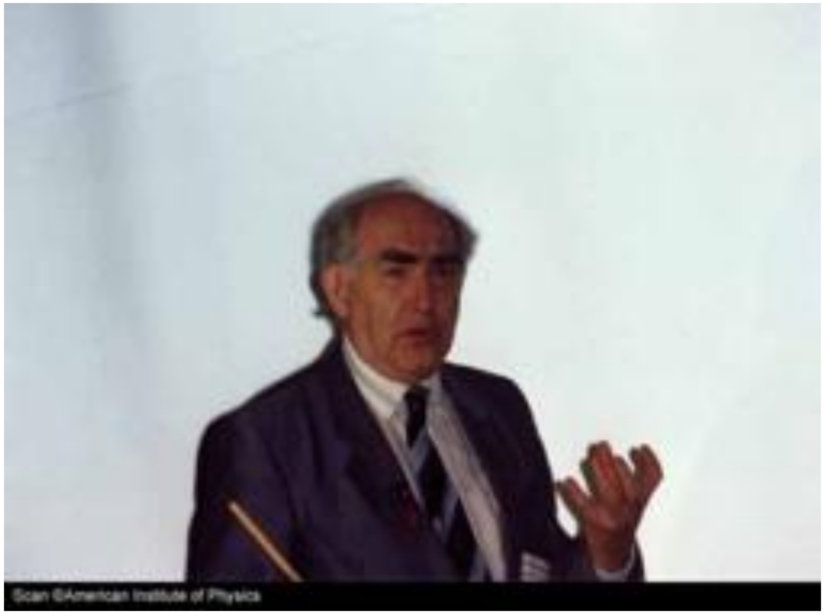
Pairing in Cuprates and Fe-based Superconductors: is it so simple as it is claimed - EPI vs Coulomb pairing mechanism?

M. L. Kulic,

Goethe University Frankfurt/Main, Germany

This talk is devoted to our unforgetable teachers and friends ***Vitalii Lazarevich Ginzburg*** and ***Evgenii Grigorievich Maksimov***



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OUTLINE

1. *HTSC in cuprates and Fe-based*

1986 : cuprates SC - $T_c \approx 100$ K ($YBa_2Cu_3O_7$) ⇒ single-band metal Fermi surface

$$\text{d-wave pairing} \Rightarrow \Delta_{d_{x^2-y^2}}(\boldsymbol{k},\omega) \approx \Delta^0(\omega)(\cos k_x - \cos k_y)$$

2008 : Fe-based SC - $T_c \le 55$ K ($SmFeAsO_{1-x}F_x$) ⇒ multi-band metal Fermi surface $i = 1, 2...$

$$s_{++}\text{- or } s_{\pm}\text{- and d-wave pairing} \Rightarrow \Delta_1(\boldsymbol{k},\omega) = \pm\Delta_2(\boldsymbol{k},\omega)\ ?$$

2. Phonon (EPI) vs spin-fluctuation (SFI) mechanism of pairing

- similarty of phase diagrams in cuprates and Fe-based SC
- DFT (band-structure) claims EPI is unimportant!? $\lambda_{ep}^{Fe} \approx 0.2$!?
- DFT fails to explain magnetism, phonons, ARPES .... in both compounds!
- ARPES, tunneling, phonon line-widths, neutron scttering make limits on EPI and SFI!

3. Challenge for the pairing theory

- EPI "dominates" in small-q; Coulomb in large-q scattering in cuprates and Fe-based SC?
- Why robustness *of SC in presence of* ***nonmagnetic*** *impurities* in both SC?

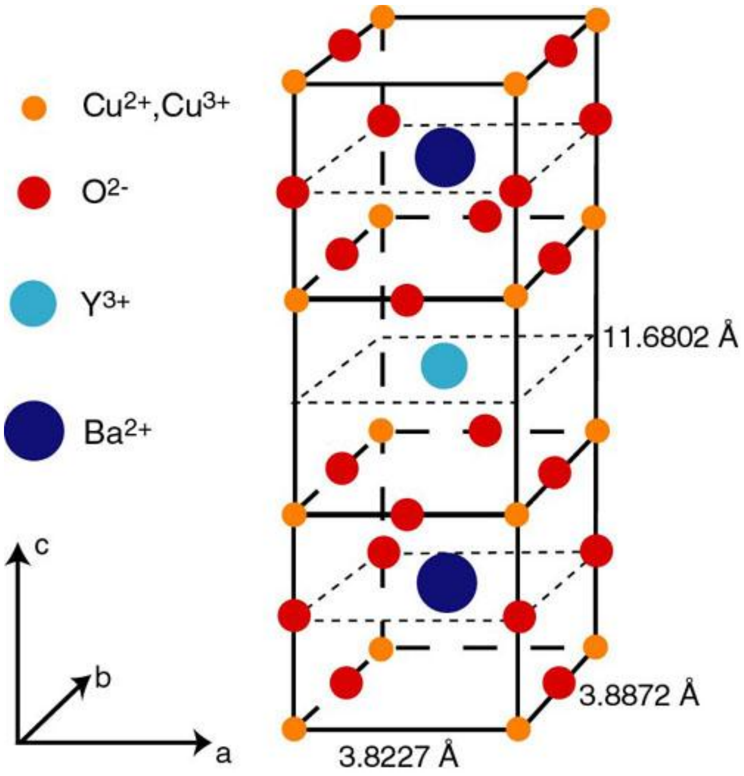
4. Conclusions

Pairing potential :
- **CUPRATES** ⇒ (small-q) phonons + Coulomb(large-q) ?
- **Fe-BASED** ⇒ equally?: phonons(intraband) + Coulomb(interband)

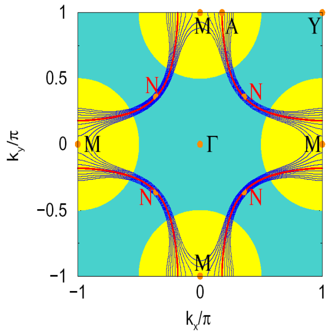
E. G. Maksimov, M.L.K., O. V. Dolgov, Advances Cond. Mat. Phys. (2010) - **B2**; (**M.L.K.** Phys.Rep. 338, p.1 (2000) - **B1**)

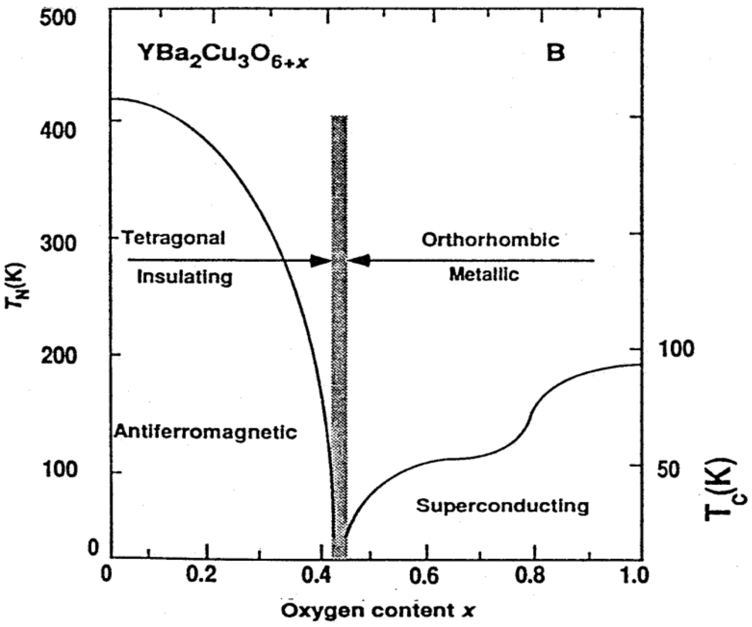
CUPRATES → YBCO – prototype of HTSC material

$YBa_2Cu_3O_7; T_c \approx 93$ K



one-band Fermi surface ⇒





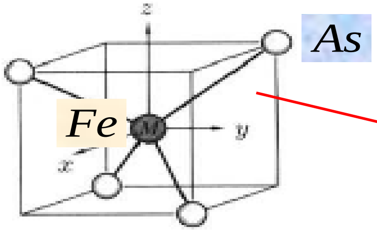
$YBa_2Cu_3O_{6+x}$ - **AF - order and Mott - insulator** due to strong correlations

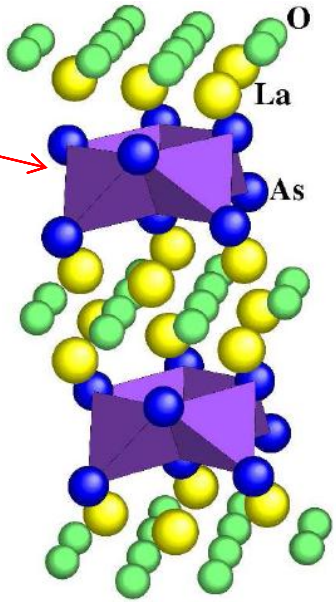
d-wave pairing ⇒ importance of magnetism for pairing?

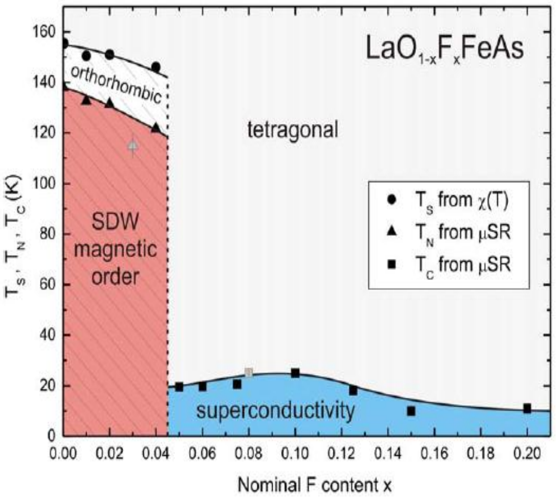
ionic - metallic structure ⇒ importance of phonons!

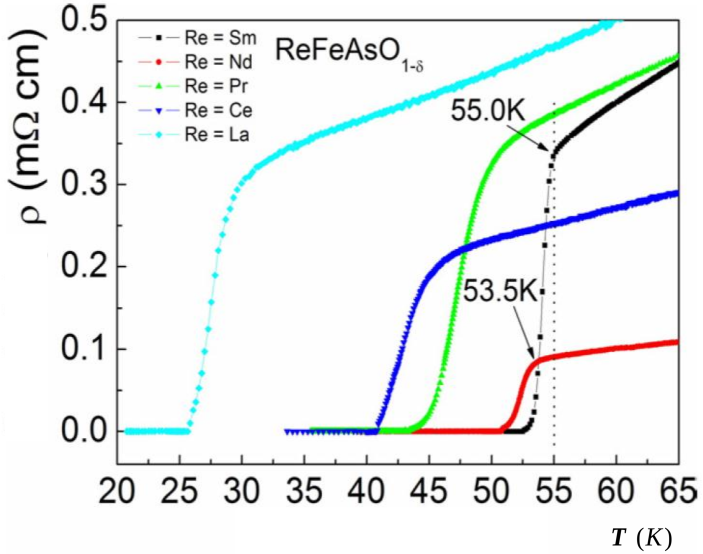
HTSC is due to phonons or Coulomb (spin - fluctuations) or both?

