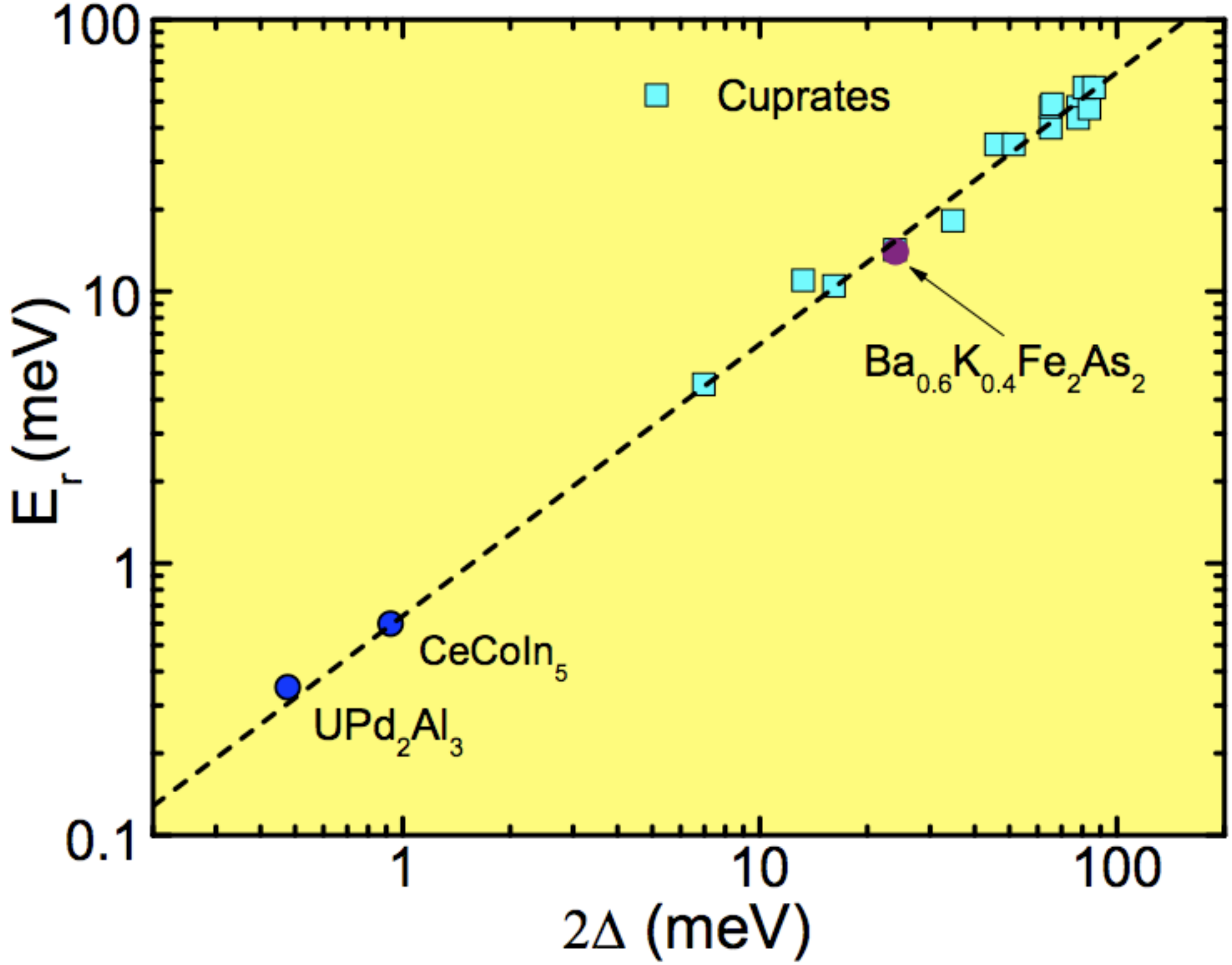
$$(1 - \frac{\Delta(k+Q)\Delta(k)}{E(k+Q)E(k)})$$



$BaFe_{1.85}Co_{.15}As_2$

Tc=25K

D.S. Inosov et al
0907.3632



100
10
1
0.1
1
10
100
E_r (meV)
2Δ (meV)
Cuprates
$Ba_{0.6}K_{0.4}Fe_2As_2$
$CeCoIn_5$
UPd_2Al_3

Common Threads:

Families of layered 2D materials with correlated itinerant d or f electrons

Common Threads:

Families of layered 2D materials with correlated itinerant d or f electrons

Competition and/or coexistence of AF and unconventional superconductivity

Common Threads:

Families of layered 2D materials with correlated itinerant d or f electrons

Competition and/or coexistence of AF and unconventional superconductivity

Neutron scattering resonance implies a sign change of the gap $\Delta(k+Q) = -\Delta(k)$

Common Threads:

Families of layered 2D materials with correlated itinerant d or f electrons

Competition and/or coexistence of AF and unconventional superconductivity

Neutron scattering resonance implies a sign change of the gap

$$\Delta(k+Q) = -\Delta(k)$$

The same electrons that are involved with superconductivity are involved with magnetism

3. The Models

The Models

Multi-orbital Hubbard Models

$$H_0 = \sum_{i,n,\sigma} \epsilon_n n_{in\sigma} + \sum_{i,j,\sigma} \sum_{n,m} t_{ij}^{nm} d_{n\sigma}^{\dagger}(i) d_{m\sigma}(j)$$

The Models

Multi-orbital Hubbard Models

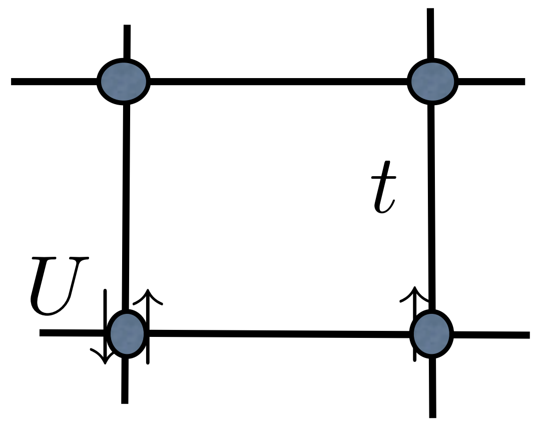
$$H_0 = \sum_{i,n,\sigma} \epsilon_n n_{in\sigma} + \sum_{i,j,\sigma} \sum_{n,m} t_{ij}^{nm} d^\dagger_{n\sigma}(i) d_{m\sigma}(j)$$

$$H_{int} = U \sum_{in} n_{i,n\uparrow} n_{i,n\downarrow} + \frac{V}{2} \sum_{i,n,m} n_{in} n_{im}$$

$$-\frac{J}{2} \sum_{i,n,m} S_{in} * S_{im} + \frac{J'}{2} \sum_{i,n,m} \sum_{\sigma} d^\dagger_{in\sigma} d^\dagger_{in-\sigma} d_{im-\sigma} d_{im\sigma}$$

4. The properties of the models

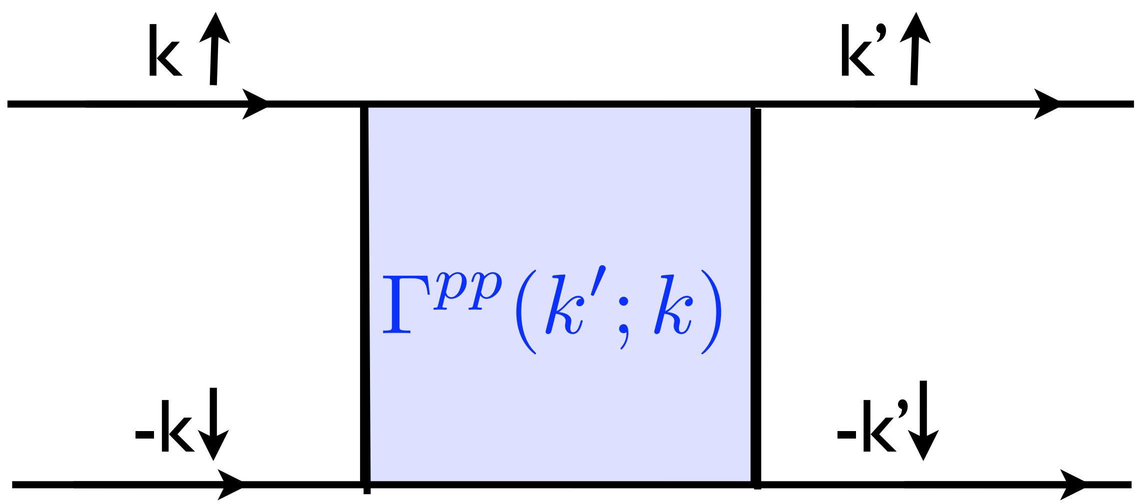
The Hubbard Model



$$H = -t \sum_{<i,j>\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

U/t $\qquad$ n =1-x

The effective pairing interaction is given by the irreducible particle-particle vertex

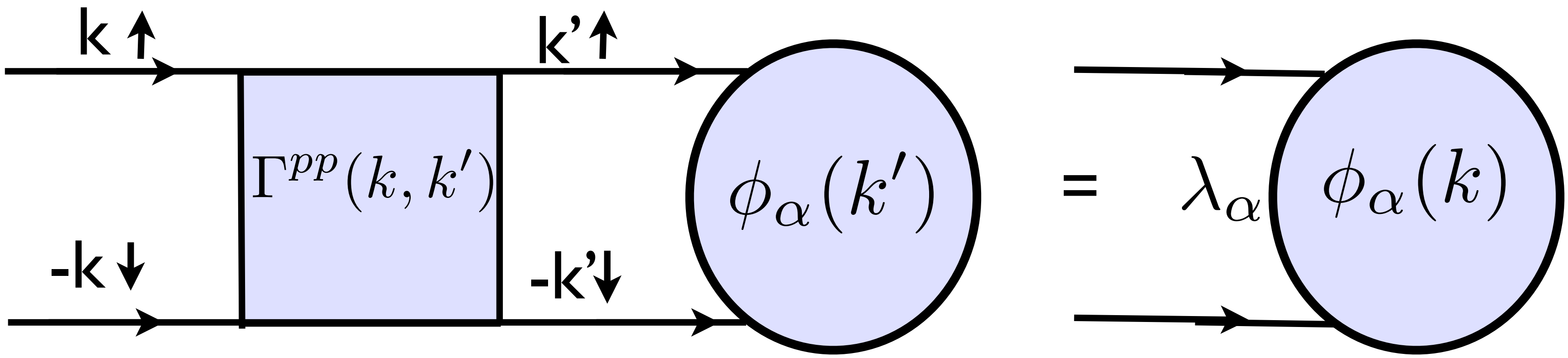


Here k=(k,iω_n). The momentum transfer is k'-k and the Matsubara energy transfer is $i\omega_{n'} - i\omega_n$.

