Thermodynamic properties of Fe-based superconductors

Christoph Meingast

Institute for Solid State Physics
Karlsruhe Institute of Technology

**DFG - Schwerpunktprogramm - Hochtemperatursupraleitung in Eisenpniktiden (SPP1458)*

F. Hardy, A. Böhmer, P. Burger, T. Wolf, R. Heid, R. Eder, P. Schweiss, P. Adelmann
IFP, KIT, Karlsruhe

W. Schranz, University of *Vienna*

M. Jackson, C. Paulsen
Institut Néel, CNRS-MCBT, Grenoble

D. Aoki
CEA Grenoble, SPSMS-INAC, Grenoble

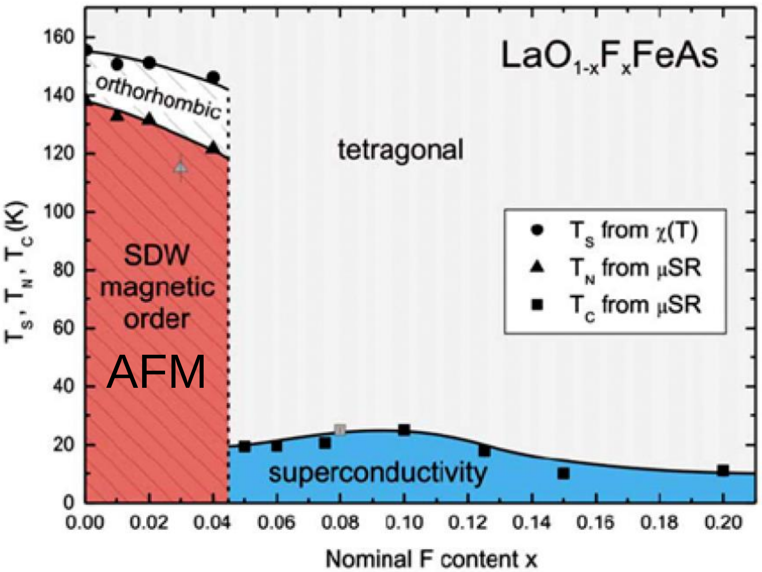
J. Schmalian
TKM, KIT, Karlsruhe

Y. X. Yao
Ames Laboratory

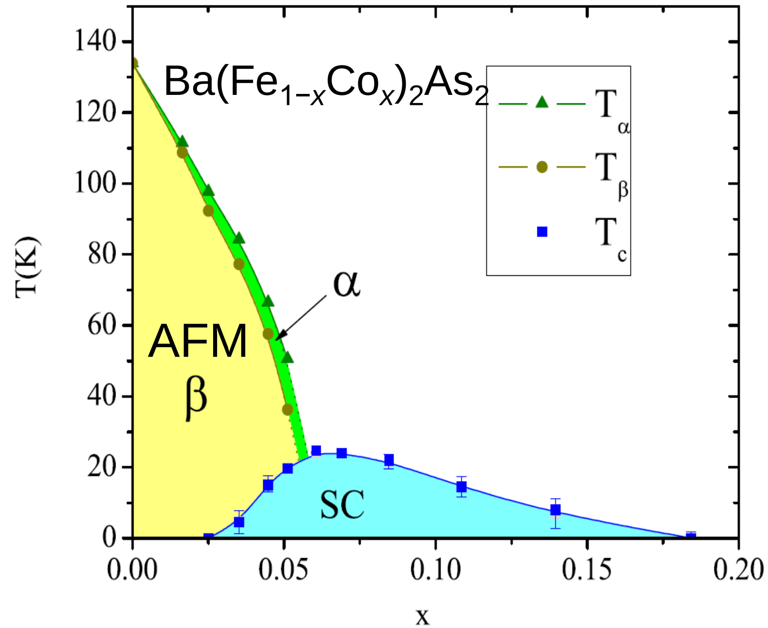
G. Kotliar
Rutgers University

Phase diagrams

H. Luetkens et al., arXiv:0806.3533



Chu et al. PRB**79**, 014506 (2009)



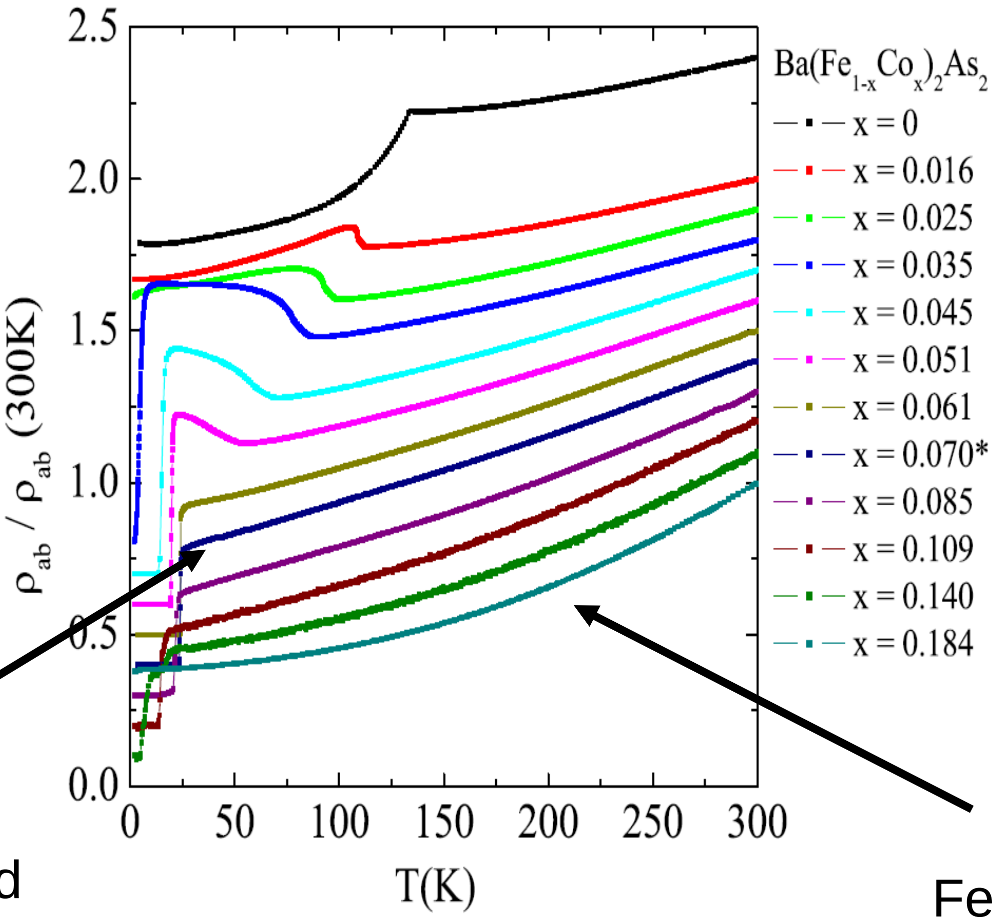
- superconductivity arises near a magnetic instability

- similar phase diagrams for other unconventional superconductors
  e.g. cuprates, heavy fermions, organics, ….

- **questions:** Is there a magnetic quantum critical point (QCP)?
  Is the pairing due to the magnetic fluctuations around the QCP?

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

Chu et al. PRB**79**, 014506 (2009)

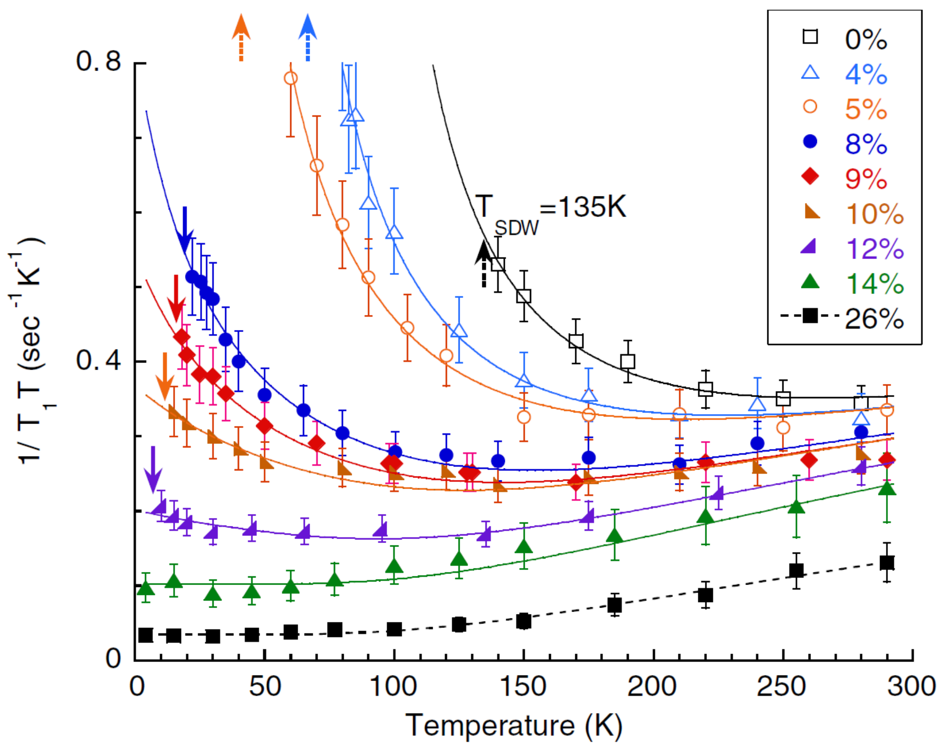


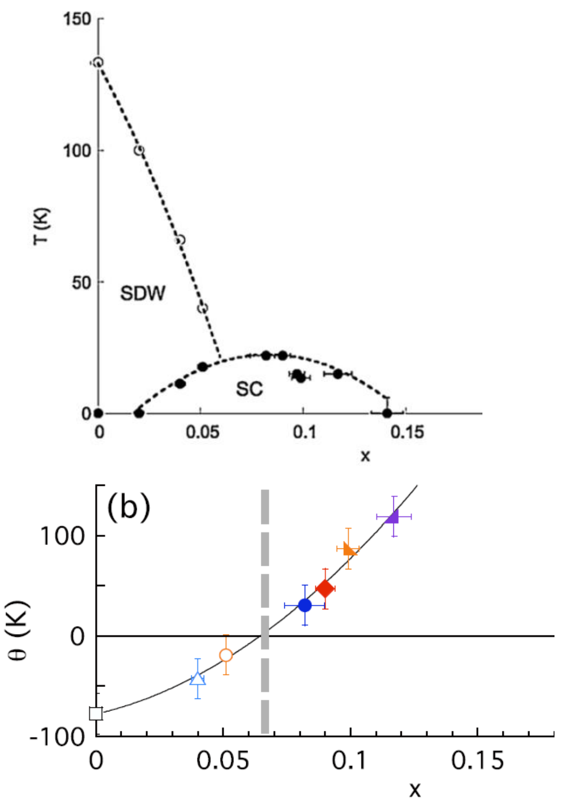
~ T
Non-Fermi liquid
\`strange metal'

~ T^2
Fermi liquid

NMR: AFM QCP from spin fluctuations in Co-Ba122

Ning et al. PRL 2010





- Spin-lattice relaxation rate diverges at -θ (Curie-Weiss law): $\frac{1}{T_1 T} = \frac{C}{T+\theta}$
- θ crosses zero smoothly at the critical concentration

Thermodynamics

- **electronic heat capacity**
  - entropy, phase transitions, superconducting gaps, fluctuations,…
  - **QCP** - diverging effective mass?

- **electronic thermal expansion**
  - pressure dependence of entropy
  - **QCP** - diverging Grüneisen parameter?
    sign change of Grüneisen parameter?

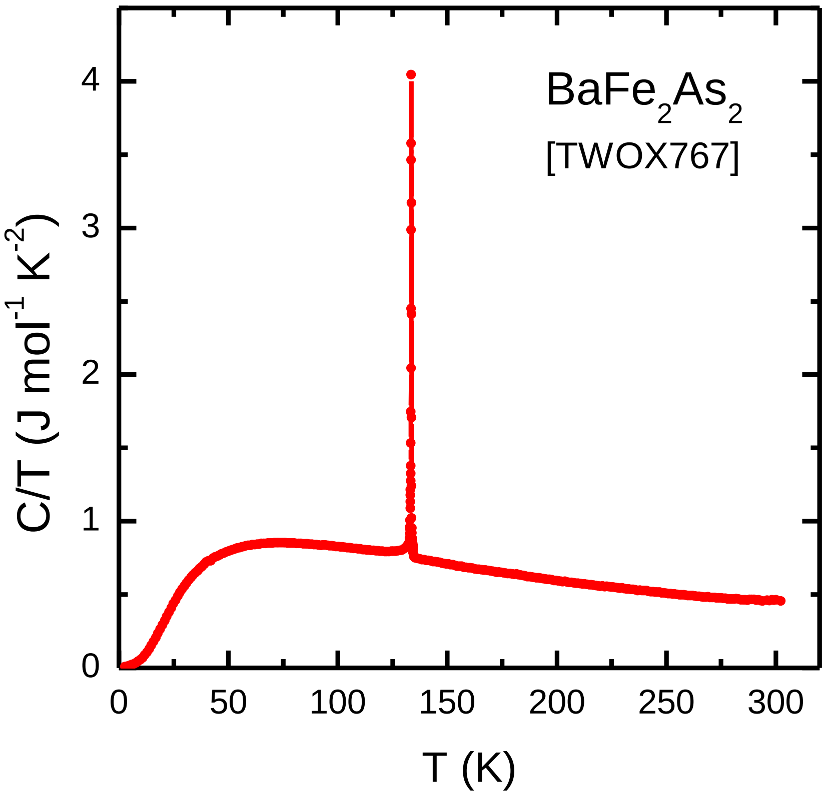
- **This talk:**
  – Co-Ba122 - quantum critical behavior?
  – shear modulus (nematicity) - compare Co- and K-doping
  – KFe_2As_2 - most strongly correlated Fe-based material?

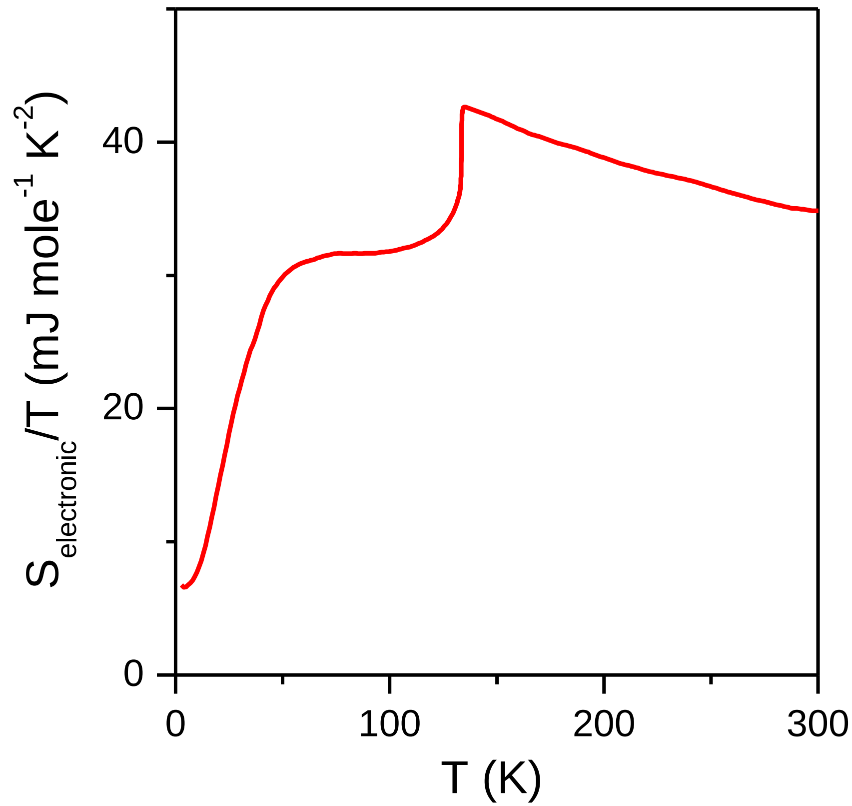
Co-doped Ba122

specific heat
and
thermal expansion

- CM et al. Phys. Rev. Lett. 108, 177004 (2012)
- F. Hardy, et al. Phys. Rev. B 81, 060501 (2010)
- Frédéric Hardy, et al., Phys. Rev. Lett. 102, 187004 (2009)

Specific heat of Ba122

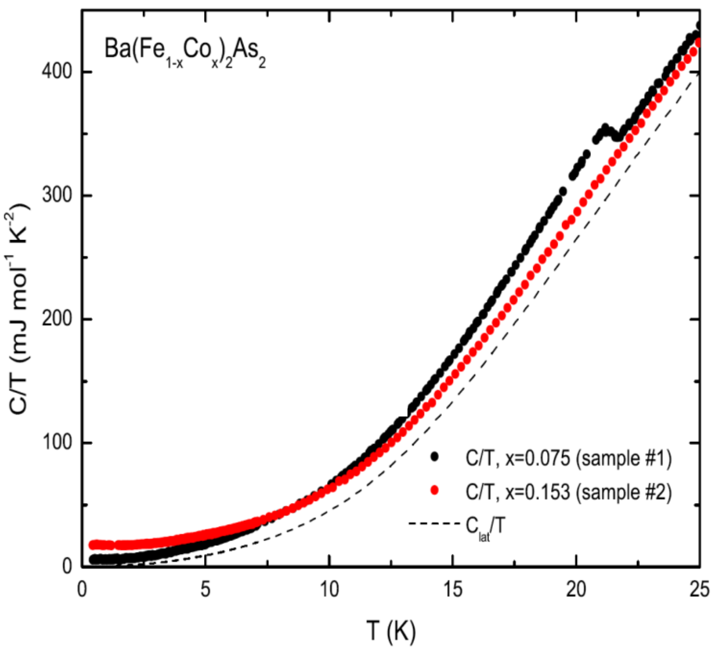


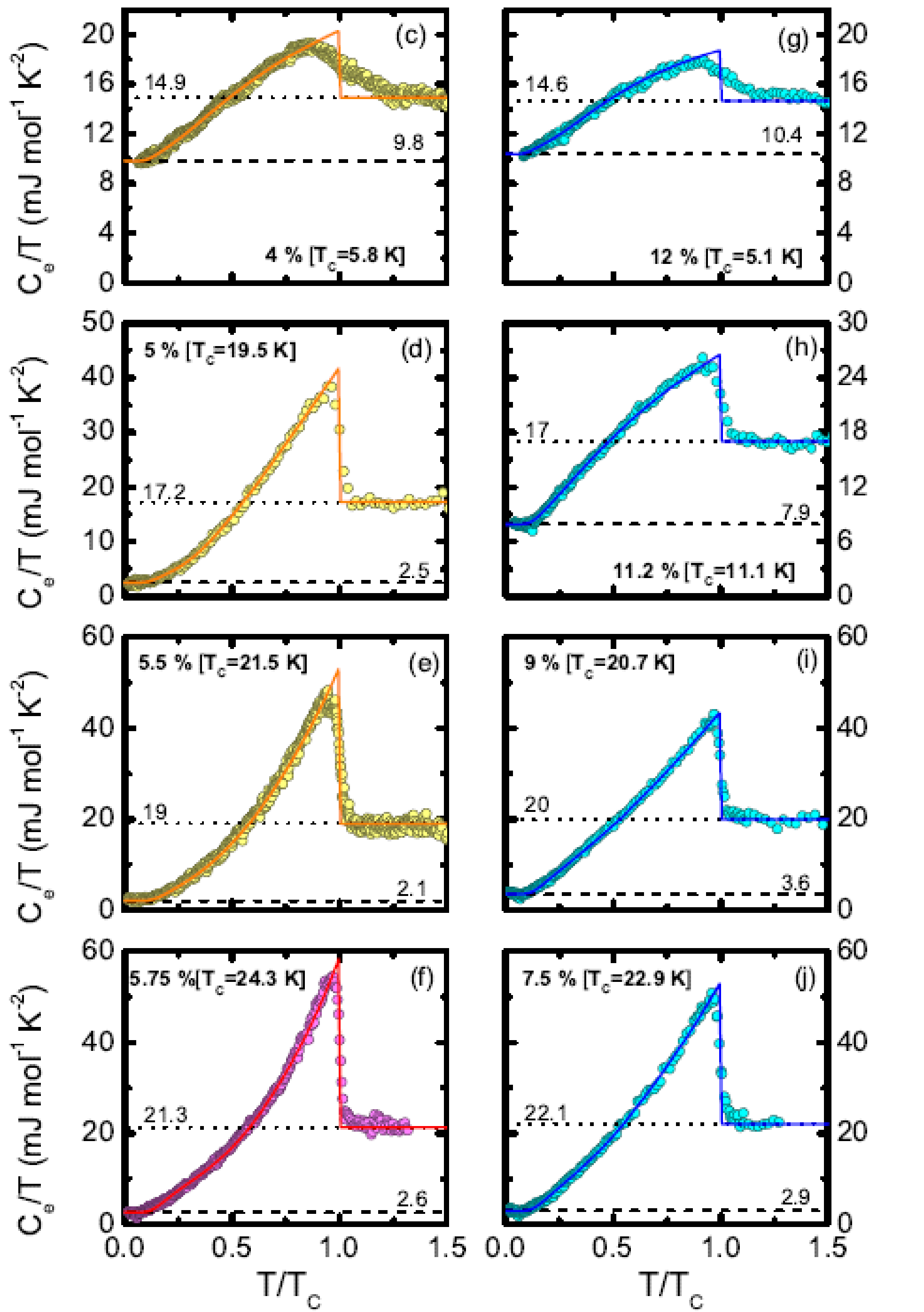


- sharp first-order SDW transition
- no visible precursors (fluctuations) above T_{SDW}
  how does this fit into NMRpicture?
- clear reduction in electronic density of states below T_{SDW}

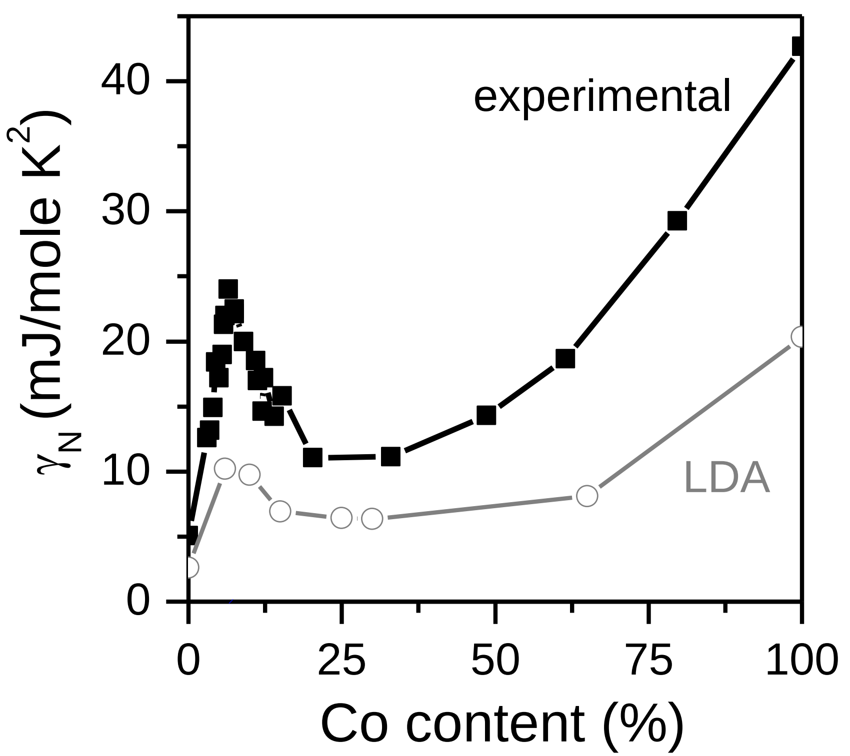
electronic heat capacity
Co-Ba122

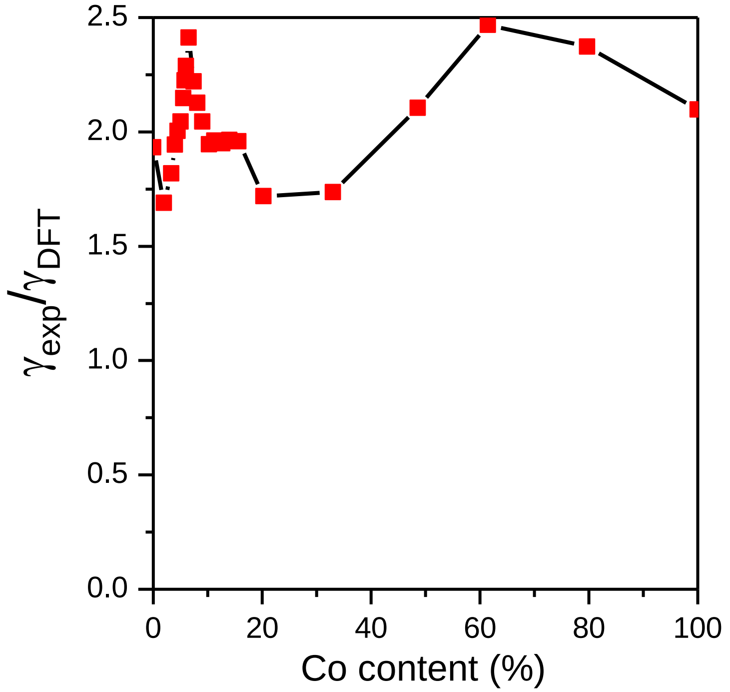
Frederic Hardy et al.
PRB 2009
EPL 2010





electronic density of states - Sommerfeld coefficient



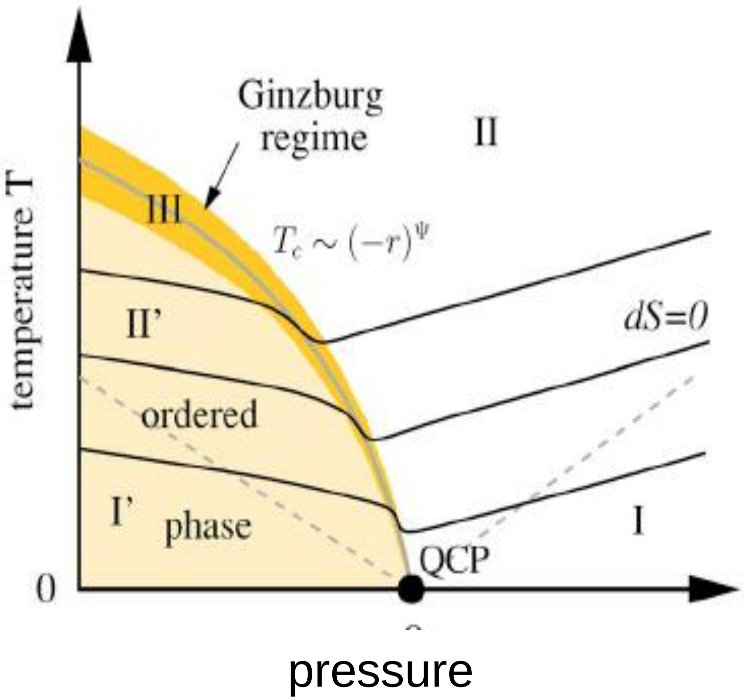


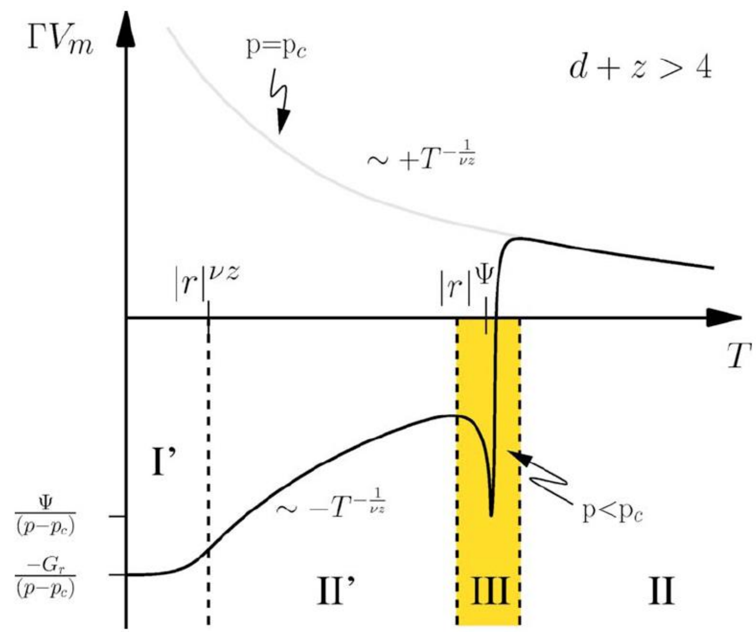
- sharp peak of γ_N at optimal doping
- DFT calculations predict similar peak (factor of 2)
  (SDW gaps FS - gap closes with doping)
- possible small mass enhancement at optimal doping