Fe-based superconductors → LaOFFeAs – prototype for ferro-pnictides



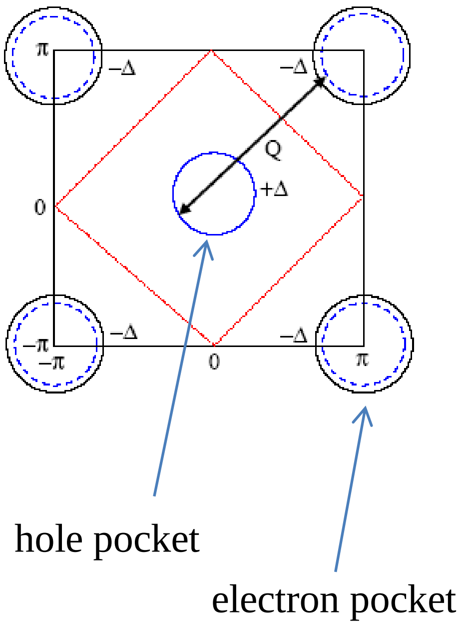






multi-band Fermi surface ⇒

$s_{\pm}$ - pairing?

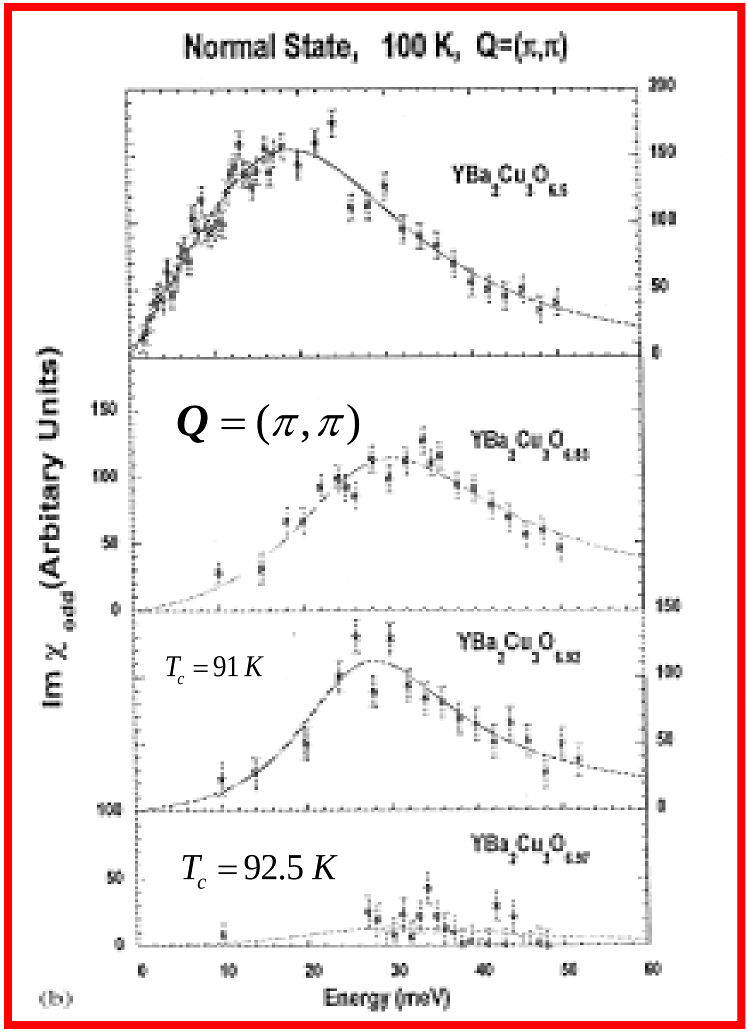


$\rho(T) = \rho_{imp} + \rho_1(T)$

$\rho_{imp} \approx 50-100\ \mu\Omega cm$ even in best ***single crystals*** !

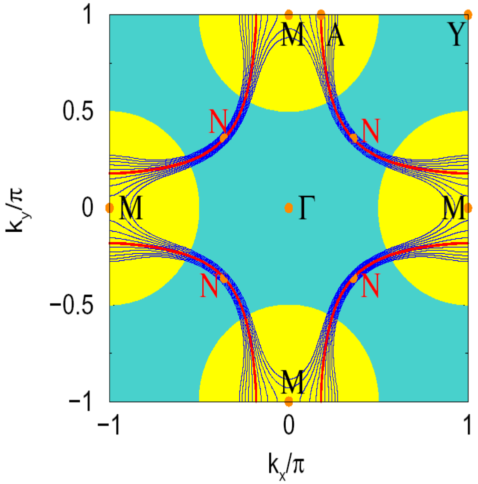
- **nonmagnetic impurities** (defects) **detrimental** for sign changing of $\Delta(\boldsymbol{k})$, like d-wave and $s_{\pm}$!?
- why is SC in Fe-based robust against the nonnagnetic impurities?

Inelastic magnetic neutron scattering against SFI mechanism



Big Change in $Im\chi$ but Small Change in T_c !

Ph. Bourges et al. (1999)



$$T_c \sim \langle \omega_{sf} \rangle \exp\{-1/\lambda_{sf}\}$$

$$\lambda_{sf} \sim g_{sf}^2 \int_0^{70-80\,meV} d\omega \frac{|\mathrm{Im}\,\chi(Q,\omega)|}{\omega} \Rightarrow T_c \text{ small !}$$

SFI-theory assumes too large $g_{sf} = (0.7 - 1)\ eV$!

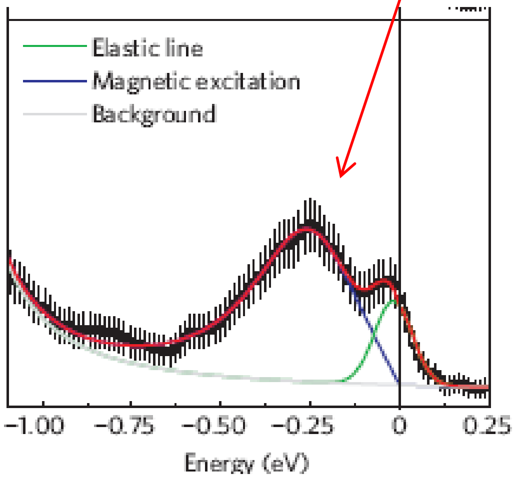
How Im $\chi(Q,\omega)$ behaves with increase of ω?

Inelastic X-ray scatt., N.Le. Tacon (2011)

Im $\chi(q=0.3,\omega) \;\Rightarrow$ peak at ω=250 meV !

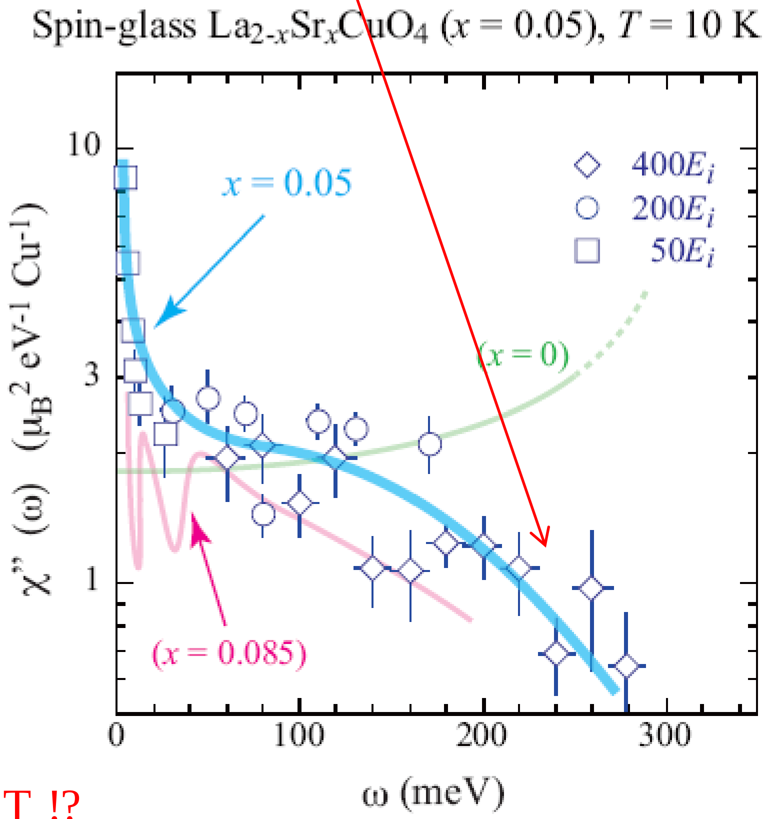
Neutron scatt. M. Fujita et al (2012)

$\int dq\,\mathrm{Im}(q,\omega)$ drops with increasing ω!



$$T_c \sim \langle \omega_{sf} \rangle \exp\{-1/\lambda_{sf}\}$$

$$\lambda_{sf} = \lambda_{sf}^{low} + \lambda_{sf}^{high} \;\Rightarrow\; T_c = ?$$

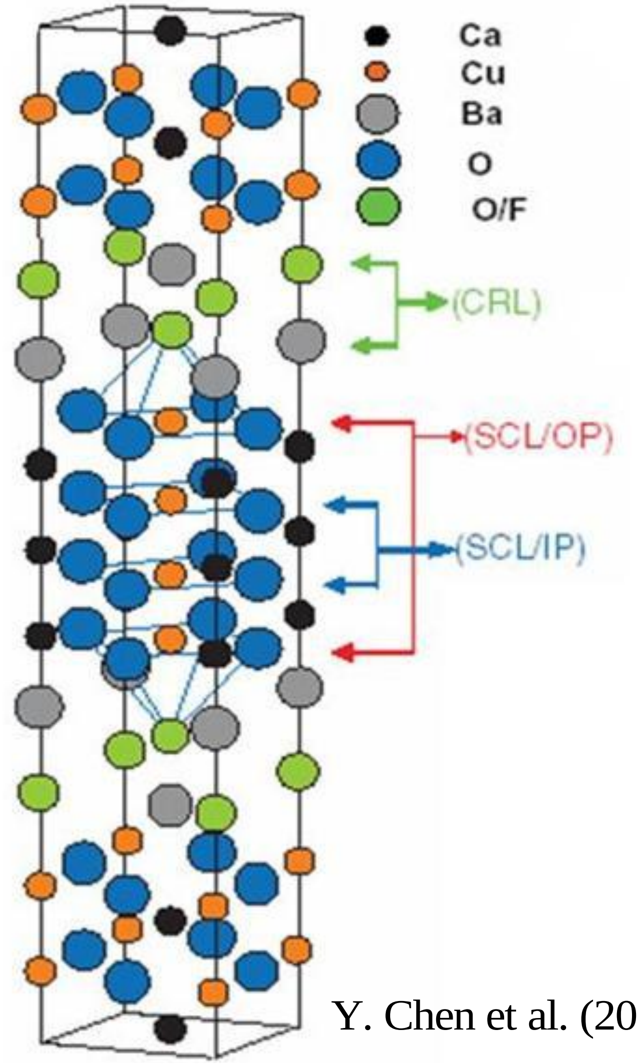


SFI solely can not give high T_c !?

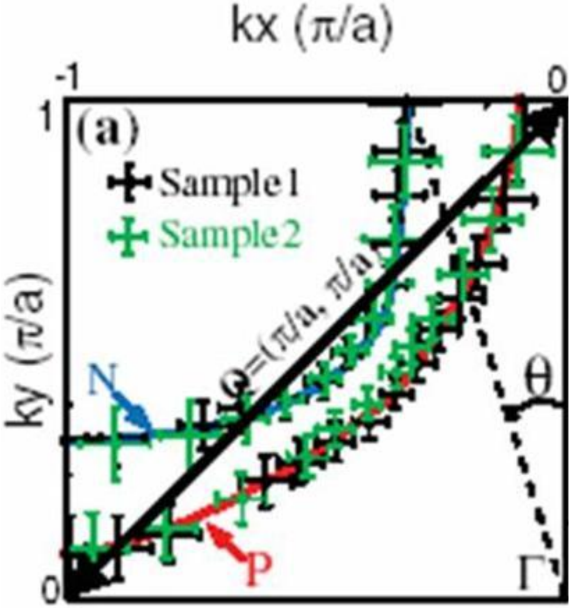
What about phonons and EPI?