Superconductivity

The Bethe-Salpeter equation for the particle-particle channel with center of mass momentum Q=0 is

$$-(T/N)\sum_{k'}\Gamma^{pp}(k,k')G_{\uparrow}(k')G_{\downarrow}(-k')\phi_{\alpha}(k') = \lambda_{\alpha}\phi_{\alpha}(k)$$



.

Superconductivity

The Bethe-Salpeter equation for the particle-particle channel with center of mass momentum Q=0 is

$$-(T/N)\sum_{k'}\Gamma^{pp}(k,k')G_{\uparrow}(k')G_{\downarrow}(-k')\phi_{\alpha}(k')=\lambda_{\alpha}\phi_{\alpha}(k)$$

The d-wave pairfield susceptibility

$$P_d(T)\approx\frac{const}{1-\lambda_{d_{x^2-y^2}}(T)}$$

.

Magnetism

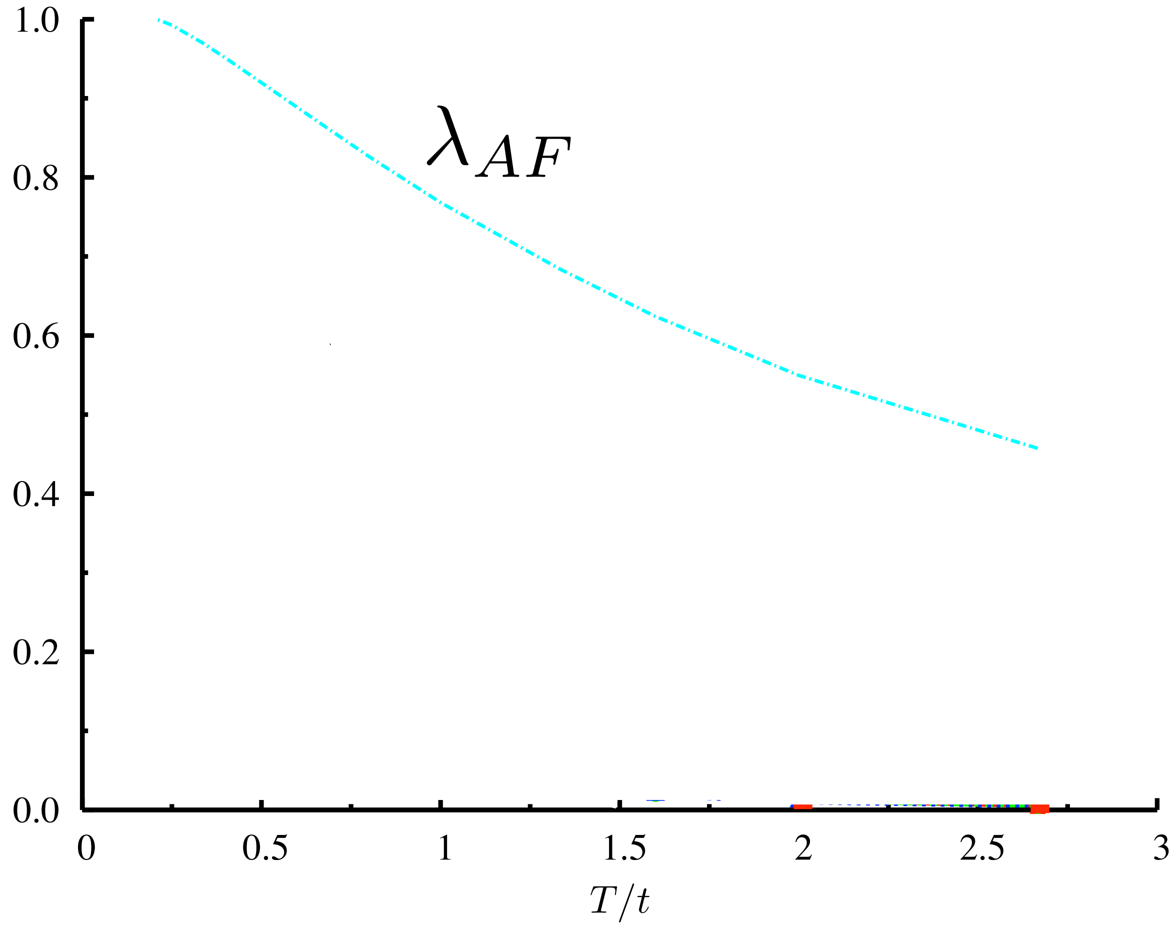
In the same way, we have for the particle-hole channel with center of mass momentum Q

$$-(T/N)\sum_{k'}\Gamma^{ph}(k,k')G(k'+Q)G(k')\psi_\alpha(k') = \lambda_\alpha\psi_\alpha(k)$$

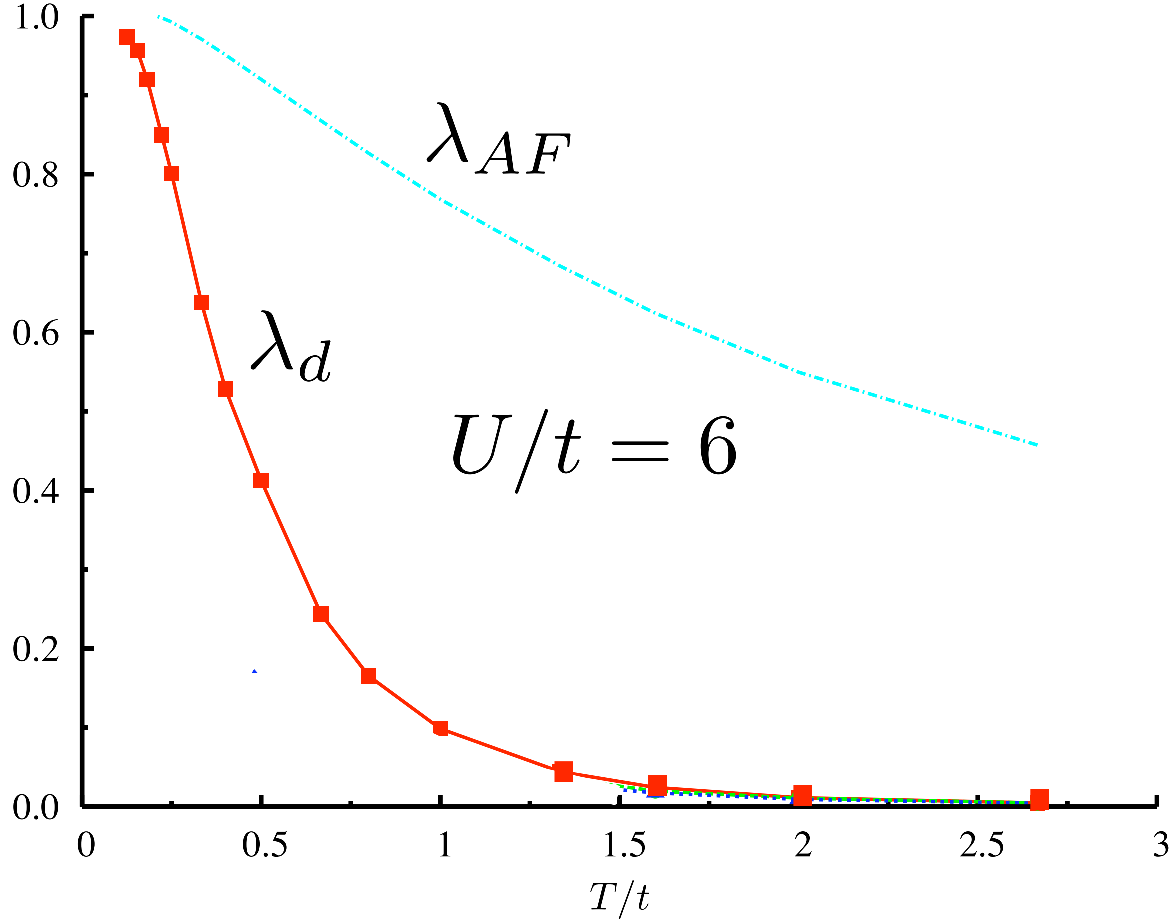
with $\Gamma^{ph}(k,k')$ the irreducible particle-hole vertex

$$\chi_{AF}(T) \approx \frac{const}{1-\lambda_{AF}(T)}$$

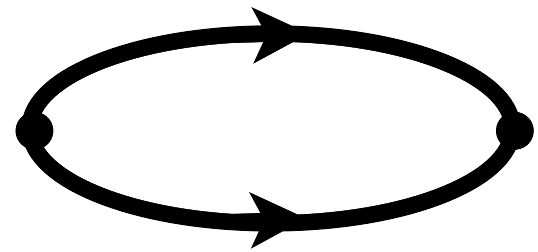
Leading eigenvalues in the particle-hole and particle-particle channels for $< n >= 1$

