Part III: SH jump & CE

Anomalous Scaling Relations & Pairing Mechanism of Fe-based SC

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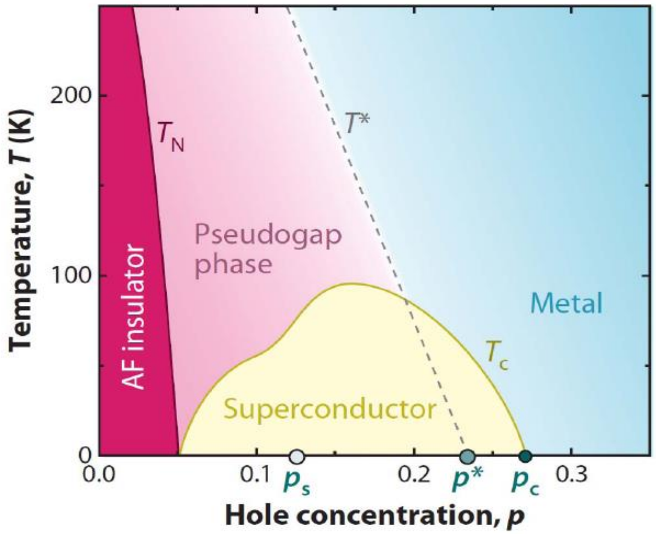
Refs:
New J Phys, 18, 023017 (2016)
arXiv:1601.01847

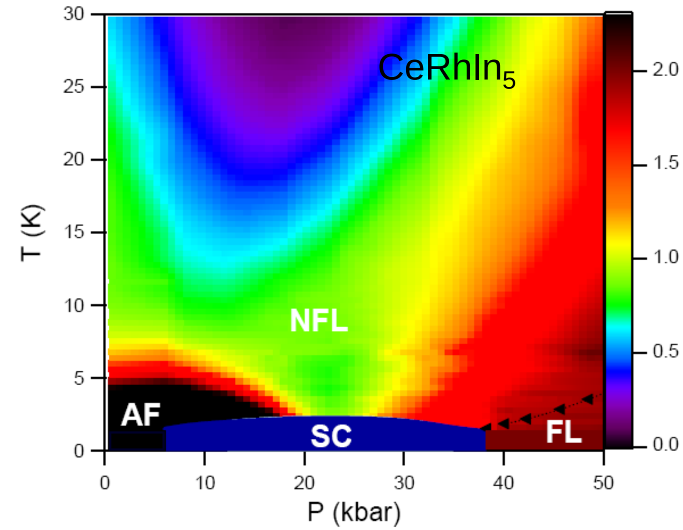
We believe : IBS are Unconventional Superconductors

Common Phase diagram of unconventional SCs

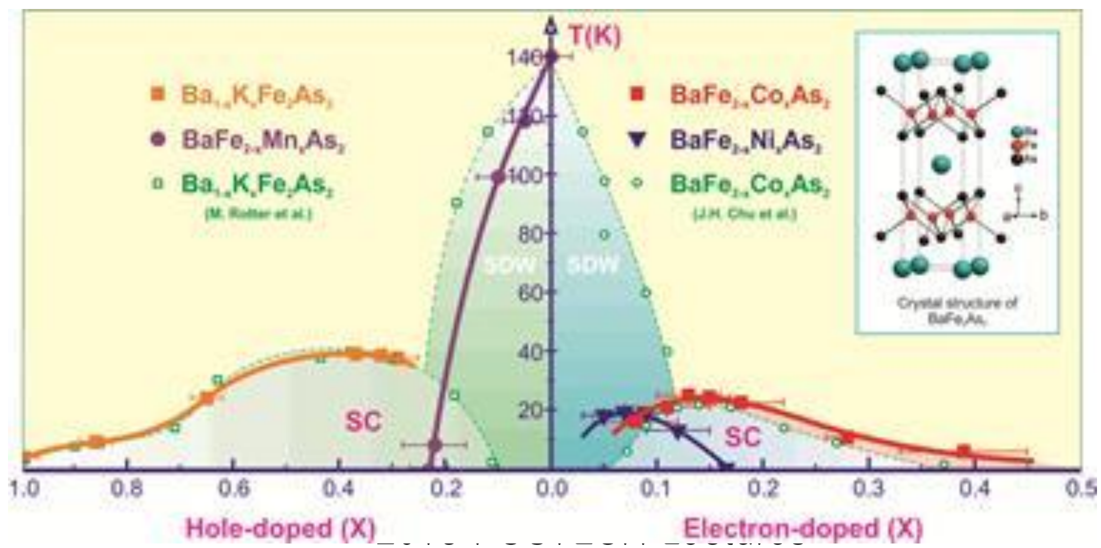
cuprate



heavy fermion



Fe-122(BaFe2 As2)



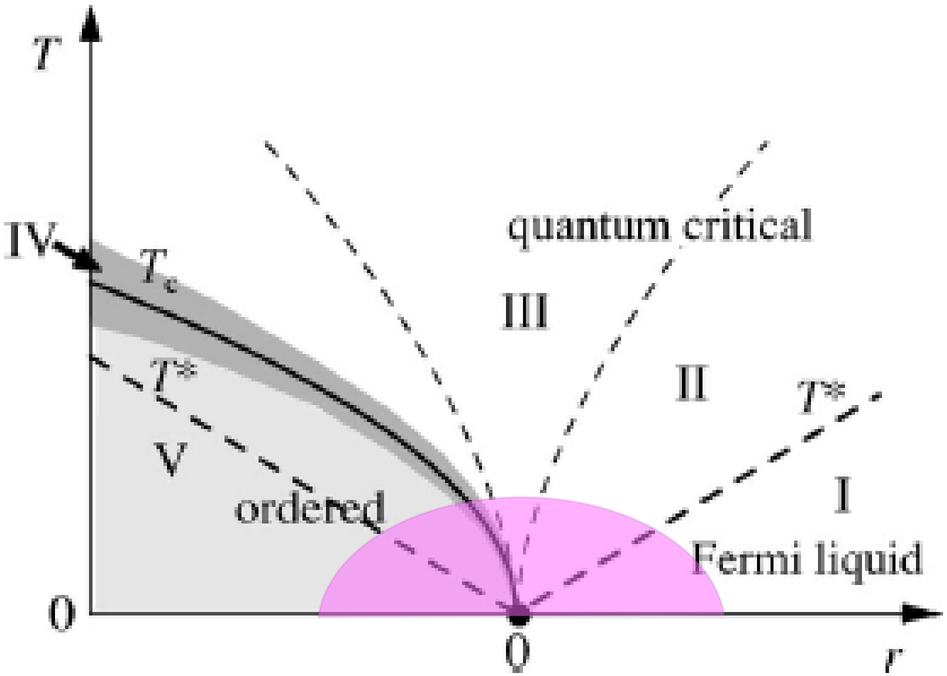
Popular belief of paradigm :

-- *Strong correlation* → *QCP (?)*

→ *NFL normal state*

→ *Un-conventional SC (perhaps high-T_c)*

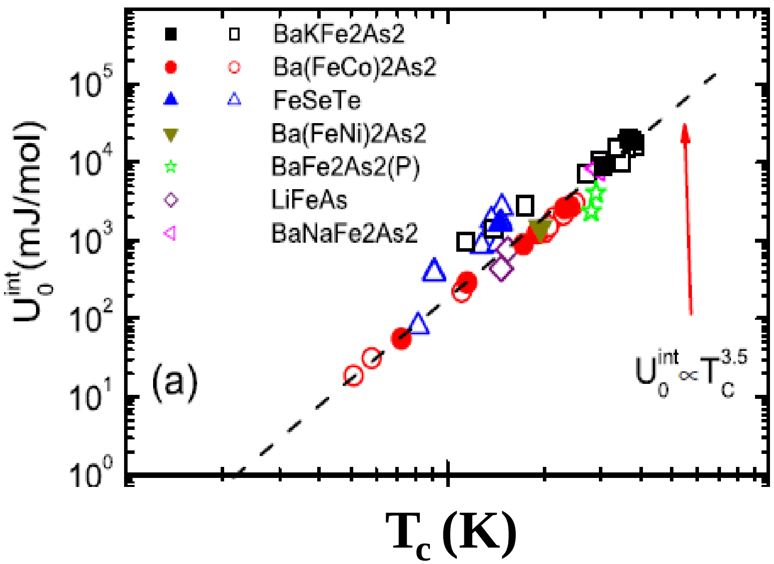
→ *Un-conventional pairing mechanism* ***(non-BCS type ?)***



Thermodynamic Evidences for Unconventional Superconductivity of IBS.

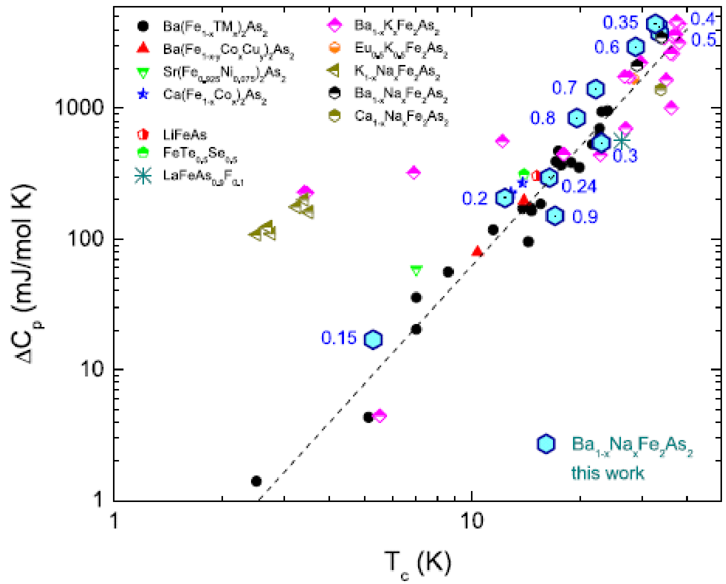
Two anomalous (non-BCS) scaling behaviors in IBS : ΔC *vs.* T_c & ΔE *vs.* T_c

→ indication of non-BCS pairing mechanism.