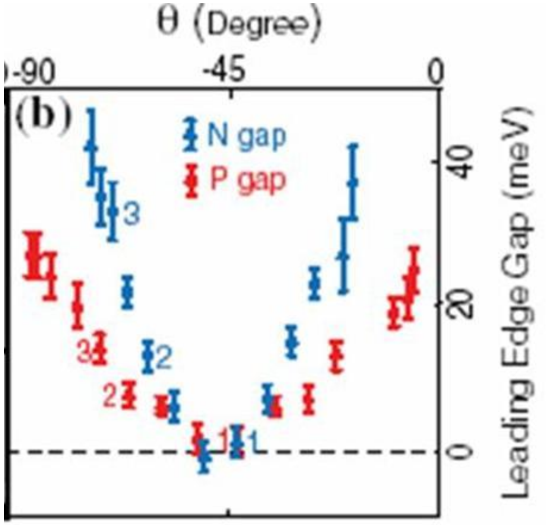
ARPES in 4-layered HTSC against SFI

$Ba_2Ca_3Cu_4O_8(O_\delta F_{1-\delta})_2$



Y. Chen et al. (2006)





$T_c \approx 60\ K$

$\frac{\Delta_N}{\Delta_P} \approx 2$!!

$\Downarrow$

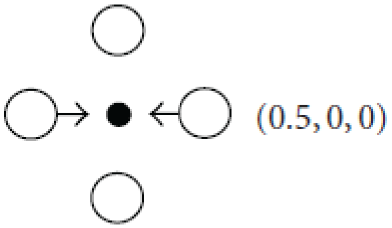
against SFI!

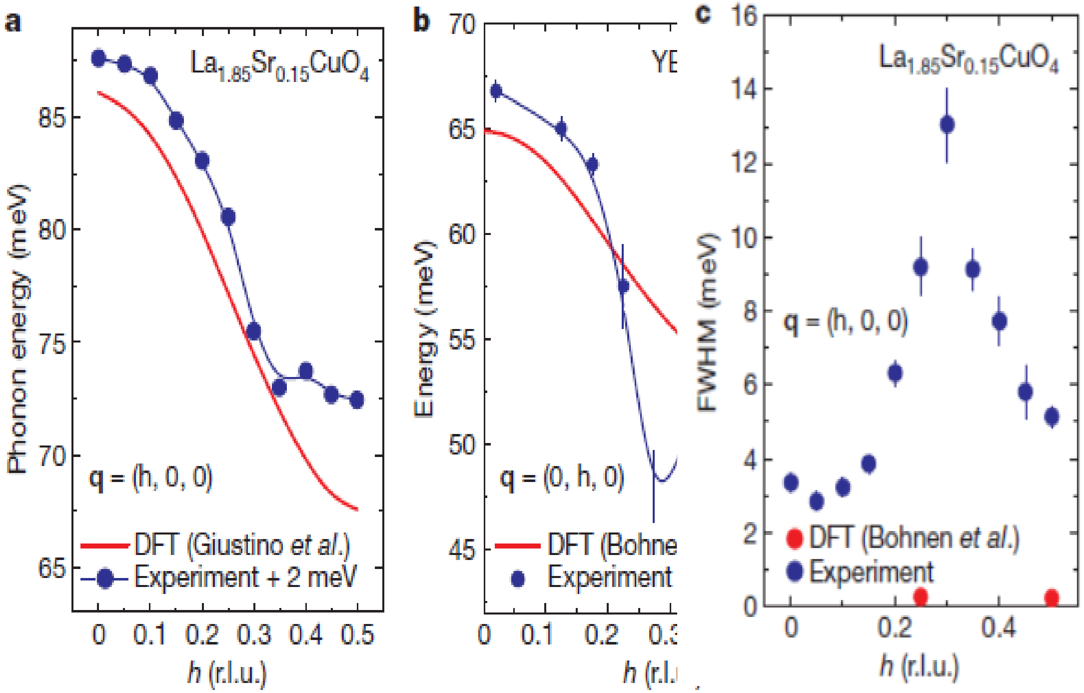
Failure of DFT for Phonon spectra in cuprates

Cuprates: DFT underestimates phonon line-widths by factor 10-20!

Bond-stretching
(longitudinal) mode

⇓





Sum-rule:

Phonon shift: $\delta\omega(\mathbf{q}) \sim \left|g_{\partial ep}(\mathbf{q})\right|^2 \mathrm{Re}\,\chi_c(\mathbf{q},\omega)$

Line-width: $\Gamma(\mathbf{q}) \sim \left|g_{\partial ep}(\mathbf{q})\right|^2 \mathrm{Im}\,\chi_c(\mathbf{q},\omega)$

$$\frac{1}{\pi N}\sum_{q\neq 0}\int_{-\infty}^{\infty} d\omega\,\mathrm{Im}\,\chi_c(q,\omega) = (1-\delta)N\begin{Bmatrix}\delta, & \text{strongly correlated}\\ 1, & \text{LDA-DFT}\end{Bmatrix}$$

$\delta(<<1)$ - doping

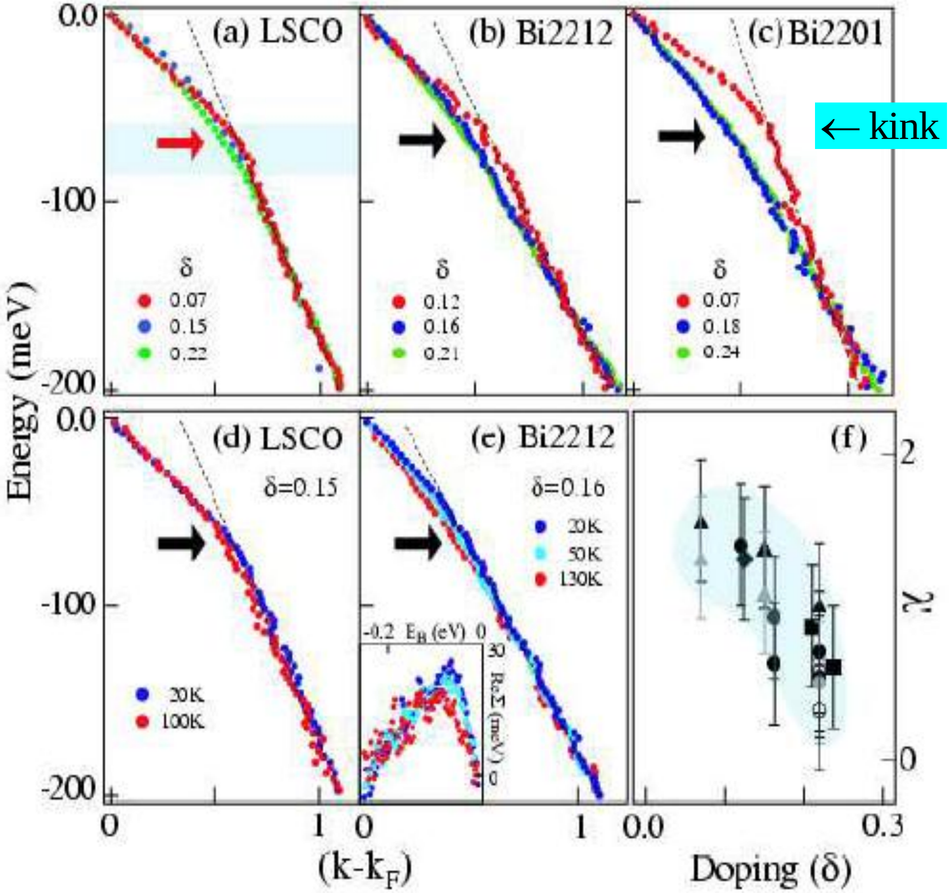
Many – body effects (due to $U >> W$) very important!

ARPES kink at the nodal (N) -point

Puzzle: $\omega_{kink}^{(s)} = \omega_{kink}^{(n)}$

isotropic EPI theory predicts: $\omega_{kink}^{(s)} = \omega_{kink}^{(n)} + \Delta_{\max}$

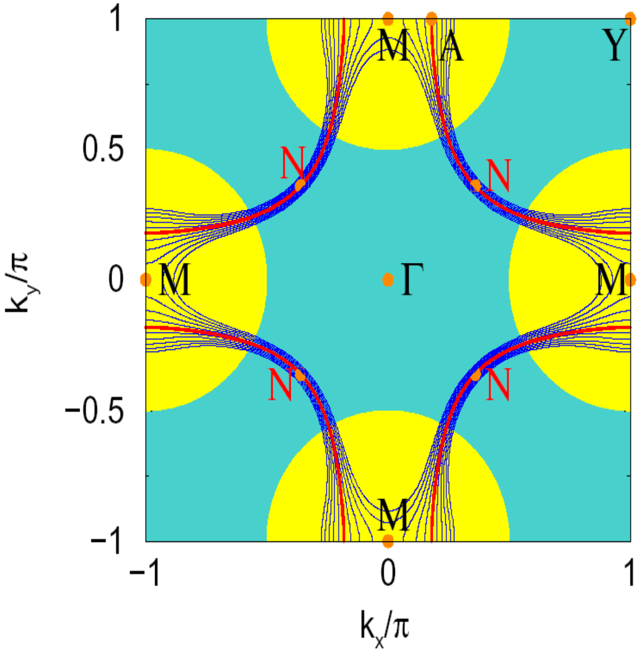
$\rightarrow$ FSP in $\alpha^2 F(\mathbf{q},\omega)$!