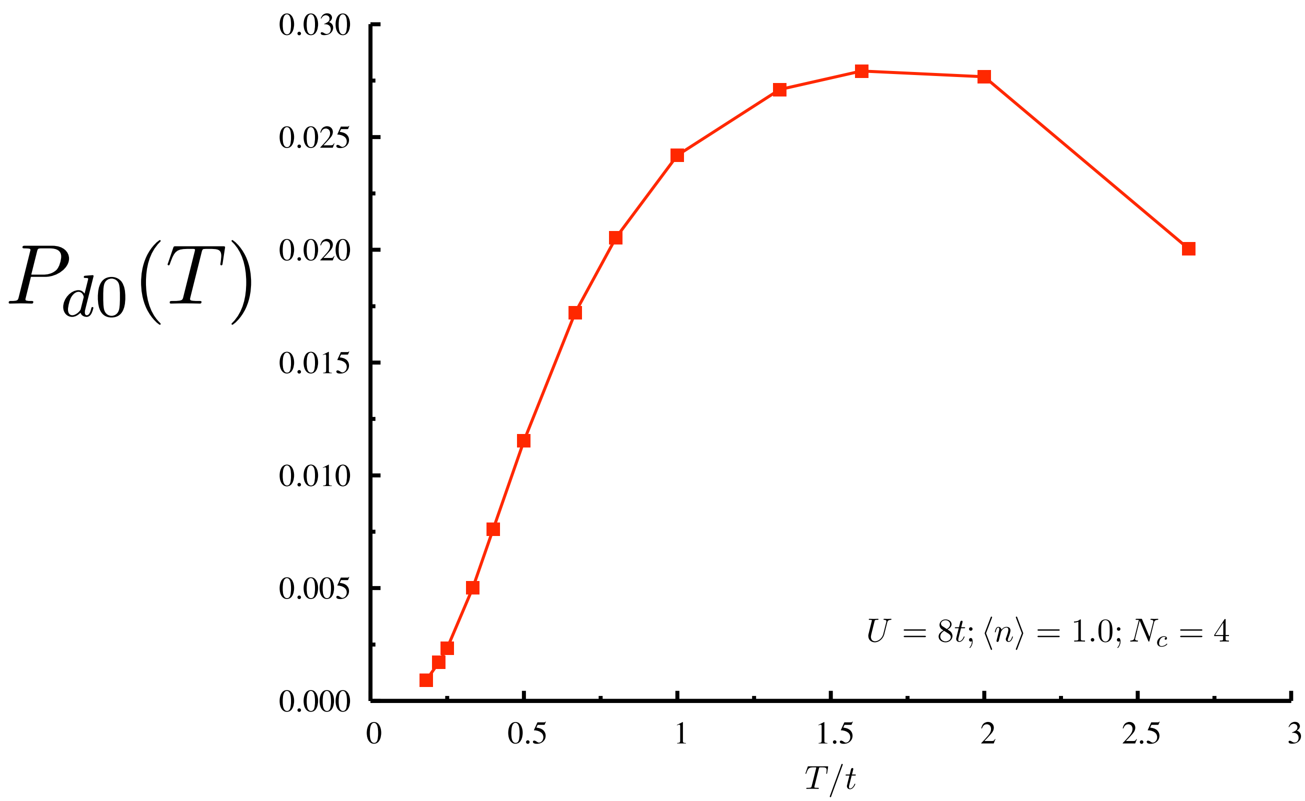


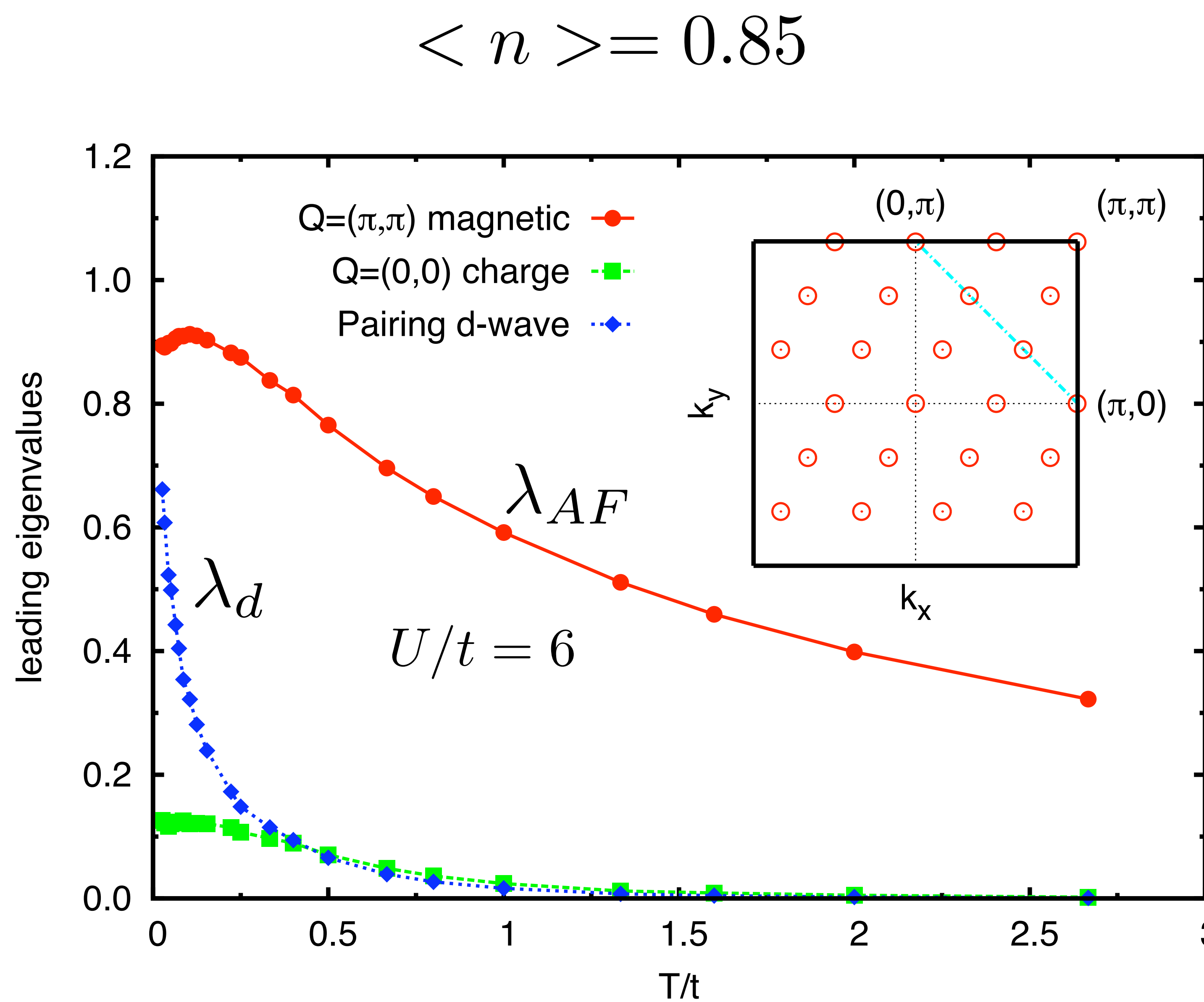
Leading eigenvalues in the particle-hole and particle-particle channels for $< n >= 1$



