On the problem of mass renormalization in Fe pnictides

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Outline

1.Introduction
2.Some theoretical aspects and background
3.Eliashberg-Migdal analysis of selected Fe pnictides
3.1. Na-doped Ca-122
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3.3 La-FeAsOF
3.4 Some remarks on other pnictides
4. Summary & Outlok

Introduction - I

The fundamental Fermi quasi-particle characteristics: **e, s=1/2, $m_*(\omega,T)$**

$$m_* = (1+\lambda)m_b$$

$$\gamma = (1+\lambda)\gamma_b$$

$$\gamma_b = \tfrac{2}{3}\pi^2 k^2_B N(0)$$

m_b-bare mass ≈ LDA band mass

λ contains **all** interactions,
among them the pairing interaction
How to map out it ?

λ -mass enhancement factor,
coupling constant (EM)

N(0) -DOS at the Fermi level

Physical quantities affected by the mass renormalization:

- Fermi velocities
- Linear electronic specific heat $C_{el} = \gamma T$

$$\omega^2_{pl} = 4/3\pi^2 ne^2/m^*$$

- Condensate density, penetration depth (plasma frequency)
- Slope of the upper critical field near T_c

Introduction-II

Enhancement vs. coupling strength relevant for superconductivity?

$m_* = (1+\lambda^*_{el\text{-}b} + \lambda^*_{el\text{-}el})m_b$

bare mass ≈ band mass

$\gamma = (1 + \lambda)\gamma_b$

λ -mass enhancement factor, coupling constant (EM)

$\gamma_b = \frac{2}{3}\pi^2 k^2_B N(0)$

N(0) -DOS at the Fermi level

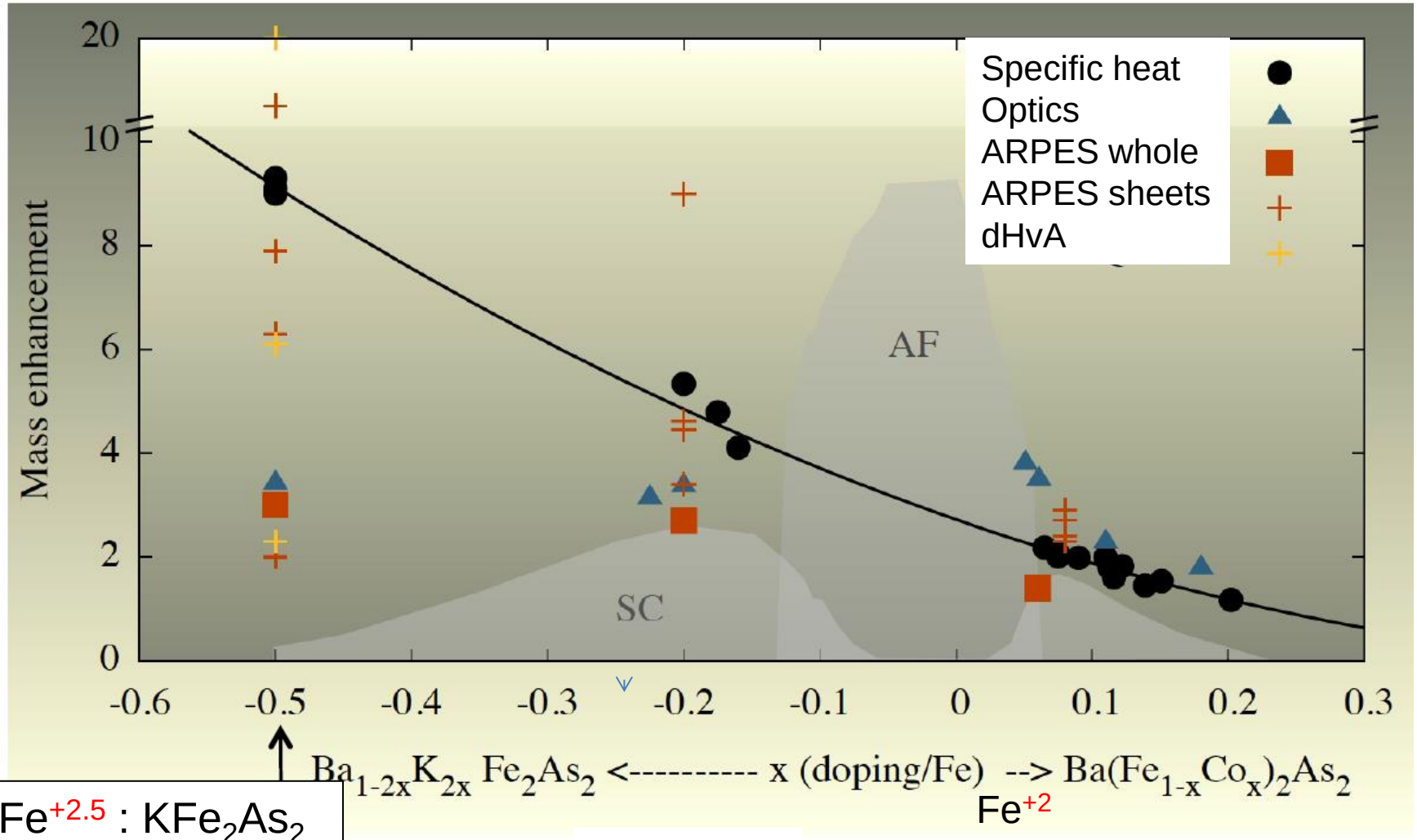
$$\mathbf{m_* = (1+\lambda_{el\text{-}b})(1+\lambda_{el\text{-}el})m_b}$$