HH Wen et al, PRB 89, 140503 (2014)

$$\Delta E \sim T_c^{3.5}$$



Bud'ko et al, PRB 79, 220516 (2009)

$$\Delta C \sim T_c^3$$

BNC scaling: $\Delta C \sim T_c^3$

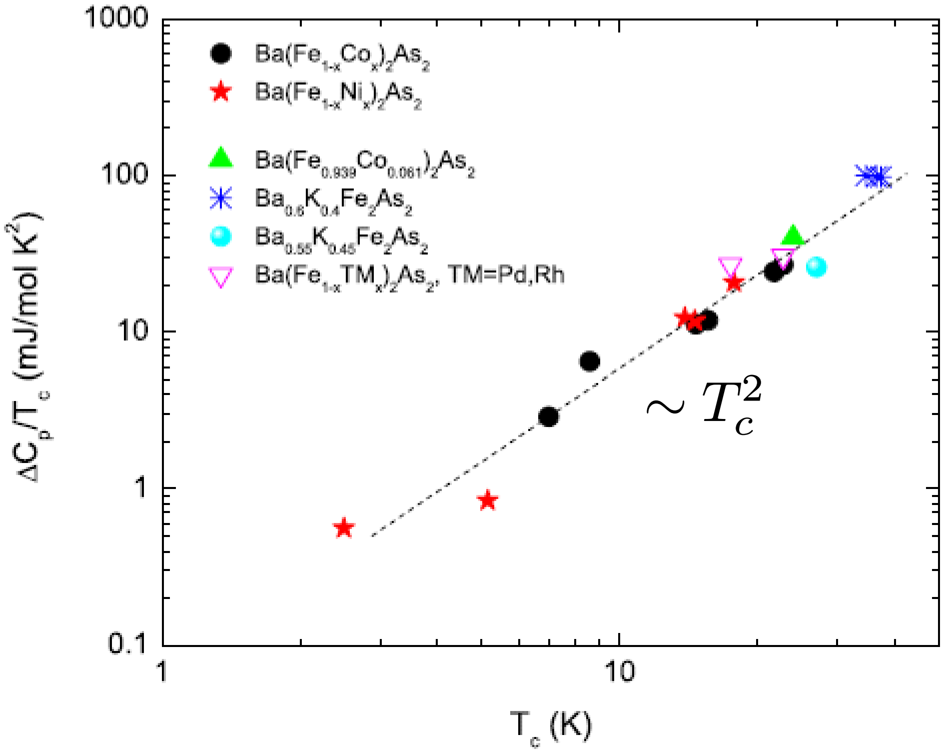
BNC scaling

Does it mean new physics (or at least Non-BCS pairing mechanism) ?

PHYSICAL REVIEW B **79**, 220516(R) (2009)

Jump in specific heat at the superconducting transition temperature in $Ba(Fe_{1-x}Co_x)_2As_2$ and $Ba(Fe_{1-x}Ni_x)_2As_2$ single crystals

Sergey L. Bud'ko, Ni Ni, and Paul C. Canfield



$\Delta C/T_c \sim T_c^2$

or $(\Delta C \sim T_c^3)$

BCS theory

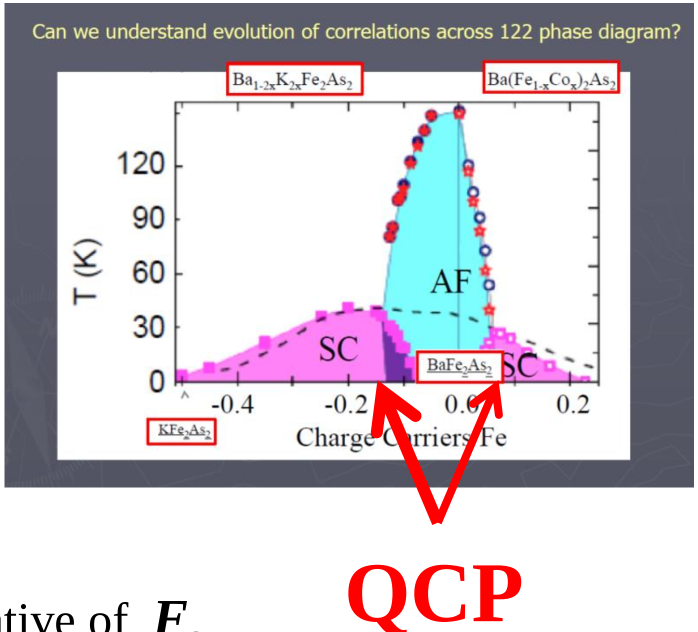
$\Delta C/T_c \sim 1.43\gamma$

(1) Zaanen claimed *(prb 80, 212502 (2009):*
ΔC ~ T_c^3 is a reflection of **C_{normal} ~ T^3**

QCP ➔ critical fluctuations is the main contribution to C(T)

Hyperscaling assumption →

$$F_s = -\rho_0\left(\frac{T}{T_0}\right)^{(d+z)/z} f\left[\frac{r}{(T/T_0)^{y_r/z)}}\right],$$



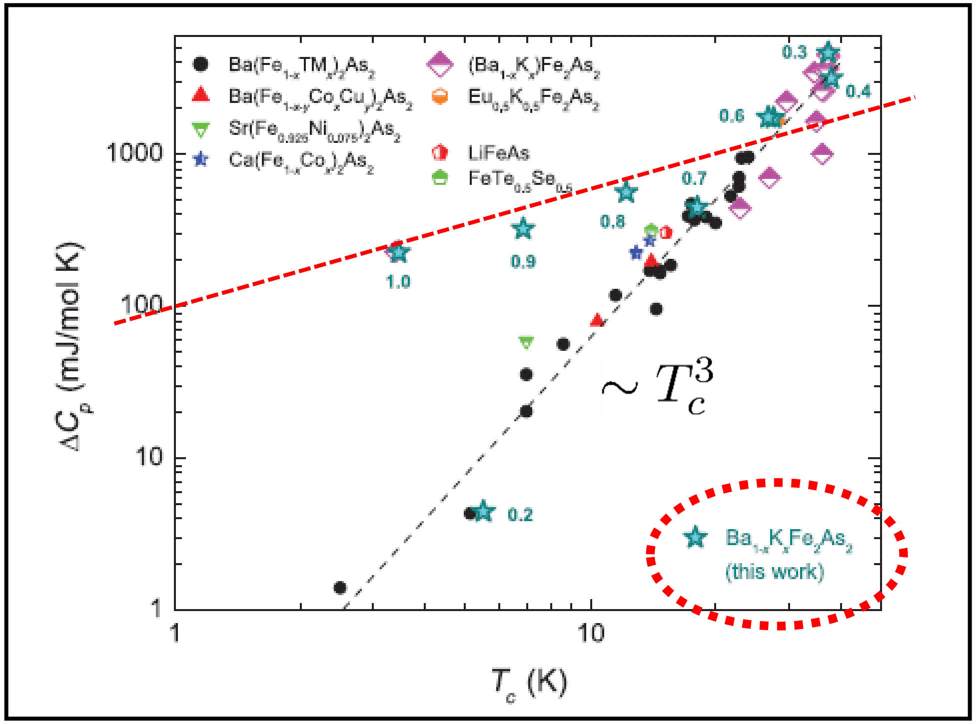
$$C_p = A_{cr}\left(\frac{T}{T_0}\right)^{d/z},$$

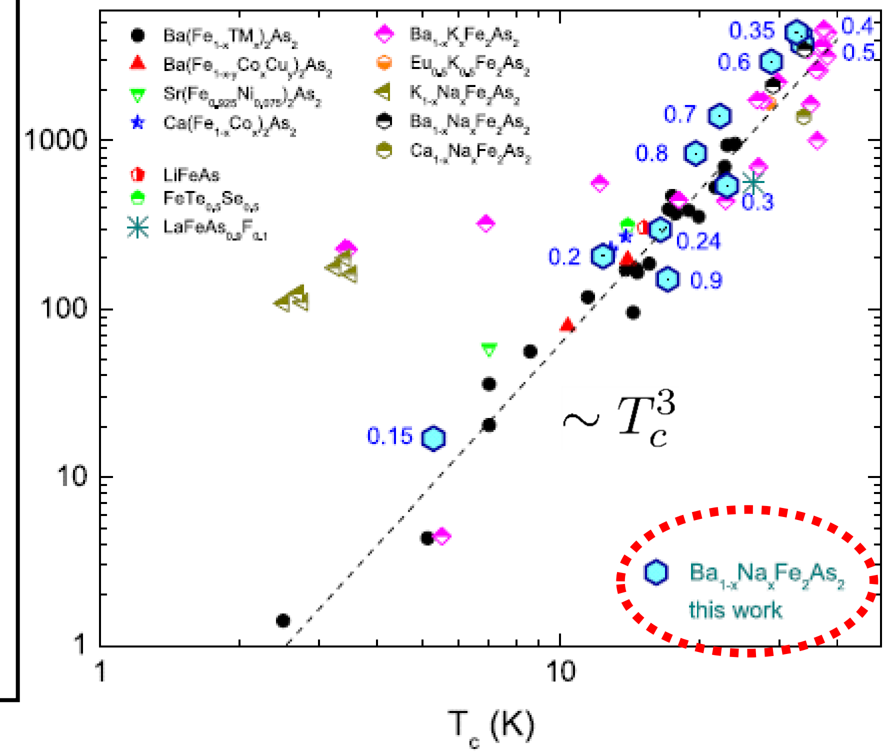
from 2nd derivative of ***F_s***

therefore, C$\sim T^3$ if $z = 1$ for $d = 3$.

Z=1 means ***dim(ω)=dim(q)*** : eg. AFM Spin wave
➔ No experimental evidence for ***ω ~ cq*** excitations over the whole doping range.