$$P_d(T) = \frac{P_{d0}(T)}{1 - \lambda_d(T)} \qquad P_{d0} =$$

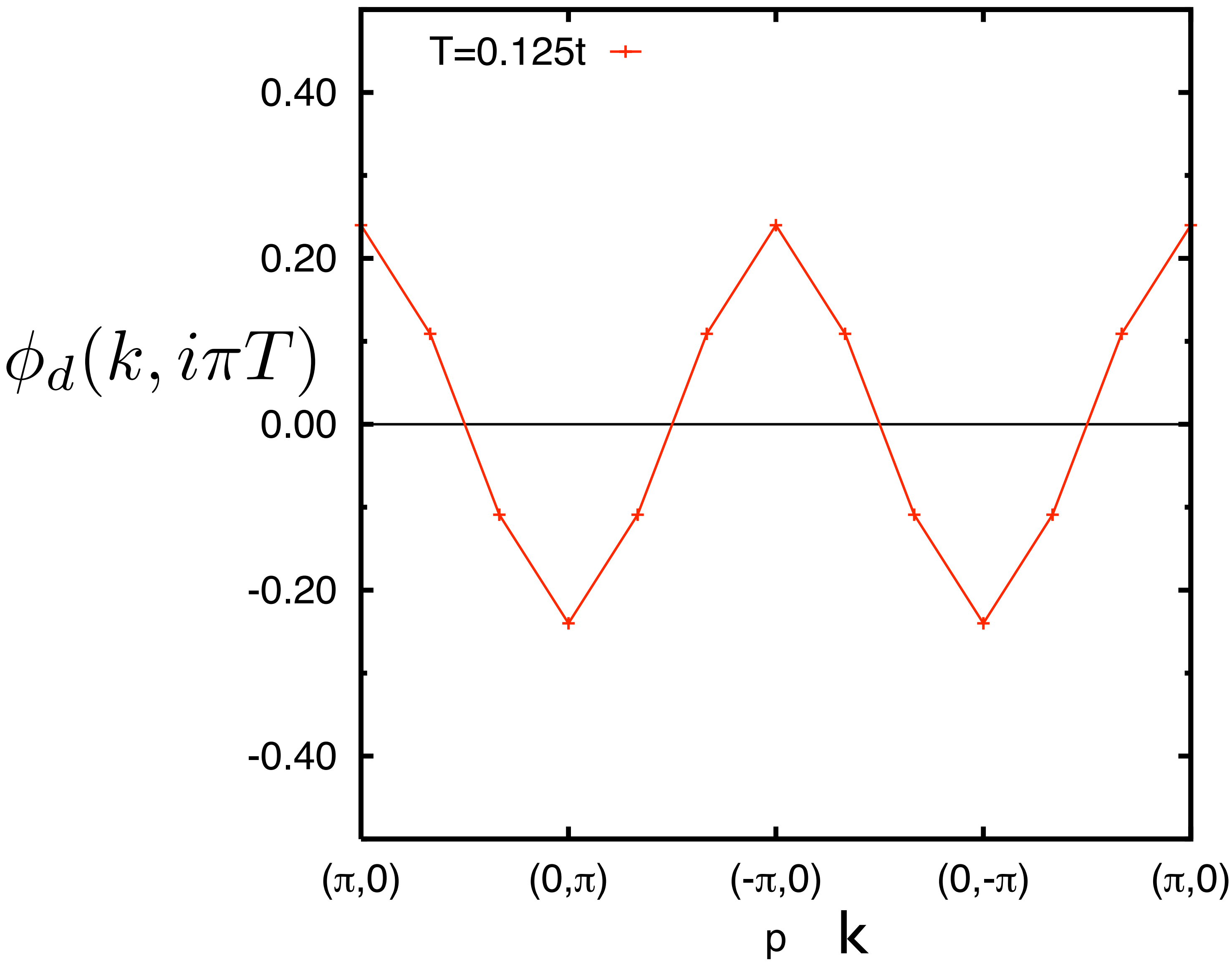




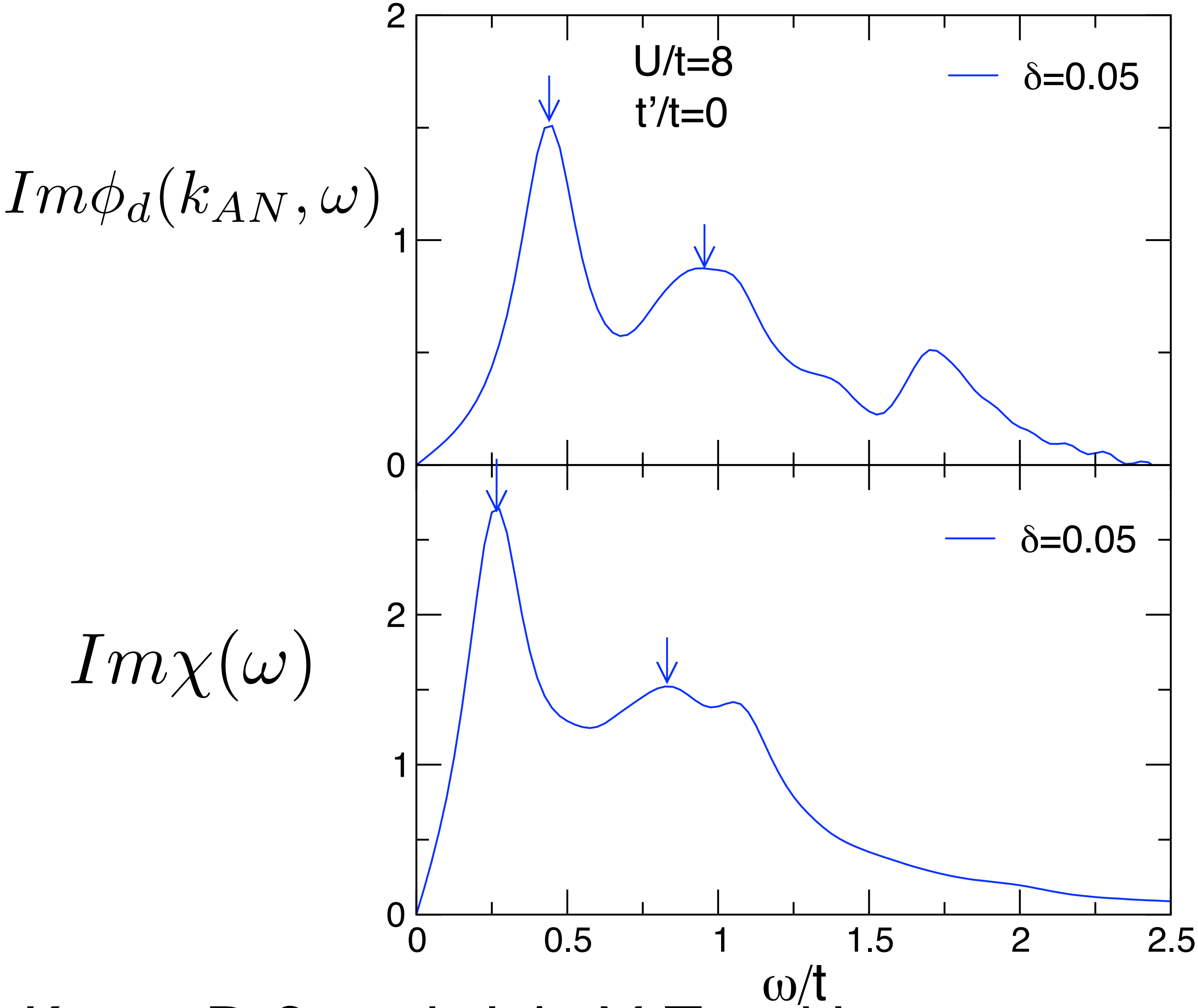


$< n >= 0.85$
Q=(π,π) magnetic
Q=(0,0) charge
Pairing d-wave
(0,π)
(π,π)
(π,0)
k_y
k_x
λ_{AF}
λ_d
$U/t = 6$
leading eigenvalues
T/t
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
0.5
1
1.5
2
2.5
3

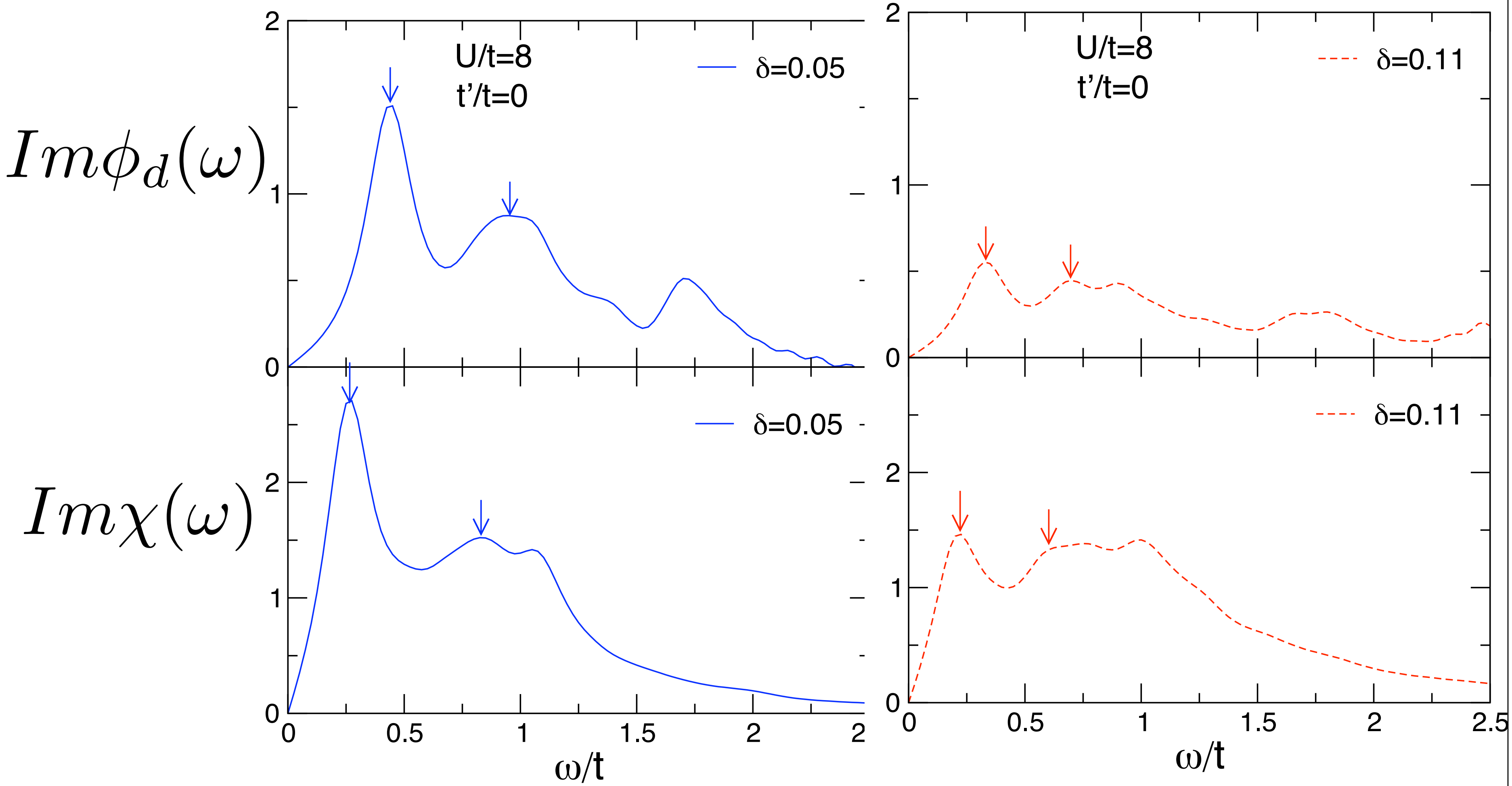
The k and ω dependence of the gap function $\phi(k, \omega)$ reflect the structure of the pairing interaction.



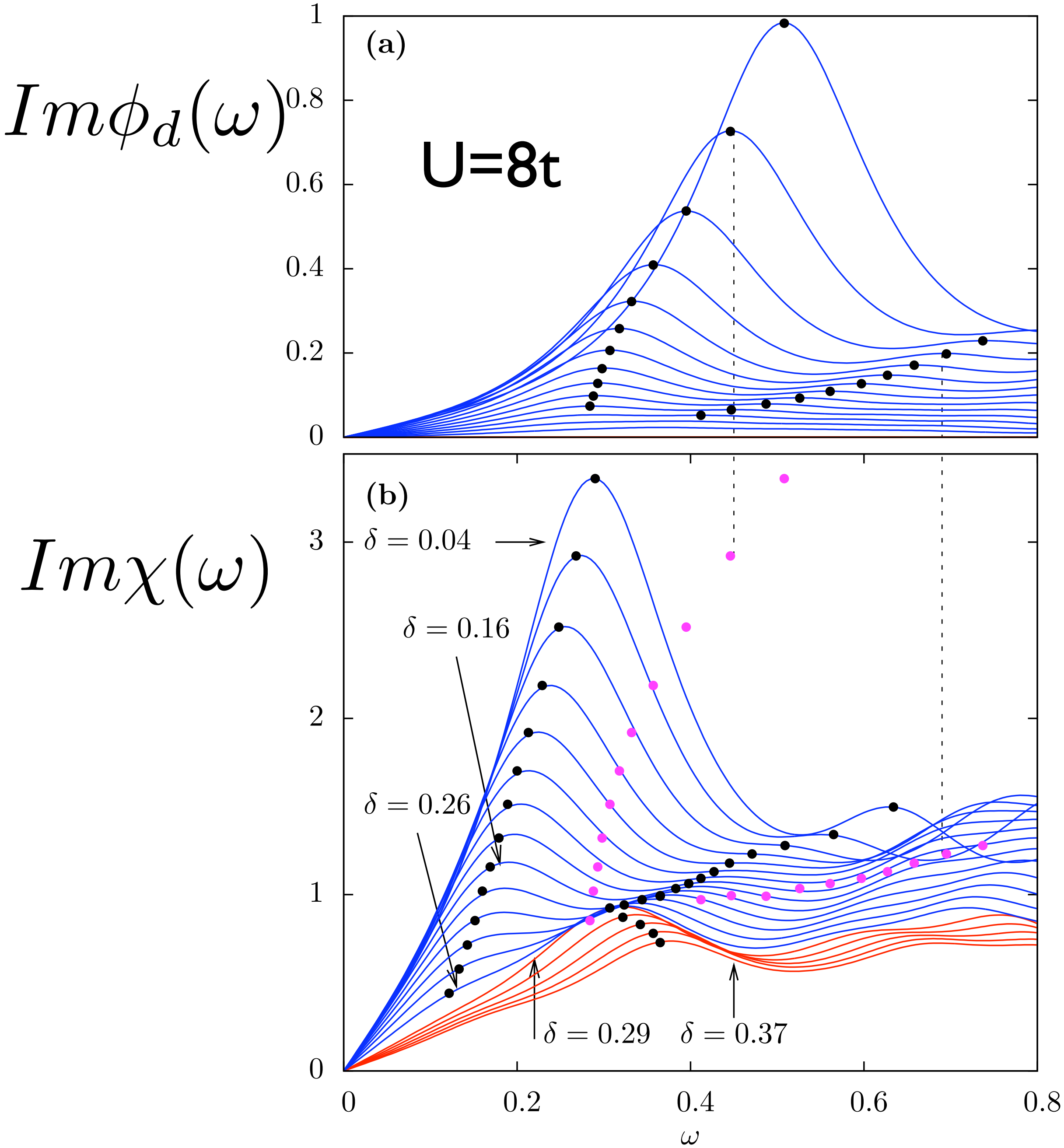
T=0.125t
0.40
0.20
0.00
-0.20
-0.40
$\phi_d(k, i\pi T)$
(π,0)
(0,π)
(-π,0)
(0,-π)
(π,0)
p k