$$\omega^2_{pl} \propto N(0)e^2\langle v^2\rangle_{FS} \propto 1/m^*$$

$$\Omega^2_{pl} \propto \Sigma_{i=1,3(5)} N_i(0)e^2\langle v^2\rangle_{FS(i)} \propto \Sigma_i 1/m^*_i$$

for multiband systems , $N_i(0)$ partial DOS

No simple correlation between T_c and mass renormalization



taken from F. de Medici

Two steps of mass renormalization

- **High**-energy: Coulomb + Hund
- **Low**-energy: el-boson interaction (spin-fluctuations, phonons, etc.) Eliashberg-Migdal theory

DMFT-prediction for pnictides:
Yin, Haule & Kotliar **(**2011)

$$m_*/m_b \approx 2.5 - 3$$

Warning: **different** renormalization for **different** orbitals (bands)! Fe $3d_{xy}$!

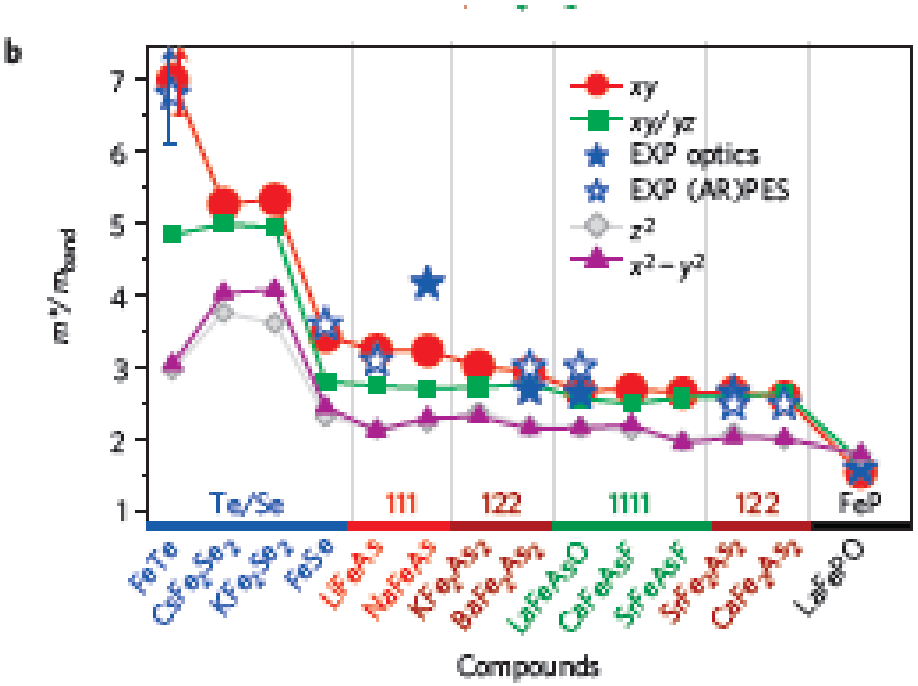


Figure 1 | Ordered magnetic moments and mass enhancements in iron-based compounds. **a**, The DFT + DMFT calculated and experimental[6–13] iron magnetic