← kink

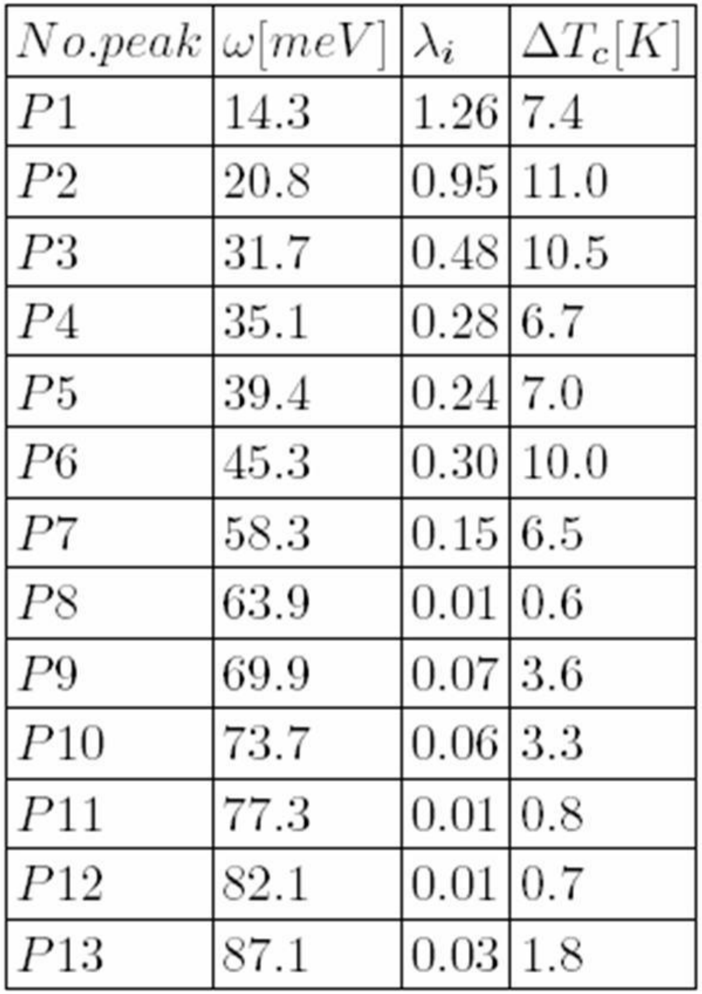
$\Delta(k_N) = 0$

$\Delta(k_A) = \Delta_{\max}$

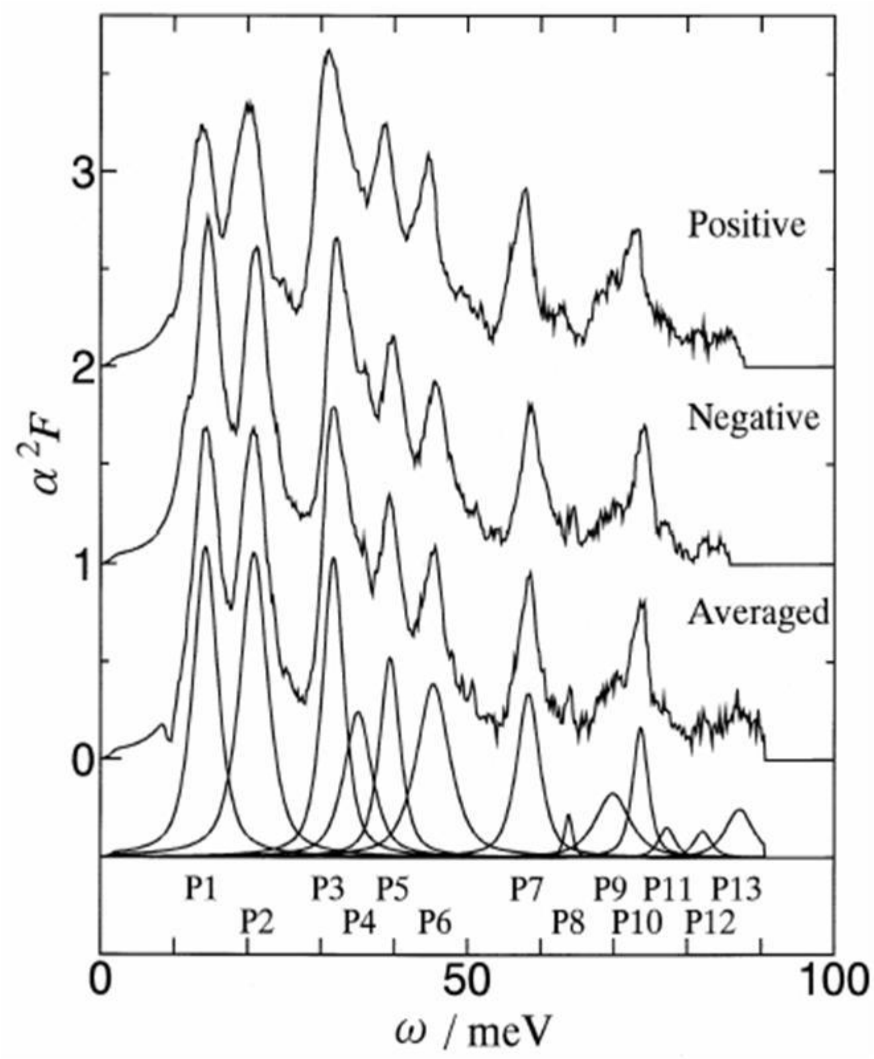


A. Lanzara et al. (2001)

In fact all phonons contribute to T_c !

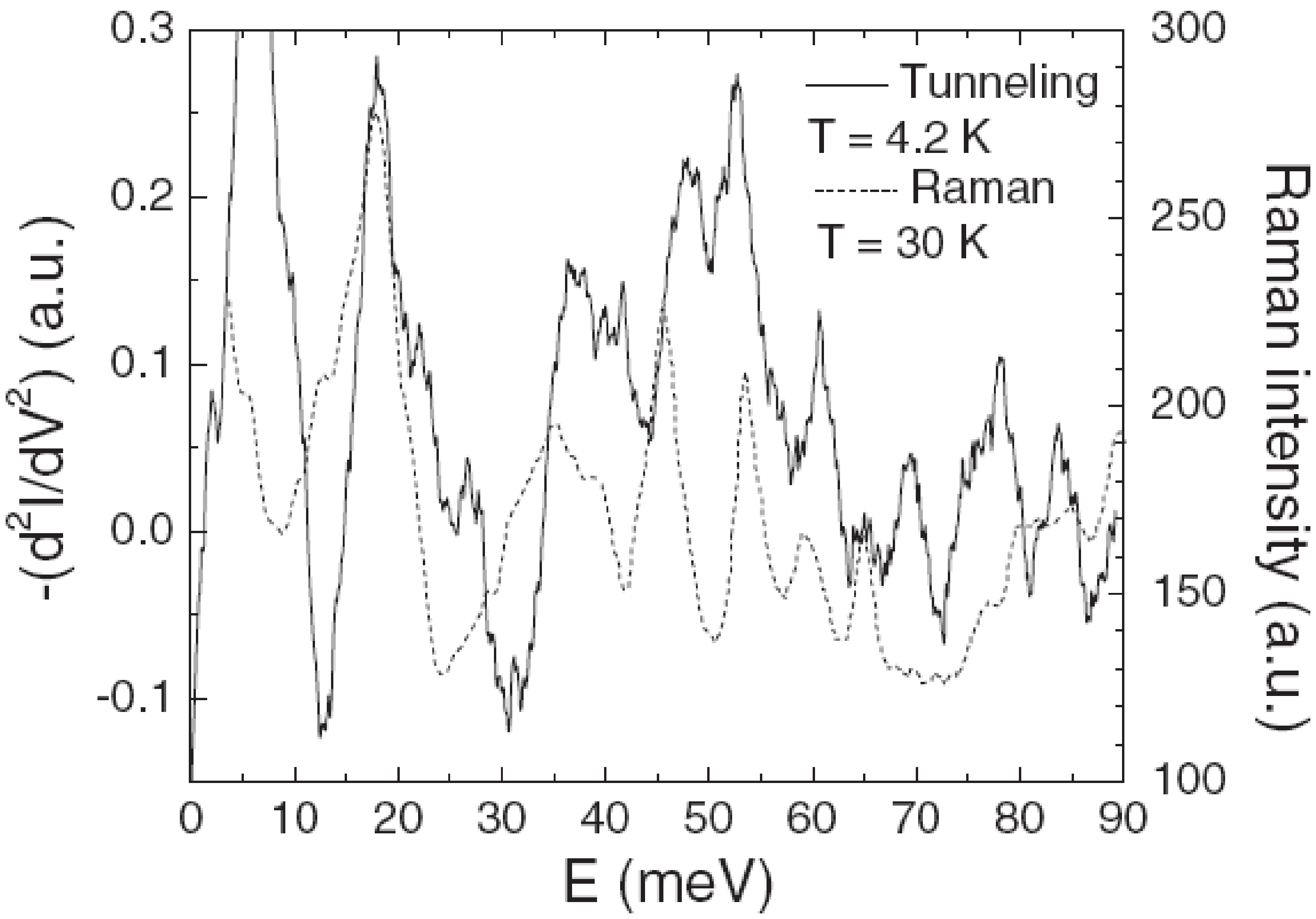


$No.peak$	$\omega[meV]$	λ_i	$\Delta T_c[K]$
$P1$	14.3	1.26	7.4
$P2$	20.8	0.95	11.0
$P3$	31.7	0.48	10.5
$P4$	35.1	0.28	6.7
$P5$	39.4	0.24	7.0
$P6$	45.3	0.30	10.0
$P7$	58.3	0.15	6.5
$P8$	63.9	0.01	0.6
$P9$	69.9	0.07	3.6
$P10$	73.7	0.06	3.3
$P11$	77.3	0.01	0.8
$P12$	82.1	0.01	0.7
$P13$	87.1	0.03	1.8



D. Shimada eta al. (1997, 2007)

Tunneling vs phonon Raman spectra in LASCO films



H. Shim et al. (2008)

Constraints on EPI imply strong q-dependence

1. **d-wave** pairing ⇒ $\Delta(\mathbf{k},\omega) \approx \Delta^{0}(\omega)(\cos k_x - \cos k_y)$
2. high $T_c \approx 160\ K$
3. rather **large EPI** coupling ⇒ $\lambda_{epi} = 1 - 2$
4. **small** $\lambda_{\mathrm{tr}} \sim 0.4 - 0.6 \quad (\rho(\mathrm{T}) \sim \lambda_{\mathrm{tr}} T)$

Asuumption: pairing is due to **SFI** ⇒ EPI is pair-breaking

Question - how large is the **bare** T_{co}^{sfi} ?

$$Z(\omega)\Delta(\mathbf{k},\omega) = \int d^3q \int \frac{d\Omega}{\Omega} V_{sfi}(\mathbf{k}-\mathbf{q},\Omega)\Delta(\mathbf{q},\omega) th\frac{\xi(\mathbf{q})}{2T_c}$$

$$\Delta(\mathbf{k},\omega) = \Delta(\omega)[\cos k_x - \cos k_y] \quad \text{and} \quad Z(\omega) \approx 1 + i\Gamma_{epi}$$

⇒

$$\ln\frac{T_c}{T_{c0}^{sfi}} = \Psi\left(\frac{1}{2}\right) - \Psi\left(\frac{1}{2} + \frac{\Gamma_{epi}}{2\pi T_c}\right)$$

$$\Gamma_{epi} \approx 2\pi\lambda_{epi} T$$

↙

- for $T_c \approx 160\ K$ ⇒ $T_{co}^{sfi} \approx (400 - 1100)\ K$!

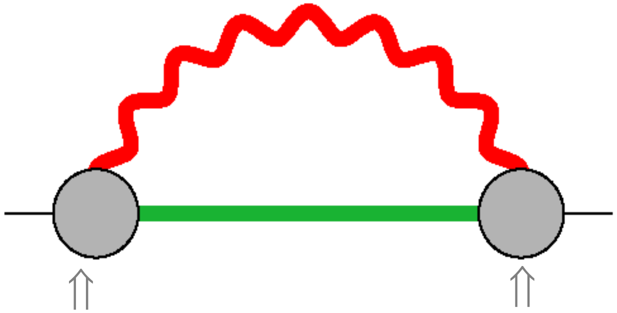
Way out ⇒ forward scattering peak (**FSP**) in EPI $\lambda_{\mathrm{epi}}(q)$

Experiment EPI must be strongly momentum dependent

Long range EPI (*forward scattering peak*) due to:

- long range due to *the Madelung energy* $\Rightarrow \dfrac{g_{ep}^{0}(\boldsymbol{k},\boldsymbol{q})}{\varepsilon(\boldsymbol{q})}$

- long range due to *strong correlations* $\Rightarrow \gamma_c(\boldsymbol{k},q)$ (vertex)

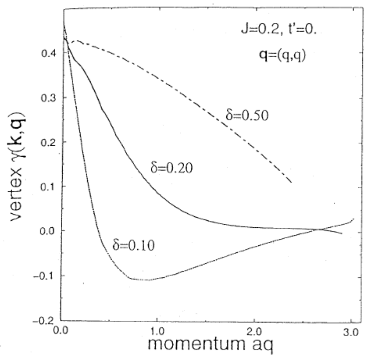


$$\gamma_c(\boldsymbol{k},\boldsymbol{q})\frac{g_{ep}^{0}(\boldsymbol{k},\boldsymbol{q})}{\varepsilon(\boldsymbol{q})} \qquad \gamma_c(\boldsymbol{k},\boldsymbol{q})\frac{g_{ep}^{0}(\boldsymbol{k},\boldsymbol{q})}{\varepsilon(\boldsymbol{q})}$$

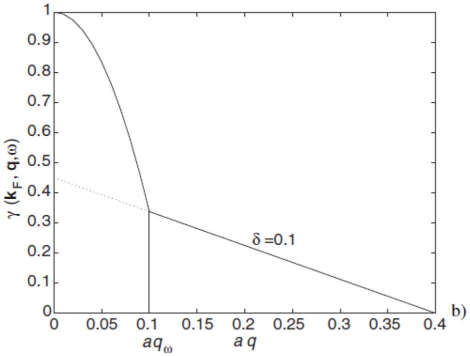
$$T_c^{(i)} \sim \left\langle \omega_{ph} \right\rangle e^{-\frac{1+\lambda_i}{\lambda_i-\mu_i^*}}$$