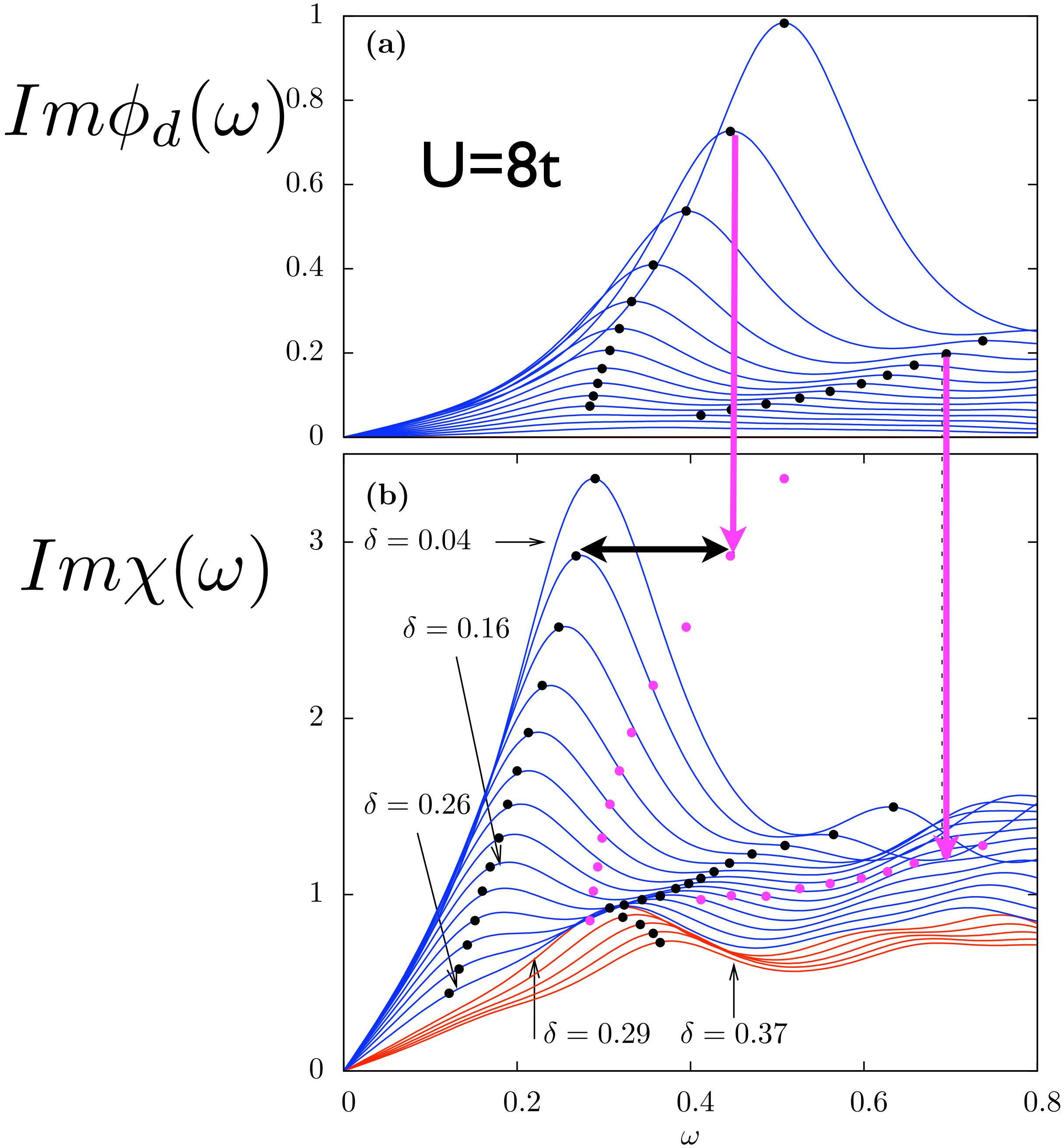
B. Kyung, D. Senechal, A.-M. Tremblay
0812.1228



$Im\phi_d(\omega)$
$Im\chi(\omega)$
U/t=8
t'/t=0
δ=0.05
δ=0.11
ω/t



$Im\phi_d(\omega)$
U=8t
(a)
(b)
$Im\chi(\omega)$
$\delta = 0.04$
$\delta = 0.16$
$\delta = 0.26$
$\delta = 0.29$
$\delta = 0.37$
ω



$Im\phi_d(\omega)$
(a)
U=8t
$Im\chi(\omega)$
(b)
$\delta = 0.04$
$\delta = 0.16$
$\delta = 0.26$
$\delta = 0.29$
$\delta = 0.37$
ω

There are many papers addressing the multi-orbital Hubbard model and the Fe superconductors

The s^{+-} gap was proposed by

I.I.Mazin, D.J. Singh, M.D.Johannes and M.H. Du, PRL '08

RPA calculations

T. Takimoto, T. Hotta and K. Ueda, PRB '04

K. Kuroki et al , PRL '08, Physica C '08, PRB '09

S. Graser et al, NJP '09

RG calculations

F. Wang et al Europhys Lett '09

A.V. Chubukov et al, PRB '08

C. Platt et al, 0903.1963

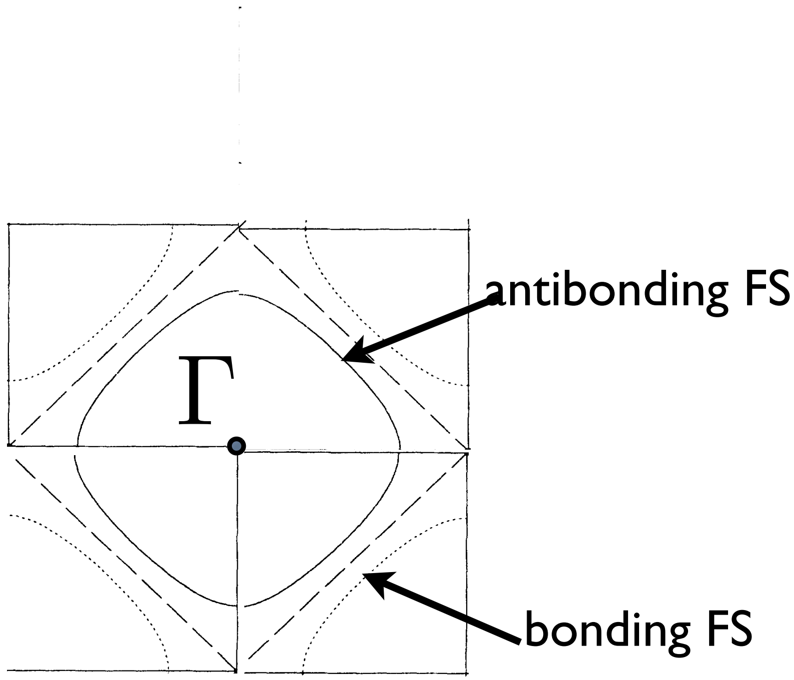
A Monte Carlo treatment of a Hubbard Model with two Fermi surfaces

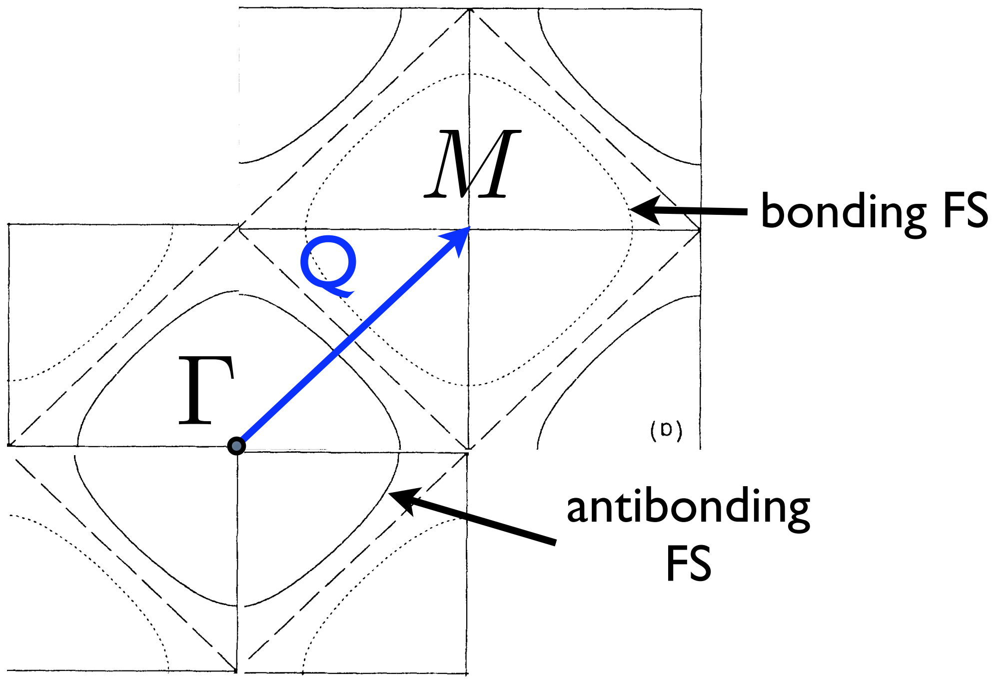
The 2-layer Hubbard model with an interlayer hopping