Grüneisen parameter near a QCP- pressure tuning

$$\Gamma^{Grüneisen} = \frac{\alpha(T)}{C_p(T)}$$

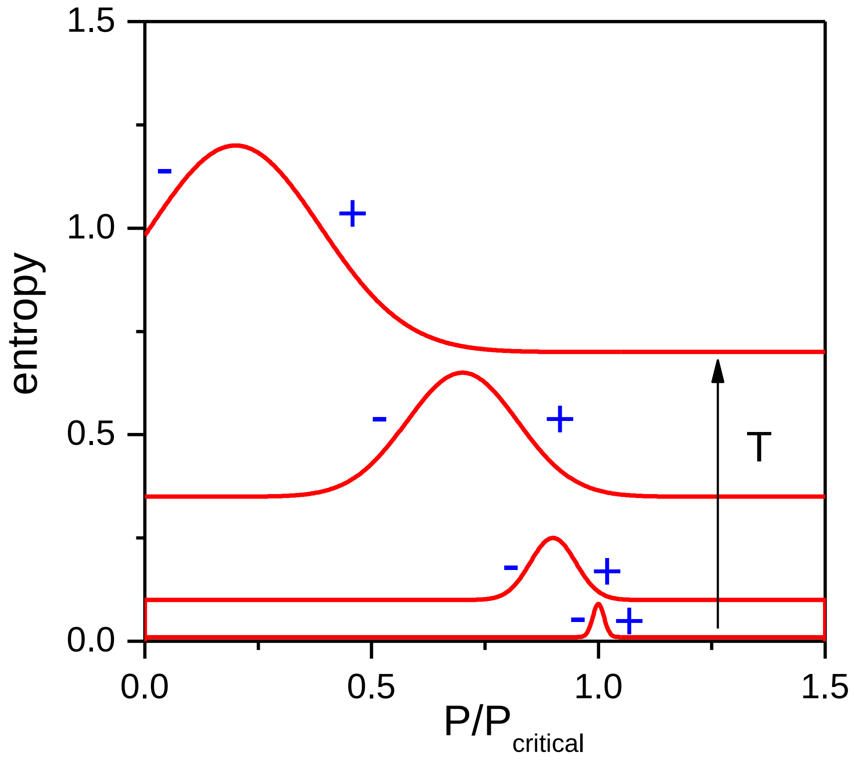
L. Zhu et al. PRL 2003
M. Garst et al. PRB 2005

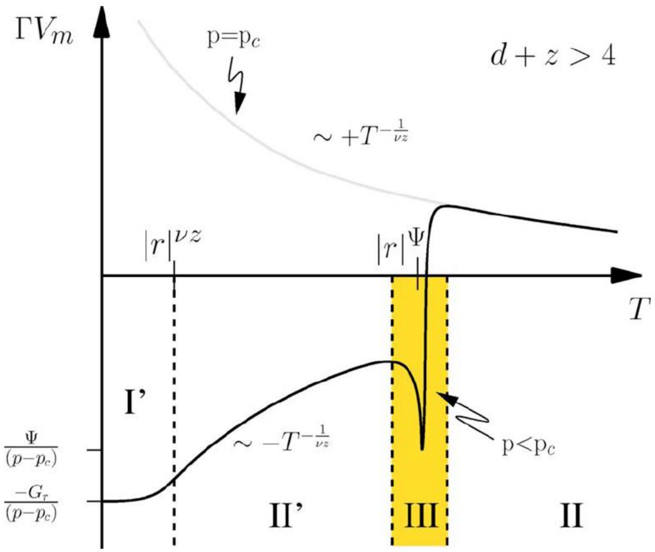




- *divergence of Grüneisen parameter at QCP*
- *sign change at finite-T transition*
- *'smoking gun' of QCP*

$$\alpha = \frac{1}{L_i}\frac{dL_i}{dT} = -\frac{dS}{dp_i}\bigg|_T$$





- accumulation of entropy along critical line ending at the QCP
  competing phases
  new emergent phases - e.g. superconductivity

thermal expansion - capacitance dilatometer

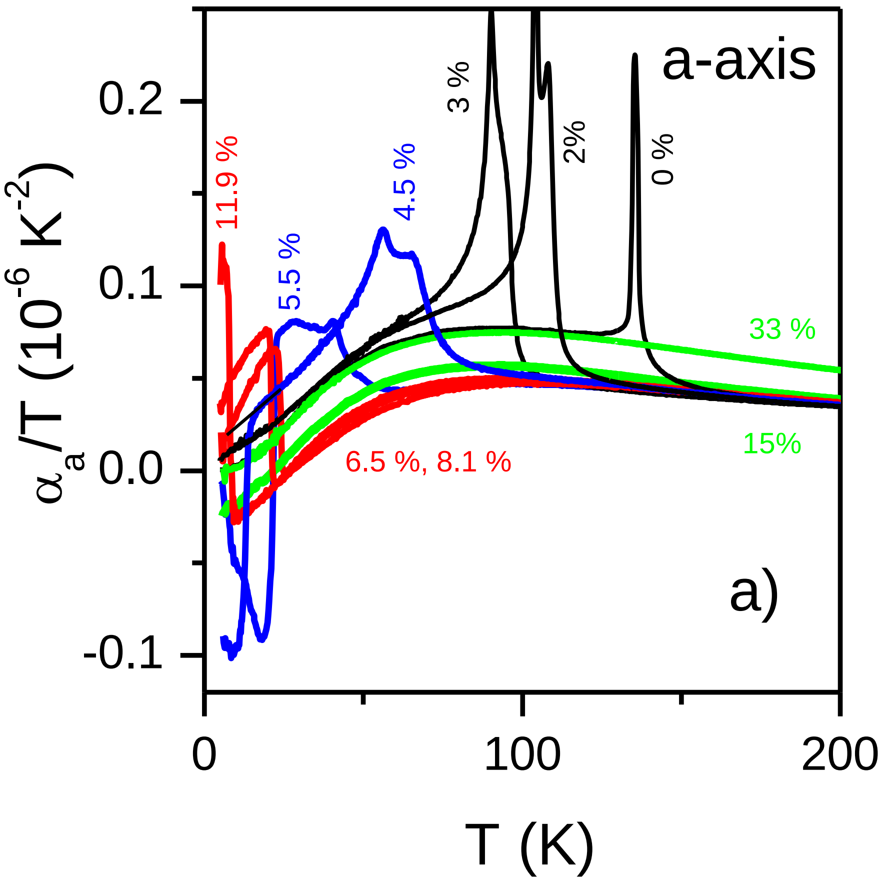
1 cm

- absolute resolution: *D L ~ 0.01 Å*
- relative resolution: *D L/L* ~ 10^{-8} - 10^{-10}

  (diffraction ~ 10^{-6})

thermal expansion of $Ba(Fe,Co)_2As_2$

CM et al. PRL 2012



Fermi liquid

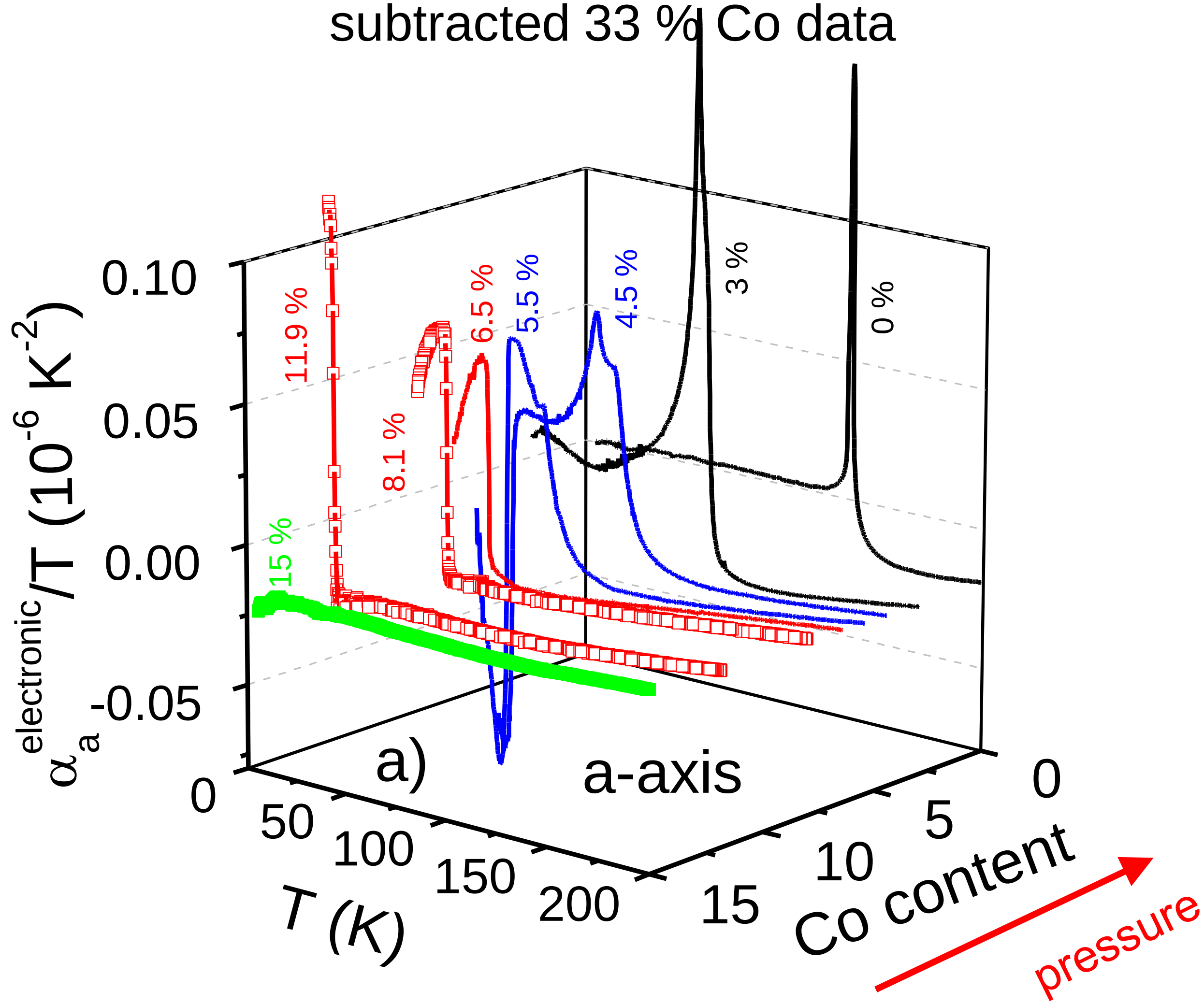
$$\alpha_i(T) = a \cdot T + b \cdot T^3 + \ldots$$

electronic phonons

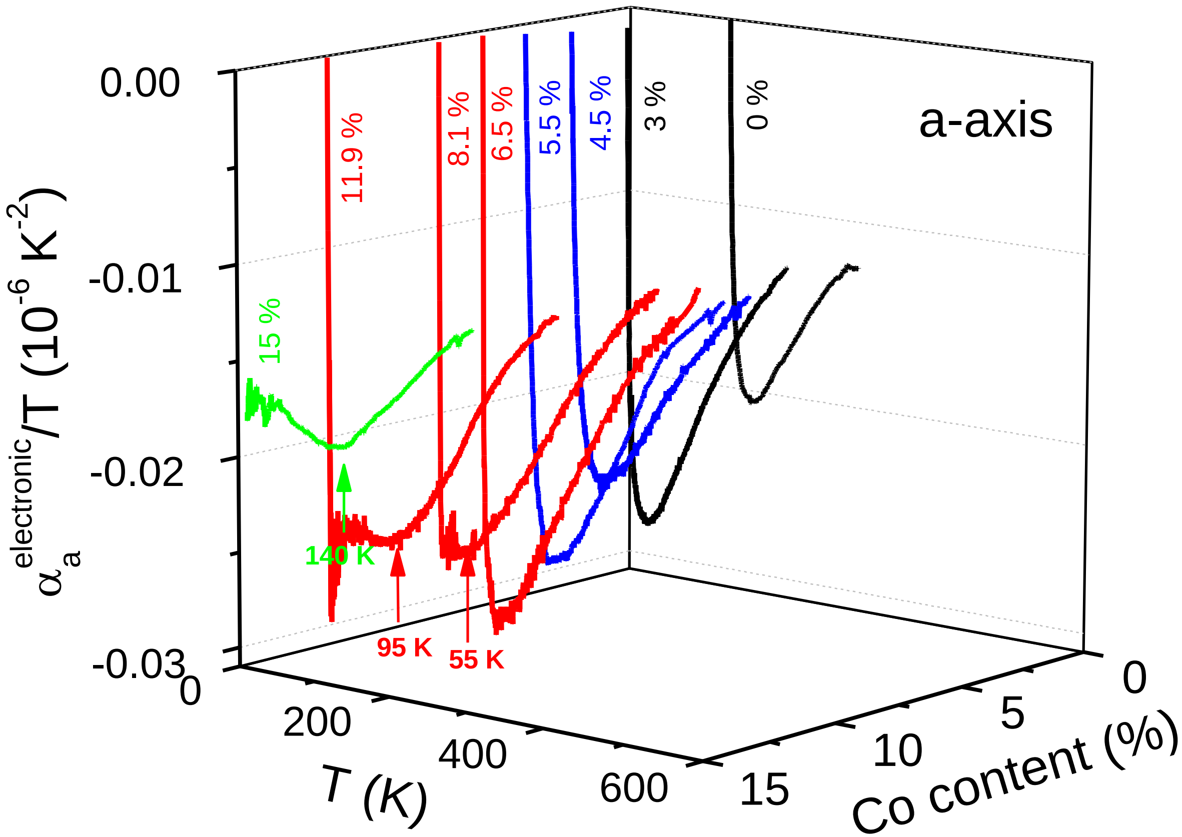
$$\left.\frac{\alpha_i}{T}\right|_{T=0} = -\frac{d\gamma_N}{dp_i}$$

- clear signatures of SDW and superconducting transitions
- use 33 % data as phonon background: nearly zero electronic signal!!

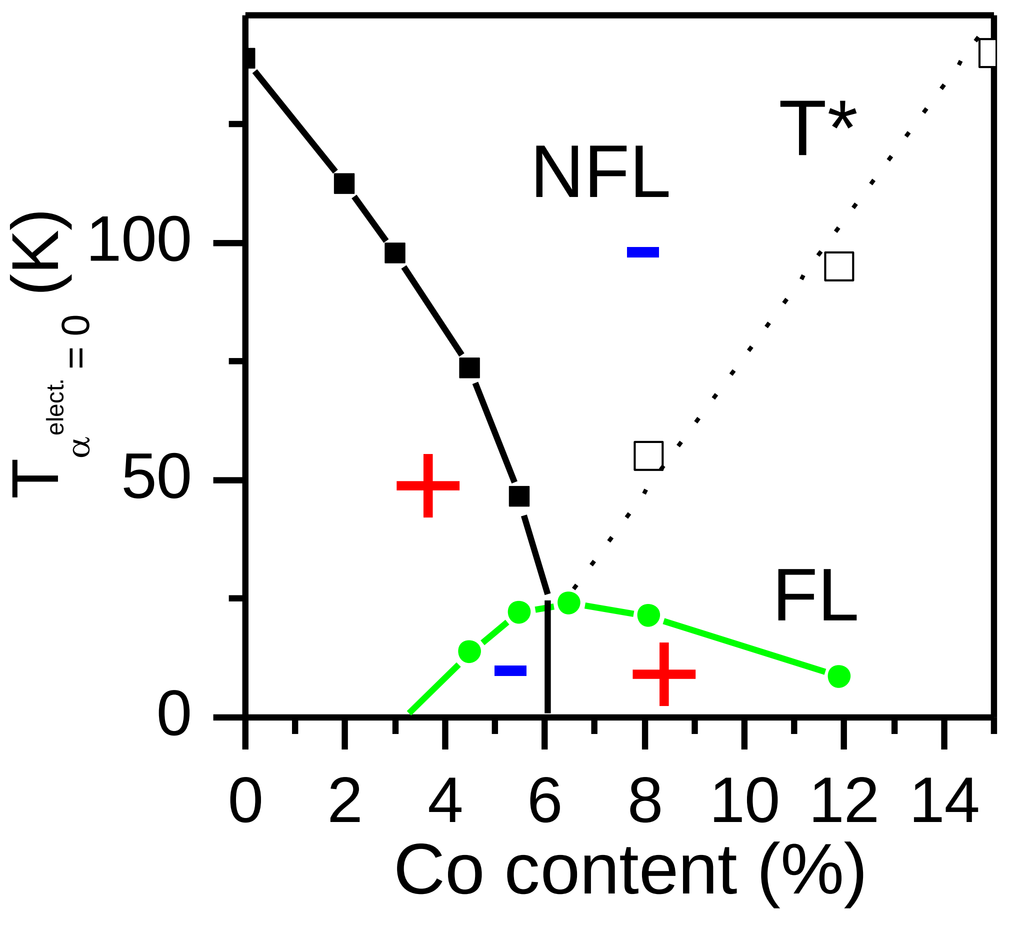
electronic/magnetic thermal expansion



- negative contribution above T_{SDW}, T_c
- sign changes at T_{SDW} and T_c



- clear evidence for non-Fermi liquid state above T_{SDW}, T_c
- possible crossover to Fermi-liquid behavior below T*

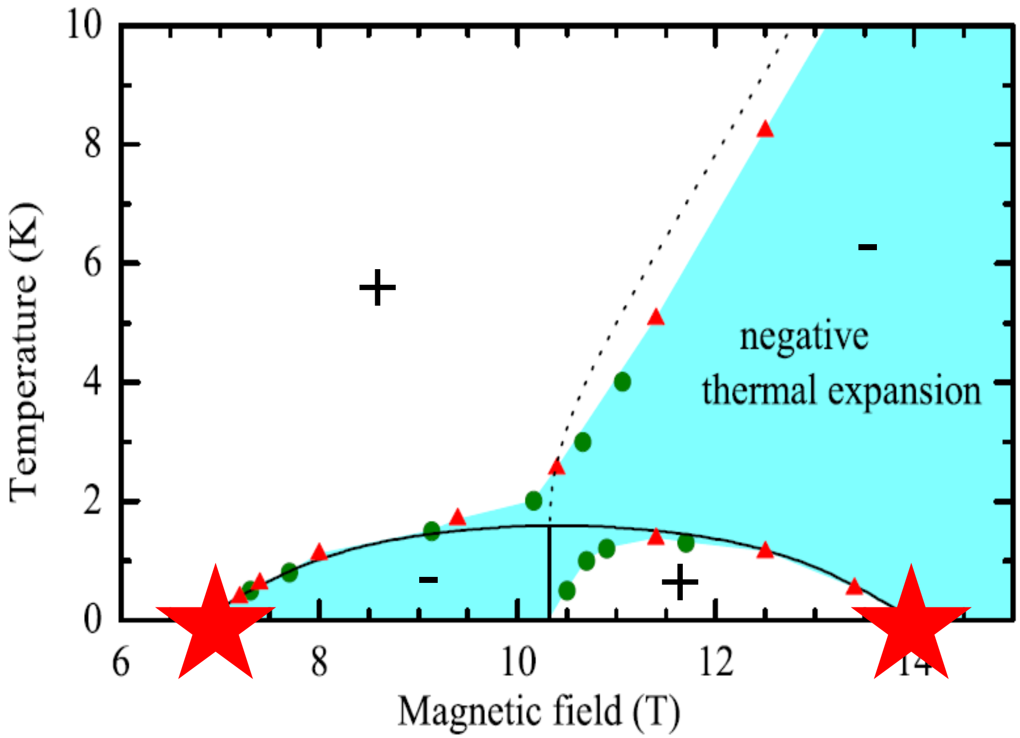


- sign changes of α(T) - expected behavior at a QCP
- superconductivity is an emergent phase and covers QCP

PRL **100,** 067208 (2008) PHYSICAL REVIEW LETTERS week ending 15 FEBRUARY 2008

Diverging Thermal Expansion of the Spin-Ladder System $(C_5H_{12}N)_2CuBr_4$

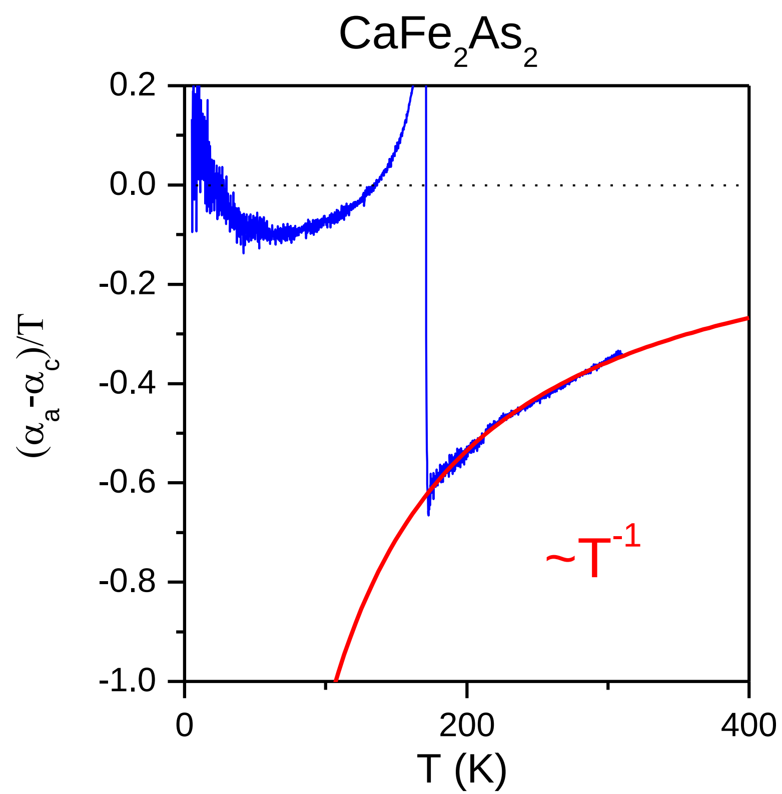
T. Lorenz,[1,*] O. Heyer,[1] M. Garst,[2] F. Anfuso,[2] A. Rosch,[2] Ch. Rüegg,[3] and K. Krämer[4]

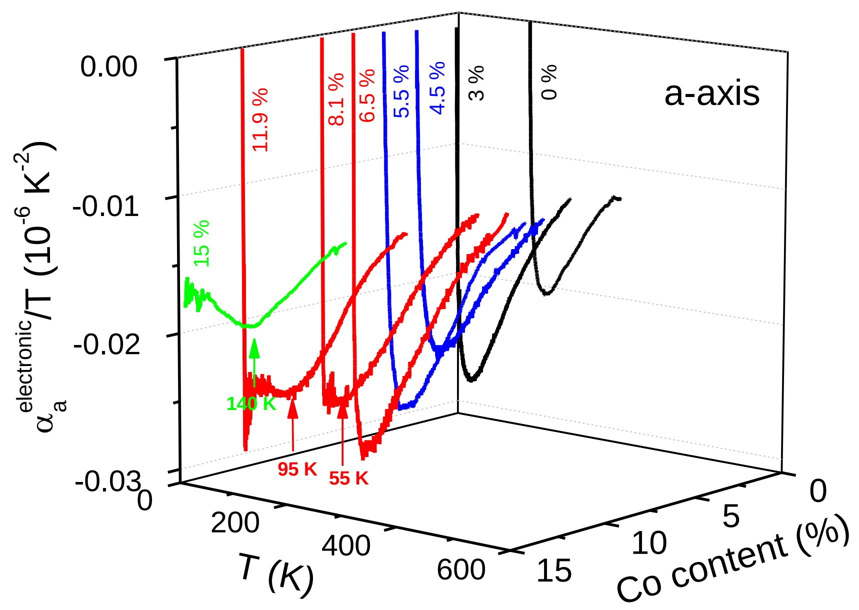


- weakly coupled 1d chains (magnetic field tuning)
- QCP ‘hidden‘ - Bose Einstein condensation of magnons

→ additional sign changes of alpha
2 QCPs (at 7 T and 14 T)

Paul Canfield





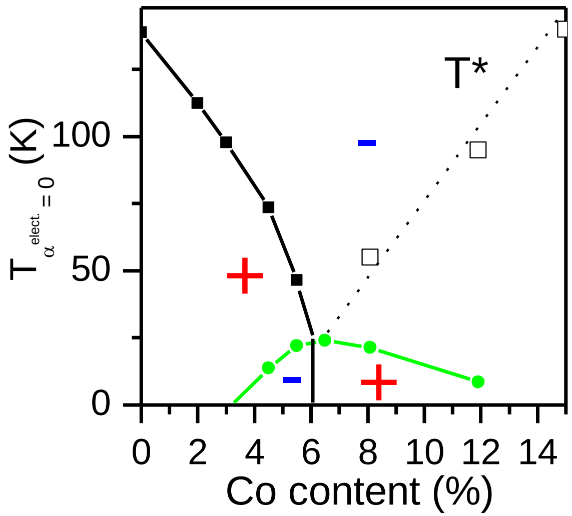
Summary - Co-Ba122

Evidence for quantum critical scenario?