- since $\lambda_d \approx \lambda_d$ and $\mu_d^* \ll \mu_s^* \Rightarrow T_c^{(d)} > T_c^{(s)}$

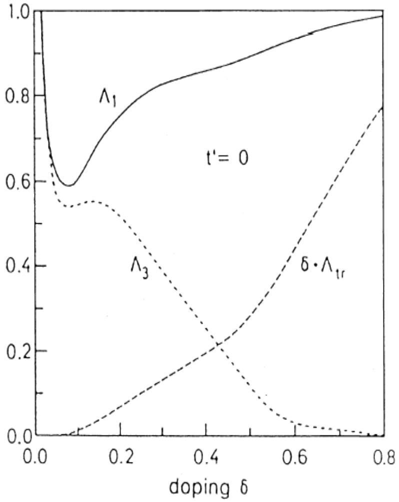
adiabatic: $\omega=0$



nonadiabatic: $\omega \neq 0$



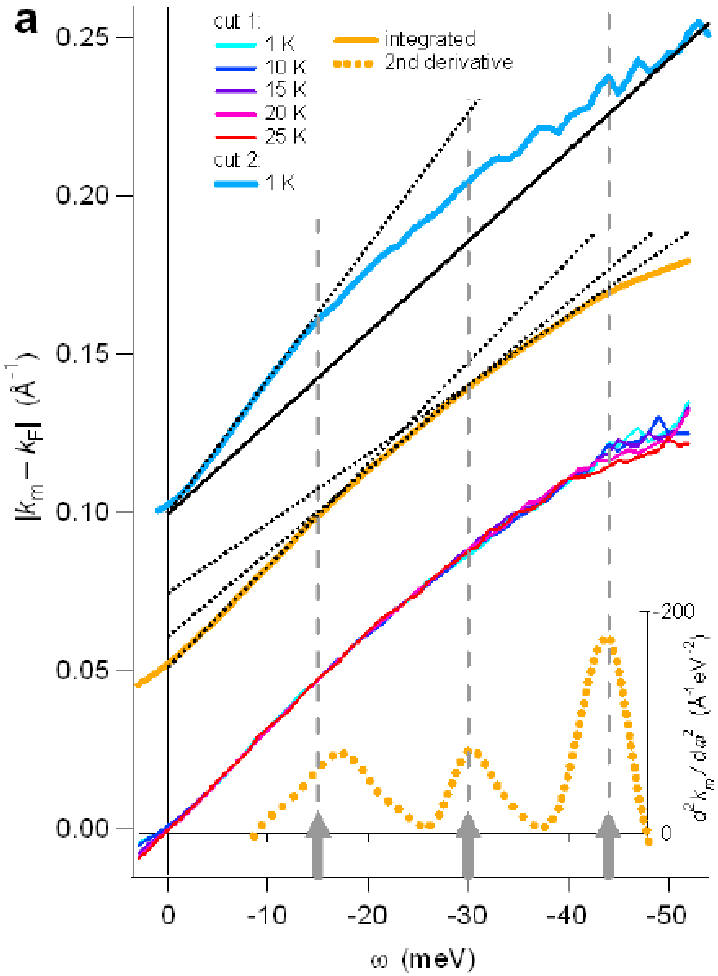
$\lambda_s \sim \Lambda_1 \qquad \lambda_d \sim \Lambda_3$



Experiments $\Rightarrow$ EPI strongly ***k***-dependent

Theory: strong correlations $\Rightarrow$ EPI peaked at small ***k***!

ARPES in *LiFeAs* with $T_c = 18$ K $\rightarrow$ $\lambda_{\text{epi}} > 1$!?



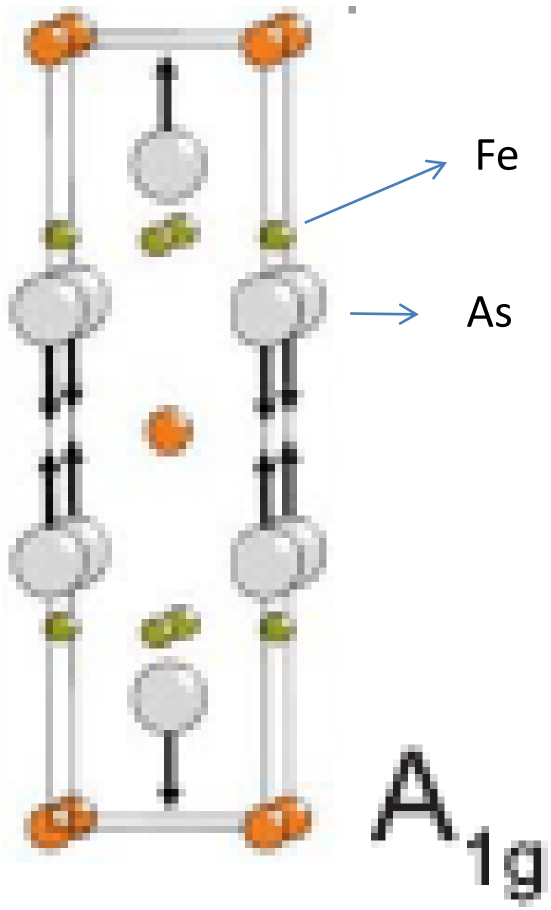
$$\lambda_{ep} = 2\int_0^\infty \frac{\alpha^2 F(\omega)}{\omega} d\omega = \sum_{\kappa=1}^{3} \lambda_{ep}^{(\kappa)} \approx 1.38$$

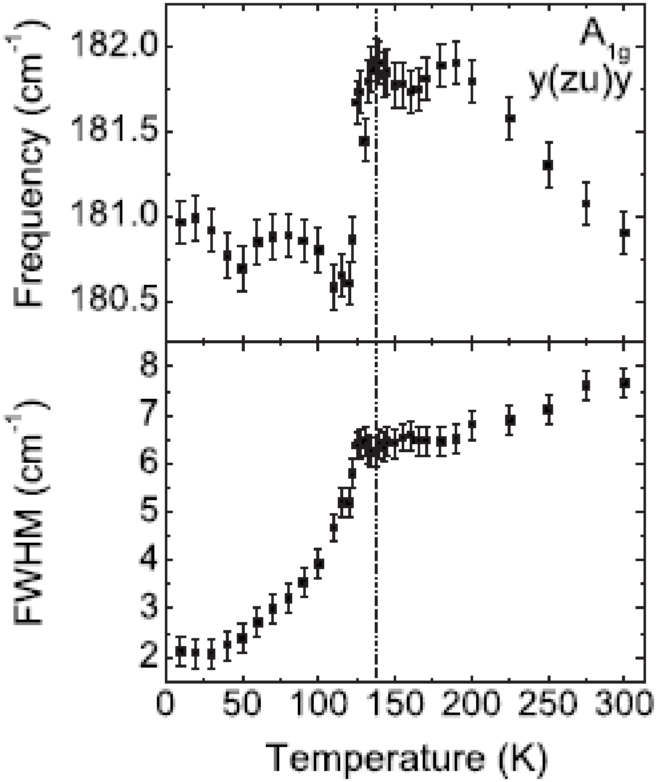
$$\lambda_{ep}^{(1,2,3)} = 0.75;\;\; 0.25;\;\; 0.38$$

- it is not sufficient to explain T_c ?
- additional coupling is needed ?

Failure of DFT for Phonon spectra in Fe-based

$BaFe_2As_2$





$$\Gamma_{LDA} \approx 0.1 N(0)\lambda_{ep}\omega^2 \approx 0.4 cm^{-1} \approx 0.1\,\Gamma_{\exp}\ !$$

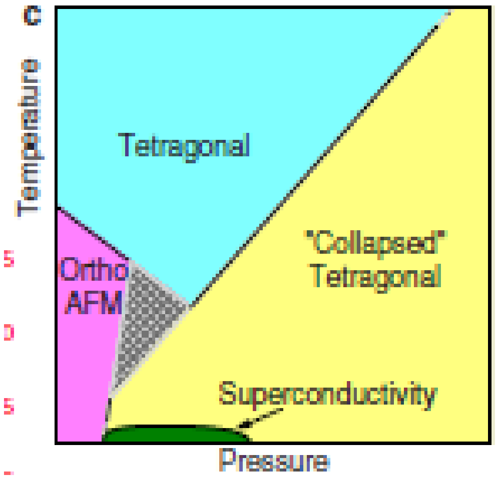
$\Rightarrow$ *many – body* effects beyond LDA important!

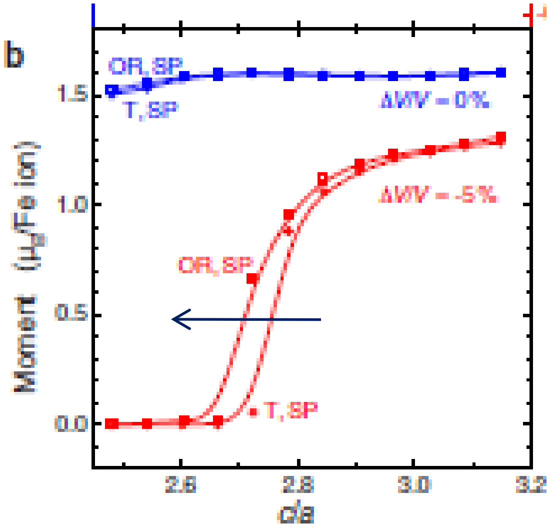
$\lambda_{ep}^{LDA} \approx 0.2$?

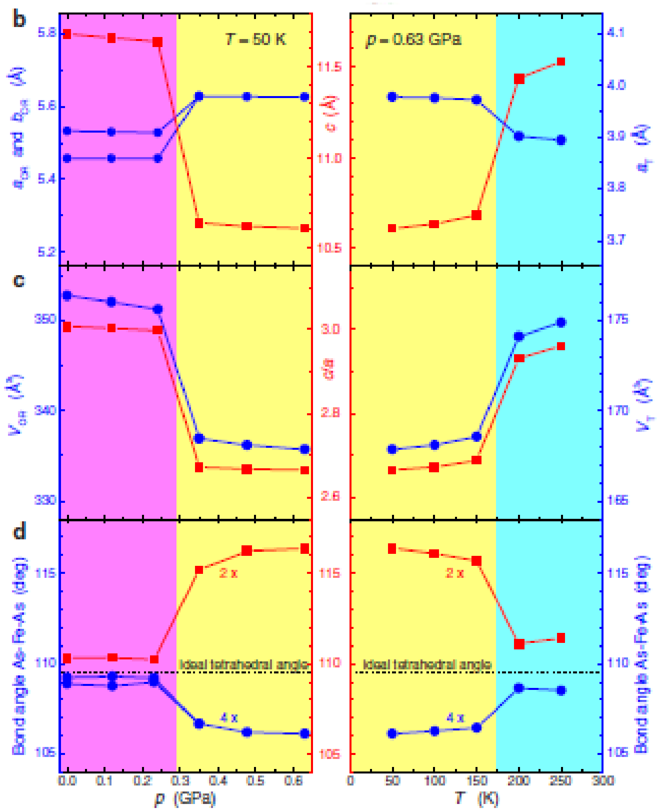
Giant magneto-elastic effects

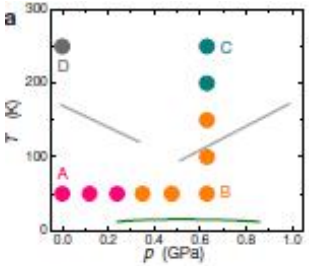
- at critical pressure P_c: orthorhombic+SDW $(m \neq 0) \Rightarrow$ collapsed tetragonal $(m = 0)$

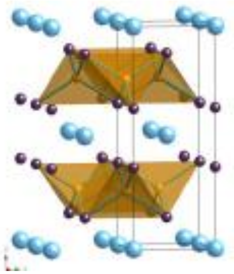
$CaFe_2As_2$











$P_c^{(\exp)} \approx 0.35\ GPa$ but $P_c^{(LDA)} \approx 5\ GPa$!