Some deviation exist, too. e.g. (Ba,**K**)Fe_2As_2





Contrast between two hole doped Ba(K,Na)Fe_2As_2

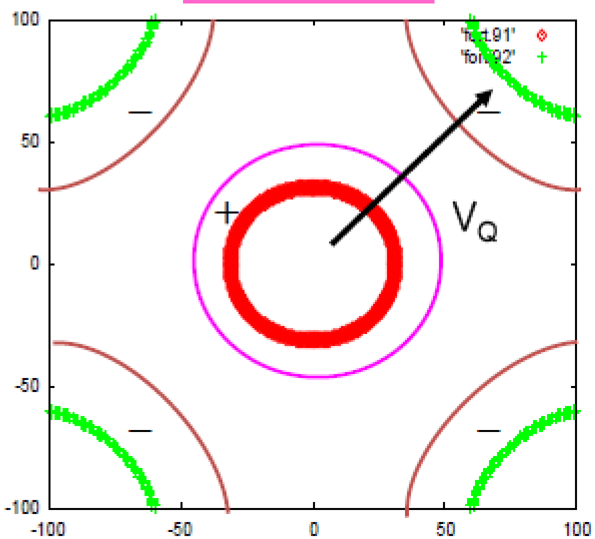
Na_imp stronger than **K_imp**

Our Theory of ΔC : A **hint** from multi band theory

$$\Delta C = N_h(0)\left(\frac{-d\Delta_h^2}{dT}\right)\bigg|_{T_c} + N_e(0)\left(\frac{-d\Delta_e^2}{dT}\right)\bigg|_{T_c}$$

$$\frac{\Delta_h}{\Delta_e} \sim \sqrt{\frac{N_e}{N_h}} \quad \text{as } T \to T_c,$$

±S-wave



Two band SC mediated by
$V_{inter\text{-}band} >> V_{intra\text{-}band}$

One band BCS theory

$$\Delta C = N(0)\left(\frac{-d\Delta^2}{dT}\right)\Big|_{T_c}$$

$$\Delta^2_{BCS}(T) \approx (3.06)^2 T_c^2 (1 - T/T_c).$$

$$\Delta C/T_c \sim N_0$$

$$T_c = \omega_D \exp[\frac{-1}{VN(0)}]$$

Two band (BCS) model

$$\Delta C = \sum_{i=h,e} N_i(0)\left(\frac{-d\Delta_i^2}{dT}\right)\Big|_{T_c}$$

If $V_{inter} \gg V_{intra}$,

$$\Delta_h = -[V_{hh}N_h\chi_h]\Delta_h - [V_{he}N_e\chi_e]\Delta_e,$$
$$\Delta_e = -[V_{ee}N_e\chi_e]\Delta_e - [V_{eh}N_h\chi_h]\Delta_h,$$

$$\frac{\Delta_h}{\Delta_e} \sim \sqrt{\frac{N_e}{N_h}} \quad \text{as } T \to T_c,$$

$$T_c \approx 1.14\Lambda_{hi} \exp\left[-1/(V_{inter}\sqrt{N_e N_h})\right].$$

$$\frac{\Delta C}{T_c} \approx 4 \times (3.06)^2 N_{tot} \cdot (\bar{N}_h \bar{N}_e).$$

$$N_{tot} = N_h + N_e \; ; \; \bar{N}_{h,e} = \frac{N_{h,e}}{N_{tot}}$$

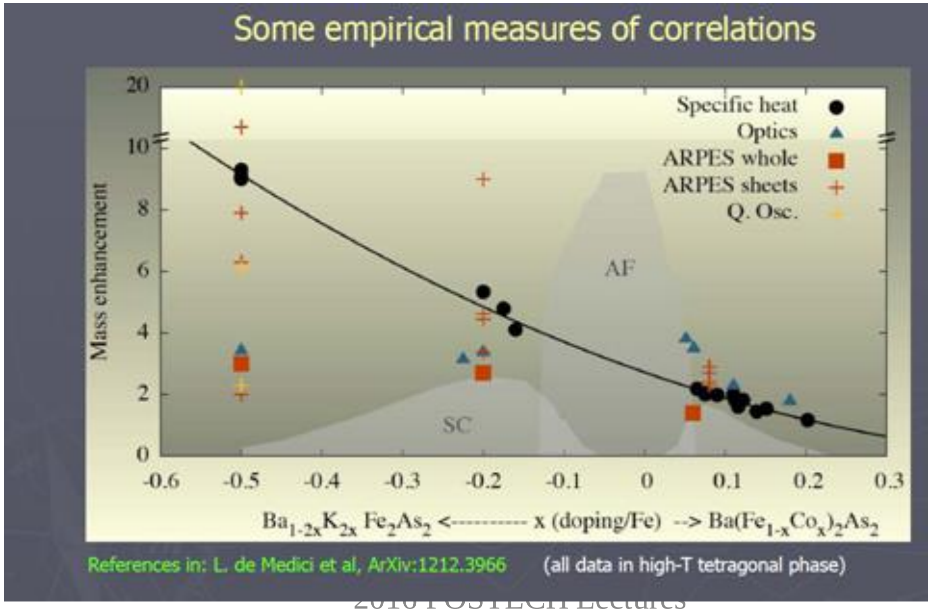
$\Delta C/T_c$ can strongly vary even with $N_{tot} = const.$

Our Model

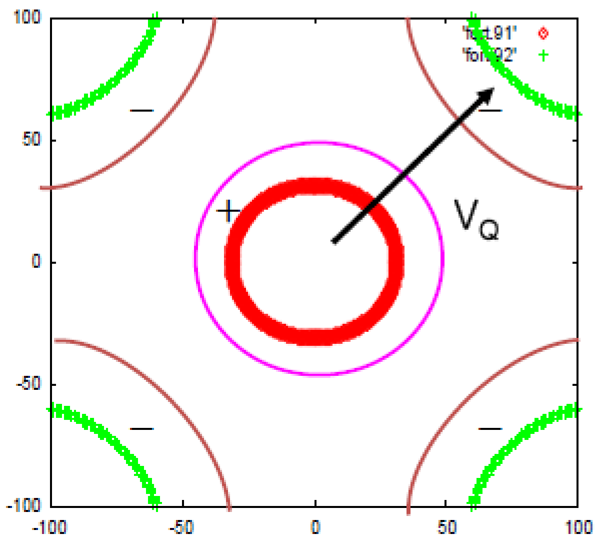
(1) **Two band BCS SC +**

(2) **Doping assumption $N_{tot} = N_h + N_e = const.$**

"N_{tot} =const." can be relaxed.



(1) Minimal Two Band model => ±S gap solution



Pairing interaction

$$V(k,k') = V_M \frac{\kappa^2}{|(\vec{k}-\vec{k}') - \vec{Q}|^2 + \kappa^2}$$

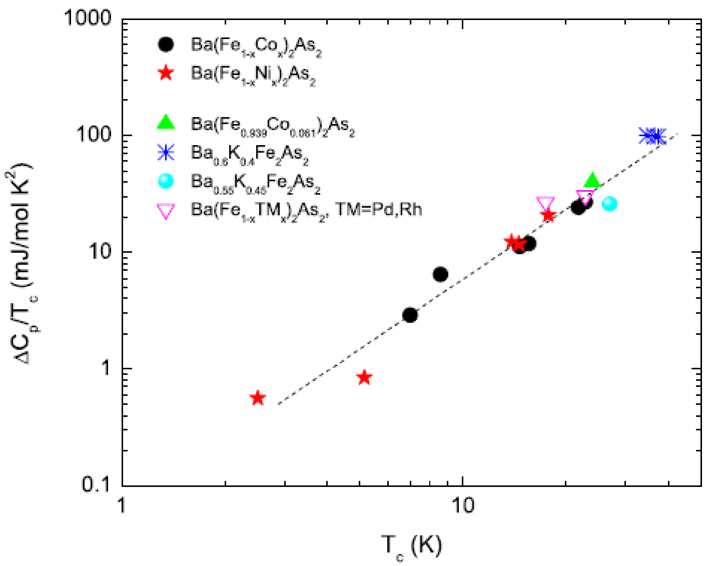
All repulsive **V_{ab} >0**

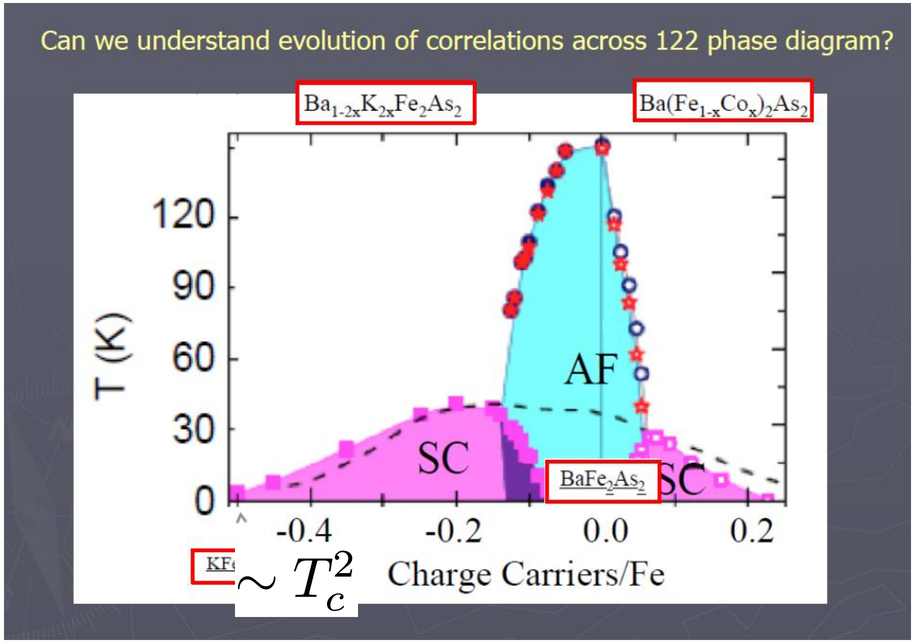
$V_{inter\text{-}band}$ > $V_{intra\text{-}band}$

Coupled Gap Eq.

$$\begin{aligned}
\Delta_h(k) &= \qquad (5)\\
&- \sum_{k'} [V_{hh}(k,k')\Delta_h(k')\chi_h(k') + V_{he}(k,k')\Delta_e(k')\chi_e(k')],\\
\Delta_e(k) &= \\
&- \sum_{k'} [V_{eh}(k,k')\Delta_h(k')\chi_h(k') + V_{ee}(k,k')\Delta_e(k')\chi_e(k')]. \qquad (6)
\end{aligned}$$