$$-t_z \sum_{i,\sigma} (d^\dagger_{1\sigma}(i) d_{2\sigma}(i) + h.c.)$$

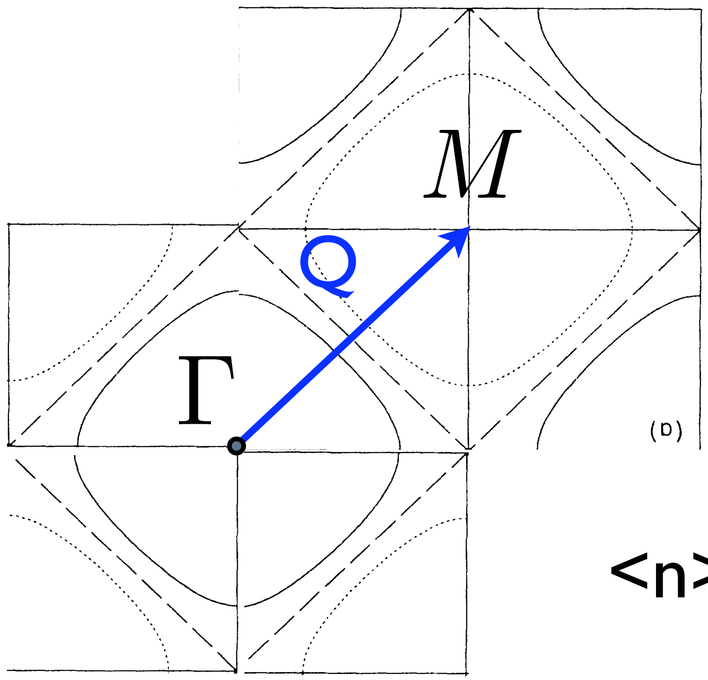
N. Bulut et al ,PRB 45, 5577

K. Bouadim et al, PRB 77, 144527

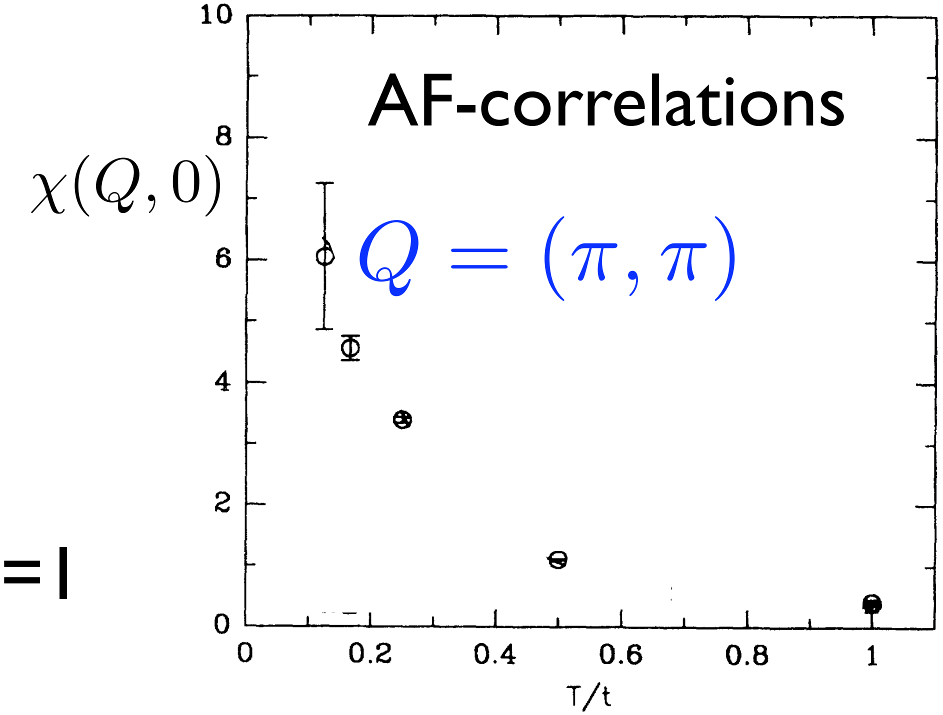

antibonding FS
Γ
bonding FS

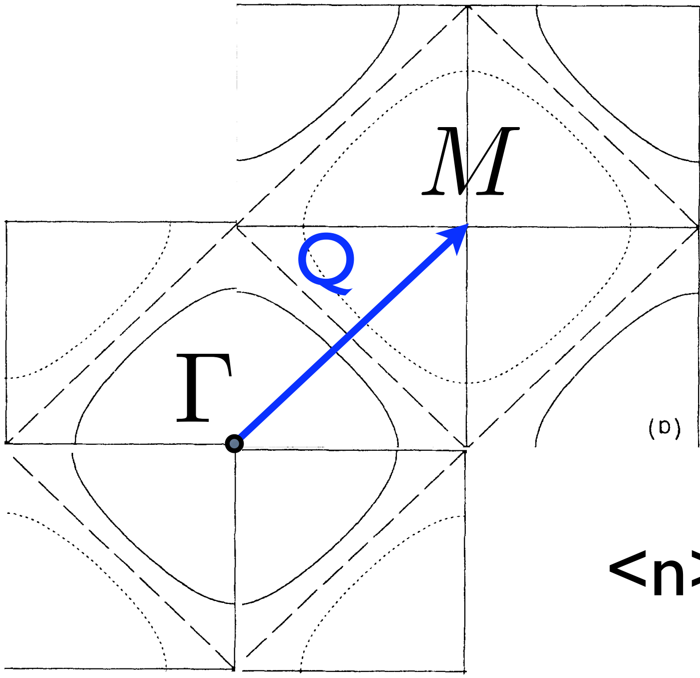


M
bonding FS
Q
Γ
(b)
antibonding
FS

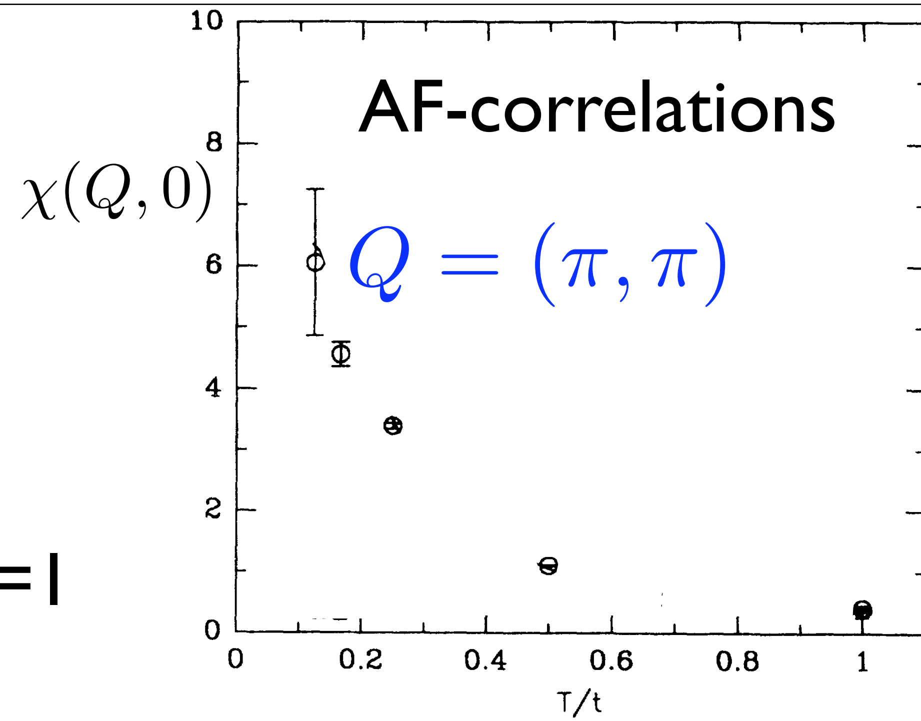


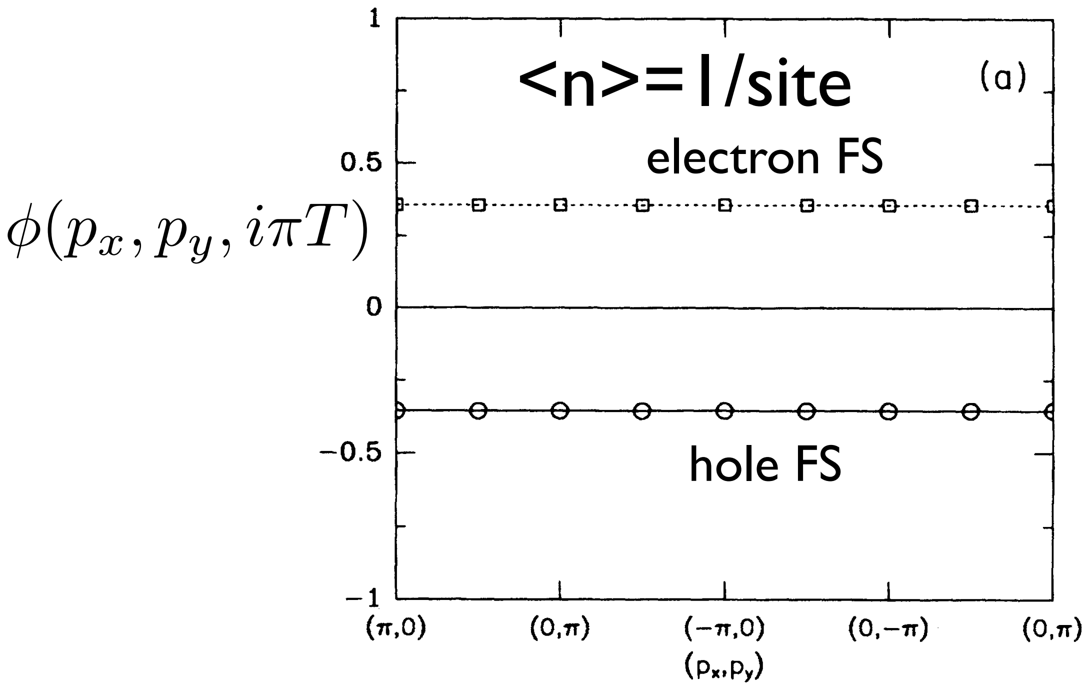
<n>=1





<n>=1

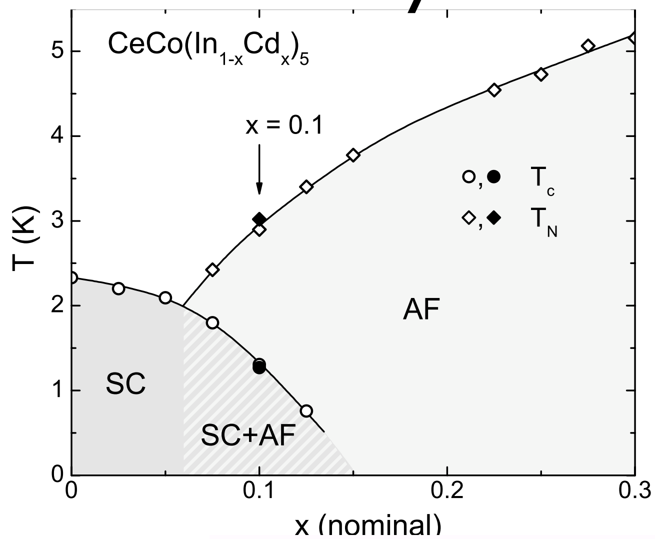


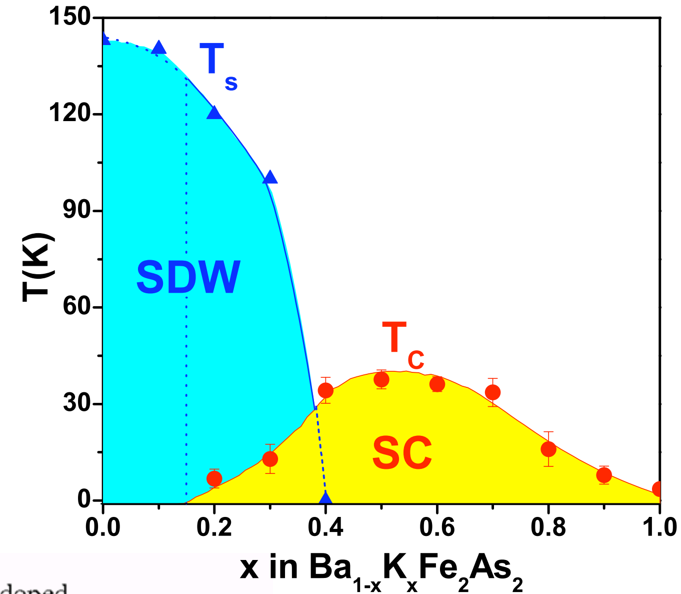


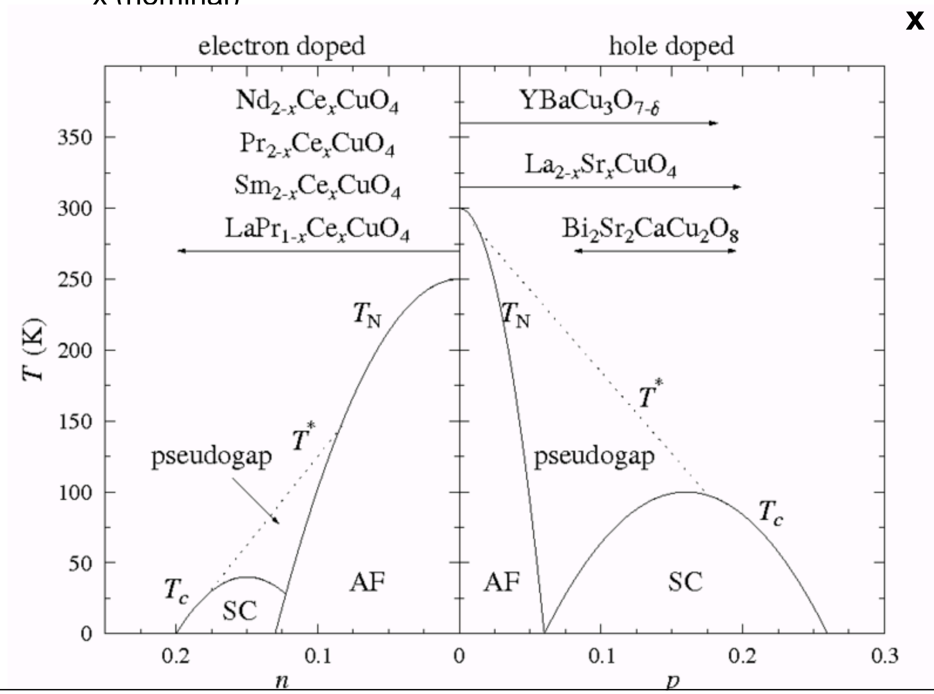
Sign-switched pairfield