- something fails in LDA?

21:28

Strong (?) ***EPI due to large As polarizability*** - many body effect

G. Sawatzky et al. EPL(2009), arXiv:0808.1390

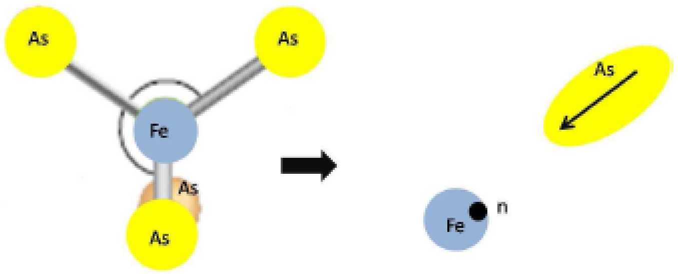


Fig. 1: Schematic picture of the polarization of the As electronic cloud due to charge fluctuations (n) on the Fe-ions. The tiny arrow on the As-ion describes the induced electronic dipole moment on As.

$$\hat{H}_0^{(pol)} = -\sum_{\mathbf{R}_{Fe}} V_P(\mathbf{R}_{Fe})\hat{n}_{\mathbf{R}_{Fe}}/2,$$

$$\hat{H}_H^{(pol)} = \sum_{\mathbf{R}_{Fe}} U^{(sc)}_{\mathbf{R}_{Fe}}\hat{n}_{\mathbf{R}_{Fe}\uparrow}\hat{n}_{\mathbf{R}_{Fe}\downarrow}$$

$$U^{(sc)}_{\mathbf{R}_{Fe}} = U_{at} - V_p(\mathbf{R}_{Fe})$$

$$V_p \approx \sum_{\mathbf{R}_{As}\in n.n.\mathbf{R}_{Fe}} \frac{\alpha_{As}e^2}{|\mathbf{R}_{Fe}-\mathbf{R}_{As}|^4}$$

$$\boxed{\alpha_{As}\sim(10-12)\ \mathring{A}^3}$$

$$\boxed{V_p\sim 10}\ \boxed{eV} \longrightarrow \boxed{U^{(sc)}\lesssim 3\ eV}$$

Strong EPI: $V_{ep} = 4V_p(\approx 40\ eV) \gg V_{ep}^{LDA}(\approx 1-2\ eV)$!

$$\boxed{\hat{H}_{ep}^{(pol)} = V_{ep}\sum_{\mathbf{R}_{Fe}} \hat{\varphi}_{\mathbf{R}_{Fe}}(\hat{n}_{\mathbf{R}_{Fe}} - \lambda\hat{\mathbf{S}}^2_{\mathbf{R}_{Fe}})}$$

$$\boxed{\hat{\varphi}_{\mathbf{R}_{Fe}} = \frac{1}{Zd}\sum_{\mathbf{R}_{As}\in n.n.\mathbf{R}_{Fe}} \mathbf{n}_{As}\cdot(\hat{\mathbf{u}}_{\mathbf{R}_{As}} - \hat{\mathbf{u}}_{\mathbf{R}_{Fe}})}$$

$$\boxed{\mathbf{n}_{As} = (\mathbf{R}^0_{Fe} - \mathbf{R}^0_{As})/d_{As-Fe}}$$

→ giant magneto-elastic effects

M.L.K., A. A. Haghighirad, EPL(2008)

Magneto-elastic coupling effects

$$\boxed{G(S_Q,\varepsilon,P) \approx \frac{\varepsilon^2}{2\kappa_{eff}} + P\varepsilon - \frac{a(\varepsilon)}{2}S_Q^2 + \frac{b}{4}S_Q^4 + \frac{c}{6}S_Q^6}$$

$\varepsilon(\equiv \delta V/V) = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$ $\boxed{a(\varepsilon) = U^{(sc)}(\varepsilon) - \chi_0^{-1}(Q,\varepsilon,T)}$ $\chi_0(Q) = N(0)f(Q)$

For small strain $\varepsilon \ll 1$ $a(\varepsilon) \approx a_0 + (\gamma_k + \gamma_p)\varepsilon;$

$$a_0 = [U^{(sc)} - \chi_0^{-1}(Q,0,T)].$$

$$\gamma_k = \chi_0^{-1}(Q,0)\,d\ln\chi_0(Q,\varepsilon)/d\varepsilon$$

$$\gamma_p = V_{ep}/r$$

$$\epsilon_d = (\delta d_{Fe-As}/d_{Fe-As}) = 0.01$$

$\varepsilon_d \approx \varepsilon/r$ with $r \sim 3-4.$

First order phase transition at P_c

$$P_c = \frac{1}{(\gamma_k + \gamma_p)\kappa_{eff}}\left(a_0 + \frac{3b_{ren}^2}{16c}\right)$$

$$\gamma_k \equiv \gamma_{LDA},\ b_{ren} = b - \kappa_{eff}(\gamma_k + \gamma_p)^2/2$$

$\gamma_p \approx 10\ \gamma_{LDA} \Rightarrow P_c$ is *due to many body effects!*

M.L.K., A. A. Haghighirad, EPL(2008)

Contribution of EPI to superconductivity

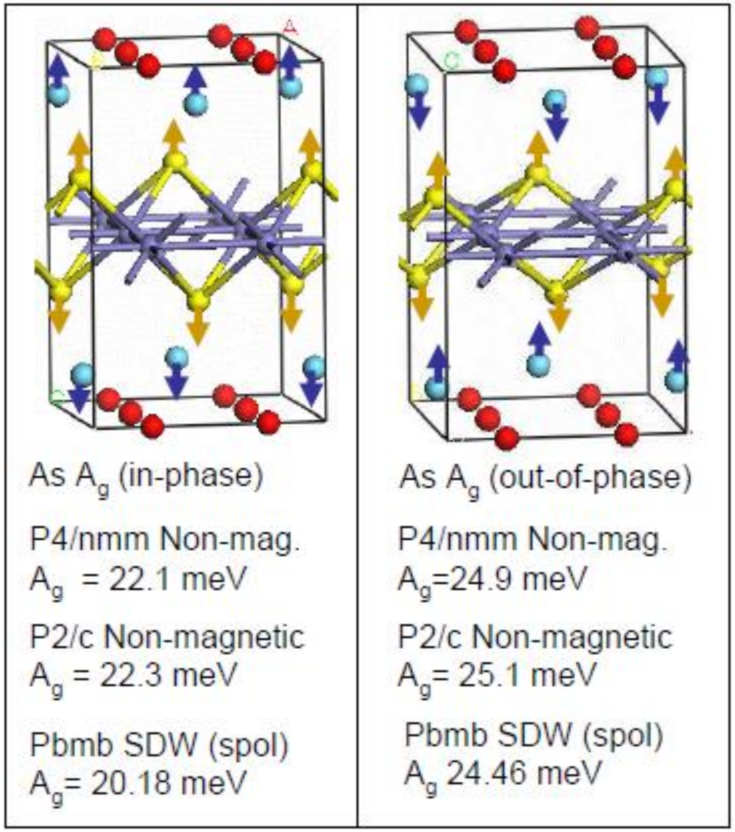


FIG. 19: (color online) Top panel shows two Arsenic c-polarized A_g modes, which are in-phase and out-of-phase with respect to As and La motions along c-axis. The bottom panel shows the mode energies for non-magnetic tetragonal (P4/nmm), non-magnetic orthorhombic distorted lattices (P2/c), and SDW magnetic configuration (Pbmb).

Strong EPI *with As* $\boldsymbol{A_{1g}}$ ***- modes***

$$\Downarrow$$

large ***intra - band*** pairing

$$\Downarrow$$

large As isotope effect

$$g^2_{A_{1g}} \approx V^2_{ep} \cos^2\theta \left\langle \hat{u}^2_{As} \right\rangle / d^2_{Fe-As} \quad \left\langle \hat{u}^2_{A_{1g}} \right\rangle \approx \hbar^2 / 2M_{As}\omega_{A_{1g}}$$

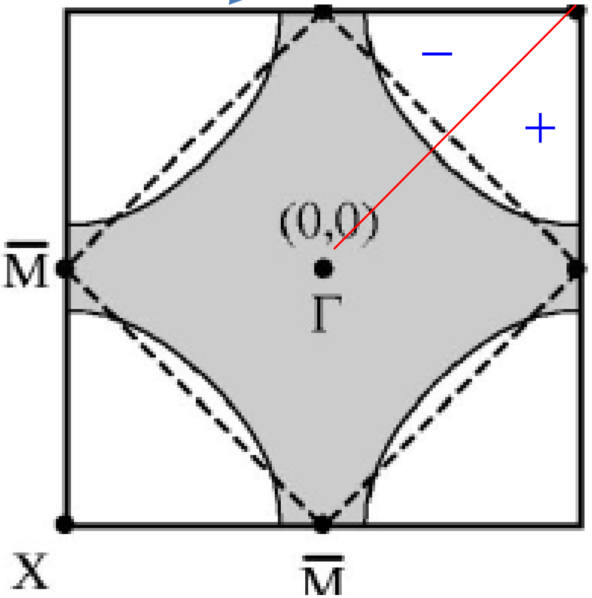
$$g^{pol}_{ep} (= \partial V_{ep} / \partial d_{As-Fe})$$

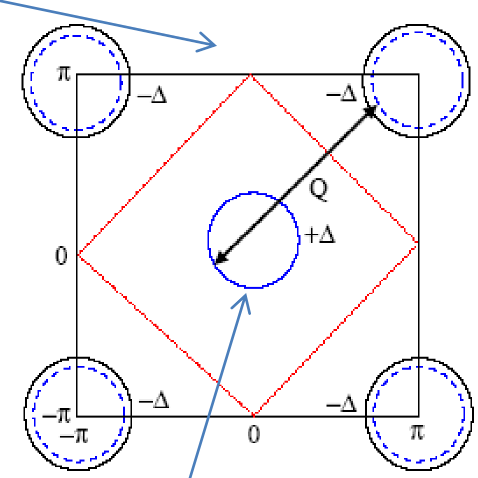
$$g^{pol}_{ep} (\sim \; 16 \; eV/\text{Å}) \gg g^{(LDA)}_{ep} (< \; 1 \; eV/\text{Å})$$

$$\lambda^{0,i}_{ep,A_{1g}} = 2N_i(0) g^2_{A_{1g}} / \omega_{A_{1g}} \sim 1$$

M.L.K., A. A. Haghighirad, EPL(2008)

Cuprates and Fe-based SC as "two-band" superconductors





hole pocket

electron pocket

$$T_c \approx \langle \omega \rangle \exp\{-1/\lambda_{\max}\}$$

$$\lambda_{\max} = \frac{\lambda_{++} + \lambda_{--} + \sqrt{(\lambda_{++} - \lambda_{--}) + 4\lambda_{+-}^2}}{2}$$

Wishfull properties: $\lambda_{++} > 0,\ \lambda_{--} > 0,\ \lambda_{+-}$ - any sign!

$\Rightarrow$ Coulomb (interband) und phonons (intraband) constructively increase T_c!