(2) Modeling of Doping



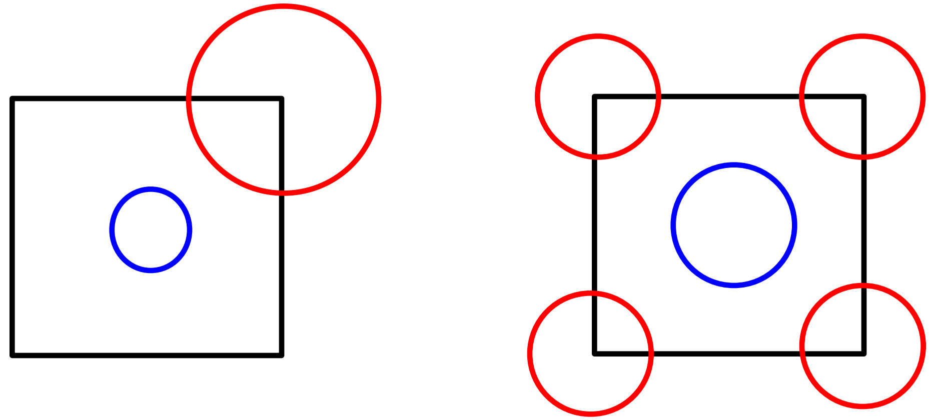


undoped **$BaFe_2As_2$** : compensated metal

→ **hole carriers = electron carriers**

($N_h \approx N_e$)

(2) Modeling of Doping: Rigid band model

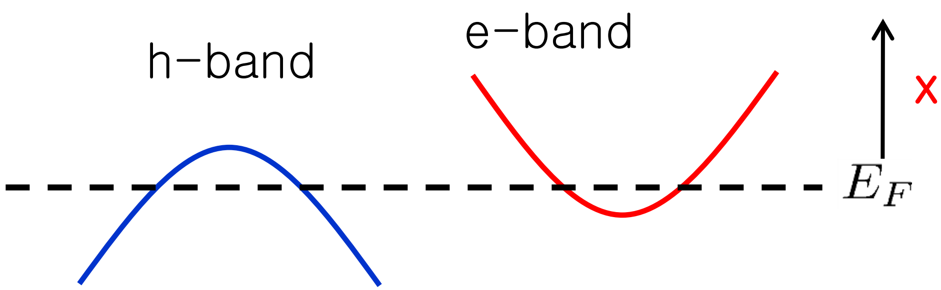


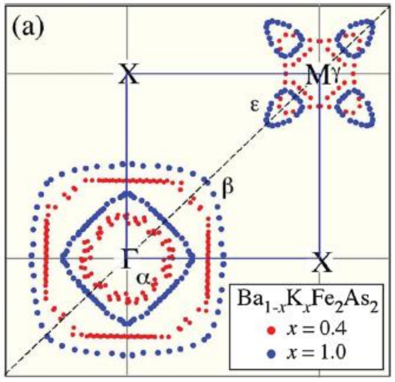
Elec. doping
$N_h < N_e$

No doping
$N_h \approx N_e$

hole doping
$N_h > N_e$

With doping, the FS size, $N_{h,e}$ (=$N_{tot} - N_{e,h}$) changes, but keeping $N_{tot} = N_h + N_e$ =const.





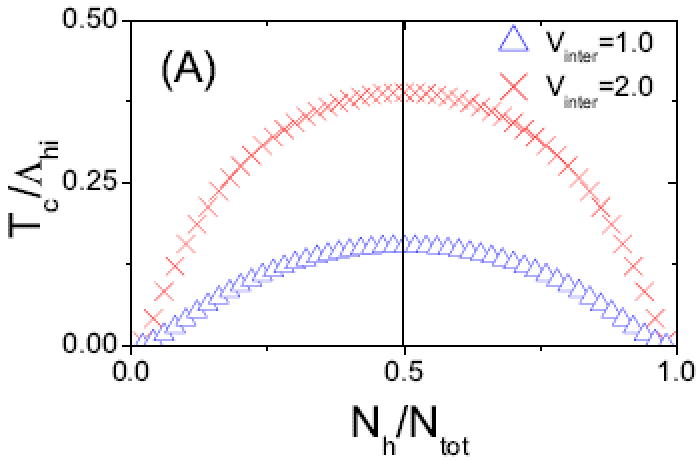
Sato et al., PRL 103, 047002 (2009)

Co, Ni doping → electron doping
K, Na doping → hole doping

Results

$$\Delta_h(k) = \qquad (5)$$
$$- \sum_{k'} [V_{hh}(k,k')\Delta_h(k')\chi_h(k') + V_{he}(k,k')\Delta_e(k')\chi_e(k')],$$
$$\Delta_e(k) =$$
$$- \sum_{k'} [V_{eh}(k,k')\Delta_h(k')\chi_h(k') + V_{ee}(k,k')\Delta_e(k')\chi_e(k')]. \qquad (6)$$

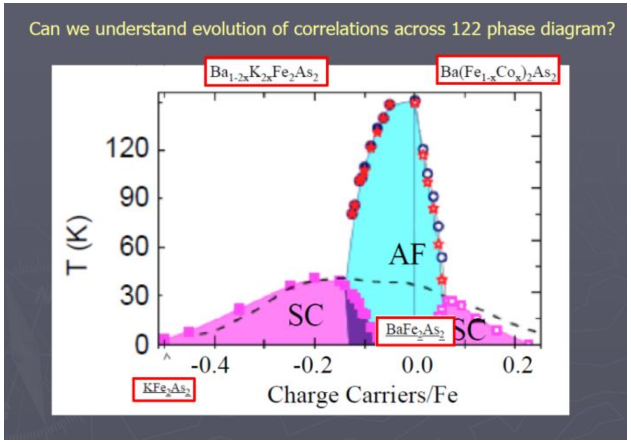
Calculations of T_c with varying N_h



Pairing interaction

$$\bar{V}^{eff}_{inter} = \bar{V}_{inter}\bar{N}_h\bar{N}_e$$
$$\bar{V}^{eff}_{intra} = \bar{V}_{intra}\bar{N}_{h,e}$$

V_{eff} varies strongly with doping.



$$0 < \bar{N}_{h,e}(x) < 1$$

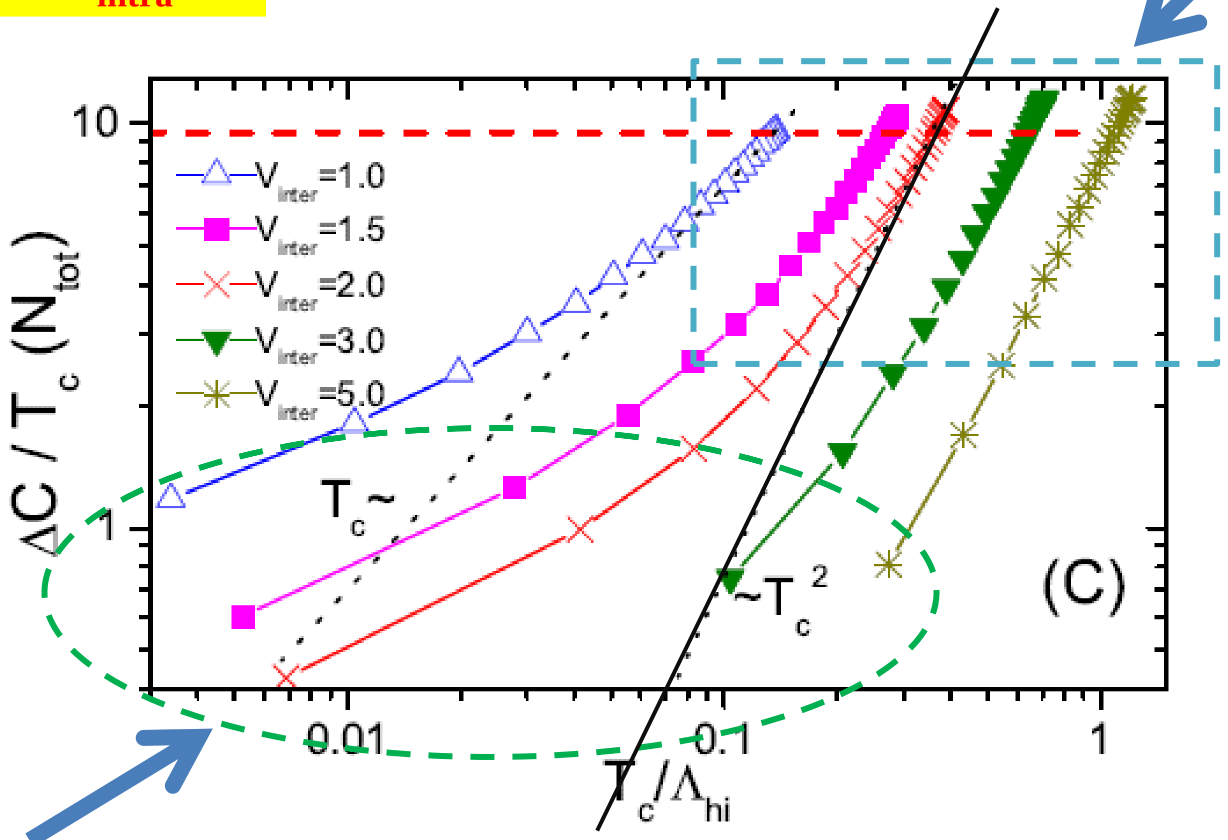
Simple model captures the Dome -shape T_c phase diagram for whole doping range.