- small enhancement of effective mass at critical doping

- NFL behavior of thermal expansion above T_{SDW} (Ca122)

- sign changes of Grüneisen parameters



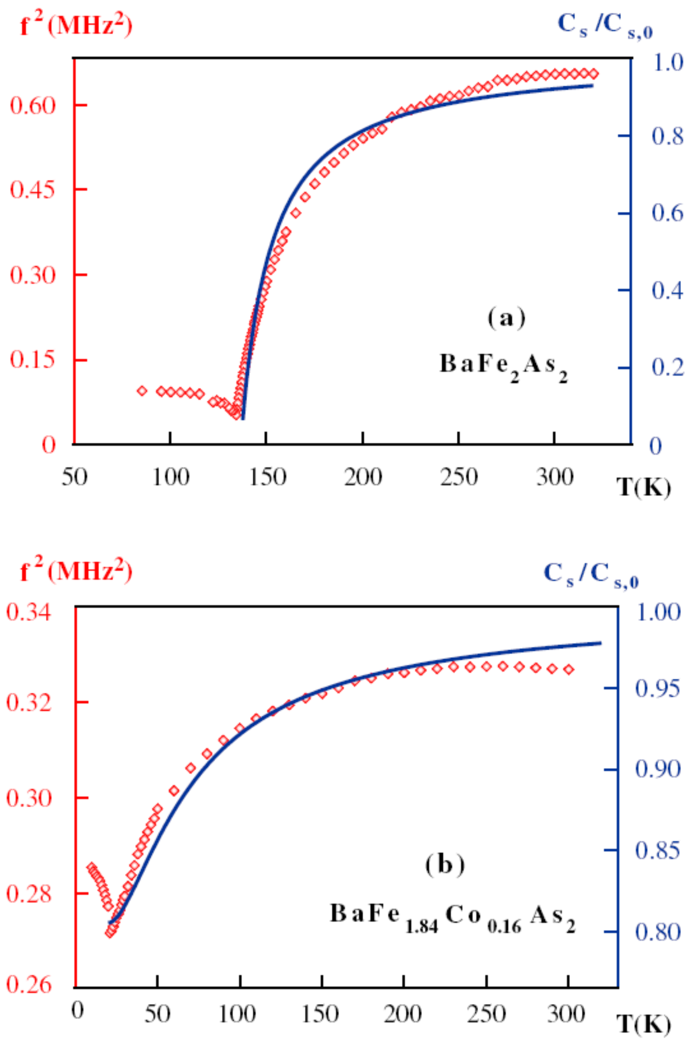
shear modulus - nematicity

Co- and K-doped Ba122

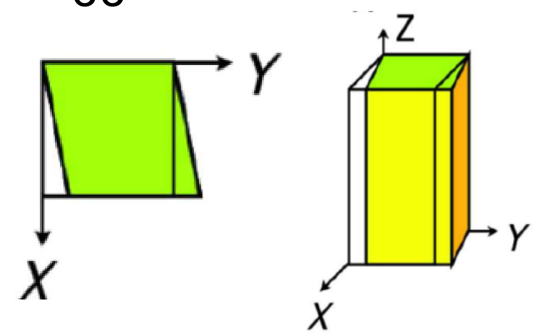
- A. E. Böhmer, et al. arXiv:1305.3515
- Rafael M. Fernandes, et al.Phys. Rev. Lett. 111, 137001 (2013)

softening of shear modulus - C_{66}

Fernandes et al. PRL 2010



C_{66}



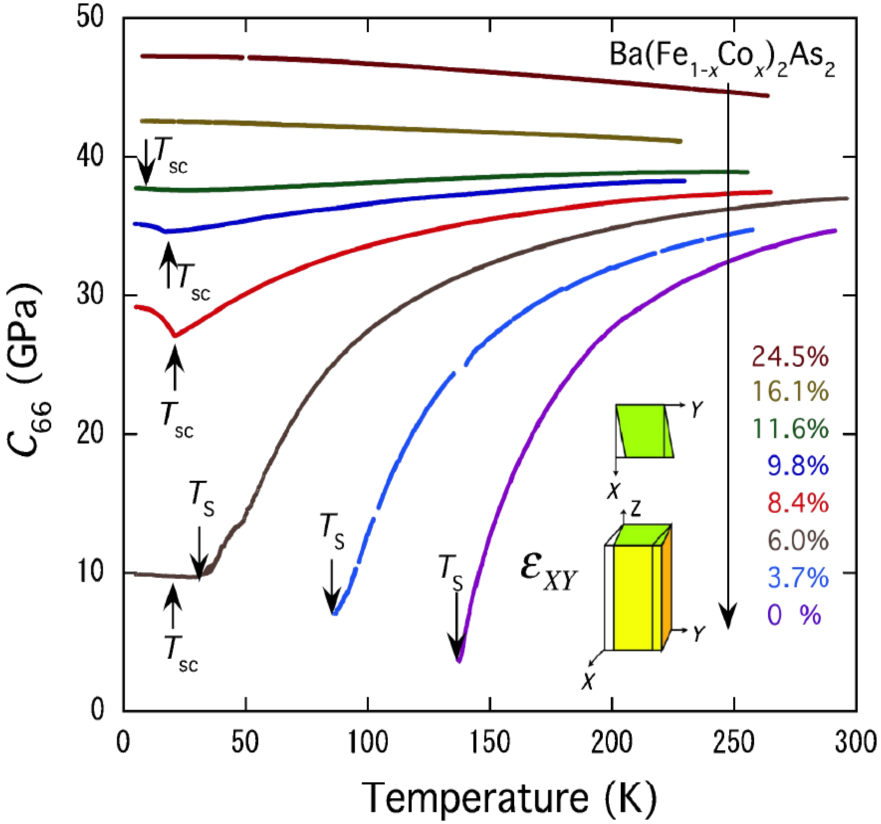
- soft mode of structural/magnetic transition

- **softening:**
  emergent magnetic/nematic fluctuations

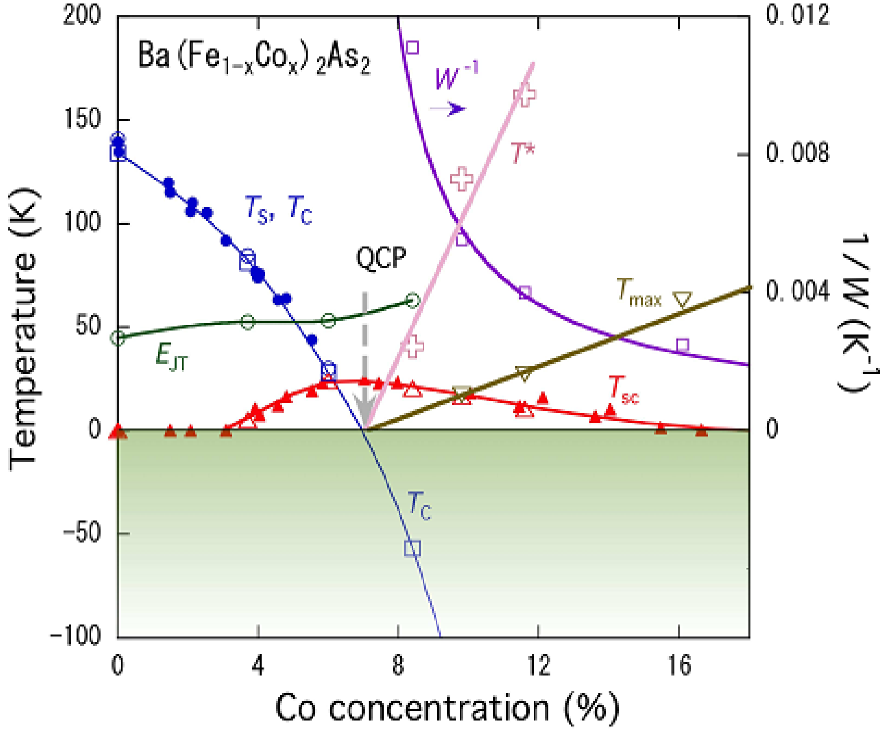
- **hardening below T_c:**
  consistent with magnetically driven nematic fluctuations and competing AFM and SC order

Structural quantum critical point in Co-Ba122

Yoshizawa et al. JPSJ (2012)



Yoshizawa et al. JPSJ (2012)

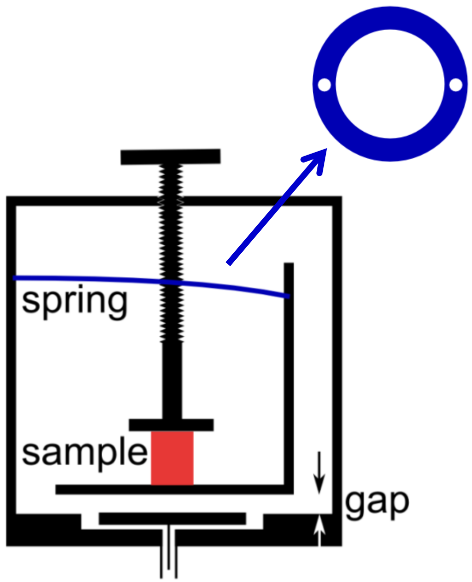


- softening observed also in overdoped tetragonal state
- evidence for 'structural' quantum critical point
- authors stressed importance of **orbital degrees of freedom**

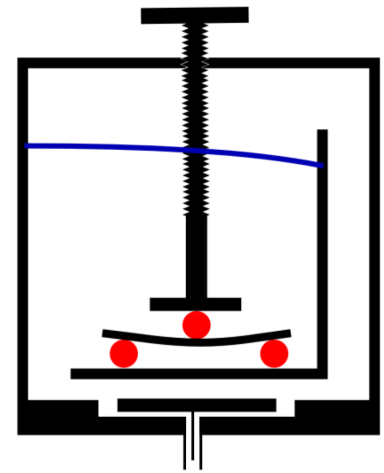
Question: Is this behavior universal in pnictides - e.g. K-Ba122?

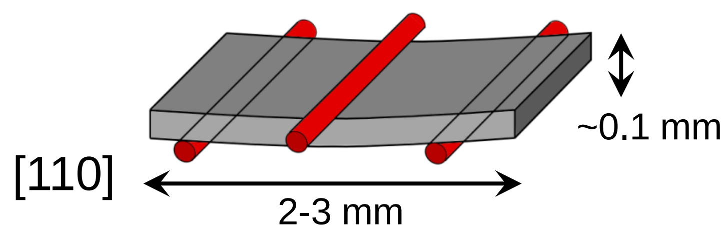
Young's modulus in a capacitance dilatometer

A. E. Böhmer, et al. arXiv:1305.3515



resolution: 10^{-11}-10^{-12} m





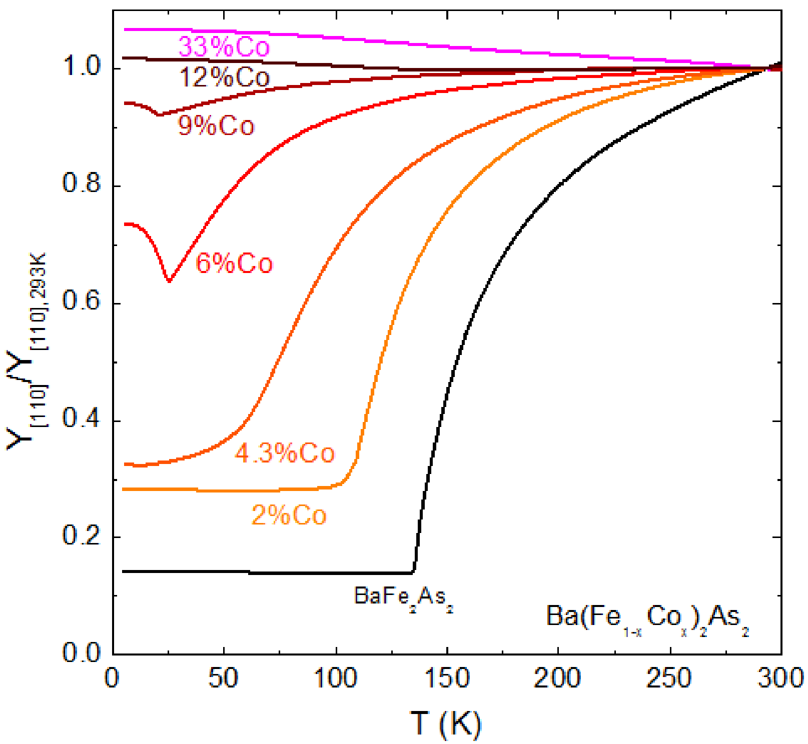
- Measure bending changes under constant force (~20 g) with high resolution vs T
- Young's modulus is directly related to C_{66} if C_{66} is small

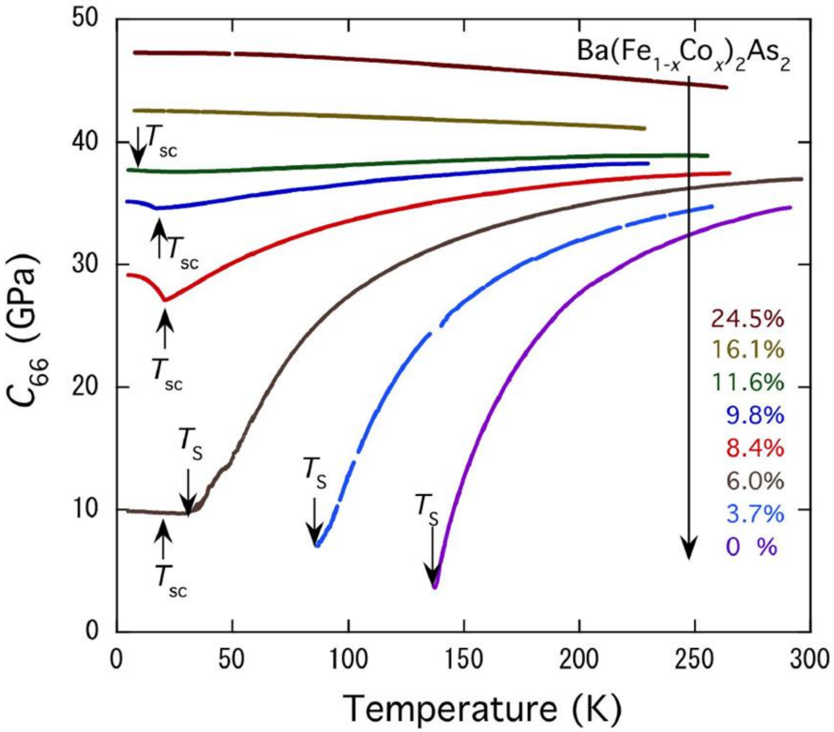
$$Y_{[110]} = 4\left(\frac{1}{C_{66}} + \frac{1}{\gamma}\right)^{-1} \text{ with } \gamma = \frac{C_{11}}{2} + \frac{C_{12}}{2} + \frac{C_{13}^2}{C_{33}}$$

e. g. Kityk et al., PRB, 2000

Young's modulus vs C_{66} from ultrasound: Co-Ba122

A. E. Böhmer, et al. arXiv:1305.3515

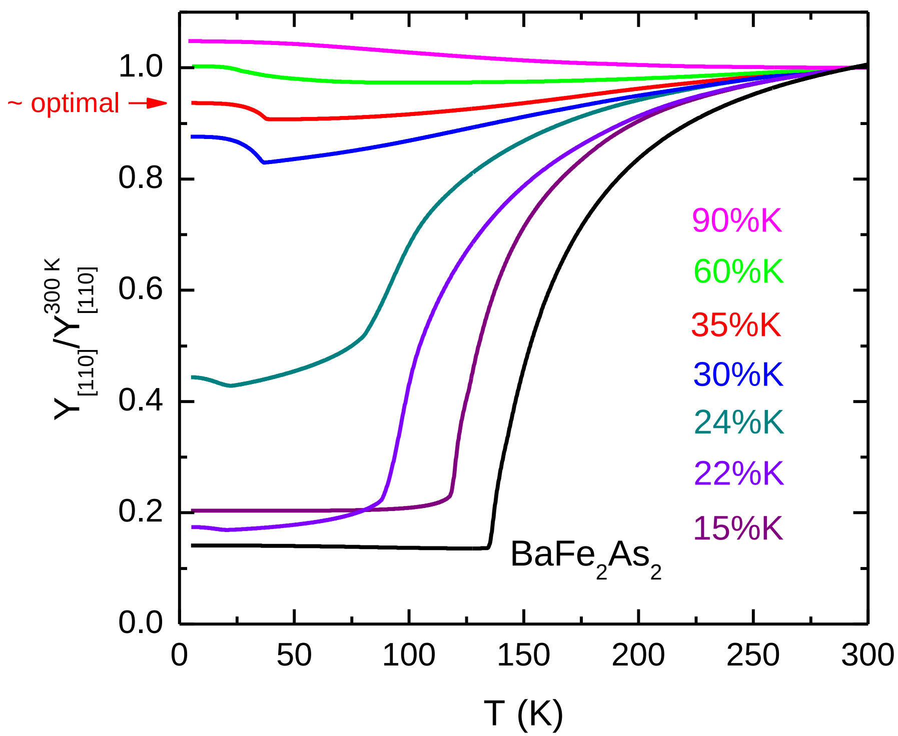




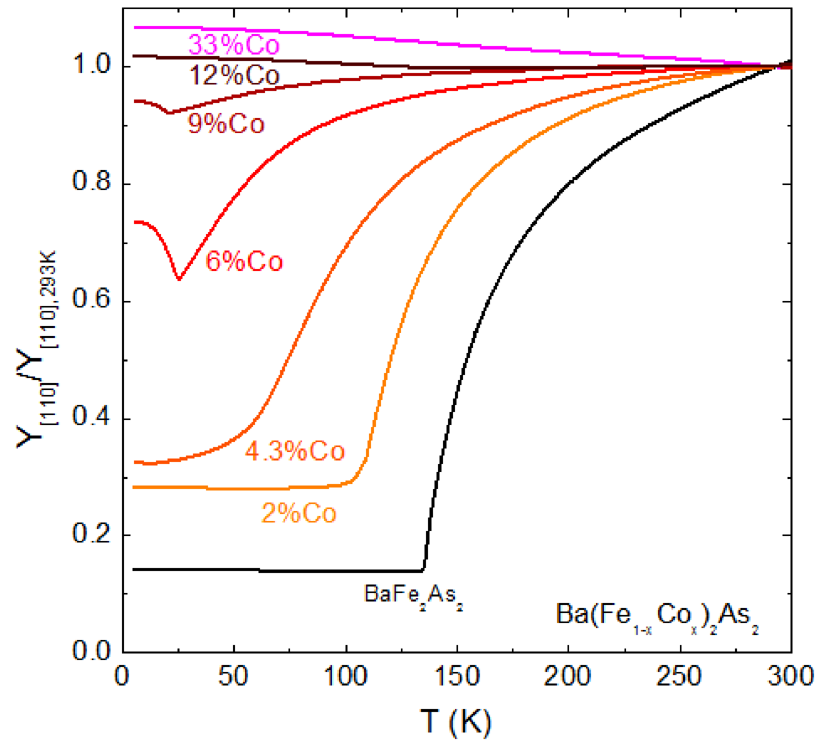
- Good qualitative agreement with C_{66} from ultrasound measurements by Yoshizawa et al.
- Young's moduli are normalized at room temperature

Young's modulus: K- and Co-doped Ba122

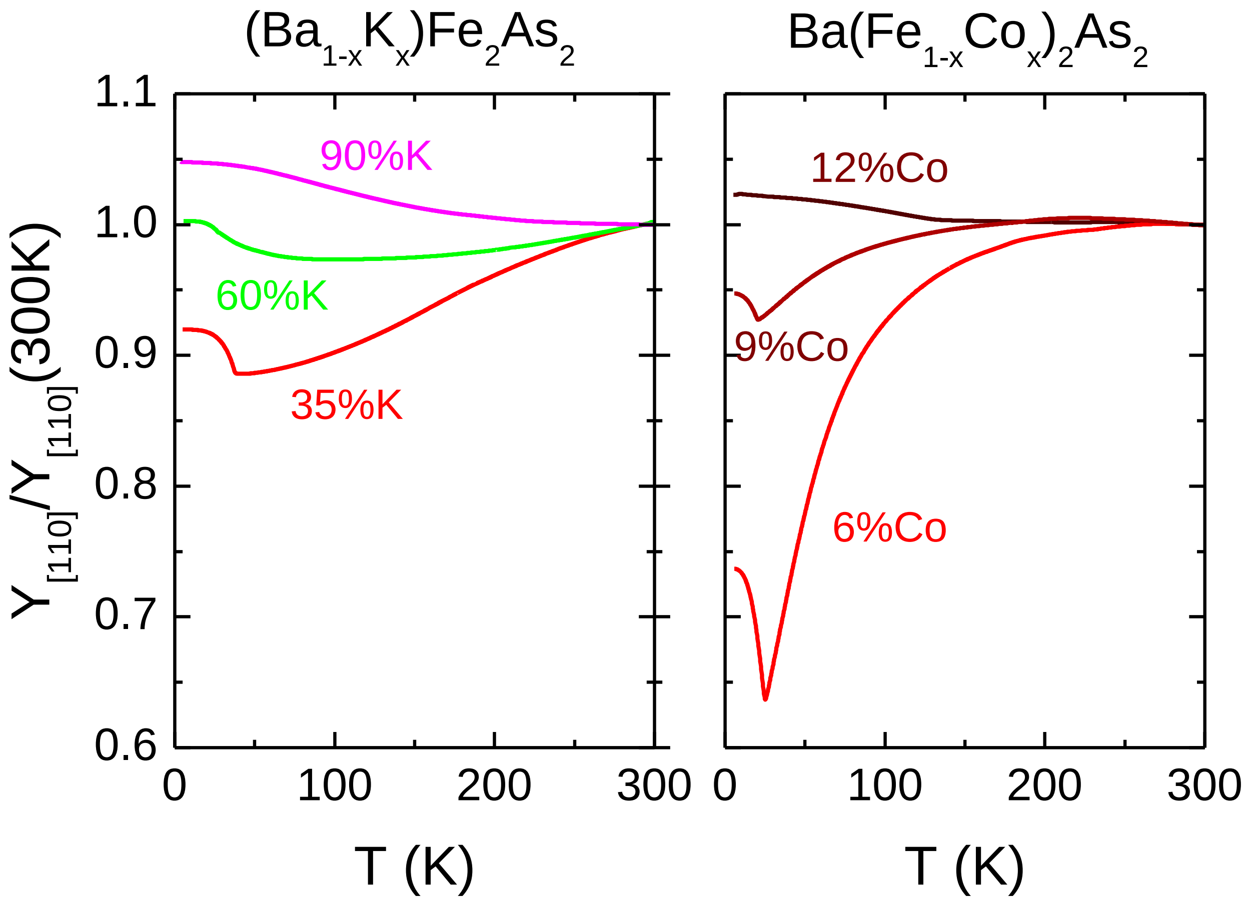
K-Ba122



Co-Ba122



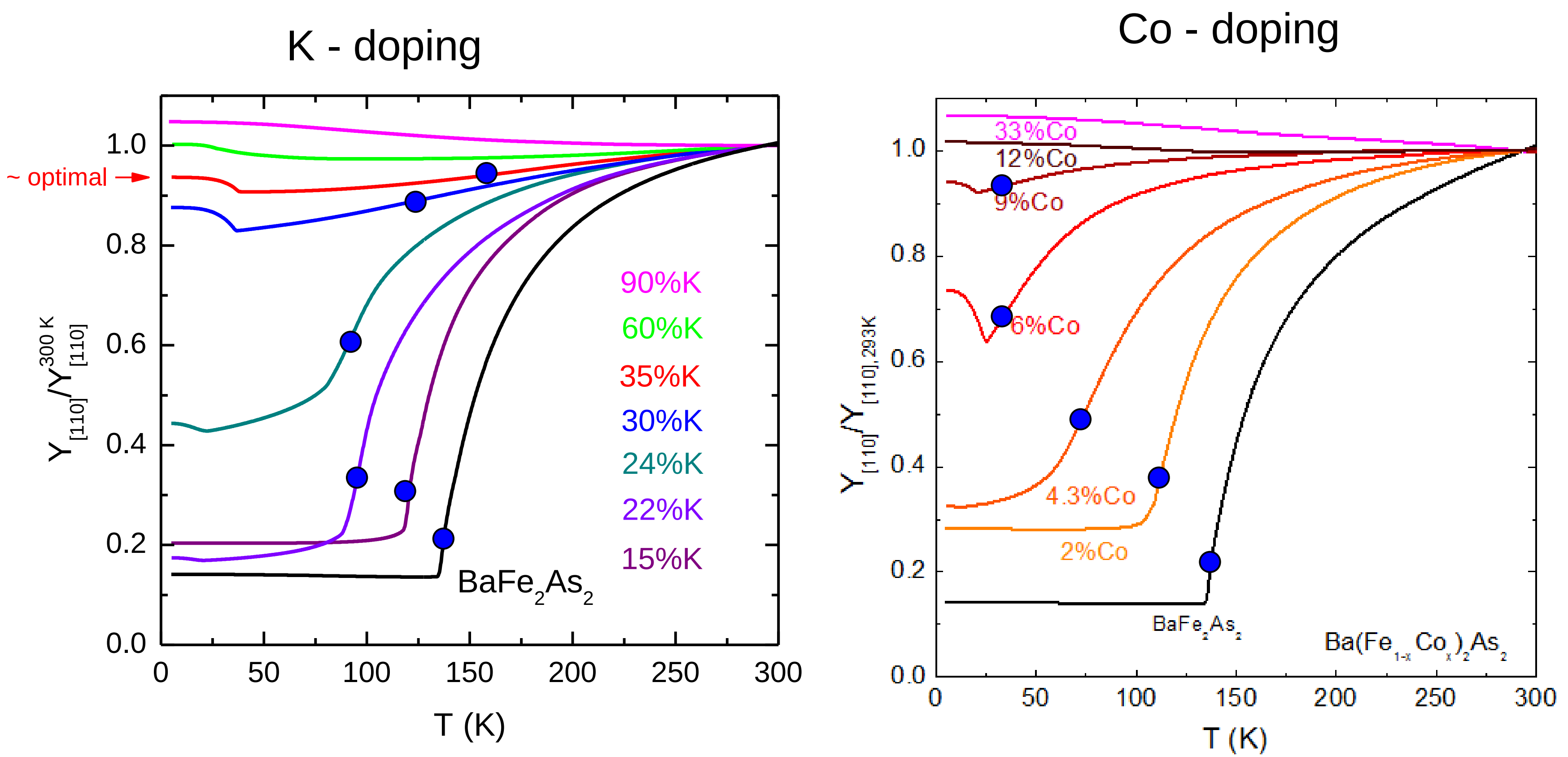
- K-Ba122 Young's moduli: qualitatively similar to Co-Ba122 data
- differences: - behavior at optimal doping less 'critical'
  - almost no hardening seen below T_c for 60 % K (T_c= 28 K) vs 9 % Co



- clear difference at optimal doping - lack of critical behavior in shear modulus for K-doping
- broad hardening for 60 % K below 100 K (not related to T_c!)