Some Common Threads

Competition and/or coexistence of AF and unconventional superconductivity

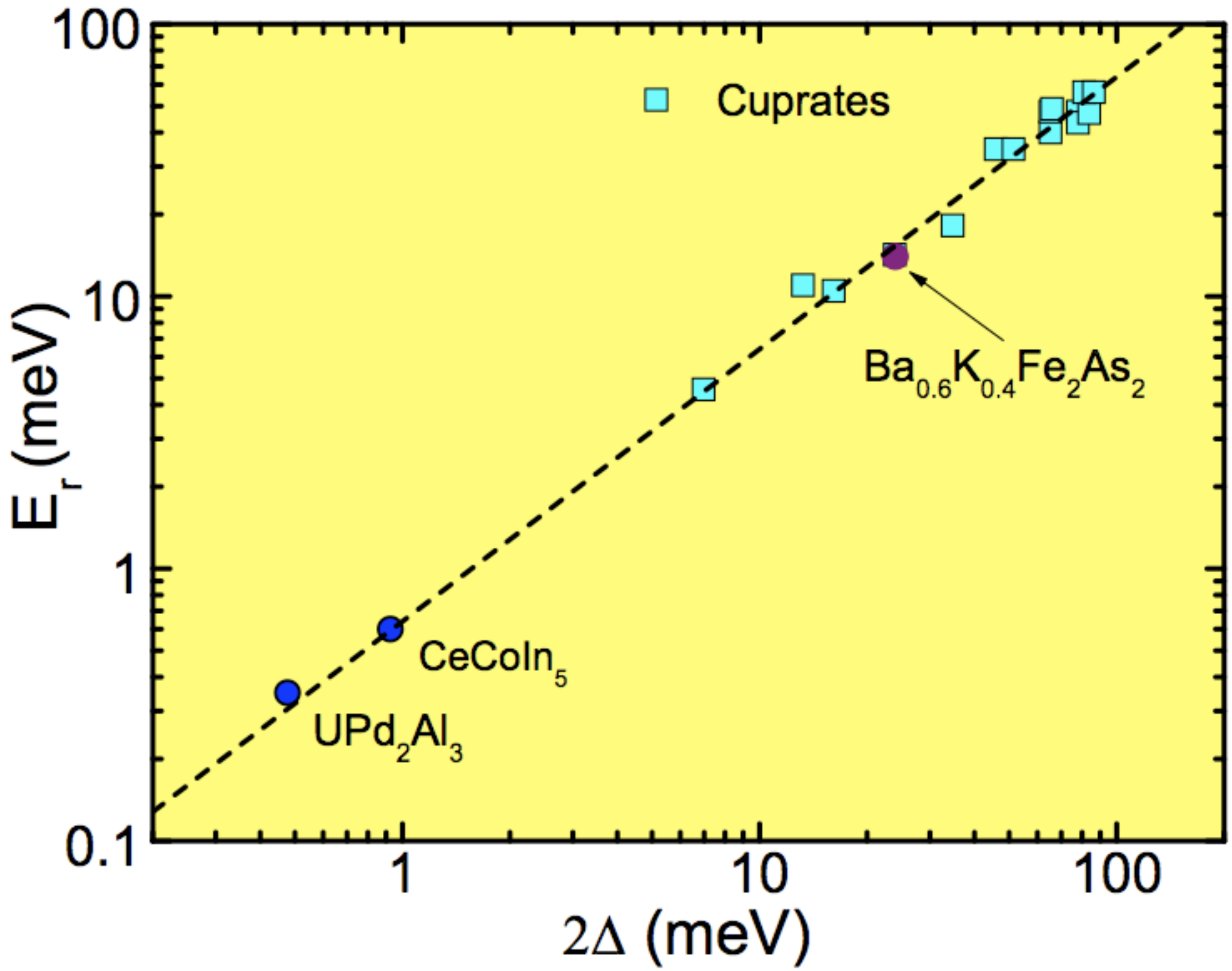


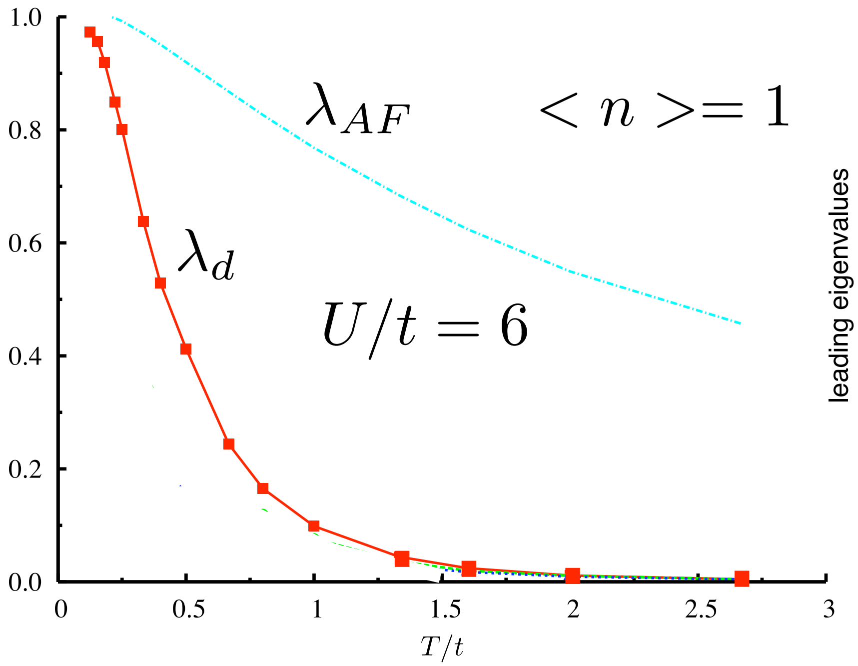


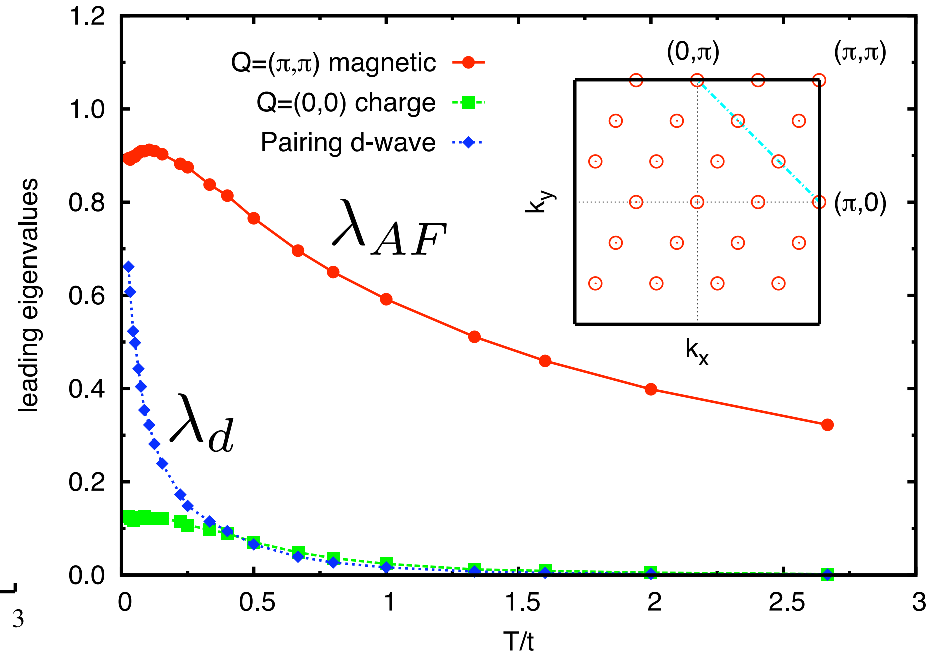


Neutron scattering resonance implies a sign change of the gap

$$\Delta(k+Q) = -\Delta(k)$$





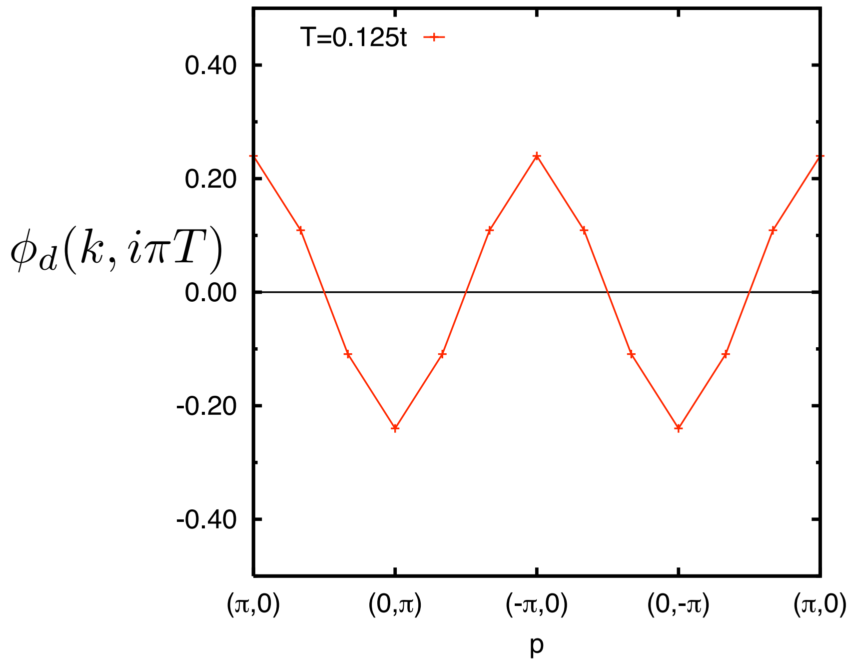


In both the materials and the models superconductivity appears when antiferromagnetism is suppressed.

In the models we see that the structure of the interaction is reflected in $\Delta(k, \omega)$