Calculation of ΔC & T_c with doping N_h

$$\Delta C = \sum_{i=h,e} N_i(0)\left(\frac{-d\Delta_i^2}{dT}\right)\Big|_{T_c}$$

1. Increasing V_{inter}, better fit the BNC scaling.
2. Near max. T_{max} ($N_h \approx N_e$), best fit the BNC scaling.

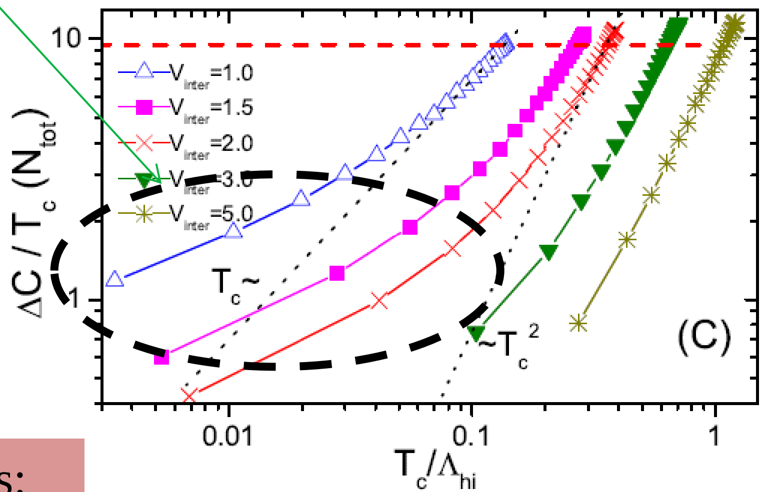
Results with V_{intra}=0:



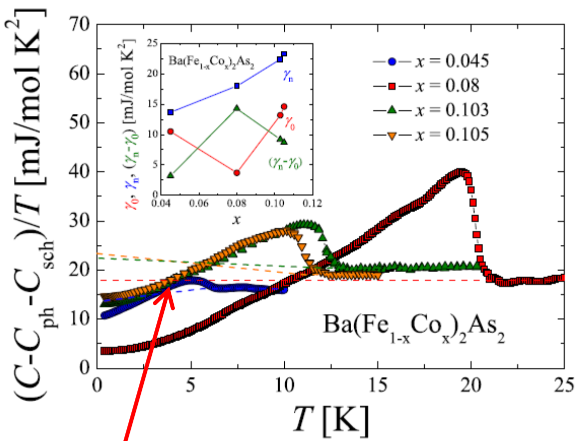
Some deviation. How to cure ?

Calculation of ΔC including impurity:

Region most deviated from BNC scaling is the region most sensitive to impurity scattering due to a small gap ($\Delta_{h,e} \ll \Delta_{e,h}$)



Gofryk et al. PRB 81 2010



Imp. Effects:

$$\Delta C = \sum_{i=h,e} N_i \left(\frac{-d\Delta_i^2}{dT}\right) \int dx \left[\frac{1}{\cosh^2(\frac{x}{2})}\right] \frac{x^2}{x^2 + (\frac{\Gamma_{tot}}{T_c})^2}.$$

Skalski et al., 136, A1500 (1957)

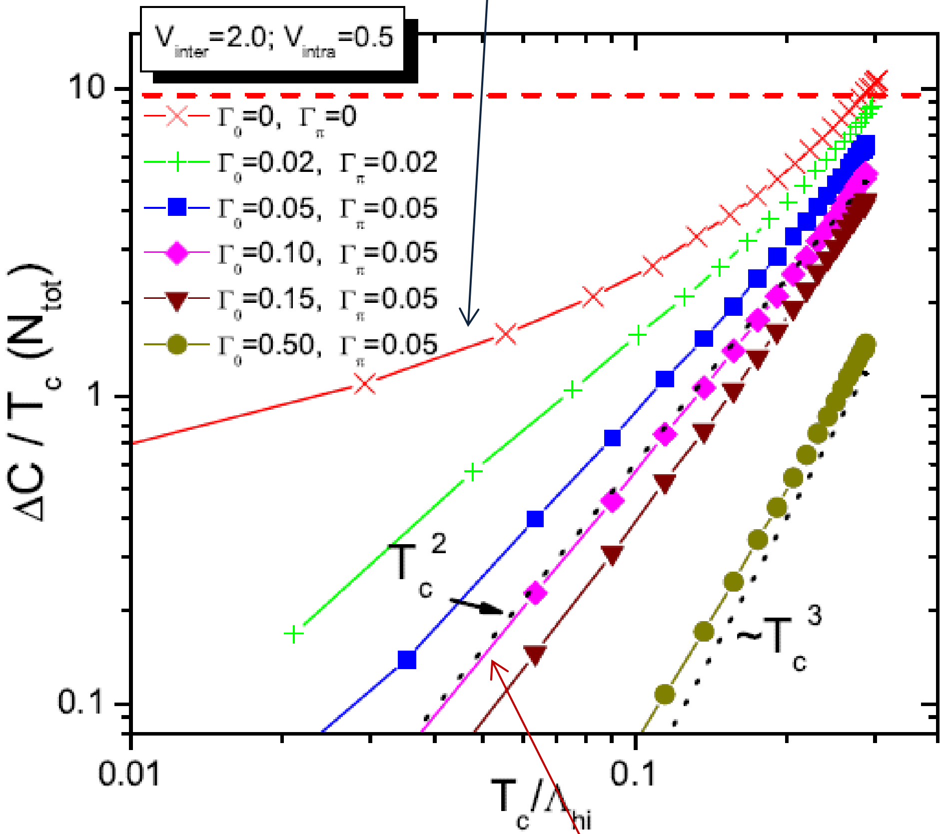
$$\Gamma_{tot} = \Gamma_0 + \Gamma_\pi$$ (**Non pair-breaking** + pair-breaking)

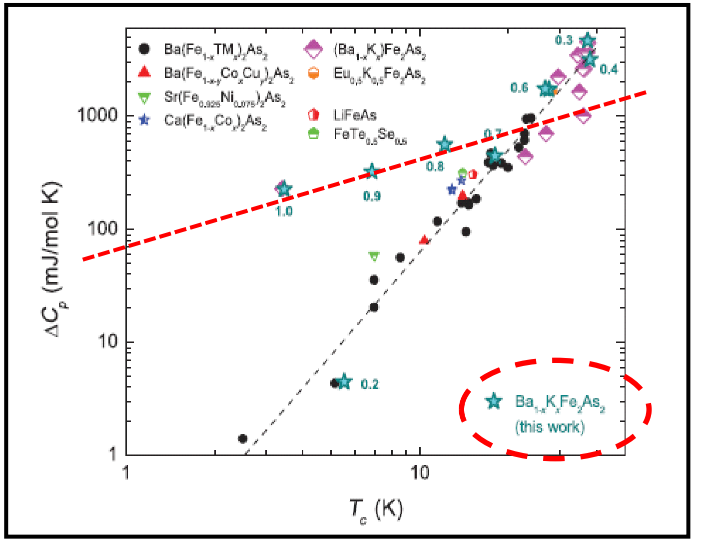
We choose $\Gamma_0 > \Gamma_\pi$ So, mainly q.p. damping

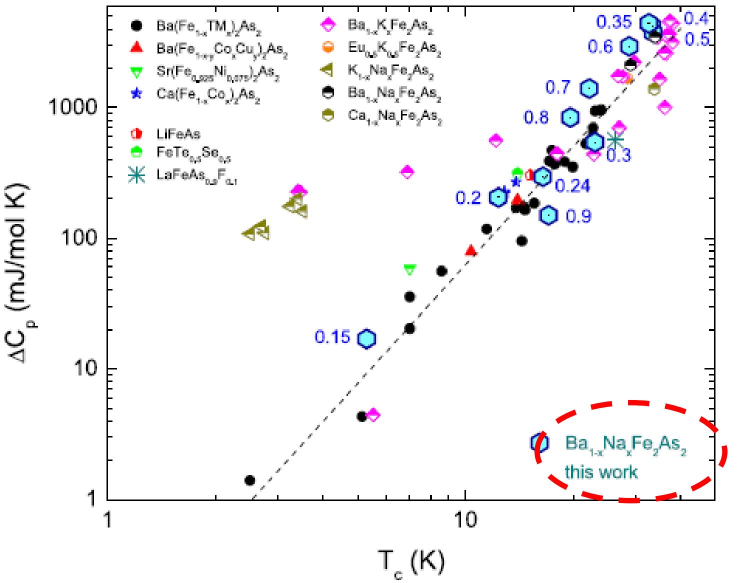
Results of ΔC including impurity:

Continuous evolution of the slope with imp.