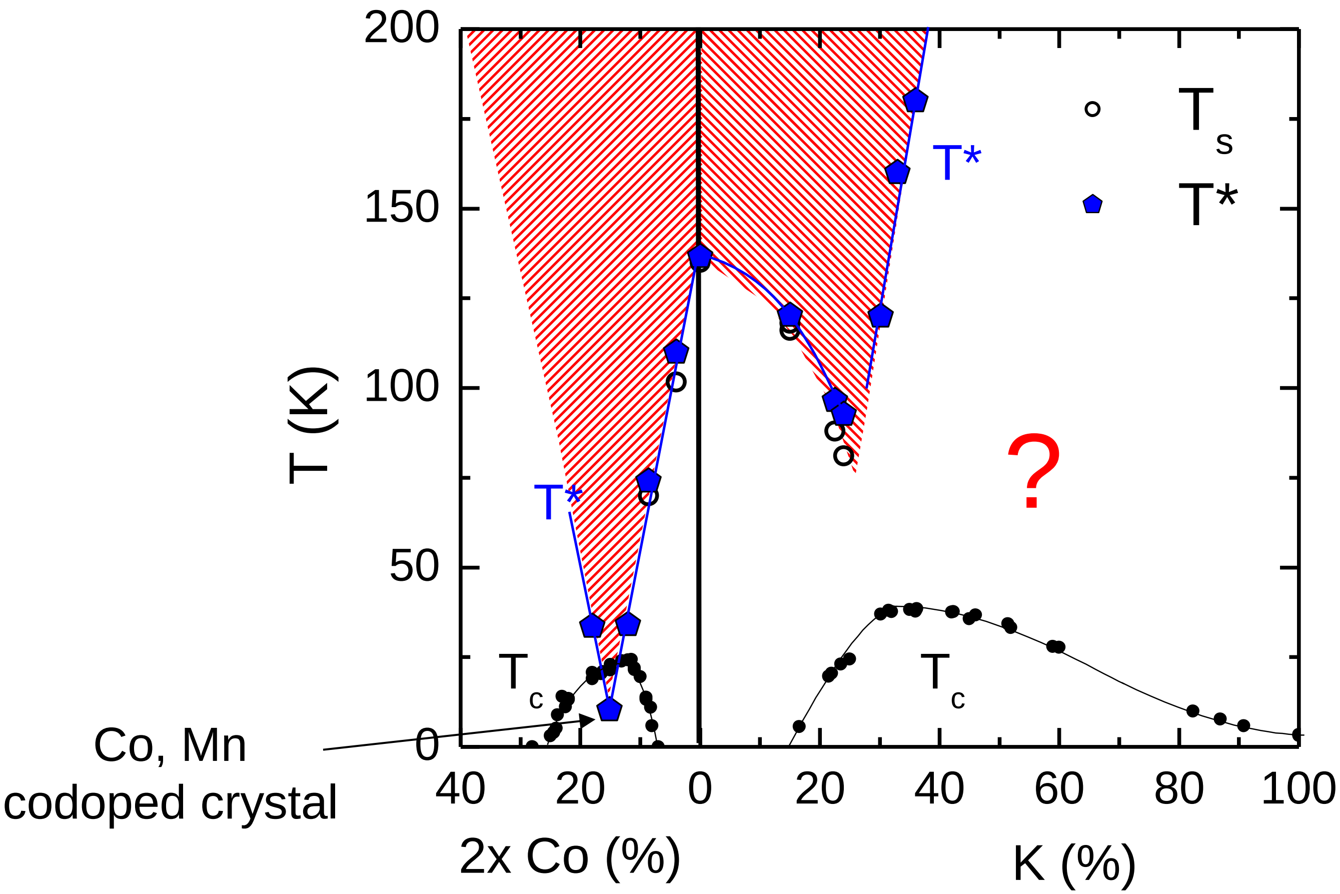
  versus softening and hardening for 9 % Co (similar reduced T_c)

Quantum critical points: K- vs Co-doping?



- Inflection points - maximum in ‘nematic susceptibility'
- plot points vs doping.

Phase diagram of 'divergent' lattice softening



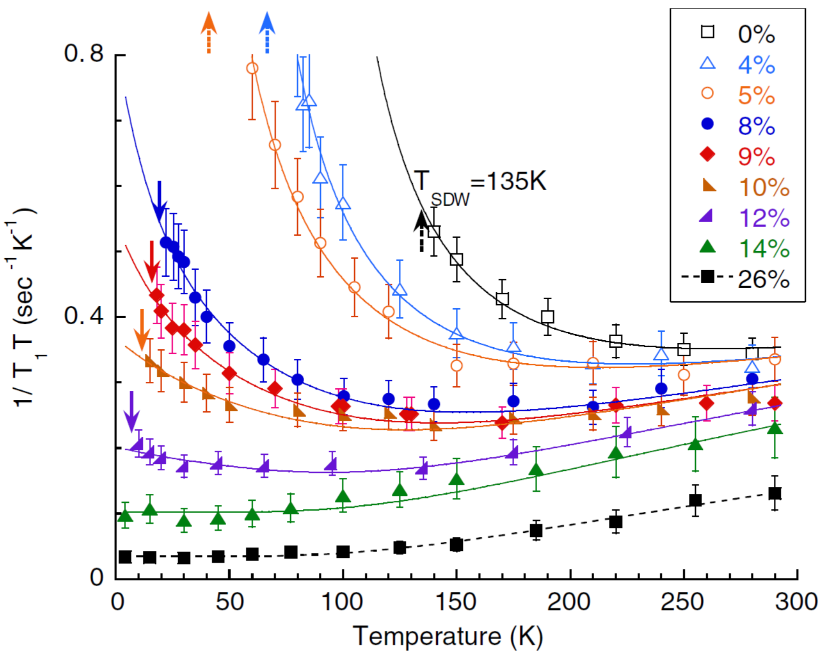
- Co - doping: resembles expected behavior at a quantum critical point
- K - doping: softening cut off already at high temperatures - lack of real QCP!
- Large region at higher K doping without large softening (and hardening)
- Question: Can one explain relatively large T_c (28 K at 60 % K) within spin mediated pairing scenario? Lack of critical softening and hardening!

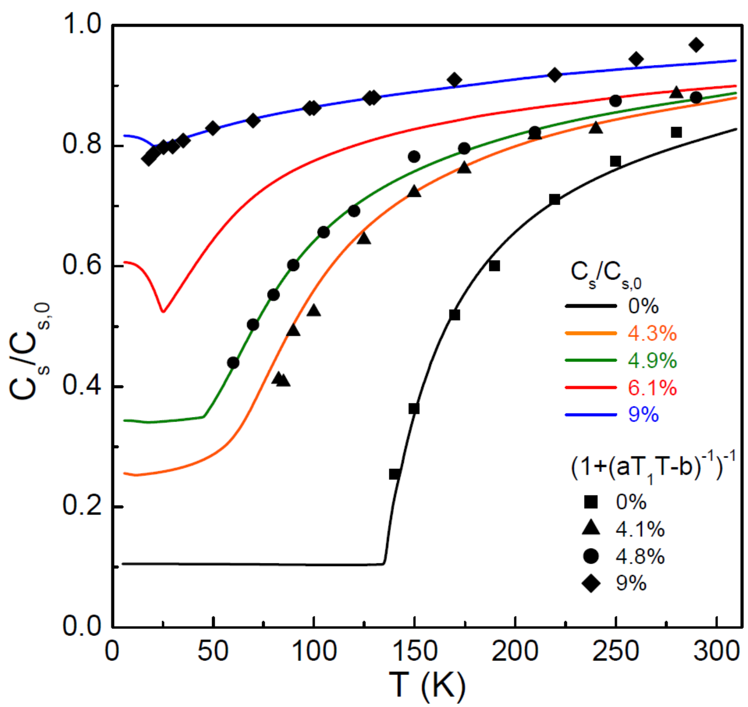
Scaling between magnetic and lattice fluctuations in a family of iron-pnictide superconductors

Rafael M. Fernandes,[1] Anna E. Böhmer,[2] Christoph Meingast,[2] and Jörg Schmalian[3]

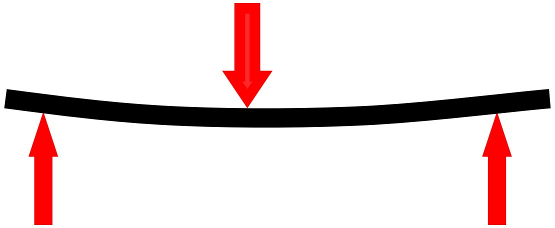
Co-Ba122

PRL 2013





$$\frac{C_s}{C_{s,0}} = \frac{1}{1 + \left[a\left(T_1 T\right) - b\right]^{-1}}$$



Conclusions - shear modulus

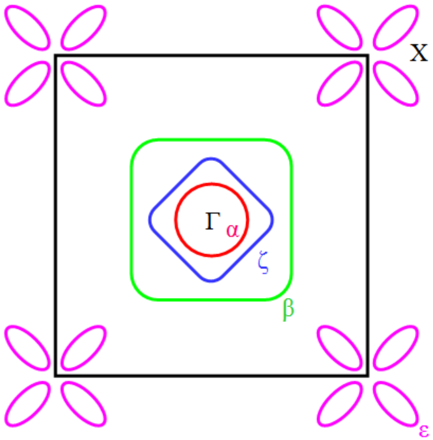
- New technique: three-point-bending in capacitance dilatometer
  - High resolution – crystals don’t need to be perfect!I
- Confirmation of ‘quantum criticality’ in $Ba(Fe,Co)_2 As_2$
- New results for $(Ba,K)Fe_2As_2$:
  - Absence of quantum criticality !
  - Maximum T_c not at the point of vanishing orthorhombic order
  - Little coupling of C_{66} shear mode with superconductivity for overdoped samples
  - Reconcile T_c=28K at 60% $(Ba,K)Fe_2As_2$ within spin-fluctuation scenario?

KFe_2As_2

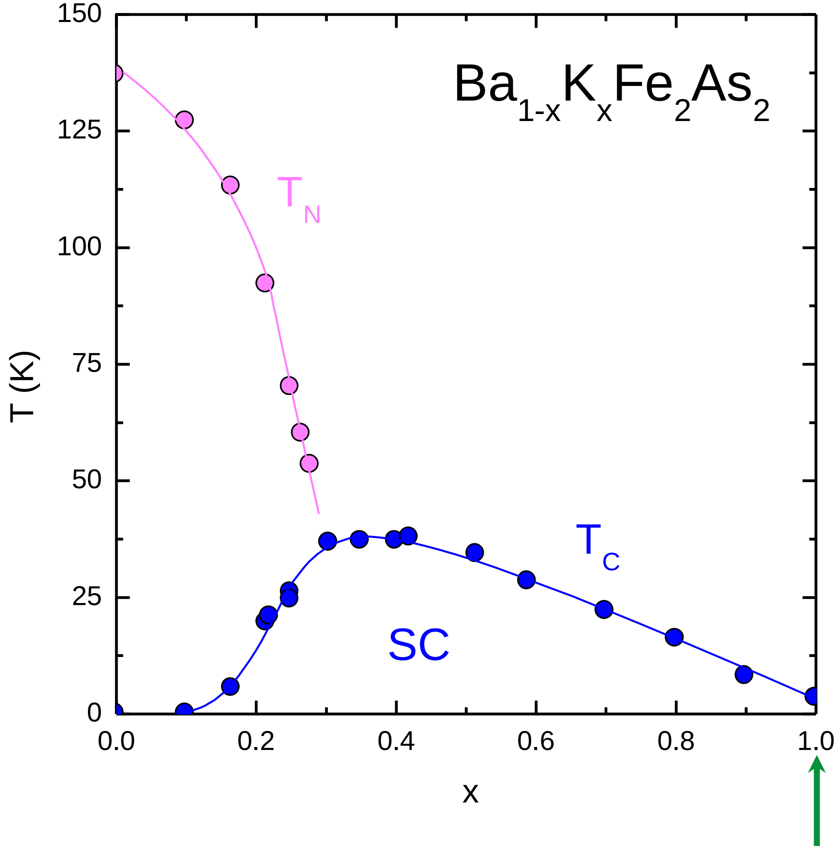
specific heat, magnetization, thermal expansion,..

- F. Hardy, et al. Phys. Rev. Lett. 111, 27002 (2013)
- P. Burger, et al. Phys. Rev. B 88, 014517 (2013)
- Frederic Hardy, et al., arXiv:1309.5654

KFe_2As_2



only *h* pockets



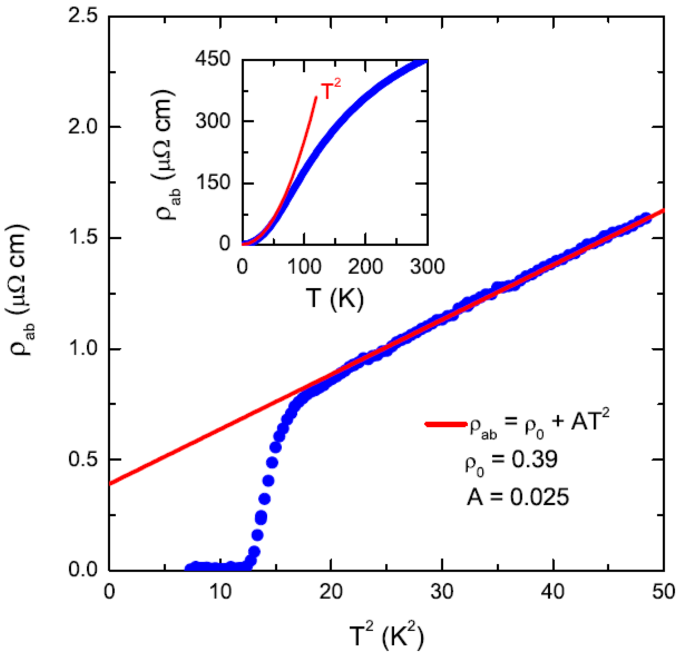
KFe_2As_2

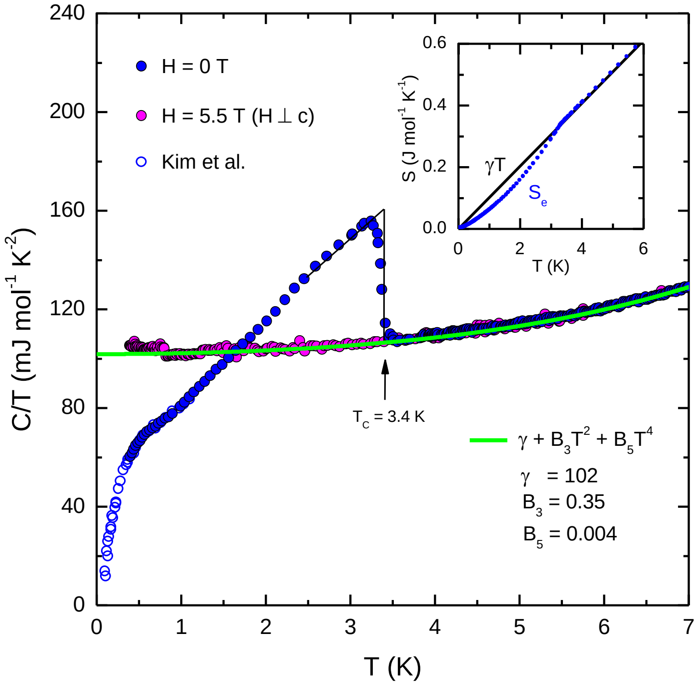
$T_C = 3.4$ K

- stoichiometric - clean system!!
- non magnetic
- strongly correlated - Hund's metal
- '3d heavy fermion metal'
- low T_c - 3.4 K (advantage!)
- nodes? (nodal-s or d-wave?)

resistivity and heat capacity

F. Hardy, et al. PRL 111, 27002 (2013)





- Fermi liquid!
- clean: RRR ~ 1000 - 2000

Sommerfeld coefficient

γ_n = 102 mJ mol^{-1} K^{-2}

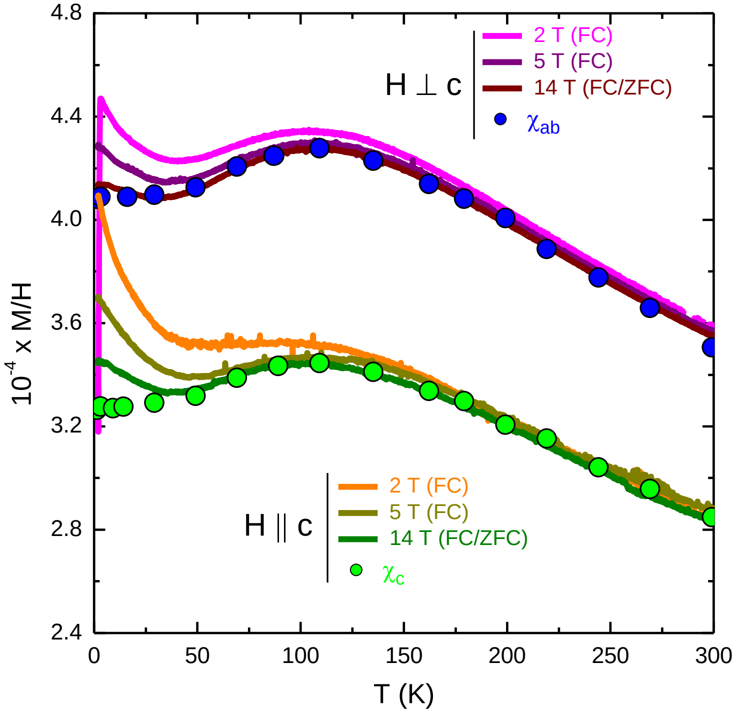
(γ_{LDA} = 10 mJ mol^{-1} K^{-2})

- strongly correlated!!
- small gap

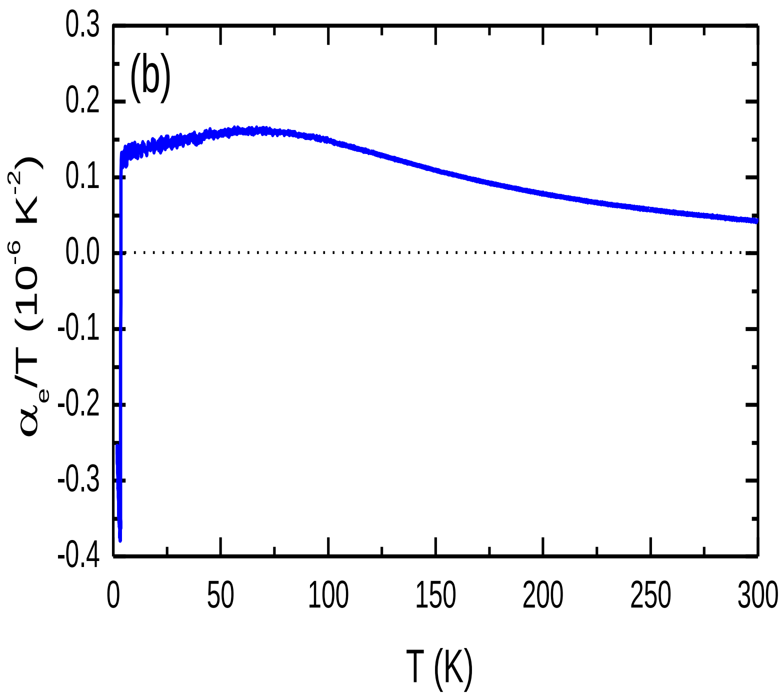
Coherence – incoherence crossover

F. Hardy, et al. PRL 111, 27002 (2013)

Susceptibility



electronic thermal expansion



Pauli susceptibility

$\chi_c = 3.3 \times 10^{-4}$

$\chi_{ab} = 4.1 \times 10^{-4}$

Similar to heavy-fermion compounds

T << T* : heavy Landau quasiparticles (FL)

T >> T* : strongly incoherent regime
local moment behavior

correlations: orbitally-selective Mott transition?

F. Hardy, et al. PRL 111, 27002 (2013)

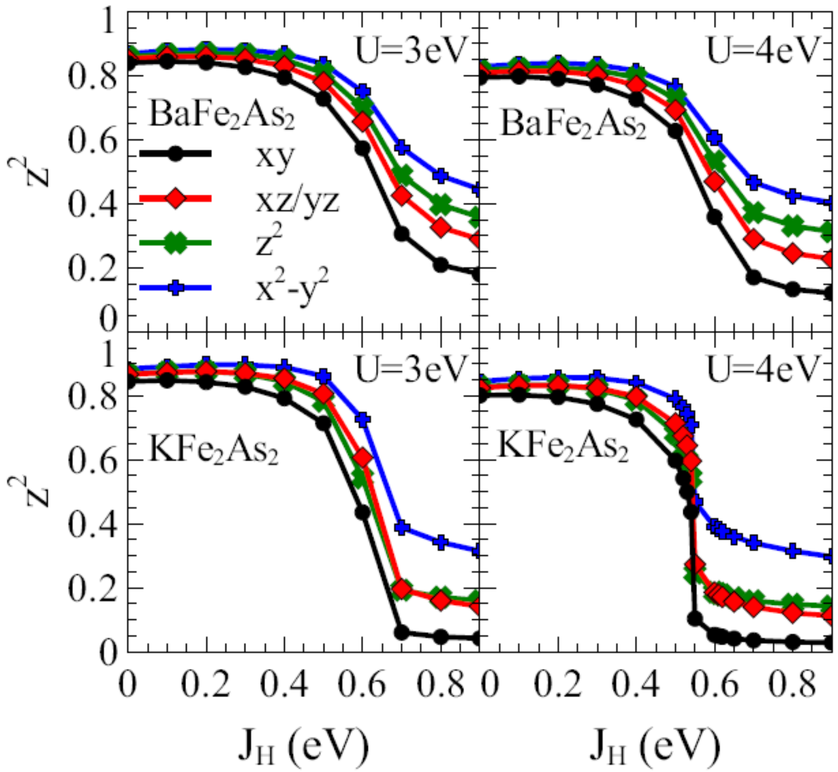


FIG. 5: (Color online) Gutzwiller slave-boson mean-field calculations of the orbitally-resolved mass-enhancement factor z_α for $BaFe_2As_2$ and KFe_2As_2, for two different values of the intraorbital Coulomb repulsion U.

J. Schmalian, G. Kotliar

LDA+DMFT: Strong Hund's coupling

Haule, et al., New J. Phys. 11, (2009) 025021

Yin, Nature Materials 10, (2011) 932

de' Medici, et al., arxiv:1212.3966 (2012)

Kondo interactions between

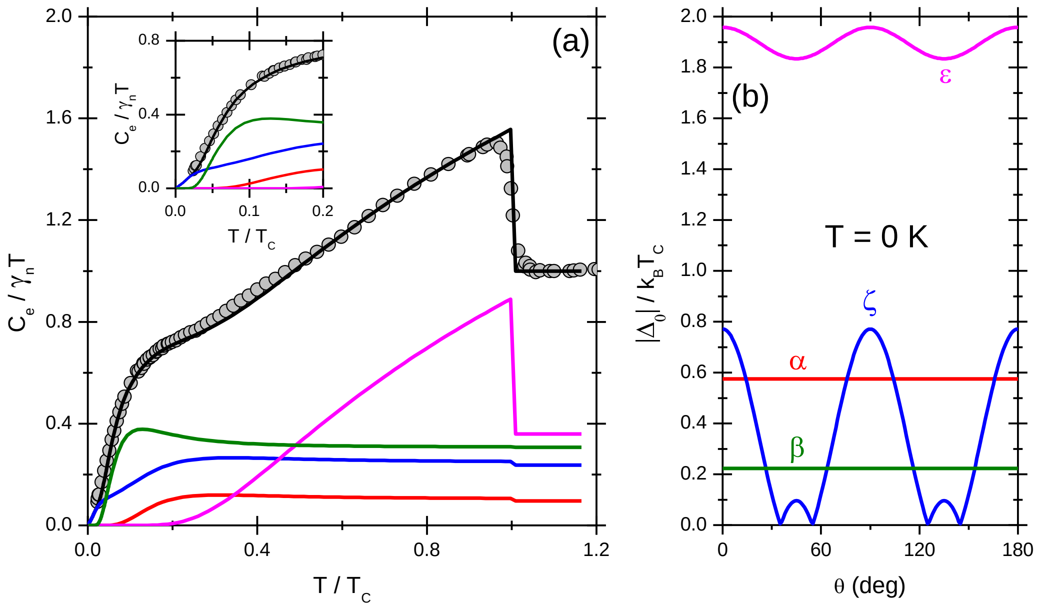
localized spins and itinerant *e*

L.P. Gor'kov et al., PRB 87 (2012) 024504

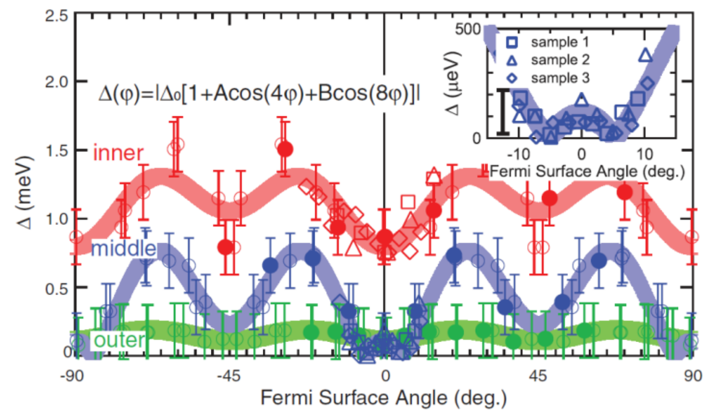
specific heat - 4-band BCS model

Frederic Hardy, et al., arXiv:1309.5654

Heat Capacity

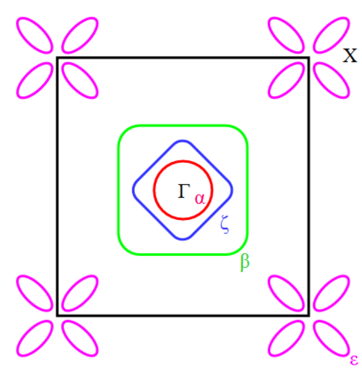


Laser ARPES



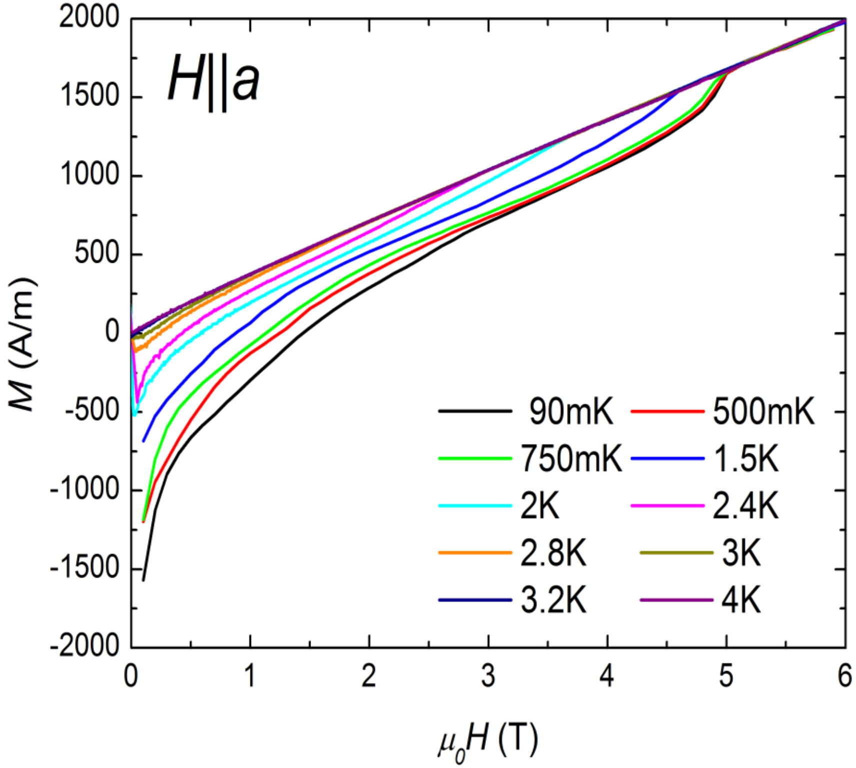
Okazaki et al., Science 337 (2012) 1314

- four-band BCS 'fit'
- density of states from de Haas-van Alphen
- consistent with ARPES (not values of Δ!)
- small gaps and nodes

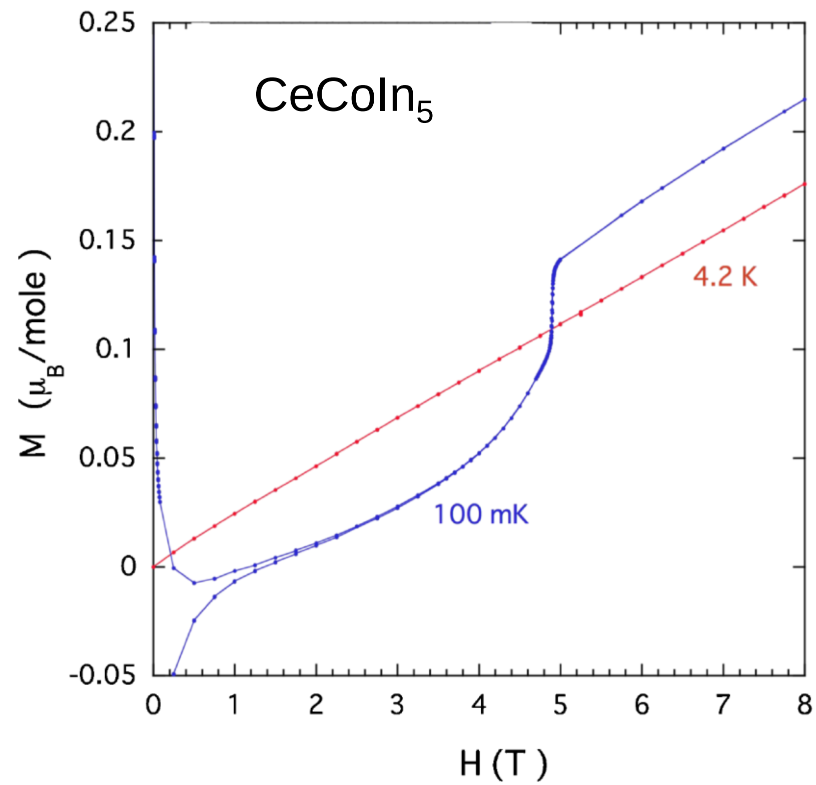


Strong Pauli-limiting behavior - KFe_2As_2 H||a

P. Burger, et al. Phys. Rev. B 88, 014517 (2013)



Paulsen et al., JPSJ 80 (2011) 053701



- strong Pauli limitation seen at low temperatures
  weakly first-order transition at H_{c2}
  FFLO?