moments in the SDW and DSDW states. Also shown is the calculated fluctuating moment in the paramagnetic (PM) state. **b**, The DFT + DMFT-calculated mass enhancement m^*/m_{band} of the iron 3*d* orbitals in the paramagnetic state and the low-energy effective mass enhancement obtained from optical spectroscopy experiments[16–19] and (angle-resolved) photoemission spectroscopy experiments[20–24].

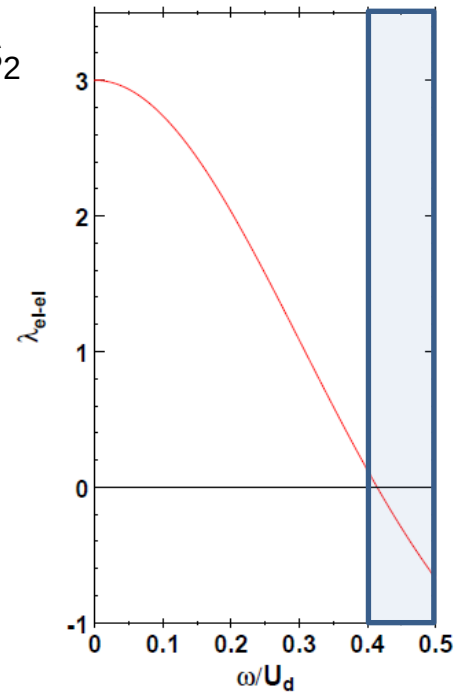
Phenomenological description of the (lower) high-energy mass renormalization

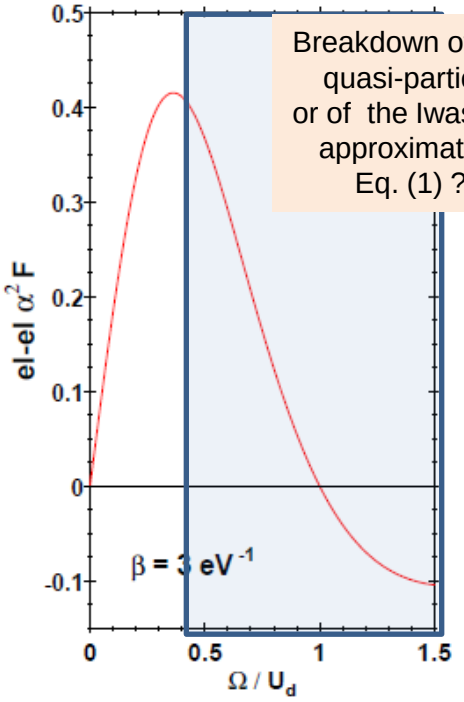
Heavily hole doped $(Ca,Na)Fe_2As_2$

$\lambda_{el\text{-}el}(0) = - \partial \mathrm{Re}\, \Sigma_{el\text{-}el}(\omega)/\partial \omega|_{\omega=0}$

$\lambda_{el\text{-}el}(0) = 0.5\beta U_d$

$= 2.5 \div 3$





Breakdown of the quasi-particle or of the Iwasawa approximation Eq. (1) ?