Strong deviation. (clean limit)
$(BaK)Fe_2As_2$





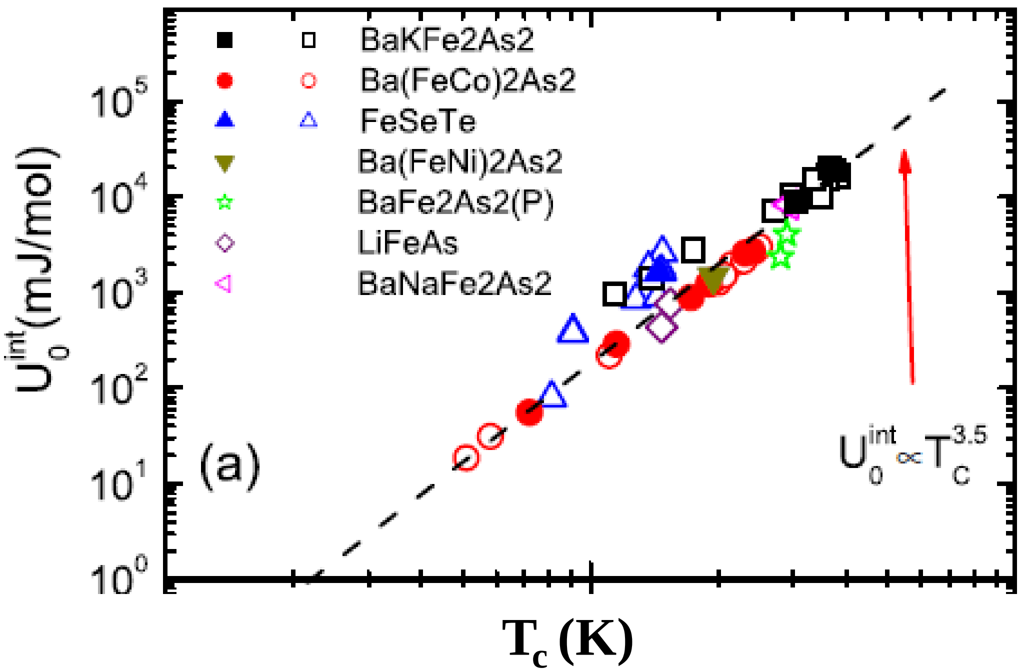


Perfect BNC scaling (non clean):
$(BaNa)Fe_22As_2$, $Ba(FeCo)_2As_2$

TECH Le

Condensation E: $\Delta E \sim T_c^{3.5}$

Condensation Energy : $\Delta E = E_n - E_{sc}$



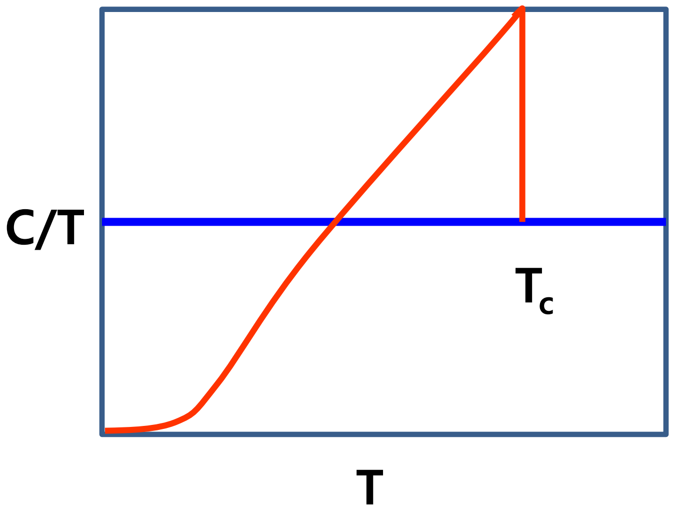
$\Delta E \sim T_c^{3.5}$

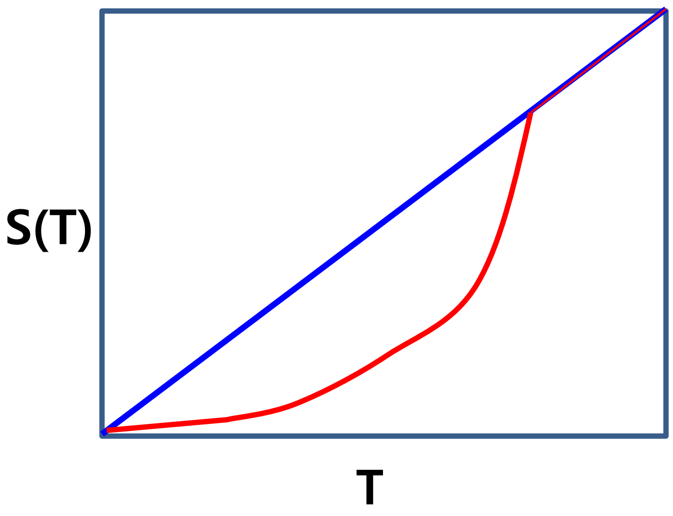
$\Delta E_{BCS} \sim T_c^2$

HH Wen et al, PRB 89, 140503 (2014)

Evidence of the Non-BCS pairing mechanism ?

Condensation Energy: $\Delta E_{cond} = E_{normal} - E_{sc}$





$$U_0^{\text{int}} = \int_0^{T_c} [S_n(T) - S_s(T)]dT$$
$$= \int_0^{T_c} dT \int_0^{T} [C_n(T') - C_s(T')]/T' dT'.$$

BCS calculations of $\mathbf{\Delta E_{cond}}$

$$\Delta E = < H >_s - < H >_n$$

$$\begin{aligned} H &= KE + PE \\ &= \sum_{k,\sigma} \xi(k) c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,l} V_{k,l} c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} c_{-l,\downarrow} c_{l,\uparrow} \end{aligned}$$

BCS theory

$$\Delta KE = [\frac{\Delta^2}{V} - \frac{1}{2} N(0) \Delta^2] > 0$$

$$\Delta PE = -\frac{\Delta^2}{V} < 0$$

$$\Delta E = -\frac{1}{2} N(0) \Delta^2 < 0$$

Subtle balance btw KE & PE

using $\Delta_{BCS} \approx T_c$.

$$\Delta E_{BCS} \sim T_c^2$$

HH Wen et al, PRB 89, 140503 (2014)

Condensation Energy of Two band BCS model

$$\begin{aligned} H &= \sum_{k\sigma} \varepsilon_h(k) h^{\dagger}_{k\sigma} h_{k\sigma} + \sum_{k\sigma} \varepsilon_e(k) e^{\dagger}_{k\sigma} e_{k\sigma} \\ &+ \sum_{kk'\uparrow\downarrow} V(k,k') h^{\dagger}_{k\uparrow} h^{\dagger}_{-k\downarrow} h_{k'\downarrow} h_{-k'\uparrow} \\ &+ \sum_{kk'\uparrow\downarrow} V(k,k') e^{\dagger}_{k\uparrow} e^{\dagger}_{-k\downarrow} e_{k'\downarrow} e_{-k'\uparrow} \\ &+ \sum_{kk'\uparrow\downarrow} V(k,k') h^{\dagger}_{k\uparrow} h^{\dagger}_{-k\downarrow} e_{k'\downarrow} e_{-k'\uparrow} \\ &+ \sum_{kk'\uparrow\downarrow} V(k,k') e^{\dagger}_{k\uparrow} e^{\dagger}_{-k\downarrow} h_{k'\downarrow} h_{-k'\uparrow} \end{aligned}$$

$$\begin{aligned} \Delta E &= < H >_s - < H >_n \\ &= \Delta KE + \Delta PE \end{aligned}$$

$$\Delta KE = \sum_k (|\xi_h(k)| - \frac{\xi_h^2(k)}{E_h(k)}) + \sum_k (|\xi_e(k)| - \frac{\xi_e^2(k)}{E_e(k)}),$$

$$\Delta PE = V_{he} b^{*h} b^e + V_{eh} b^{*e} b^h + V_{hh} b^{*h} b^h + V_{ee} b^{*e} b^e,$$

$$\begin{aligned} b_k^h &= < h_{k\uparrow} h_{-k\downarrow} > \\ b_k^e &= < e_{k\uparrow} e_{-k\downarrow} > \end{aligned}$$

with

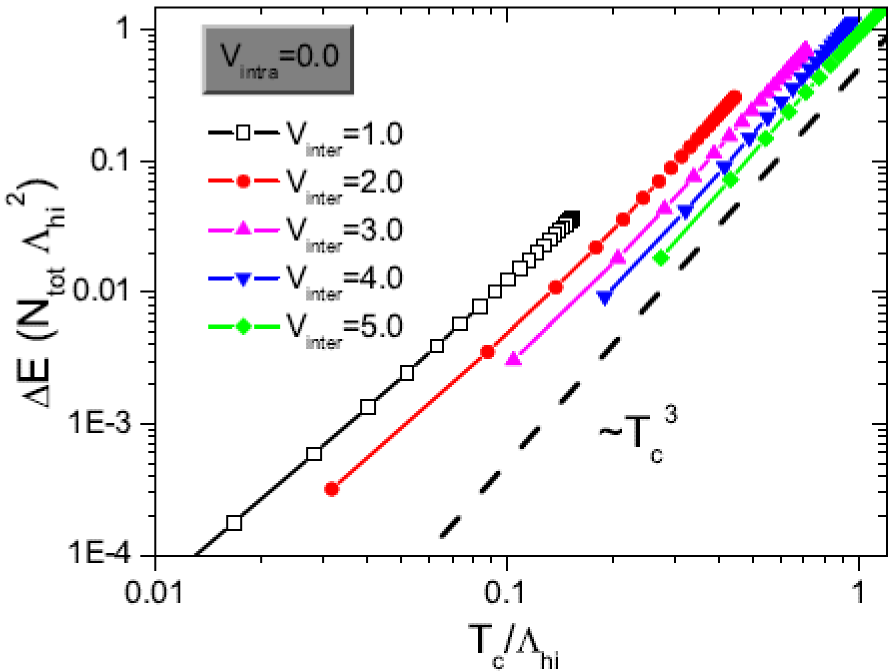
$$\begin{aligned} \Delta_h &= -\sum_k V_{hh} b_k^h - \sum_k V_{he} b_k^e \\ \Delta_e &= -\sum_k V_{eh} b_k^h - \sum_k V_{ee} b_k^e. \end{aligned}$$

$$V_{he} = V_{eh} = V_{inter};\ V_{ee} = V_{hh} = V_{intra}$$

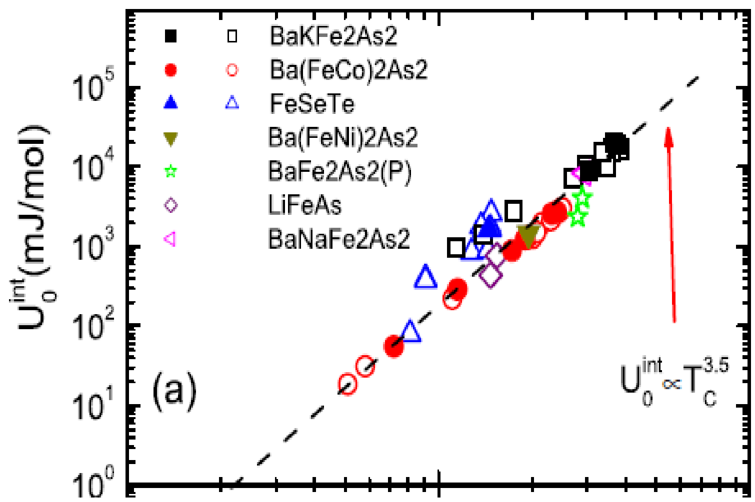
$$\Delta E = < H >_s - < H >_n \neq -\frac{1}{2} N_h \Delta_h^2 - \frac{1}{2} N_e \Delta_e^2$$