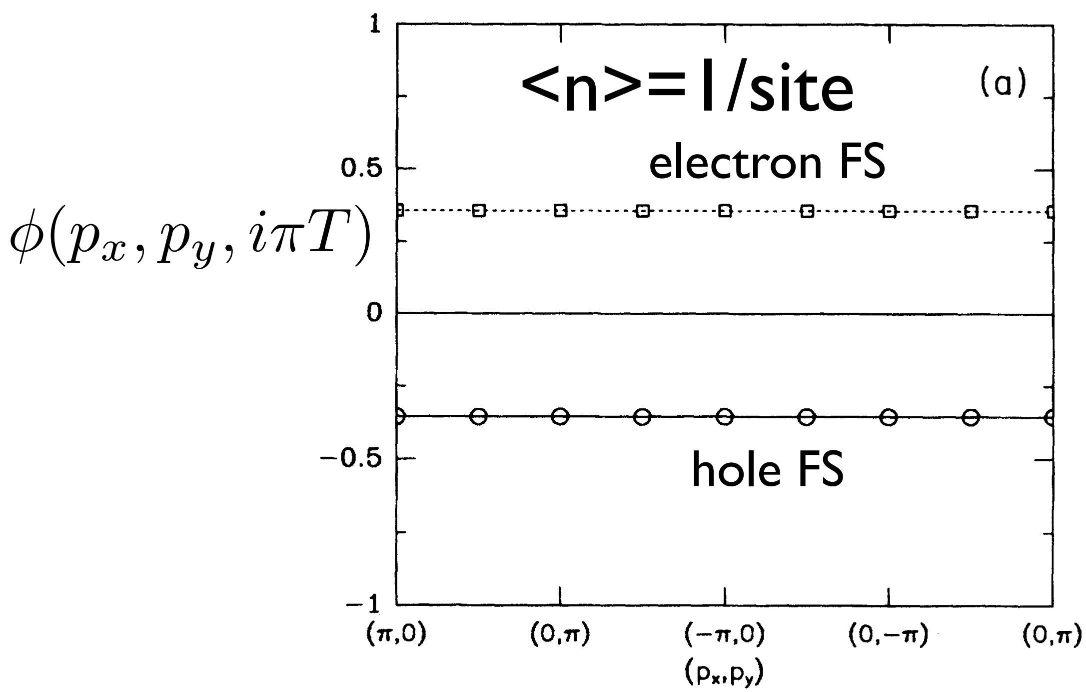
The k dependence of the gap depends upon the electronic band structure (Fermi surfaces and orbital weights).

The frequency dependence of the gap depends on the frequency dependence of the magnetic susceptibility.



Single band Hubbard

$$d_{x^2-y^2}$$

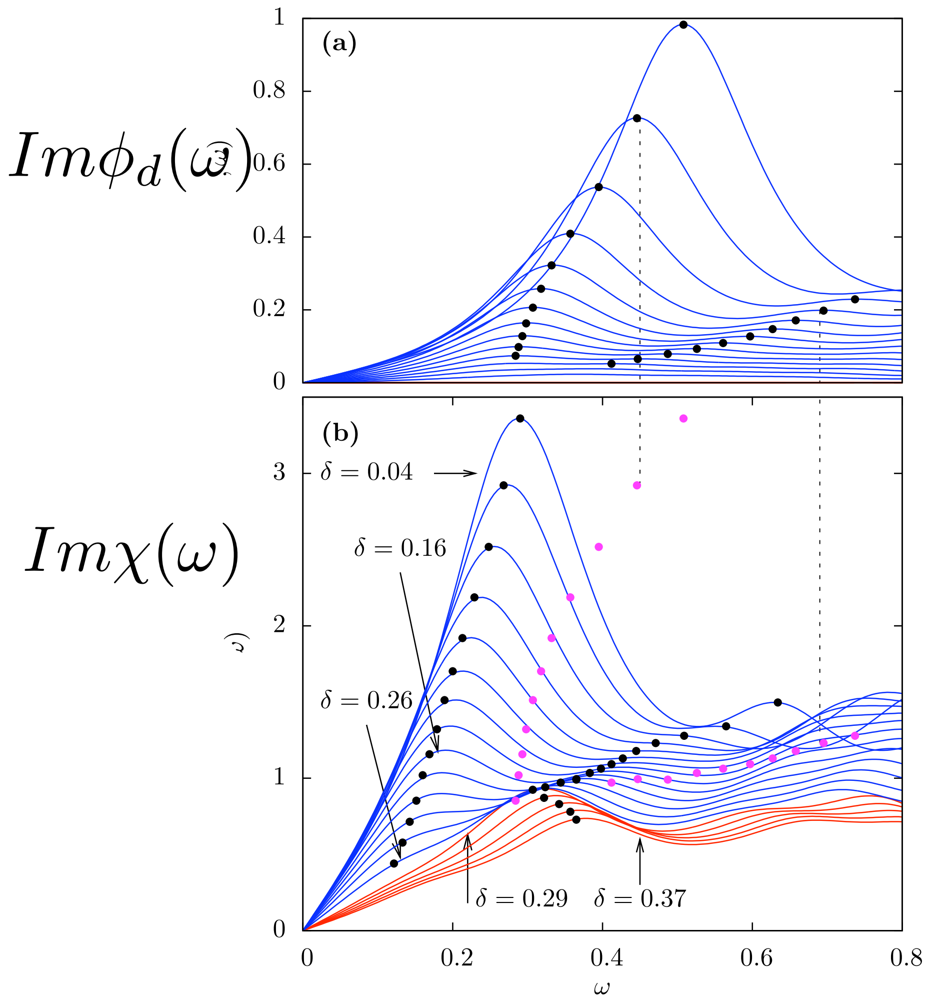


Model 2-band Hubbard

sign switched

for large t_z

The frequency dependence of the gap depends on the frequency dependence of the magnetic susceptibility.



It remains to be seen how these threads will be tied together for the real materials.