Robustness of Cuprates and Fe-based SC in presence of nonmagnetic impurities

(I) **Two-band** (toy) **model** with $\Delta_{++}(\boldsymbol{k}) = -\Delta_{--}(\boldsymbol{k})$

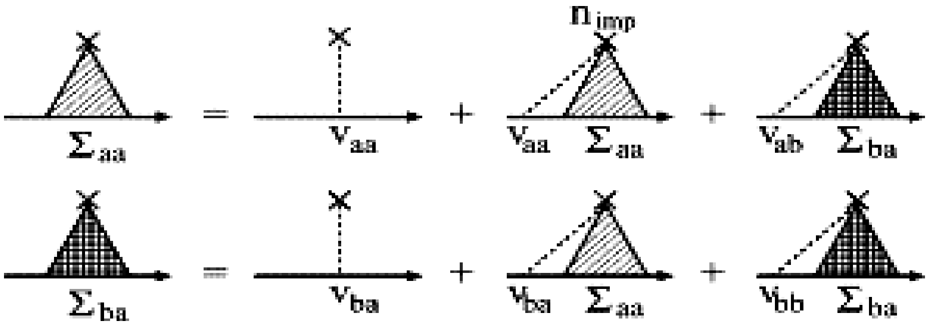
$$\rho^{-1}(T) = \frac{1}{4\pi}\sum_{i=1,2}\frac{\omega_{pl,i}^{2}}{\Gamma_i(T)}, \quad \Gamma_i(T)(=\Gamma_{ii}+\Gamma_{ij}) = \gamma_i^{(imp)} + \gamma_i^{(inel)}(T)$$

- experiments in Fe-based $\Rightarrow \gamma_{++}^{(imp)} \approx \gamma_{--}^{(imp)} \approx \gamma_{+-}^{(imp)} \sim 200-300\ K$!

$\Rightarrow$ **kills intraband gapless unconventional pairing !**

$$\hat{G}^{-1} = \hat{G}_0^{-1} - \hat{\Sigma}_{imp}(i\omega_n), \ \hat{\Sigma}_{imp} = n_{imp}\hat{T}(i\omega_n)$$

$$\hat{T}(i\omega_n) = [1 - \hat{v}\hat{G}_{loc}(i\omega_n)]\hat{v}$$



M.L.K. S. Drechsler, O.V.Dogov, (2008)
M.L.K., O. V.Dogov, (1999)

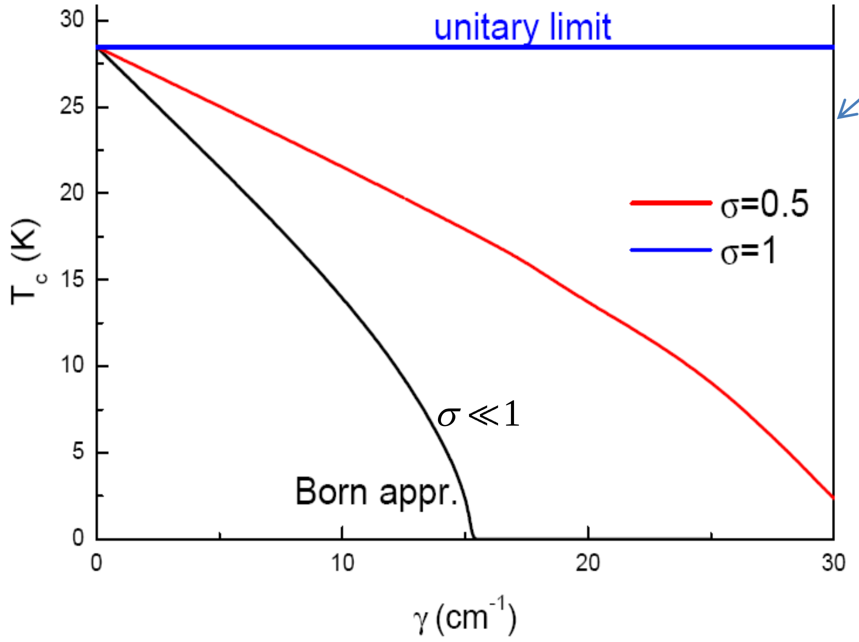
Inter - and Intra - Band Scattering: $v_{++}=v_{--}\neq 0,\ v_{+-}=v_{-+}\neq 0$

$$\ln\frac{T_c}{T_{c0}}=\psi\left(\frac{1}{2}\right)-\psi\left(\frac{1}{2}+\frac{\Gamma_{pb}}{2\pi T_c}\right)$$

$$\Gamma_{pb}=\Gamma_u\sigma_{pb},\ \Gamma_u=n_{imp}N^{-1}(0),\ \sigma_{pb}=\frac{v_{+-}^2}{[1+(\frac{v_{++}+v_{+-}}{2})^2][1+(\frac{v_{++}-v_{+-}}{2})^2]}$$

*For $(v_{++}/v_{+-})=1$ and unitary limit $v_{++}\to\infty\ \Rightarrow\ \Gamma_{pb}\to\Gamma_u$

*For $(v_{++}/v_{+-})\neq 1$ and unitary limit: $v_{++},v_{+-}\to\infty\ \Rightarrow\ \Gamma_{pb}\to 0$ (also for $v_{++}=0$)



Multi-band structure of typical Fe-based SC

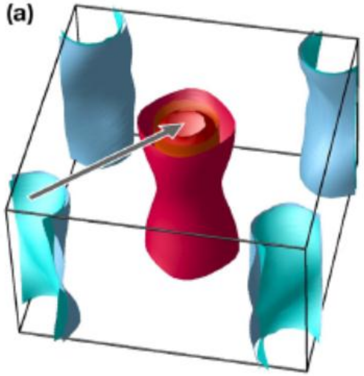
DFT in Fe-based: *good qualitative* but *bad quantitative predictions*!

- DFT overestimates magnetism: $\mu_{DFT} \sim 2\mu_B$; $\mu_{\exp} \sim 0.4\mu_B$ (in LaFeAsO)

(• DFT underestimates magnetism in cuprates: $\mu_{DFT} << \mu_{\exp}$)

- DFT for $\mu = \mu_{\exp}$ ⇒ "bad" optimized structure

(a)



$\Leftarrow$

Fermi surface of *arsenides* $Ba(Fe_{1.94}Co_{0.06})_2As_2$

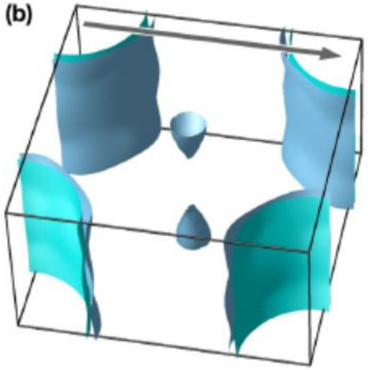
$e-h$ nesting ⇒ SDW instability - peack in $\chi_s(\mathbf{Q})$

⇒ "quasinesting" in SC compounds

⇒ $s_\pm$ pairing due to *SFI* !?

- *electron* pocket
- *hole* pocket

(b)



$\Leftarrow$

Fermi surface of *selenides* $K_{0.8}Fe_2Se_2$

NO hole pocket ⇒ no e-h nesting

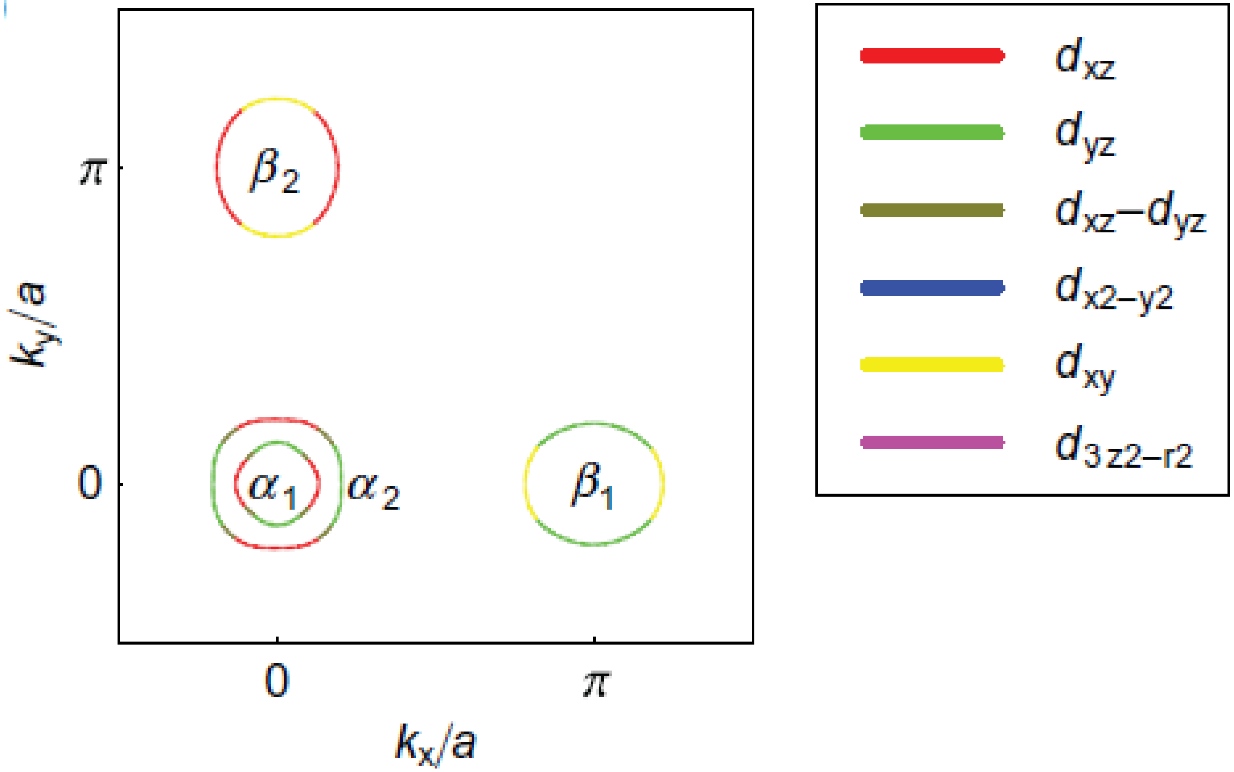
⇒ no $s_\pm$ pairng !?

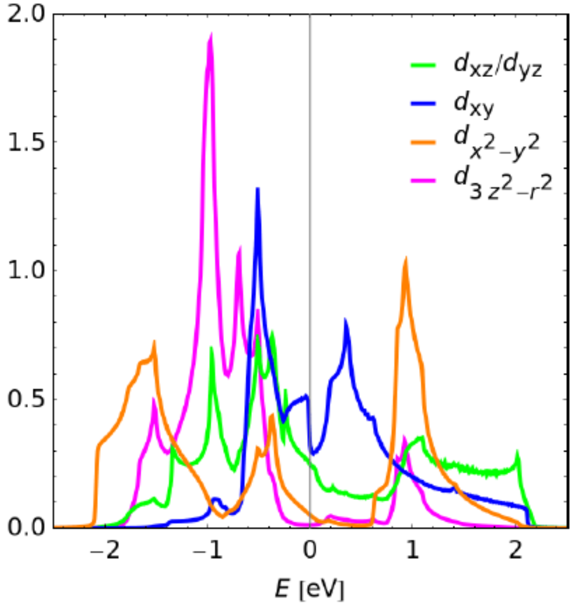
Tight binding model for *arsenide* $BaFe_2As_2$: five d-orbital model

$e-h$ nesting $\Rightarrow$ SDW instability - peack in $\chi_s(\boldsymbol{Q})$

$\Rightarrow$ "quasinesting" in SC compounds

$\Rightarrow s_{\pm}$ pairing due to *SFI* !?