Calculation with V_{intra}=0

Calculations

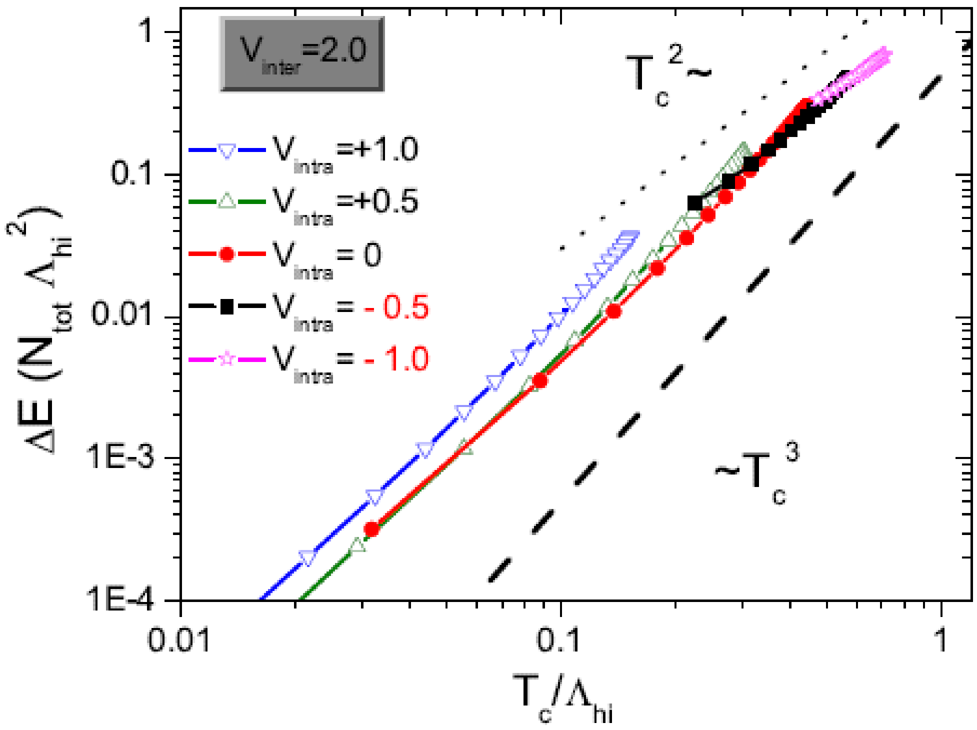


Experimental results



Genuine two band model (V_{intra}=0) follows $\Delta E \sim T_c^3$, but not $\sim T_c^{3.5}$

Effect of $V_{intra} \neq 0$



1. **Attractive V_{intra}** (<0) makes **ΔE** more BCS-like (**~T_c^2**)
2. **Repulsive V_{intra}** (>0) makes **ΔE** steeper (**~T_c^3**)

General Trend of the Scaling relations of ΔE *vs* T_c

1. Ising or Heinsenberg magnet (MFT): $\Delta E \sim T_c \sim O(J)$

→ **$\Delta KE = 0$** and **$\Delta E = \Delta PE$**

2. BCS SC: $\Delta E \sim T_c^2$

→ **$\Delta KE > 0$, $\Delta PE < 0$** and **$\Delta E = \Delta KE + \Delta PE$**

$$\begin{cases} \Delta KE = [\frac{\Delta^2}{V} - \frac{1}{2}N(0)\Delta^2] > 0 \\ \Delta PE = -\frac{\Delta^2}{V} < 0 \end{cases}$$

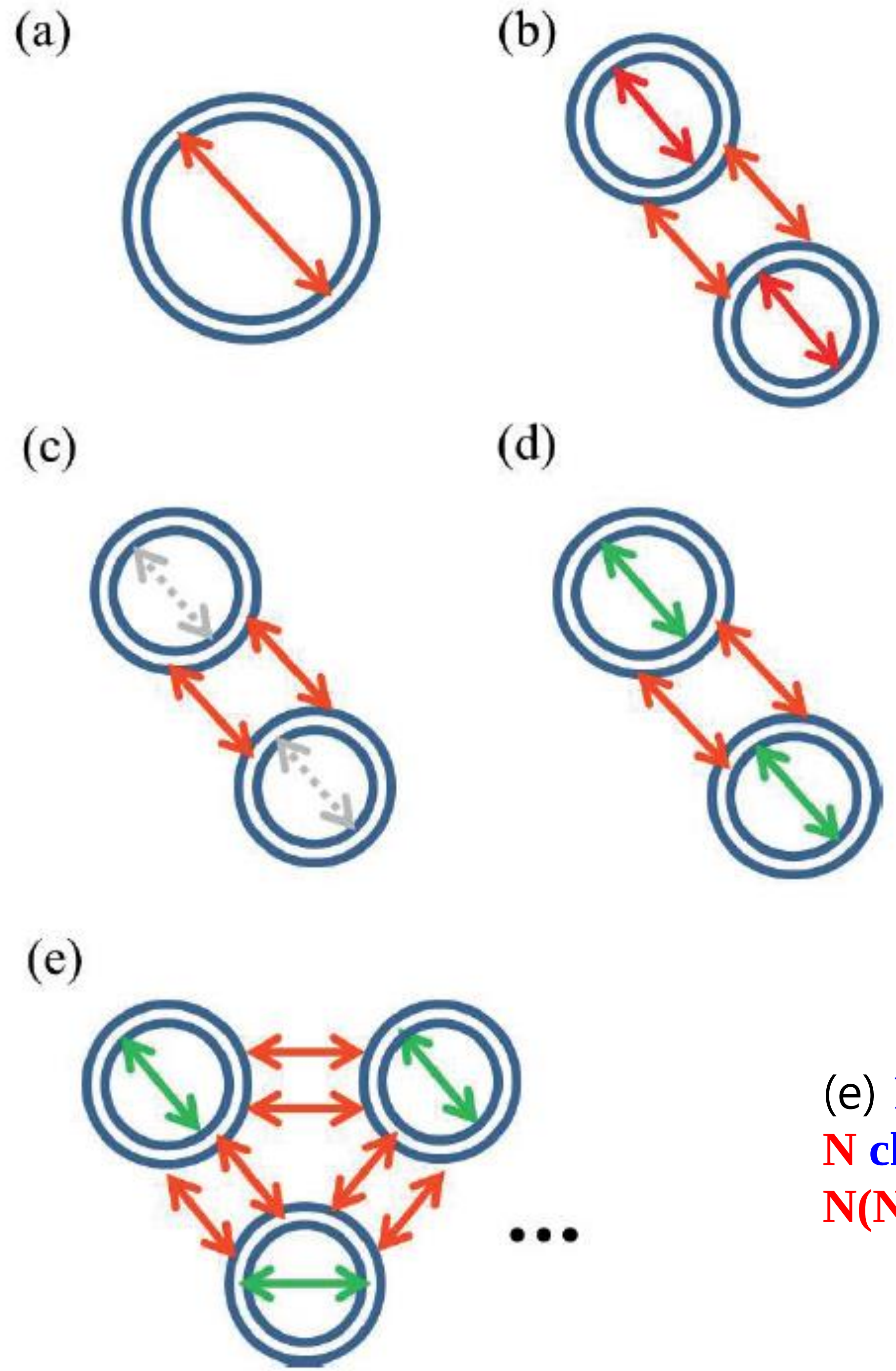
Speculation: $\Delta E \sim T_c^{\beta}$ (**$\beta > 2$**)

if **ΔKE loss >> ΔPE gain**

Indeed, this is the case for the multiband superconductor

→ **ΔPE gain** is not fully exploited.

$\beta = 2$



Single band BCS :

$\Delta KE_s > 0$

$\Delta PE_s < 0$

$\beta > 2$

(c) **$\Delta KE = \Delta KE_s$,**

$|\Delta PE| < |\Delta PE_s|$

(d) **$\Delta KE = \Delta KE_s$,**

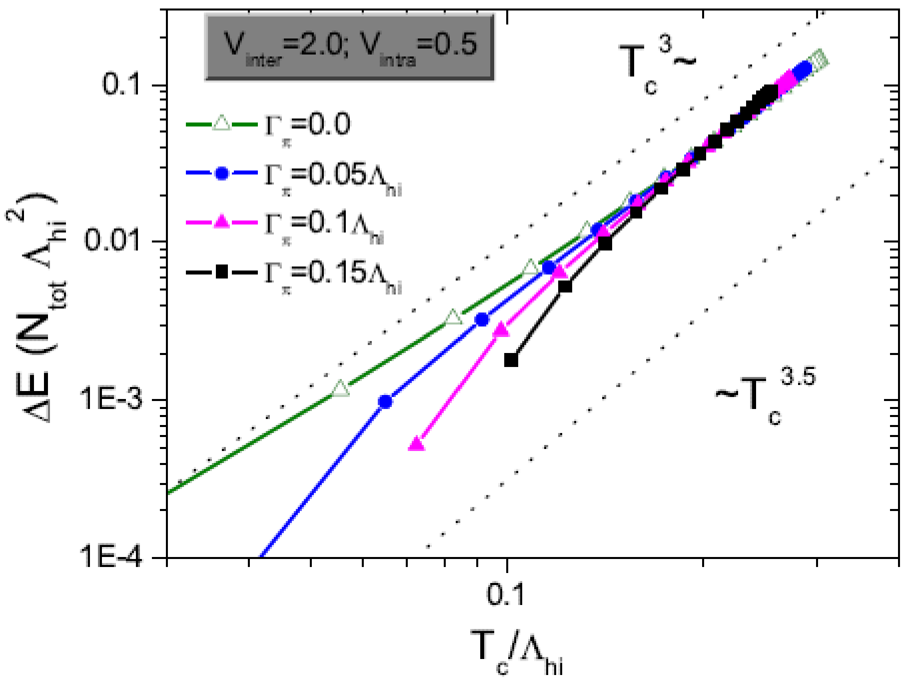
$|\Delta PE| << |\Delta PE_s|$

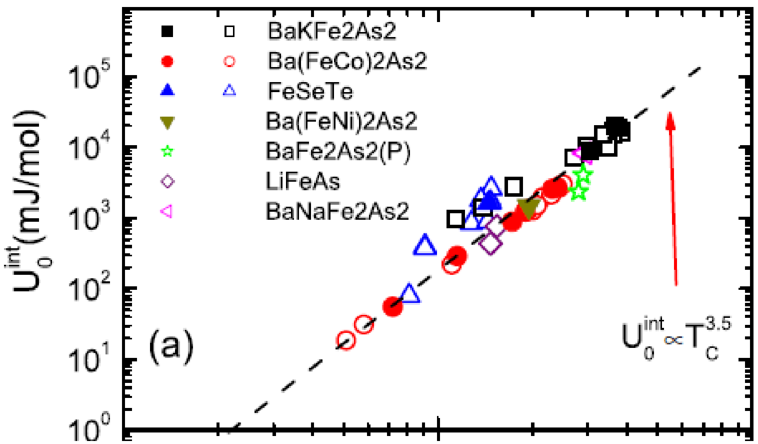
(e) **Reduces to a single band**

N channels of V_{inter}

N(N-1) channels of V_{intra}

Impurity scattering makes ΔE *vs.* T_c steeper.





because the imp effect suppresses more effectively $\Delta_{h,e}$ than T_c .