- similar to $CeCoIn_5$

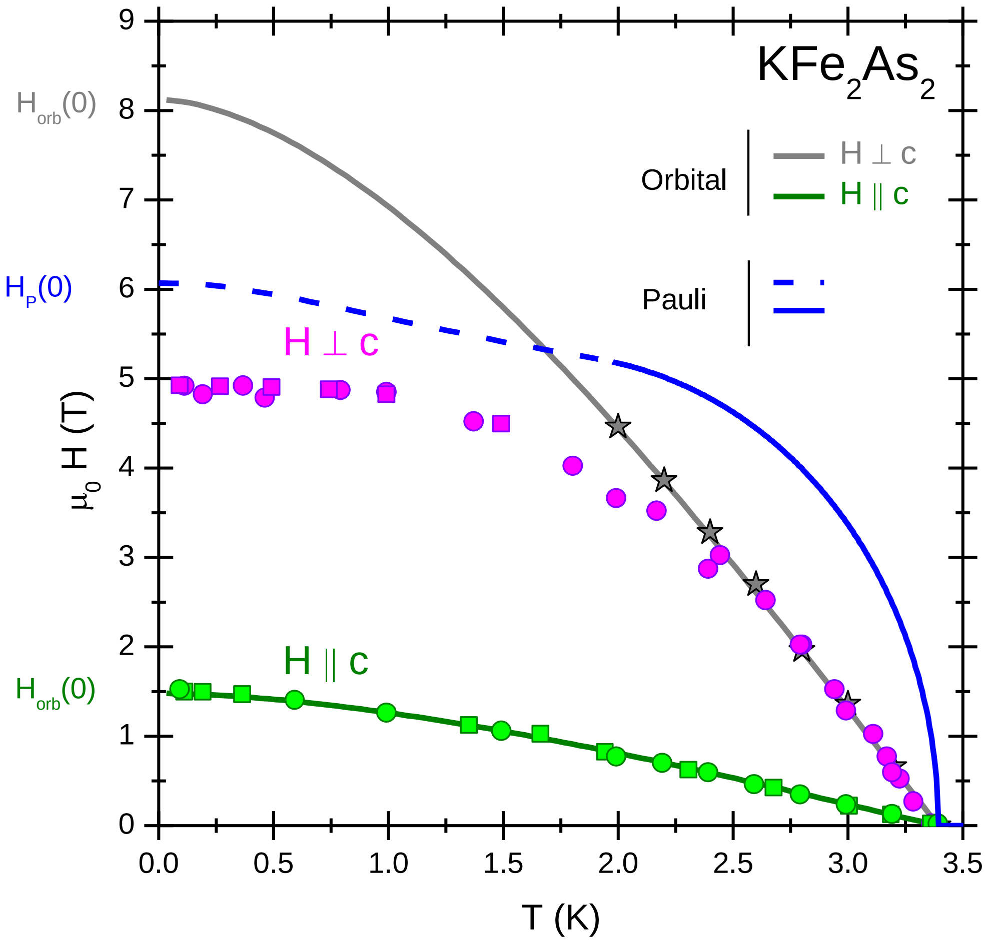
H-T phase diagram

Simple approximation of Pauli field
- single band
- ignore vortices….

$$H_p = \sqrt{\frac{1}{\chi_n}} H_c$$

$H_c = 0.072$ T
$\chi_n^a = 4.1\ 10^{-4}$
$\chi_n^c = 3.2\ 10^{-4}$
(Hardy et al PRL 2013)

$H_p = 3.5 - 3.9$ T



Maki parameter: $\alpha_M \approx 1.9$

Conclusions - K122

- Strong ‘Hund’ correlations
- Coherence-incoherence crossover
- **Large *s*-wave gap -** several tiny energy gaps
- Strong paramagnetic effects - Pauli limited H_{c2} (FFLO?)

Thanks

Superconducting state

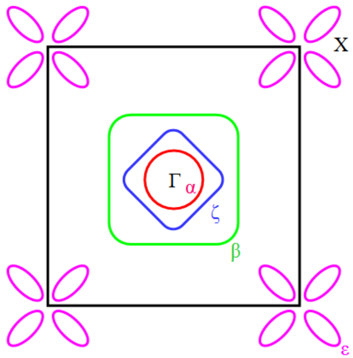
4-band BCS analysis (*s*-wave)

Hardy, et al., unpublished

Maiti et al., PRB 85 (2012) 014511

$$V_{ij}(\phi,\phi') = V_{ij}^{0} + V_{ij}^{1}\left(\cos 4\phi + \cos 4\phi'\right)$$

$$\Delta_i(\phi,T) = \Delta_i^0(T) + \Delta_i^1(T)\cdot\cos 4\phi$$



Enforcing DOS from dHvA/ARPES exp.

Angle-indep. intraband

$$V_{\alpha\alpha}^{\ 0} = V_{\beta\beta}^{\ 0} = V_{\zeta\zeta}^{\ 0} = V_1$$

$$V_{\varepsilon\varepsilon}^{\ 0} = 2.5\cdot V_1$$

Angle-indep. interband

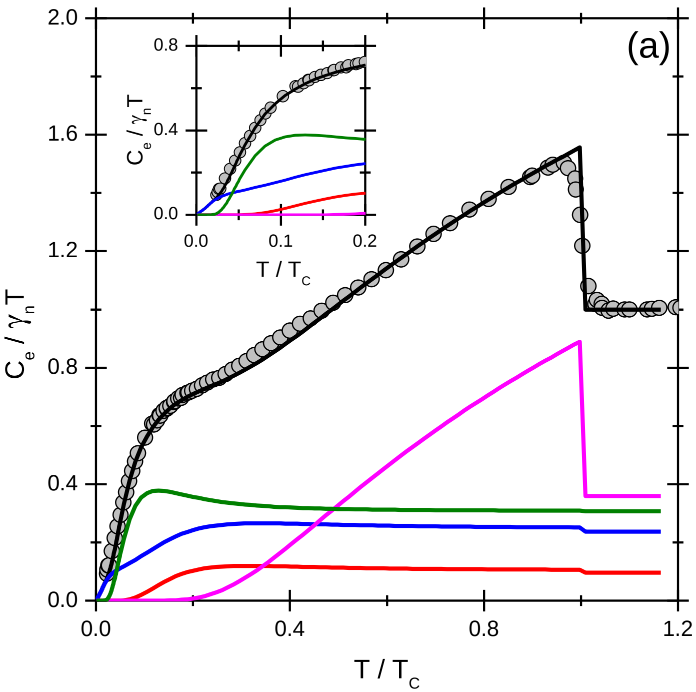
$$V_{\alpha\beta}^{\ 0} = V_{\alpha\zeta}^{\ 0} = V_{\beta\zeta}^{\ 0} = 0.7\cdot V_1$$

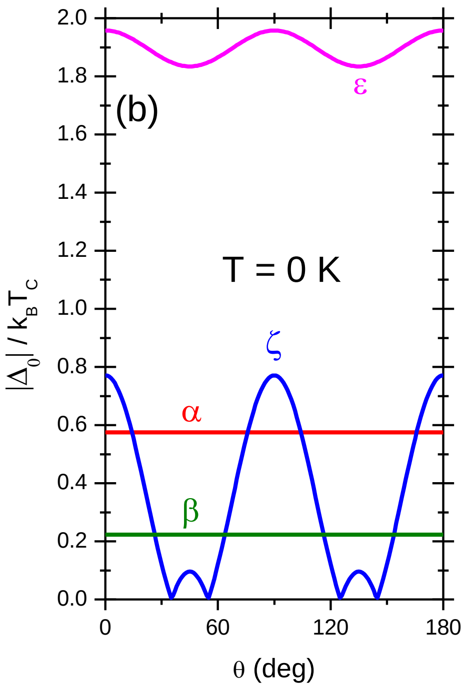
$$V_{\alpha\varepsilon}^{\ 0} = -0.5\cdot V_1$$

$$V_{\zeta\varepsilon}^{\ 0} = -0.15\cdot V_1$$

Angle-dependent interband

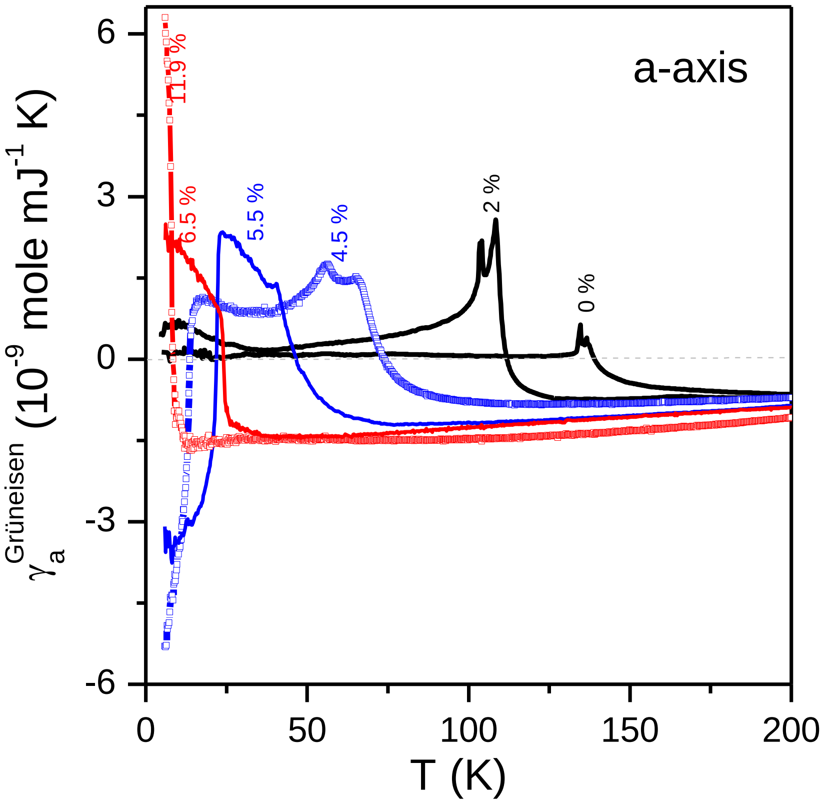
$$V_{\zeta\varepsilon}^{\ 1} = -0.6\cdot V_1$$

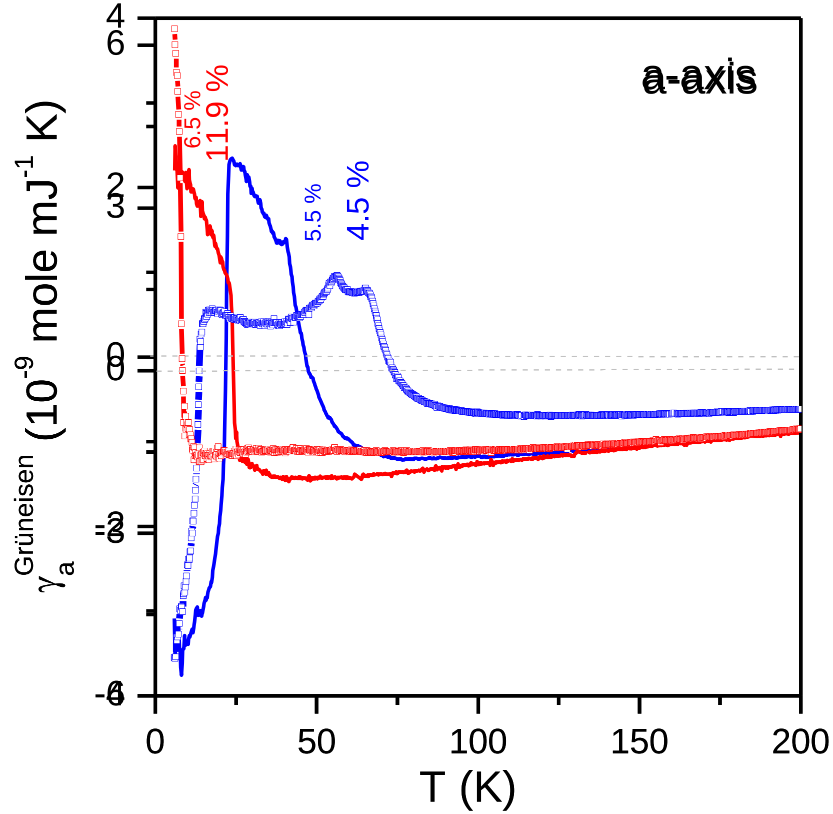




electronic Grüneisen parameter

$\alpha^{electronic}/C^{electronic}$

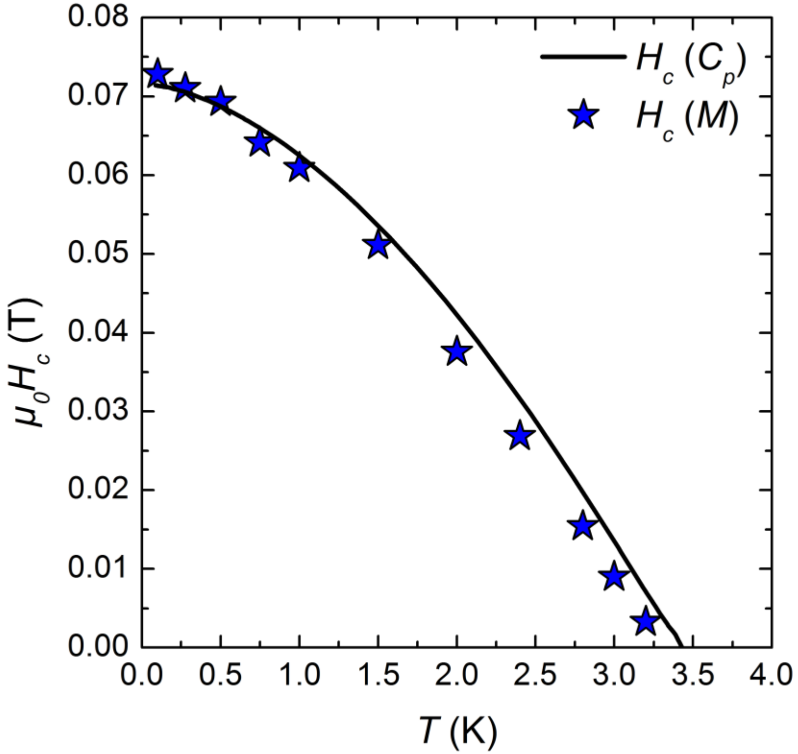




- sign change of Grüneisen parameter at T_{SDW} and T_c
- 'diverging' Grüneisen parameter near onset and end of sc dome - new QCPs!
- similar Grüneisen parameters for 5.5% and 6.5 % Co point to an intimate connection between SDW and SC states!

Thermodynamical critical field from reversible magnetization

$$\int_0^{H_{c2}} (M_s - M_n) dH = -\frac{H_c^2}{2}$$

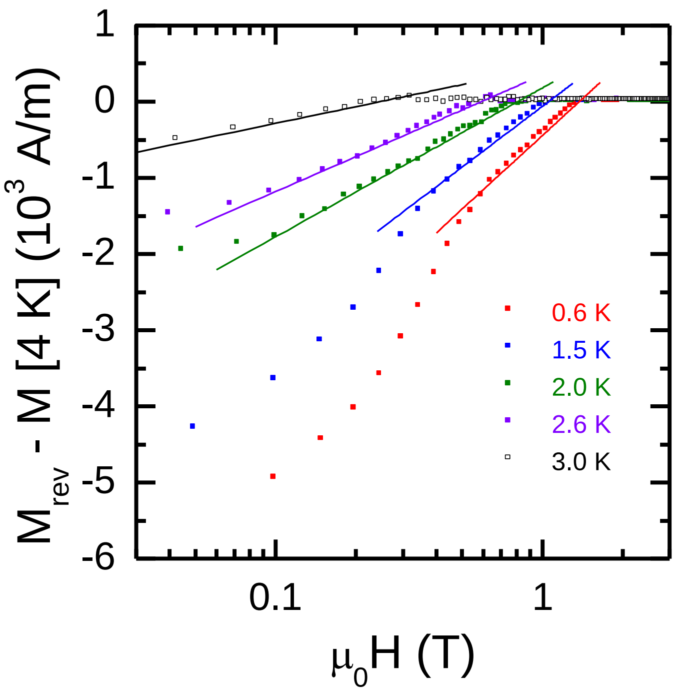


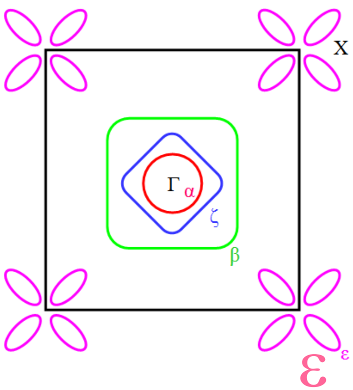
- good agreement with H_c from heat capacity data

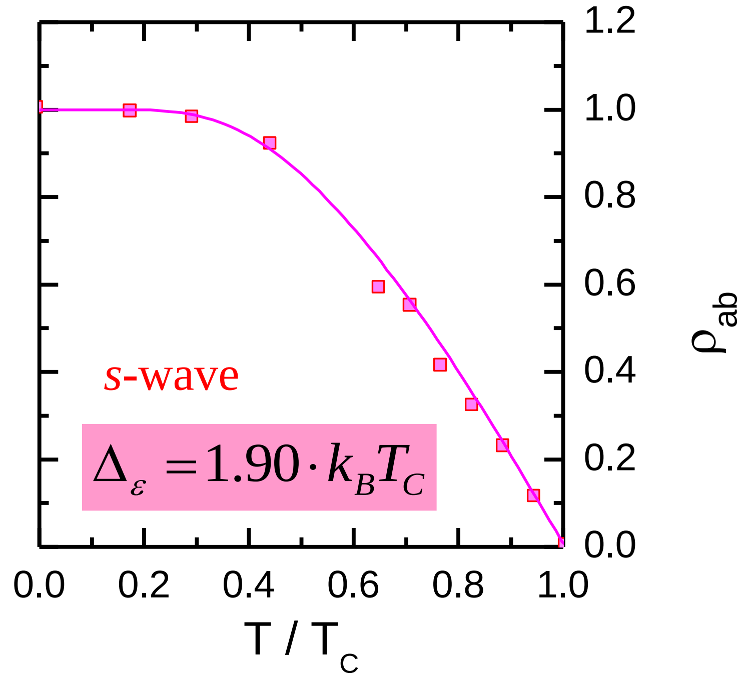
- no spurious magnetic contributions in C_p

Magnetization in the mixed state, H || c

Reversible magnetization







$$\Delta_\varepsilon = 1.90 \cdot k_B T_C$$

$H_{C2} > H > H_{C1}$

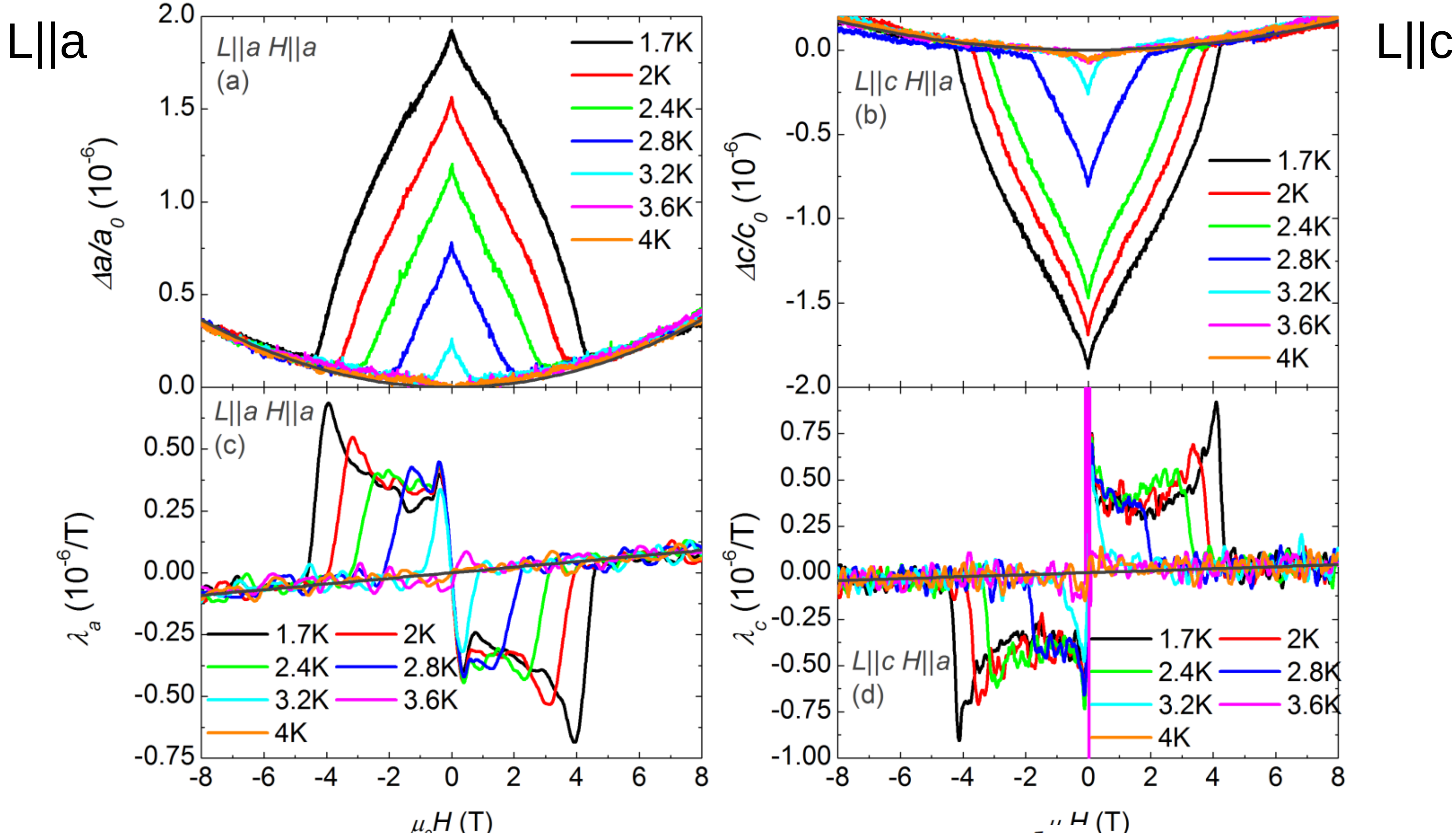
$$\mu_0 M = -\frac{\phi_0}{8\pi\lambda_{ab}^2} \ln\left(\beta \frac{H_{C2}}{H}\right)$$

$$\rho_{ab}(T) = \frac{\lambda_{ab}^2(0)}{\lambda_{ab}^2(T)}$$

Near H_{C2}: only sensitive to the large gap because vortices related with small gaps have already overlapped

de Gennes, Superconductivity of Metals and Alloys (1966)
Kogan et al., PRB 38R (1988), 11958