Orbital fluctuations compete with spin fluctuations - H.Kontani(2009)

EPI increase orbital fluctuations giving rise to s_{++} – *pairing*! No sign change! - H.Kontani(2009)

Assumption: SC due to orbital and spin fluctuations, EPI in first order neglected

$$\lambda_{\mathrm{E}}\Delta_{ll'}(k) = \frac{T}{N}\sum_{k',m_i} W_{lm_1,m_4l'}(k-k') \times G_{m_1m_2}(k')\Delta_{m_2m_3}(k')G_{m_4m_3}(-k')$$

$$\hat{W}(q) = -\tfrac{3}{2}\hat{\Gamma}^s\hat{\chi}^s(q)\hat{\Gamma}^s+\tfrac{1}{2}\hat{\Gamma}^c\hat{\chi}^c(q)\hat{\Gamma}^c+\tfrac{1}{2}(\hat{\Gamma}^s-\hat{\Gamma}^c)$$

multiorbital susceptibility $\chi^c(q)$ may be significuntly increased even by small EPI !

$\Rightarrow$ favors s_{++} !

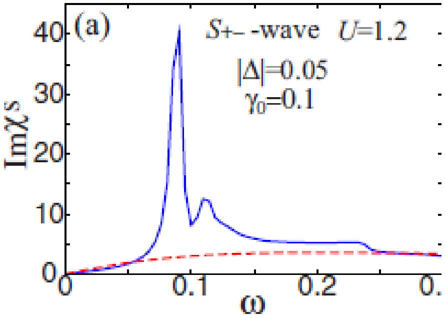
Transition from $s_\pm$ to s_{++} in the presence of impurities

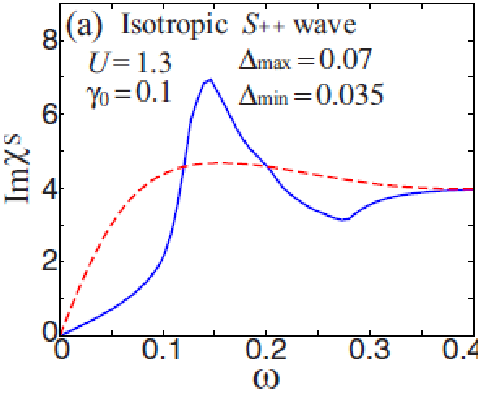
$\Rightarrow$ **multiorbital fluctuations are important**!

$s_\pm$ vs s_{++} pairing

$s_\pm$ very fragile against impurities

$s_\pm$ and s_{++} show magnetic resonance but $s_\pm$ is **sharper**





Five d-orbital model – Violation of Anderson‘s theorem for s+- !!

S.Onari & H.Kontani, PRL **103**, 177001 (2009)

For **5 d-orbitals** $|\alpha\rangle$:

$$\langle\alpha|\hat{T}(i\omega_n)|\beta\rangle = \langle\alpha|[1-\hat{I}\hat{G}_{loc}(i\omega_n)]^{-1}\hat{I}|\beta\rangle$$

In the **band** basis: $\hat{T}_{\boldsymbol{k},\boldsymbol{q}} = \hat{I}_{\boldsymbol{k},\boldsymbol{q}} + (1/N)\sum_{\boldsymbol{p}} \hat{I}_{\boldsymbol{k},\boldsymbol{p}}\hat{G}_{\boldsymbol{p}}\hat{T}_{\boldsymbol{p},\boldsymbol{q}}$

$$g = 0.66\frac{m}{m^*}\rho_{imp}[\mu\Omega cm]/T_{c0}[K],$$

$$\Downarrow$$

- for $g > g_c^{s+-} = 0.23 \;\Rightarrow\; T_c^{s+-} = 0$!

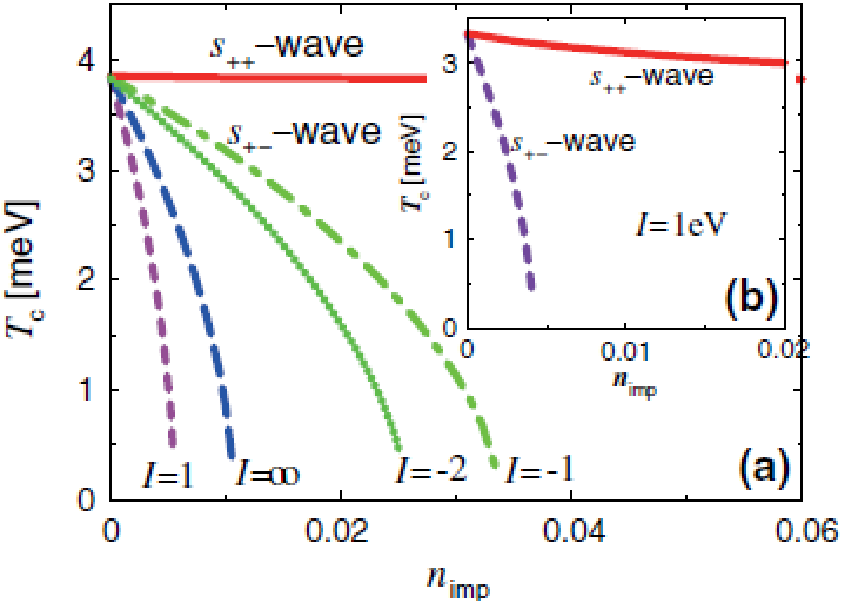
In $Sm(Fe_{1-x}Ru_x)AsO_{0.85}F_{0.15}$, $T_{c0} = 50\ K$,

$T_c(x=0.36) = 15\ K,\ T_c(x=0.75) = 0\ K,\ \dfrac{m}{m^*} = 0.5$

For $\rho_{imp}^{\exp}(x=0.05) = 250\ \mu\Omega\text{cm},\ T_c = 42\ K$

$$\Downarrow$$

g=1.5 $\gg g_c^{s+-} = 0.23$ and $s_\pm$ **cannot survive**!



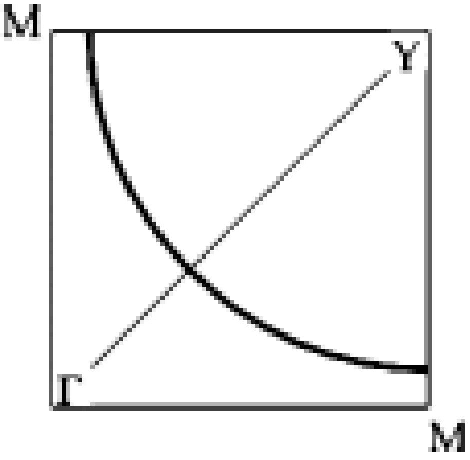
Coexistence of SC (s++ and s+-) and SDW

Problem similar to HTSC (M.L.K et al. (1995))

sign change of $F_{\uparrow\downarrow}(\boldsymbol{k},\omega)$

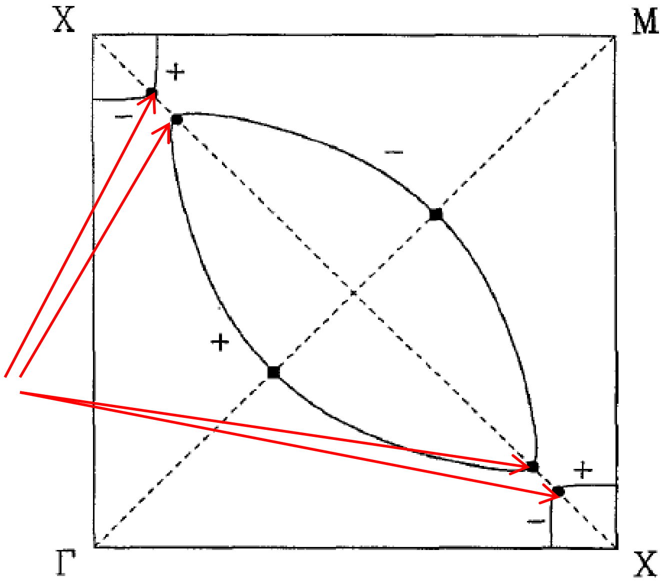
(a) - SDW order $h_{ex}(\mathrm{r}) = h^0_{ex}\cos(\boldsymbol{Qr})$, $\boldsymbol{Q} = (\pi,\pi)$

- s-wave SC with Δ=const



spectrum $E(\boldsymbol{k}) \approx \sqrt{\xi_{\boldsymbol{k}}^2 + \tilde{\Delta}_{\boldsymbol{k}}^2}$

accidental nodes for $\tilde{\Delta}_{\boldsymbol{k}} = 0$



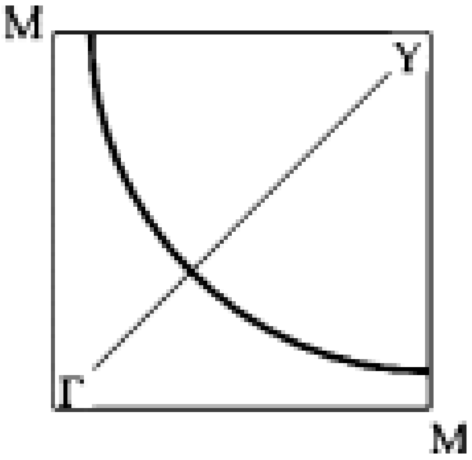
$\Downarrow$

- density of states $N(E) \approx N(0)\left(\dfrac{h_{ex}}{v_F Q}\right)\dfrac{E}{\Delta}$
- power law behavior $P(T) \sim T^n$

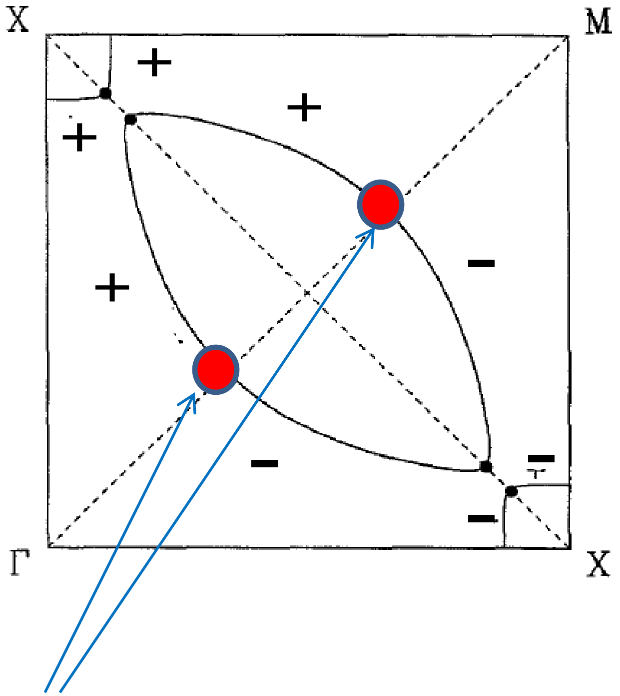
(b) - **SDW order** $h_{ex}(\mathrm{r})=h^0_{ex}\cos(\boldsymbol{Qr})$, $\boldsymbol{Q}=(\pi,\pi)$

- **d - wave SC** with $\Delta(\boldsymbol{k})=-\Delta(\boldsymbol{k}+\boldsymbol{Q})$ (also **holds for s$_\pm$** !)

sign change of $F_{\uparrow\downarrow}(\boldsymbol{k},\omega)$



spectrum $E(\boldsymbol{k})\approx\sqrt{\xi_{\boldsymbol{k}}^2+\Delta_{\boldsymbol{k}}^2}$



- standard d-wave nodes $\Delta(\boldsymbol{k})=0$
- no accidental nodes in $\Delta(\boldsymbol{k})$

$s_\pm$ and d-wave SC coexist much easier with SDW

CONCLUSIONS

1. Pairing in cuprates and Fe-based SCis due to
c**onstructive interference** (**CI**) between EPI and Coulomb

2. In cuprates EPI is important ingredient in pairing
* d-wave is due to inteplay between EPI and Coulomb
* small-q ("intraband") scattering dominated by EPI
* large-q ("interband") scattering dominated by Coulomb

3. In Fe-based SC EPI dominates in intraband pairing
* intraband (small-q) scattering due to EPI
* interband (large-q) scattering is probably dominated by Coulomb

4. **CI** phenomenon is prereqisite for higher T_c?