Conclusions:

1. **BCS theory of two band model** straightforwardly reproduces the anomalous power laws of $\boldsymbol{\Delta C}$ ***vs.*** $\boldsymbol{T_c}$ and $\boldsymbol{\Delta E}$ ***vs.*** $\boldsymbol{T_c}$ **.**

2. It is almost **impossible to invent any other theories** to explain these two scaling behaviors simultaneously.

2. **Strong Correlation Effects in Normal state do** exist in Fe-based SC compounds. And it renormalizes : pairing interactions (V_{inter}, V_{intra}), q.p. m^*, N_{ren}, etc

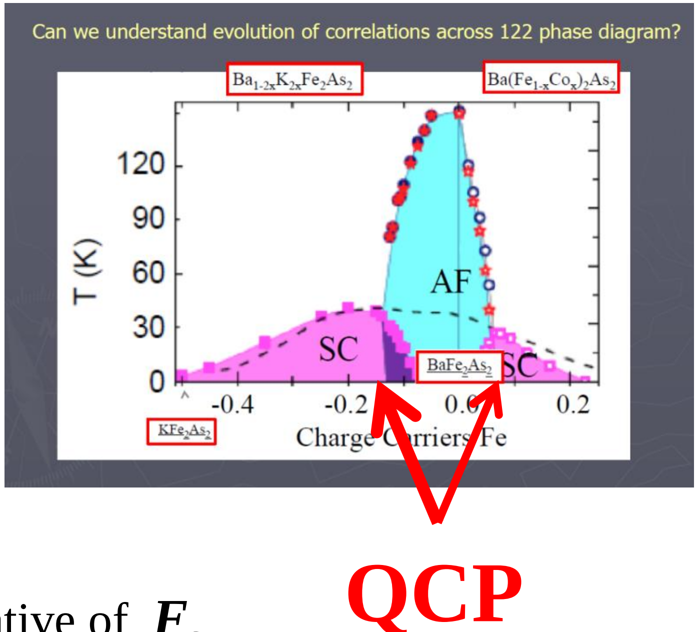
3. However, **the SC transition itself seems to follow the conventional BCS pairing mechanism**.

4. Shall we call them BCS SC ?

Previous theories to explain $\mathbf{\Delta C \sim T_c^3}$:
Kogan, Zaanen, and Chubukov et al.

(1) Zaanen claimed *(prb 80, 212502 (2009):*
ΔC ~ T_c^3 is a reflection of **C_{normal} ~ T^3**

QCP ➔ critical fluctuations is the main contribution to C(T)



Hyperscaling assumption →

$$F_s = -\rho_0 \left(\frac{T}{T_0} \right)^{(d+z)/z} f\left[\frac{r}{(T/T_0)^{y_r/z}} \right],$$

$$C_p = A_{cr} \left(\frac{T}{T_0} \right)^{d/z},$$

from 2nd derivative of ***F_s***

therefore, C~ T^3 if $z = 1$ for $d = 3.$

Z=1 means ***dim(ω)=dim(q)*** : eg. AFM Spin wave
➔ No experimental evidence for ***ω ~ cq*** excitations over the whole doping range.

(2) Kogan *PRB 81, 184528 (2010)*

: **$\Delta C \sim T_c^3$** is a general behavior of very dirt limit superconductors

if $\Gamma \gg T_c$

$$\Delta C = \frac{4\pi^4 k_B^4 N(0)\tau_m^2}{3\hbar^2} T_c^3,$$

However, we believe that this claim is based on the inconsistent approximation.

In BCS, if $\Gamma << T_c$ $\quad \Delta F \propto -N(0)\frac{\Delta^4}{T_c^2}$

$$\Delta_{BCS}^2(T) \approx T_c^2(1 - T/T_c).$$

$$\Delta C/T_c \propto \frac{\partial^2 \Delta F}{\partial T^2} \sim N(0)$$

Kogan's app, if $\Gamma >> T_c$ $\quad \Delta F \propto -N(0)\frac{\Delta^4}{\Gamma^2}$

$$\Delta_{BCS}^2(T) \approx T_c^2(1 - T/T_c).$$

$$\Delta C = \frac{4\pi^4 k_B^4 N(0)\tau_m^2}{3\hbar^2} T_c^3,$$

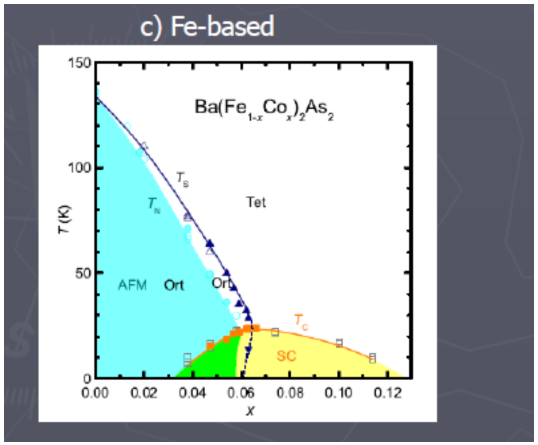
Correct app, for $\Gamma >> T_c$ $\quad \Delta F \propto -N(0)\frac{\Delta^4}{\Gamma^2}$

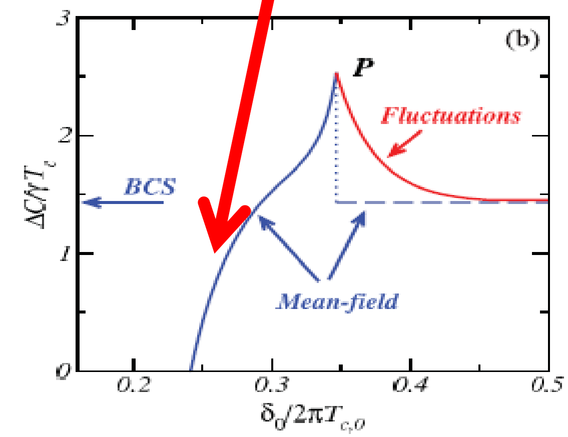
$$\Delta_{dirty}^2(T) \approx \Gamma^2(1 - T/T_c).$$

$$\Delta C/T_c \propto \frac{\partial^2 \Delta F}{\partial T^2} \sim N(0)\frac{\Gamma^2}{T_c^2}$$

(3) Chubukov+coworkers *(PRB 84, 140502 (2011))* focused only on SDW+SC region.

Simply showed that *when SDW order **M** develops, **ΔC** steeply decreases.*





$$\frac{\mathcal{F}(\Delta, M_0)}{N_F} = \frac{\mathcal{F}_0}{N_F} + \alpha_\Delta(M_0, T)\Delta^2 + \eta(M_0, T)\Delta^4,$$

Solved coupled gap Eq with $\mathbf{M}_{\mathbf{AFM}}$ & $\boldsymbol{\Delta}_{\mathbf{sc}}$

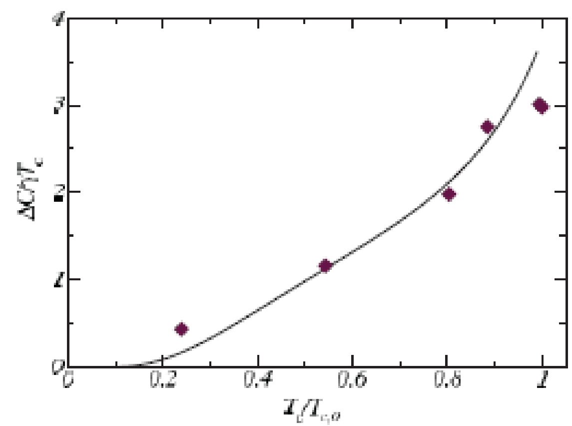


FIG. 4. (Color online) A comparison between the calculated $\Delta C/T_c$ and the experimental data from Ref. 4 for $Ba(Fe_{0.925}Co_{0.075})_2As_2$ for dopings below the optimal one. We used $T_{m,0}/T_{c,0} = 1.45$ and $\delta_2/2\pi T_{c,0} = 0.174$.

Probably, not very wrong, but not much information

One band BCS theory

$$\Delta C = N(0)\left(\frac{-d\Delta^2}{dT}\right)\Big|_{T_c}$$

$$\Delta^2_{BCS}(T) \approx (3.06)^2 T_c^2 (1 - T/T_c).$$

$$\Delta C/T_c \sim N_0$$

$$T_c = \omega_D \exp[\tfrac{-1}{VN(0)}]$$

Two band (BCS) model

$$\Delta C = \sum_{i=h,e} N_i(0)\left(\frac{-d\Delta_i^2}{dT}\right)\Big|_{T_c}$$

If $V_{inter} \gg V_{intra}$,

$$\begin{aligned}\Delta_h &= -[V_{hh}N_h\chi_h]\Delta_h - [V_{he}N_e\chi_e]\Delta_e,\\ \Delta_e &= -[V_{ee}N_e\chi_e]\Delta_e - [V_{eh}N_h\chi_h]\Delta_h,\end{aligned}$$

$$\frac{\Delta_h}{\Delta_e} \sim \sqrt{\frac{N_e}{N_h}} \quad \text{as } T \to T_c,$$

$$T_c \approx 1.14\Lambda_{hi} \exp\left[-1/(V_{inter}\sqrt{N_e N_h})\right].$$

$$\frac{\Delta C}{T_c} \approx 4 \times (3.06)^2 N_{tot} \cdot (\bar{N}_h \bar{N}_e).$$

$$N_{tot} = N_h + N_e \ ; \ \bar{N}_{h,e} = \frac{N_{h,e}}{N_{tot}}$$

$\Delta C/T_c$, T_c can strongly vary even with $N_{tot} = const.$