Magnetostriction measurements: H||a

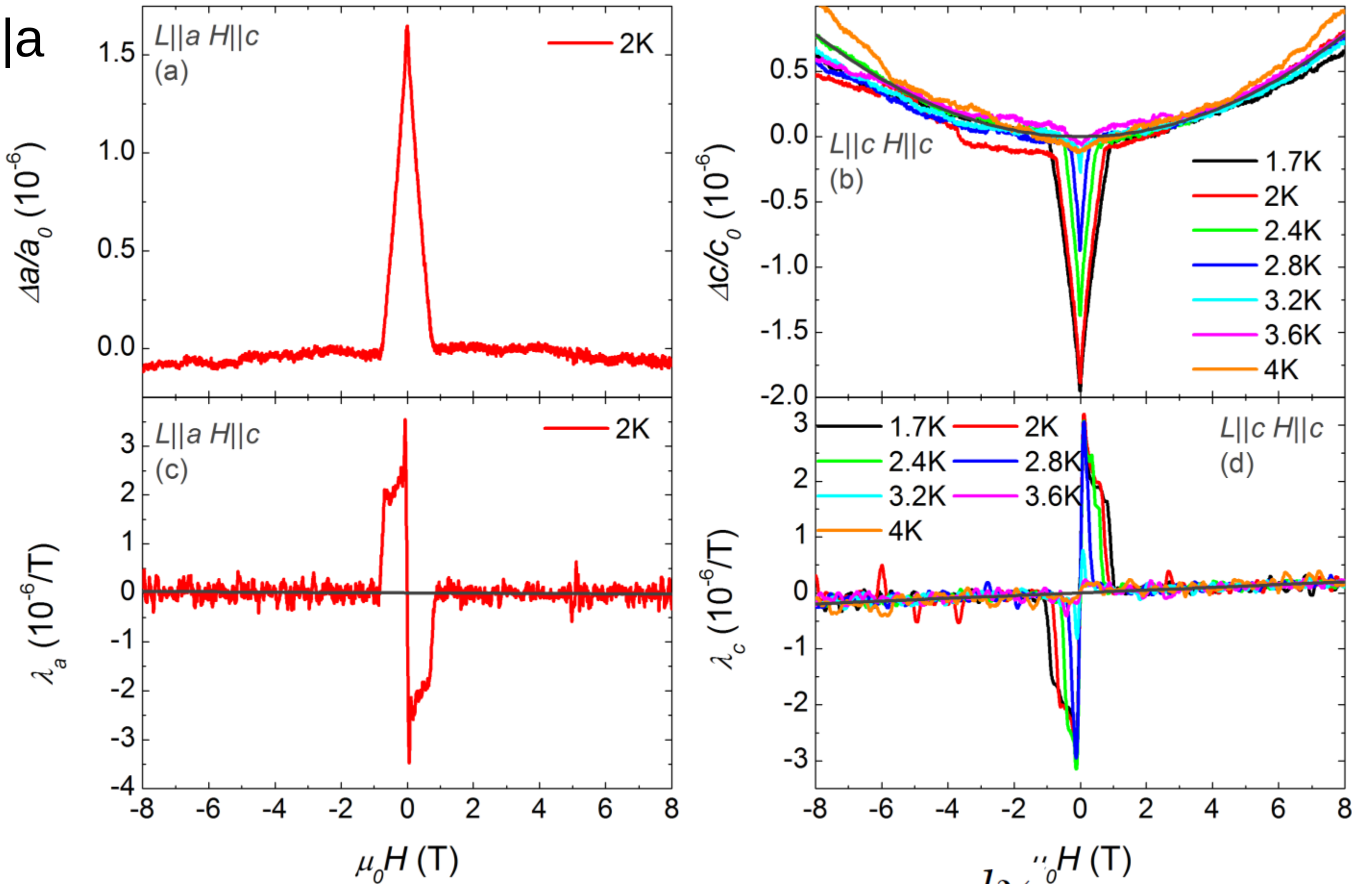


- paramagnetic signal: $\frac{d\chi}{dp_i}$
- strong Pauli limiting for H||a $\frac{dH_c}{dp_i}$
- $d\kappa/dp_i \ll dHc/dp_i$

Magnetostriction measurements: H||c

L||a

L||c

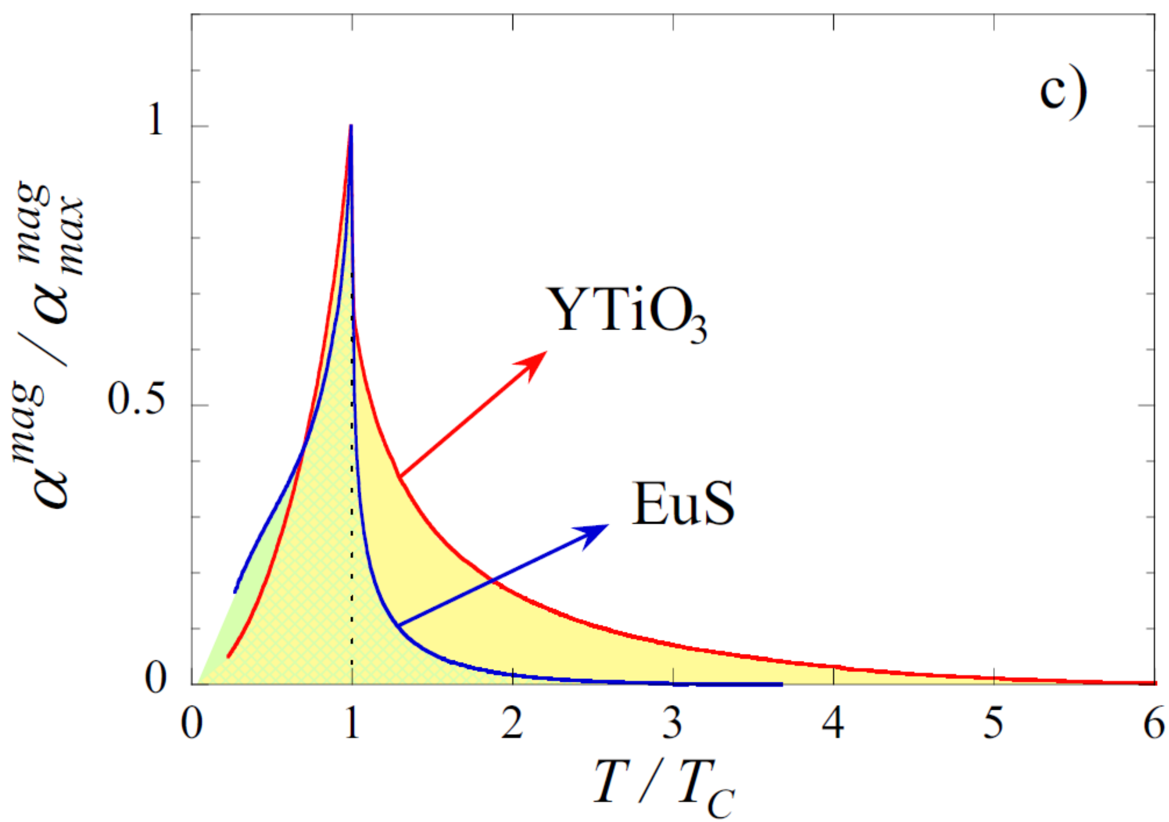


- paramagnetic signal: $$\frac{d\chi}{dp_i}$$
- weak Pauli limiting for H||c $$\frac{dH_c}{dp_i}$$
- $d\kappa/dp_i \ll dH_c/dp_i$

PHYSICAL REVIEW B **79**, 054431 (2009)

Ferromagnetism and lattice distortions in the perovskite $YTiO_3$

W. Knafo,[1,2,3] C. Meingast,[1] A. V. Boris,[4,5] P. Popovich,[4] N. N. Kovaleva,[4,5] P. Yordanov,[4] A. Maljuk,[4,6] R. K. Kremer,[4]
H. v. Löhneysen,[1,2] and B. Keimer[4]



Pressure dependencies

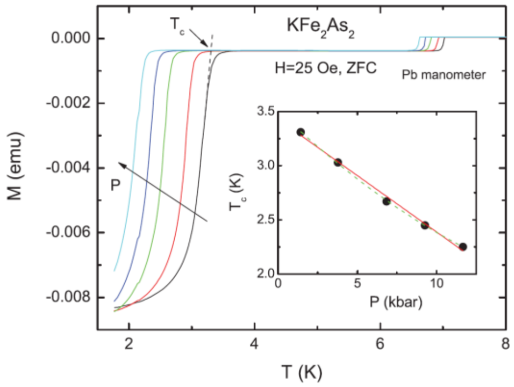
Pressure along	$d\gamma_n/dp_i$ [mJ/mol K^2 GPa]	**dT_c/dp_i [K/GPa]**	**dH_c/dp_i [T/GPa]**	$d\chi^a/dp_i$ [1/GPa]	$d\chi^c/dp_i$ [1/GPa]
a-axis	-7.7	**-1.9**	-0.049	-1.4×10^{-5}	4.1×10^{-6}
c-axis	-4.81	**2.10**	0.046	-6.7×10^{-6}	-3.0×10^{-5}

$dT_c/dP \approx -1$ K/GPa

$dT_c/dp_c \approx +1.1$ K/GPa

- superconductivity couples strongly to c/a ratio
  (opposite sign for Co-Ba122)
  normal state less anisotropic

- fair agreement with Bud'ko et al.



Bud'ko et al. PRB **86**, 224514 (2012)

Normalized pressure dependencies

[1/GPa]	$1/\gamma_n\, d\gamma_n/dp_i$	$1/T_c\, dT_c/dp_i$	$1/H_c\, H_c/dp_i$	$1/\chi^a\, d\chi^a/dp_i$	$1/\chi^c\, d\chi^c/dp_i$
a-axis	-0.076	-0.56	-0.71	-0.035	0.013
c-axis	-0.047	0.61	0.66	-0.016	-0.096
volume	-0.20	-0.51	-0.75	-0.086	-0.070

- largest relative pressure effects: T_c and H_c
- T_c and H_c closely related
–γ and χ much smaller
- detailed analysis complicated due to multiband nature
(too many parameters)

Volume Grüneisen parameters

B = 50 GPa (DFT, Rolf Heid)

	$- d\ln\gamma_n / d\ln V$	$- d\ln T_c / d\ln V$	$- d\ln H_c / d\ln V$	$- d\ln \chi^a / d\ln V$	$- d\ln \chi^c / d\ln V$
volume	- 8.9	- 23	- 34	- 3.9	- 3.1

classical superconductors	$- d\ln T_c / d\ln V$	$- d\ln \gamma / d\ln V$
Al	-17	-1.8
Pb	-3	-1.7
Nb	0	-1.5

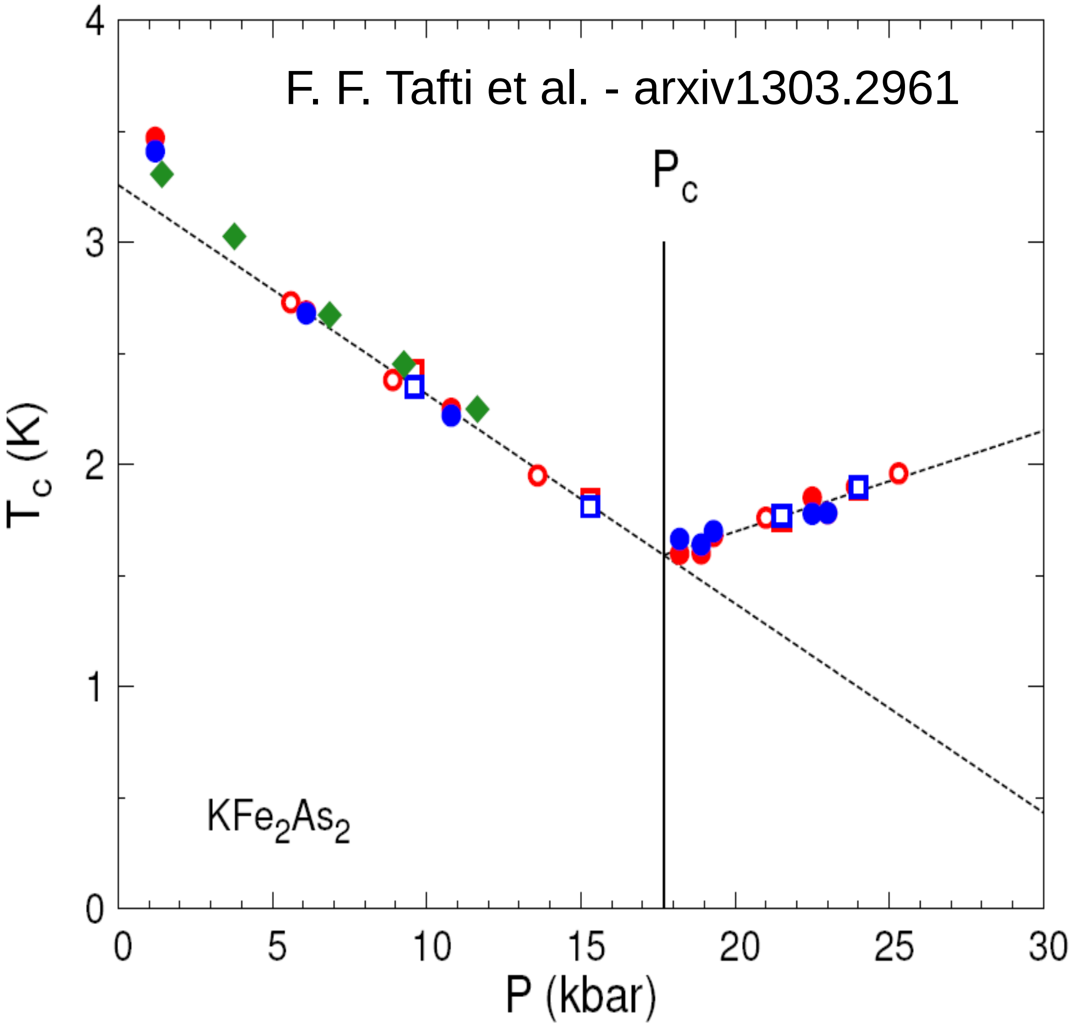
Boughton, Olsen, Palmy 1970

U-based superconductors	$- d\ln T_c / d\ln V$	$- d\ln \gamma / d\ln V$
UPt_3	- 65	- 50
URu_2Si_2	-59	- 40
UBe_{13}	-21	- 52

J. Flouquet et al. Physica C, 1991

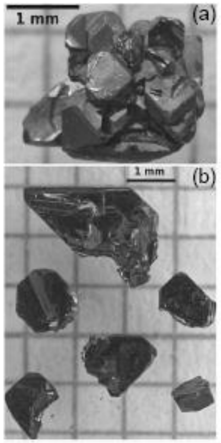
- same signs of T_c and γ Grüneisen parameters as other SC's
- intermediate absolute values of Grüneisen parameters
- does not match trend with Ba doping (T_c increases, γ decreases)

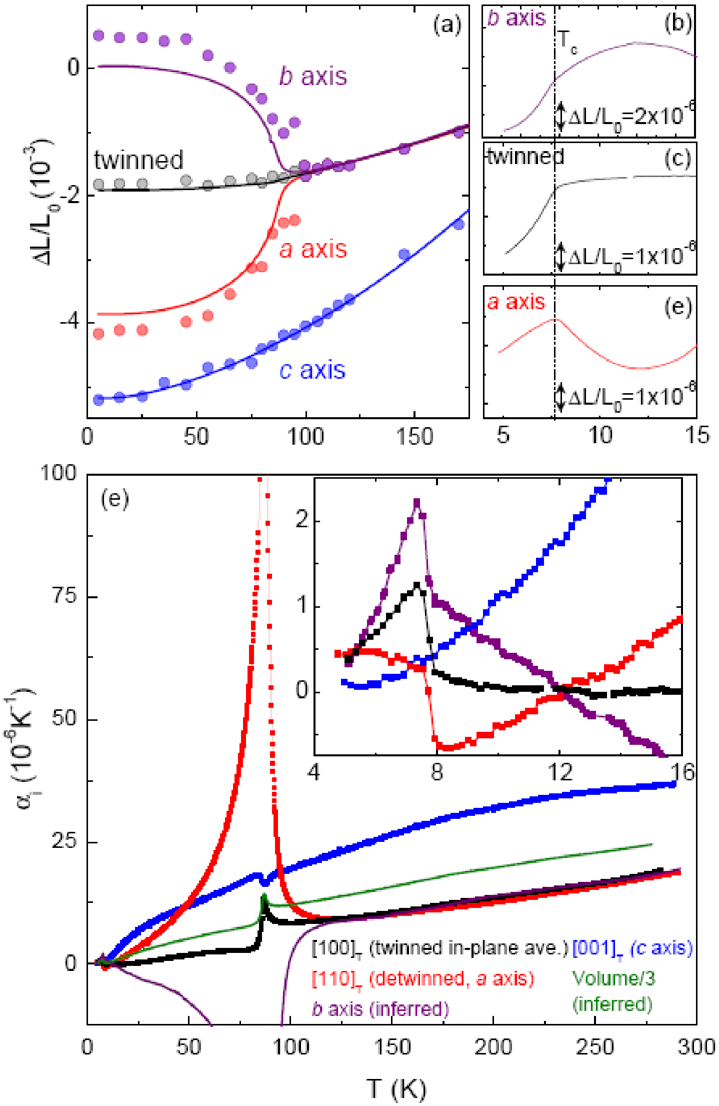
change of pairing symmetry under pressure?



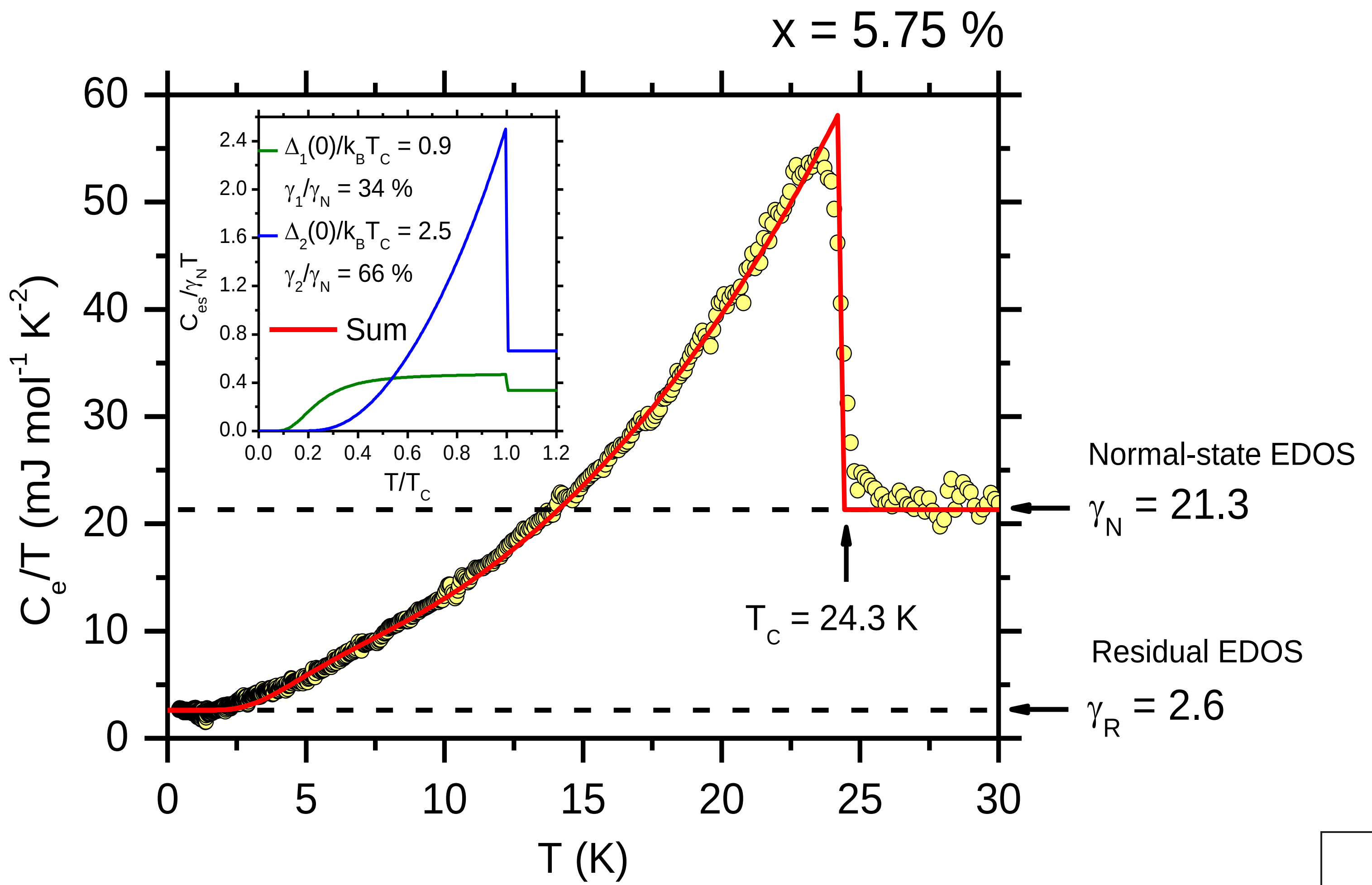
Uniaxial pressure effects in FeSe

Anna Böhmer et al. arxiv 1303.2026v1

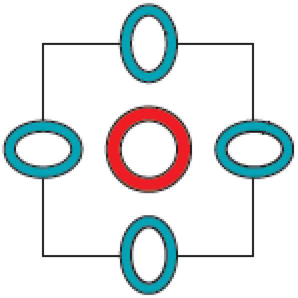




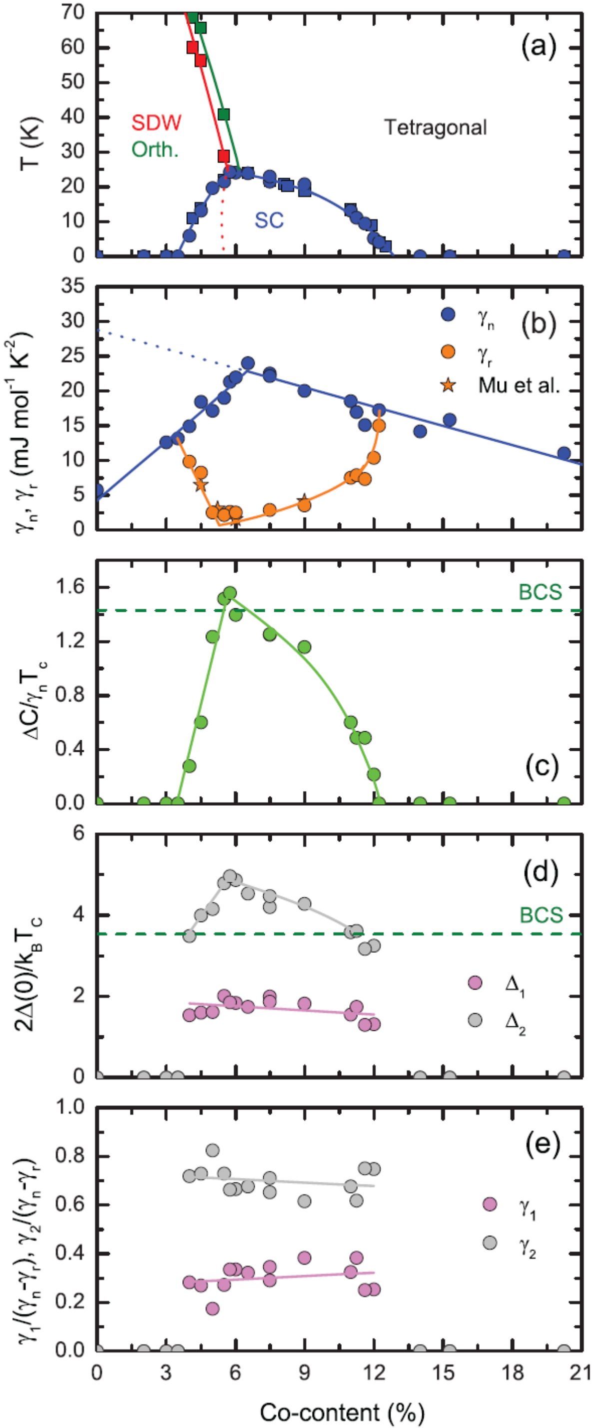
Two gap (s-wave) Analysis



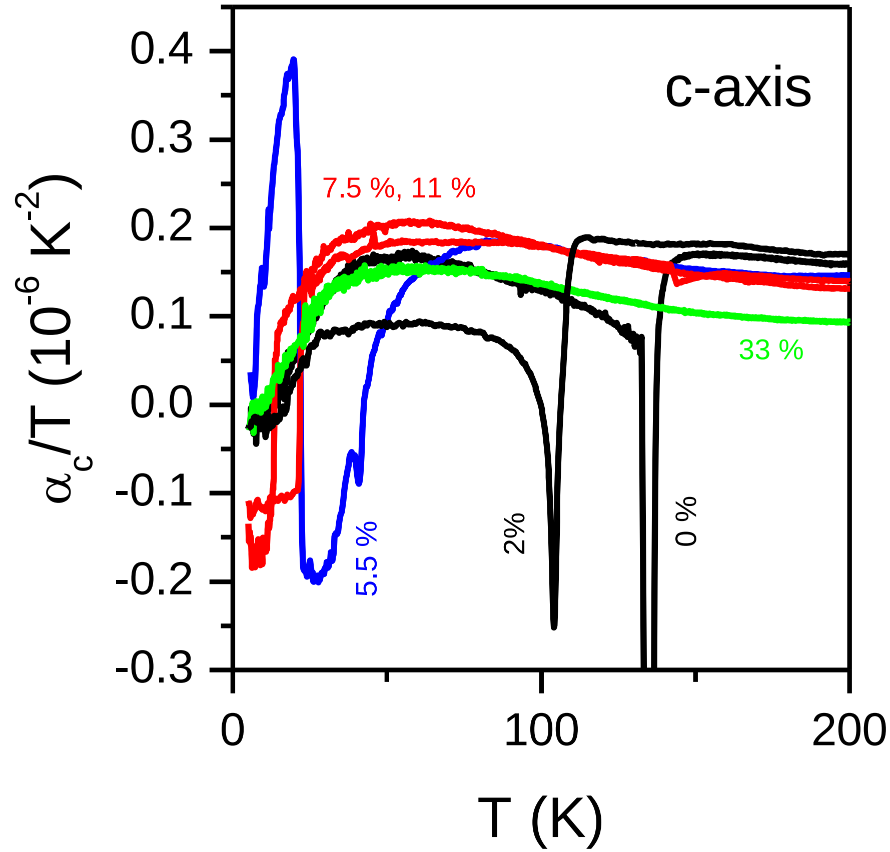
- two s-wave gaps provide very good fit of data
- consistent with proposed s+- state



s±-wave



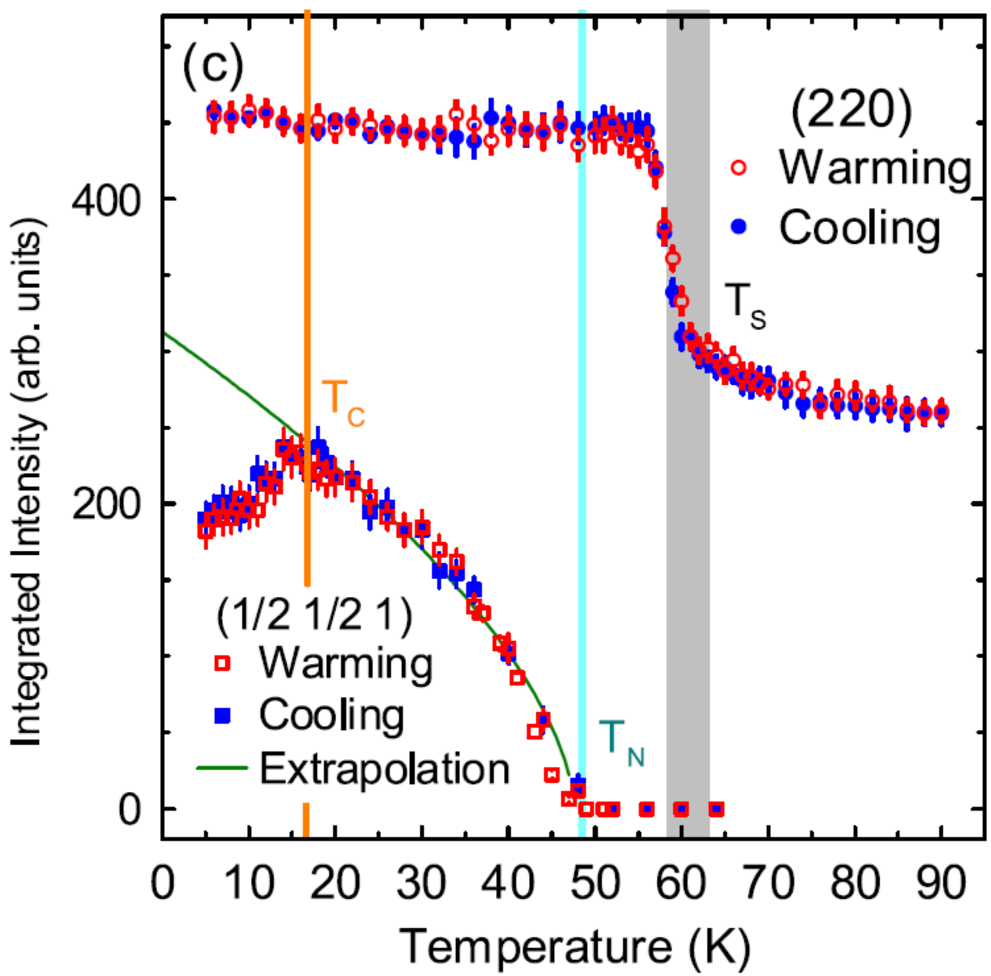
(a)
T (K)
SDW
Orth.
Tetragonal
SC
(b)
γ_n, γ_r (mJ mol^{-1} K^{-2})
γ_n
γ_r
Mu et al.
(c)
$\Delta C/\gamma_n T_c$
BCS
(d)
$2\Delta(0)/k_B T_C$
BCS
Δ_1
Δ_2
(e)
$\gamma_1/(\gamma_n-\gamma_r)$, $\gamma_2/(\gamma_n-\gamma_r)$
γ_1
γ_2
Co-content (%)



c-axis
7.5 %, 11 %
33 %
5.5 %
2%
0 %
0.4
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
0
100
200
T (K)
α_c/T (10^{-6} K^{-2})

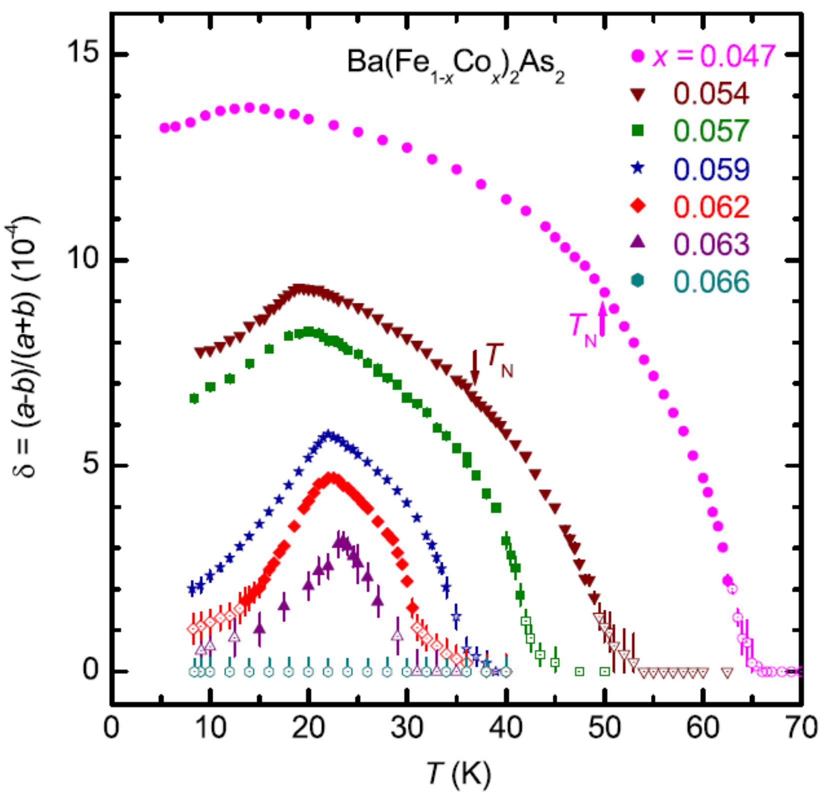
Coexistence of Competing Antiferromagnetic and Superconducting Phases in the Underdoped $Ba(Fe_{0.953}Co_{0.047})_2As_2$ Compound Using X-ray and Neutron Scattering Techniques

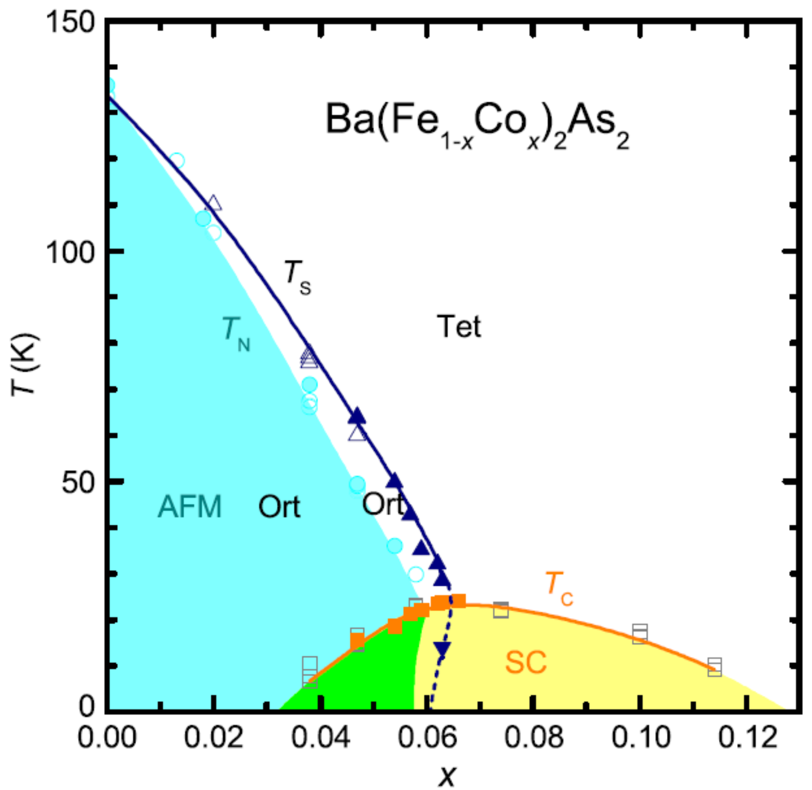
D. K. Pratt, W. Tian, A. Kreyssig, J. L. Zarestky, S. Nandi, N. Ni, S. L. Bud'ko, P. C. Canfield, A. I. Goldman, and R. J. McQueeney



Anomalous Suppression of the Orthorhombic Lattice Distortion in Superconducting $Ba(Fe_{1-x}Co_x)_2As_2$ Single Crystals

S. Nandi, M. G. Kim, A. Kreyssig, R. M. Fernandes, D. K. Pratt, A. Thaler, N. Ni, S. L. Bud'ko, P. C. Canfield, J. Schmalian, R. J. McQueeney, and A. I. Goldman*





Specific heat and thermal expansion

Gibbs free energy: $$G = U - TS + pV$$

specific heat:

$$C_p = \left.\frac{dQ}{dT}\right|_p = -T\left(\frac{\partial^2 G}{\partial T^2}\right) = T\left.\frac{dS}{dT}\right|_p$$

Volume thermal expansion:

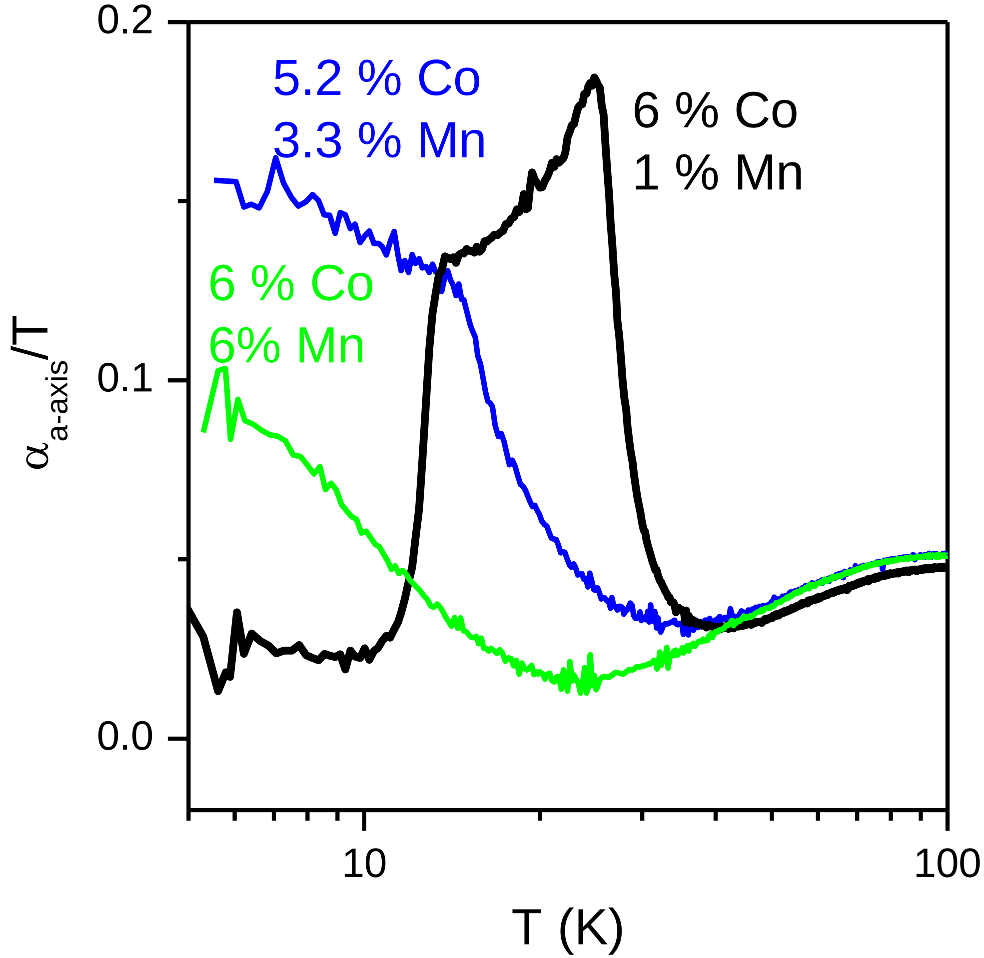
$$\beta = \frac{1}{V}\frac{dV}{dT} = \frac{1}{V}\frac{\partial^2 G}{\partial P \partial T} = \kappa_T \left.\frac{dS}{dV}\right|_T$$

- for superconductors
  - bulk superconductivity?
  - Sommerfeld coefficient
  - nature of energy gap
    (s, d, ...multigap)
  - strong or weak coupling?

- pressure dependences (uniaxial!)
- Grüneisen parameter
- Ehrenfest Relation:

$$\frac{dT_c}{dp_i} = \frac{\Delta\alpha_i V_m}{\Delta C_p / T_c}$$

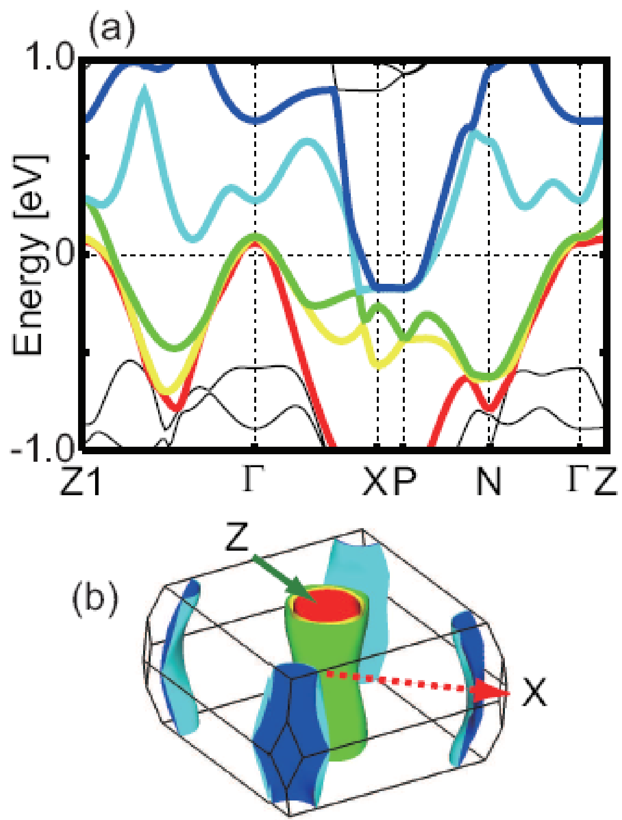
Suppression of superconducting dome in $Ba(Fe_{0.94-x}Co_{0.06}Mn_x)_2As_2$



First-Principles Calculations + Eliashberg

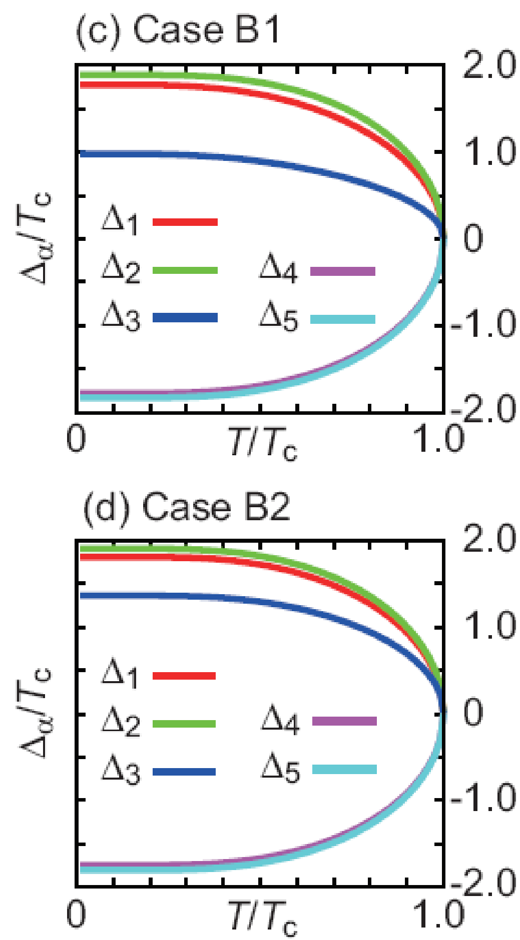
First-principles-based ±s-wave modelling for iron-based superconductors: Studies for specific heat and nuclear magnetic relaxation rate

N. Nakai,[1,2,*] H. Nakamura,[1,2,3] Y. Ota,[1,2] Y. Nagai,[3,4] N. Hayashi,[1,5] and M. Machida[1,2,3]



$N_1 : N_2 : N_3 : N_4 : N_5$

$=0.393 : 0.642 : 0.490 : 0.420 : 0.384$



L. Benfatto et al.

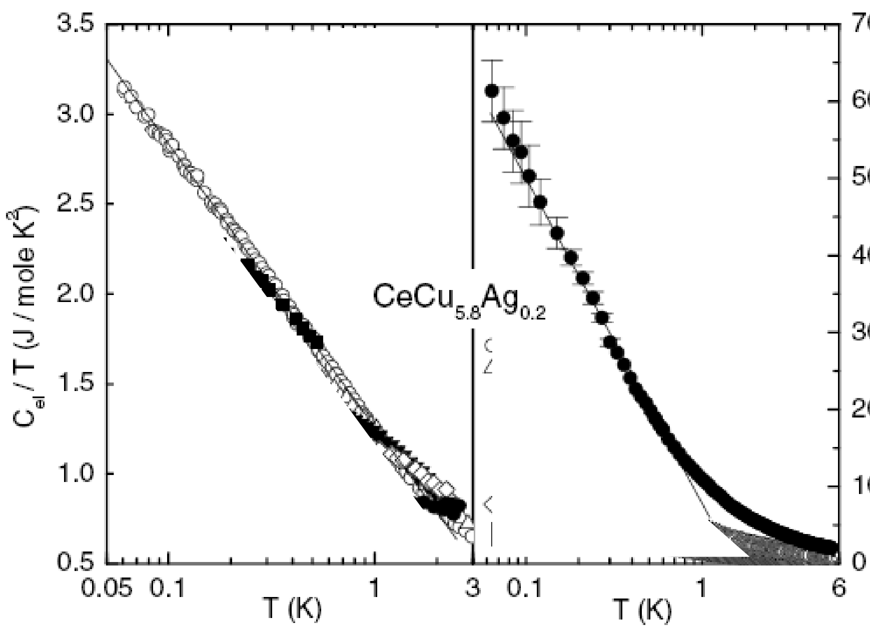
Grüneisen parameter at a QCP?

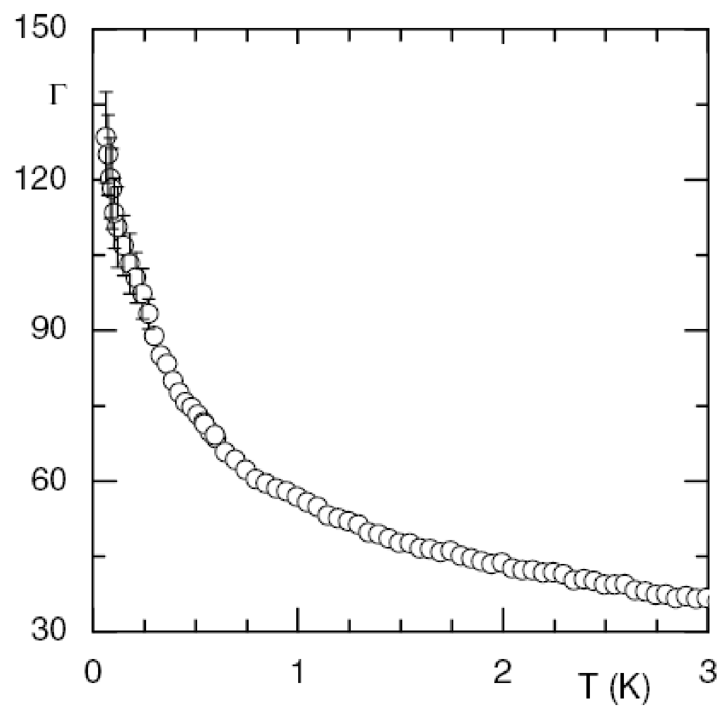
$$\Gamma = \frac{3\alpha V_{mol}}{C_p \kappa_S}$$

phonons $$\Gamma = -\frac{V}{\omega_{Debye}} \frac{\partial \omega_{Debye}}{\partial V} \approx const.$$

CeCuAg: *Küchler et al. PRL 93 (2004)*

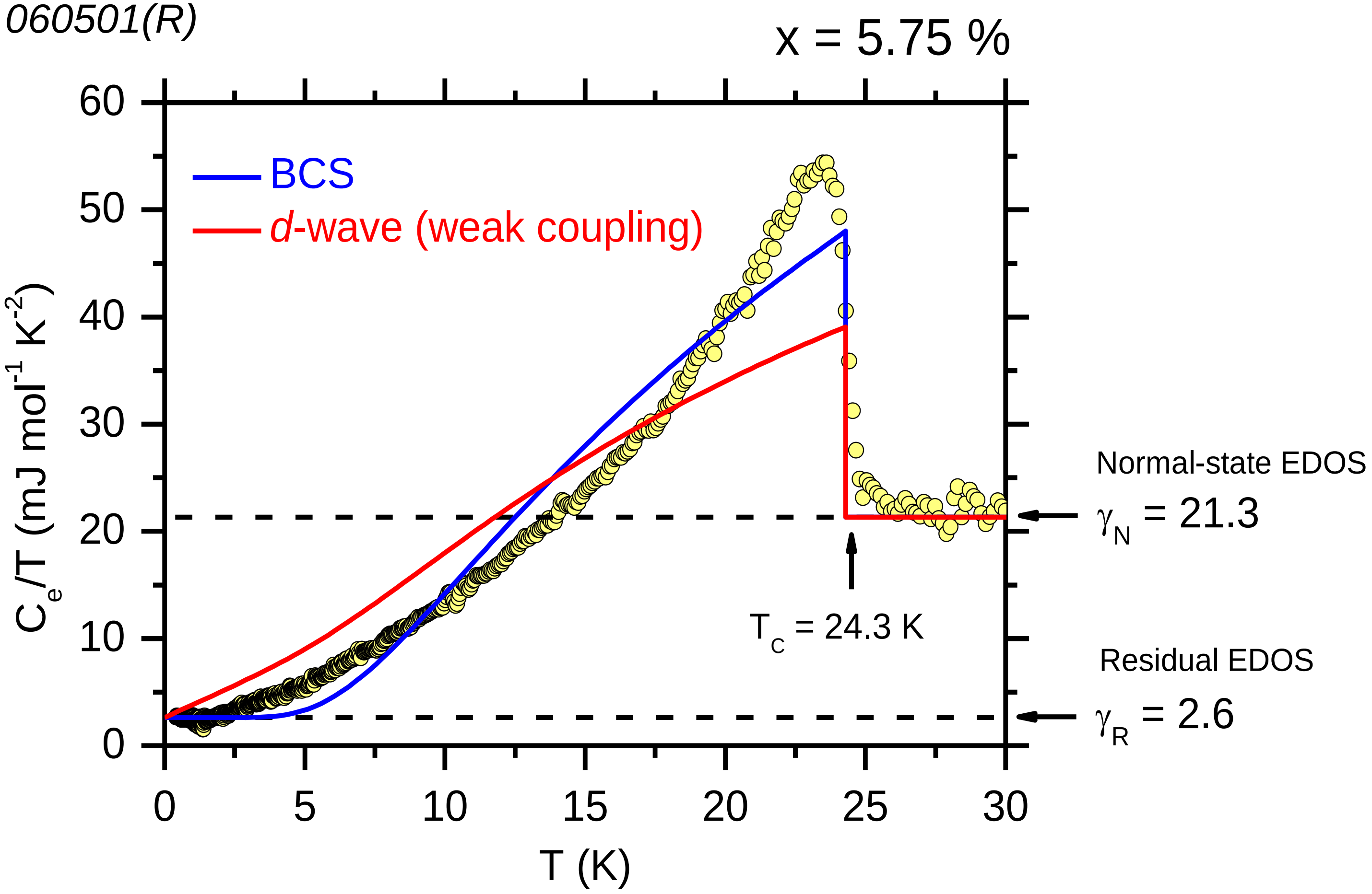
C_p/T a/T $G_{Grüneisen} = a\ /\ C_p$





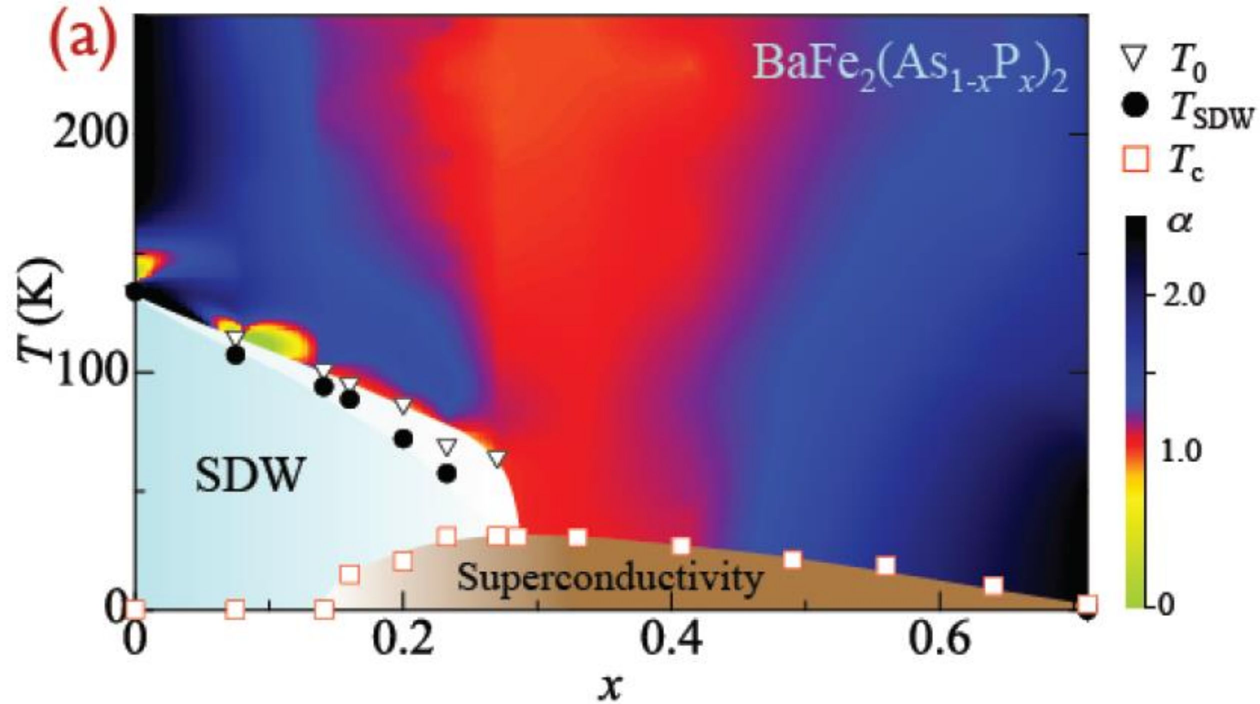
electronic specific heat of $Ba(Fe,Co)_2As_2$

*F. Hardy et al., PRB **81** (2010) 060501(R)*



- some residual electronic term at low T (need to measure below 2 K!!)
- simple single-band d-wave or s-wave fits do not work

S. Kasahara et al., Phys. Rev. B 81, 184519 (2010)



r ~ T^a

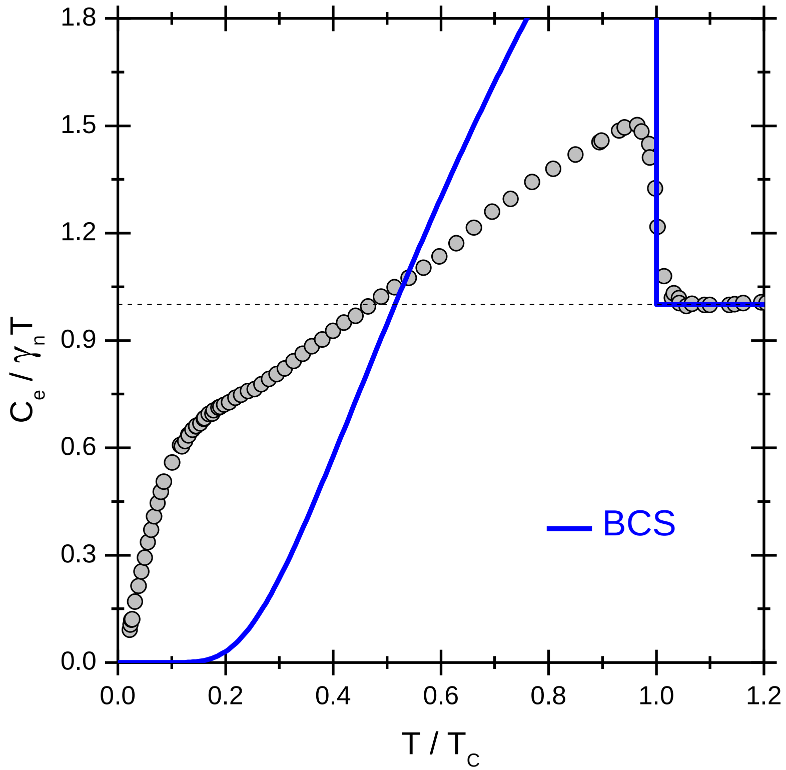
- nearly linear resistivity at optimal doping!
- similar behavior found in cuprates and heavy fermions

- **need thermodynamic data showing non-Fermi liquid behavior**

Superconducting state

KFe_2As_2

Hardy et al., unpublished

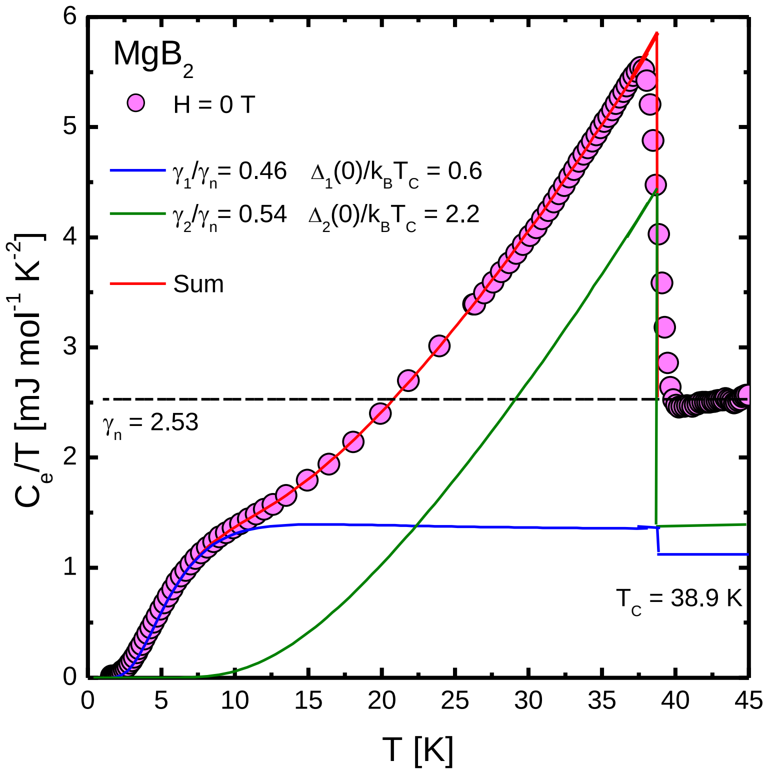


T_C = 3.4 K

γ_n = 102 mJ mol^{-1} K^{-2}

MgB_2

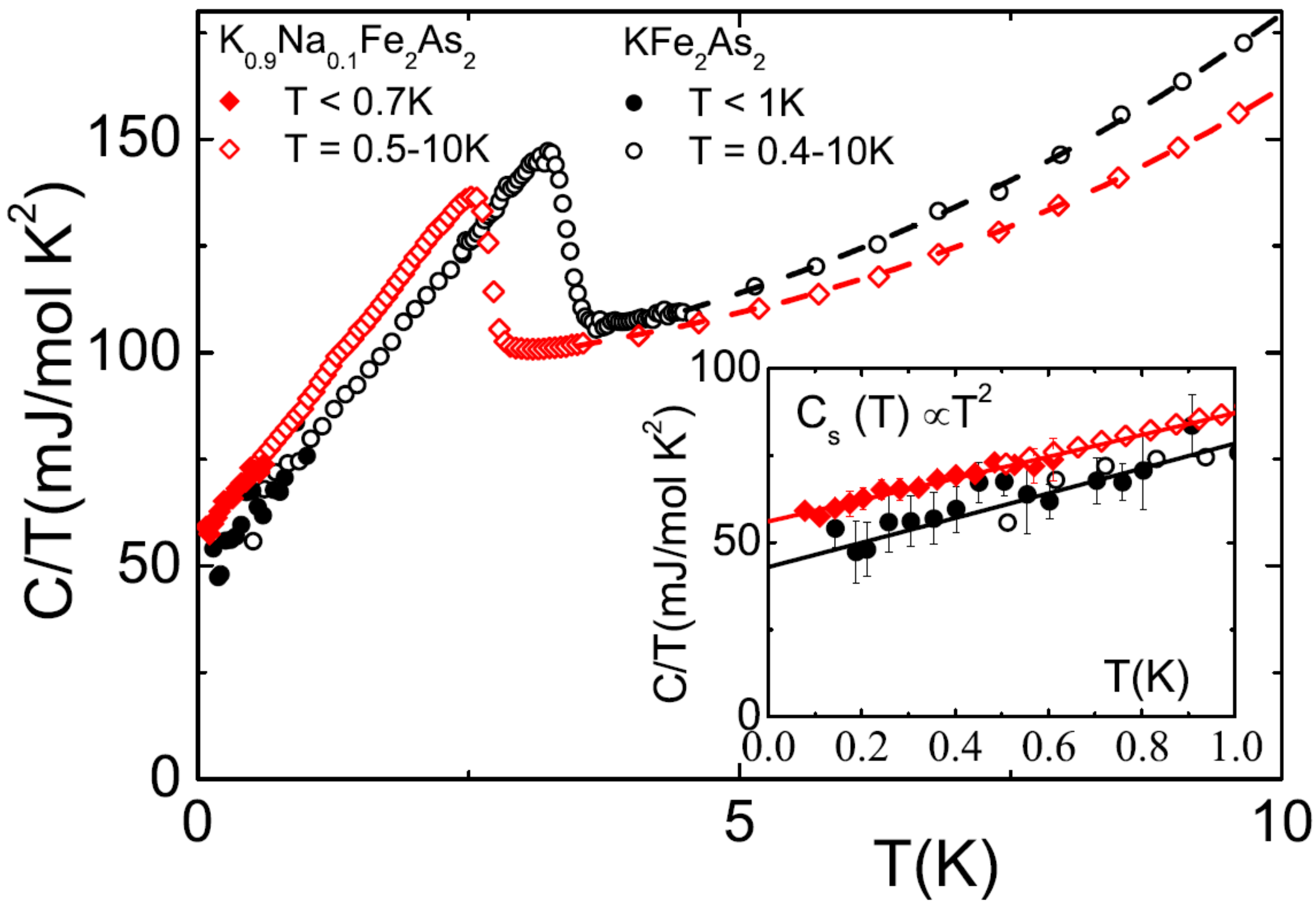
Bouquet et al., PRL 109 (2012) 087001



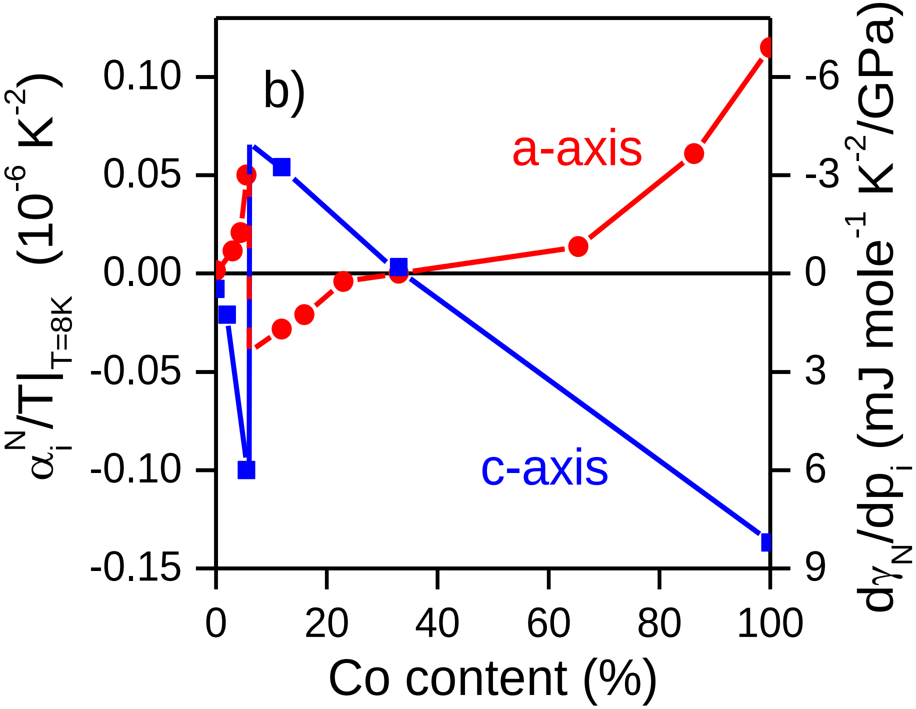
T_C = 39 K

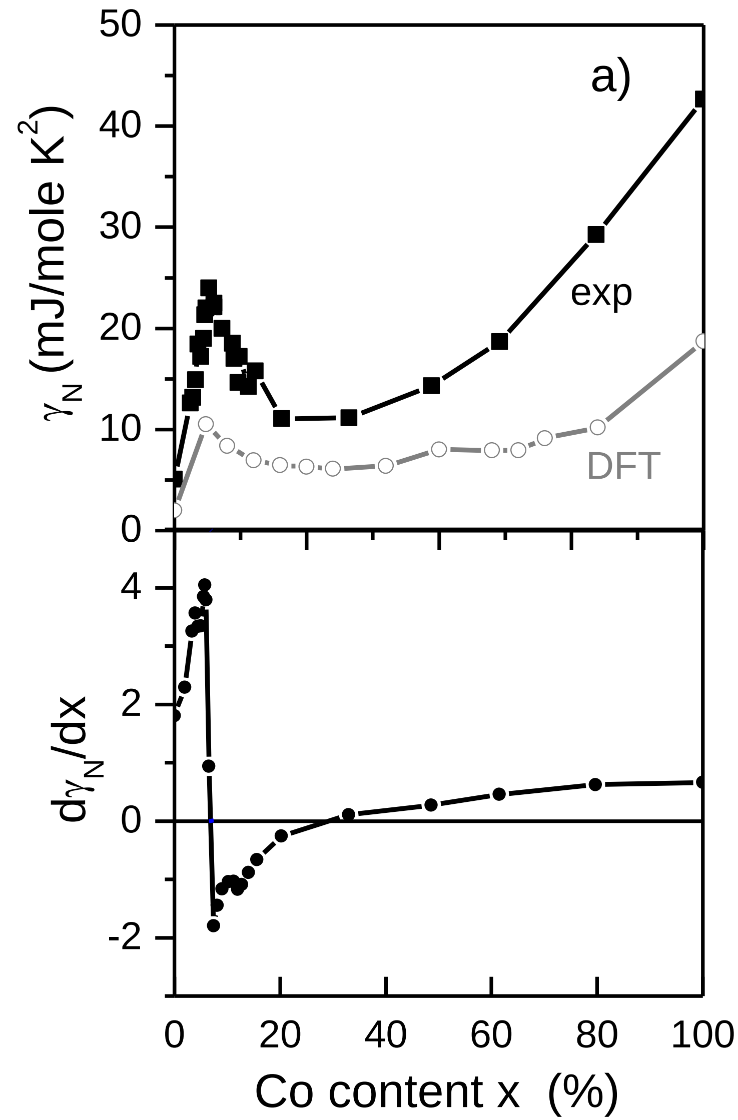
γ_n = 2.5 mJ mol^{-1} K^{-2}

M. Abdel-Hafiez et al. arxiv1301.5257



$$\frac{\alpha_i}{T} = -\frac{d\gamma}{dP_i}$$



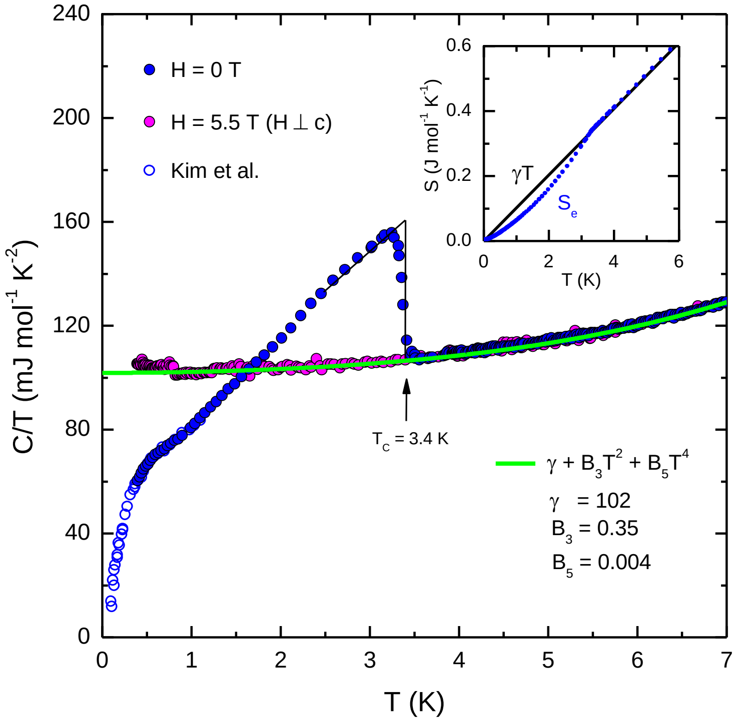


- doping and pressure are closely related: dg/dp ~ - dg/dx
- uniaxial pressure is a good tuning parameter
- 33% Co good background - dg/dp = 0

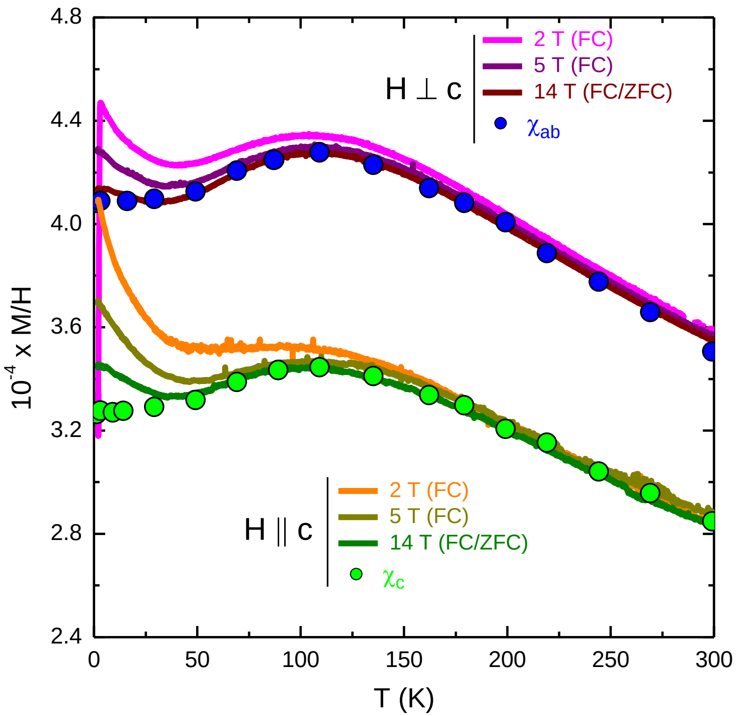
Heat capacity and susceptibility

F. Hardy, et al. PRL 111, 27002 (2013)

Heat Capacity



Susceptibility



Sommerfeld coefficient

γ_n = 102 mJ mol^{-1} K^{-2}
(γ_{LDA} = 10 mJ mol^{-1} K^{-2})

Pauli susceptibility

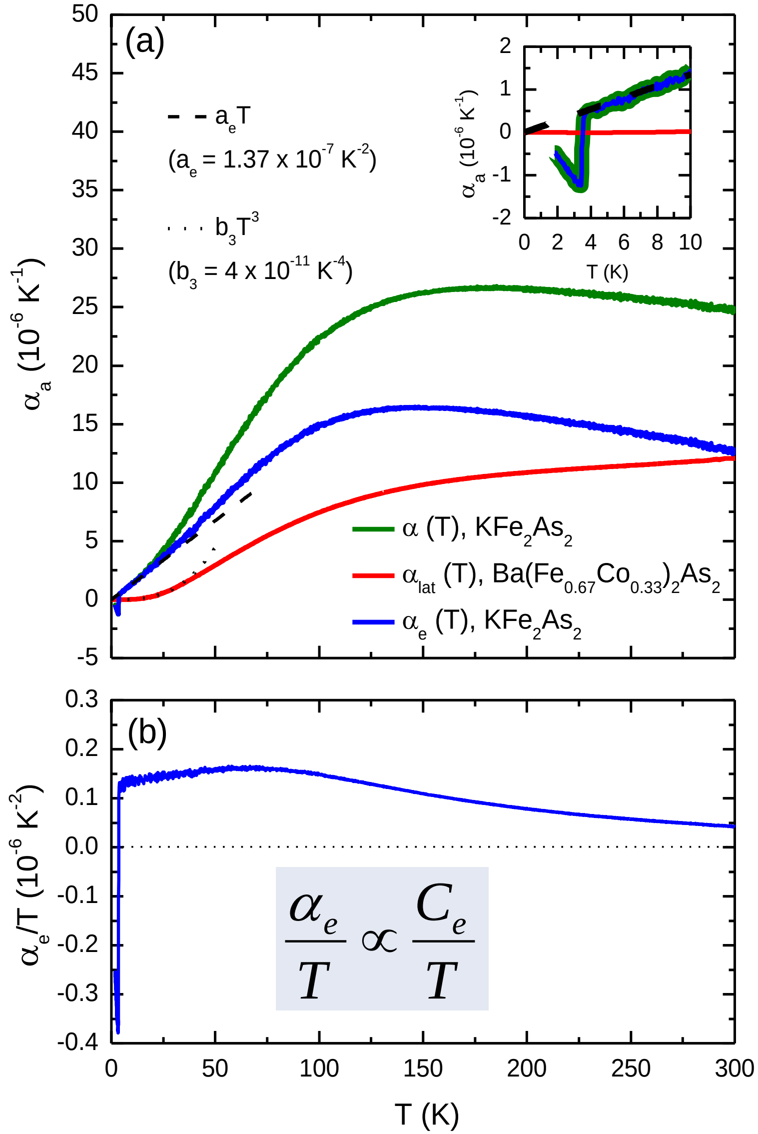
χ_c = 3.3 x 10^{-4}
χ_{ab} = 4.1 x 10^{-4}

Confirm heavy QP (dHvA, ARPES)

Coherence – incoherence crossover

Thermal expansion

F. Hardy, et al. PRL 111, 27002 (2013)



Existence of strong correlations

Similar to heavy-fermion compounds and ruthenates

Evidence for coherence-incoherence crossover

T << T* : heavy Landau quasiparticles
(Fermi liquid)

T >> T* : strongly incoherent regime
local moment behavior
non-linear heat capacity

LDA+DMFT: Strong Hund's coupling

Haule, et al., New J. Phys. 11, (2009) 025021

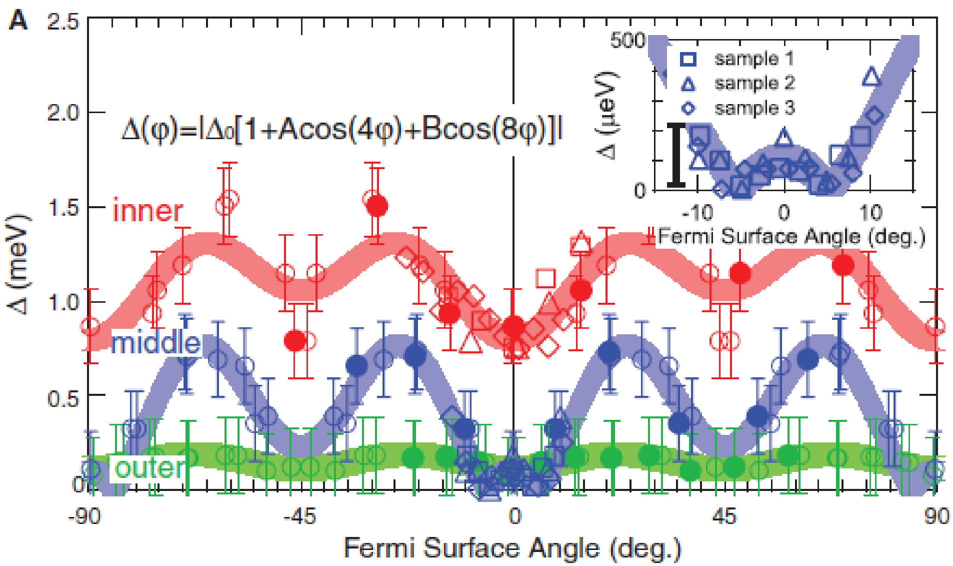
Yin, Nature Materials 10, (2011) 932

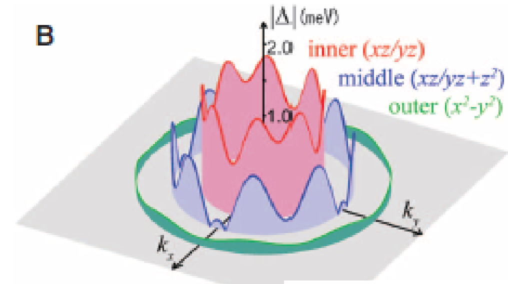
de' Medici, et al., arxiv:1212.3966 (2012)

Kondo interactions between localized spins and itinerant *e*

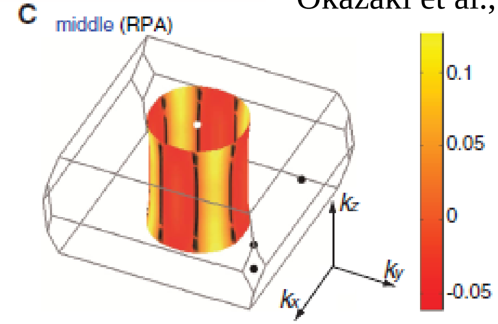
L.P. Gor'kov et al., PRB 87 (2012) 024504

Laser ARPES – KFe_2As_2





Okazaki et al., Science 337 (2012) 1314

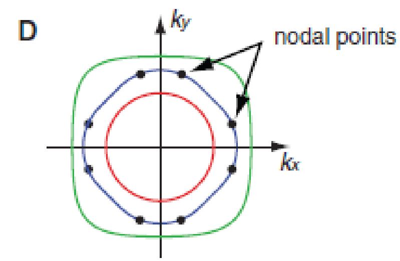


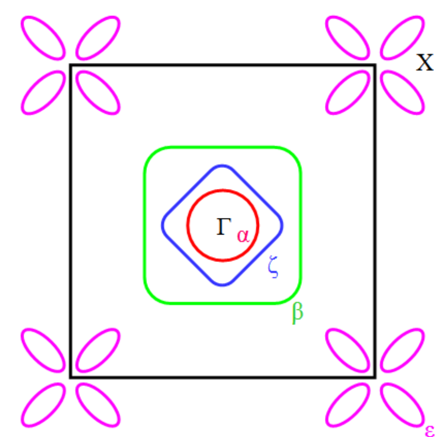
T = 1.5 K

Three gaps around Γ- point observed

Gap around X- point not observed

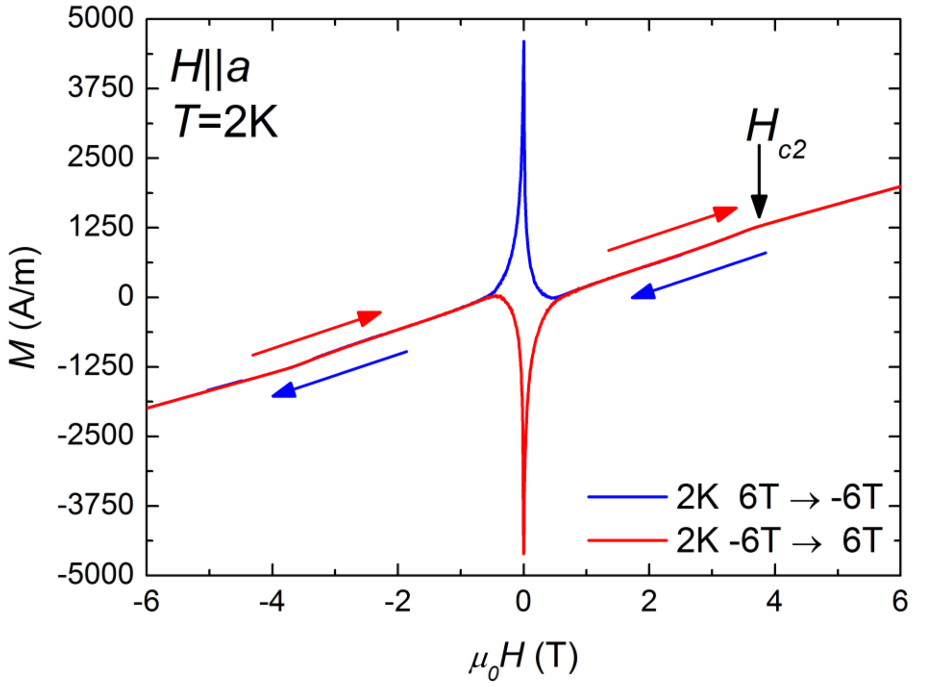
Accidental Nodes (*s*-wave)





	Δ_0 (meV)	$2\Delta_0/k_BT_c$	A	B
Inner FS	1.11 ± 0.05	7.58 ± 0.34	−0.12 ± 0.06	−0.17 ± 0.05
Middle FS	0.41 ± 0.05	2.80 ± 0.34	−0.40 ± 0.14	−0.85 ± 0.18
Outer FS	0.15 ± 0.06	1.02 ± 0.41	−0.01 ± 0.57	−0.26 ± 0.58

Magnetization of KFe_2As_2: H||a



- reversible down to small fields
  reversible magnetization: $M = (M^+ + M^-)/2$

- large paramagnetic signal