Self-energy:

$$\Sigma_{el\_el} = g\omega/(\omega^2+i\eta^2)^2 \quad , \qquad (1)$$

$g = 0.5\beta\eta^2$

$\eta \approx U_d = 2$ eV

$\lambda_{el\text{-}el}(0) = 2.5 \div 3$

Fe 3*d*

β - empirical factor

Iwasawa (2013) *4d*-metal Sr_2RuO_4

$\lambda_{el\text{-}el}(0) = 1.6 \div 1.9$

$U_d = 1.2 \div 1.5$ eV

$\beta = 2.53$ eV^{-1}

Our quantitative approach

- Comparison of DOS (specific heat) and dHvA
- Comparison of calculated and unscreened plasma frequencies at high-temperature and low-temperature as seen in the penetration depth or the μSR – data at T -> 0

With an unscreened plasma frequency of Ω_{pl}=1.33 eV derived from reflictivity data for an optimally doped La-1111 polycrystalline sample we obtained

$\lambda_{tot,el-b} = \lambda_{sf} + \lambda_{ph} \approx 1$ **to 1.2** i.e. **no strong coupling** (Drechsler2008)

Bare (LDA) plasma frequencies

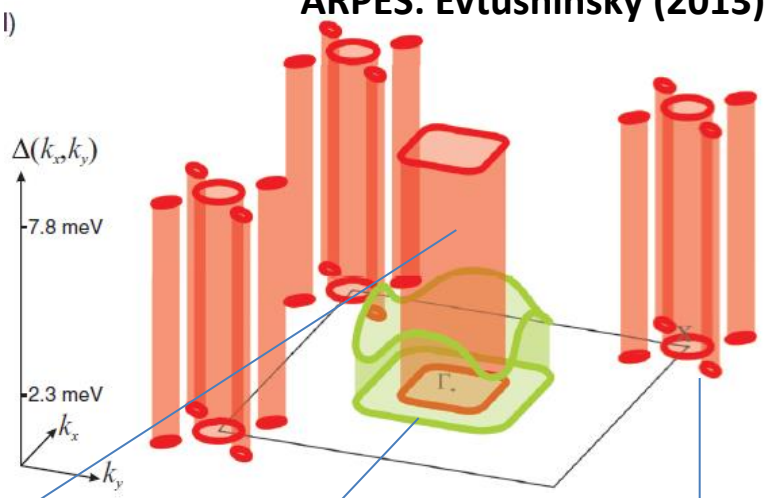
material	DFT $\|\|$ (ab)	ε_∞ (exp)	$\|\| \Omega_{pl}$ (exp)	mass ratio
LaOFeAs	**1.95. ÷2.3**	**10**	**1.29-1.33** (0.6)	**2.3 - 2.6**
$SrFe_2As_2$	**2.8**	**14**	**1.9**	**2.2**
$La_xSr_{1-x}Fe_2As_2$	**2.8**			
$SrFe_{2-x}Co_xAs_2$	**2.7**			
$BaFe_2As_2$	**2.63**	**14.9**	**1.58- 2.07**	**1.6 - 2.77**
$K_xBa_{1-x}Fe_2As_2$	**2.63**		1.5; **1.6, 1.9** ±0.2	**1.92 - 2.7**
$CaFe_2As_2$	**2.95**			
KFe_2As_2	**2.9**		**2.27 - 1.94**	**1.63-2.23**
NaFeAs	**2.68**			
LiFeAs	**2.9**			
LaOFeP	**2.37-2.57**	10	**1.85**	**1.64 – 1.95**
α - Fe	**6.85**		**3.72 - 4.9**	**1.95 - 3.4**

Our estimate for the high-energy mass renormalization

$Ca_{0.32}Na_{0.68}Fe_2As_2$ -I

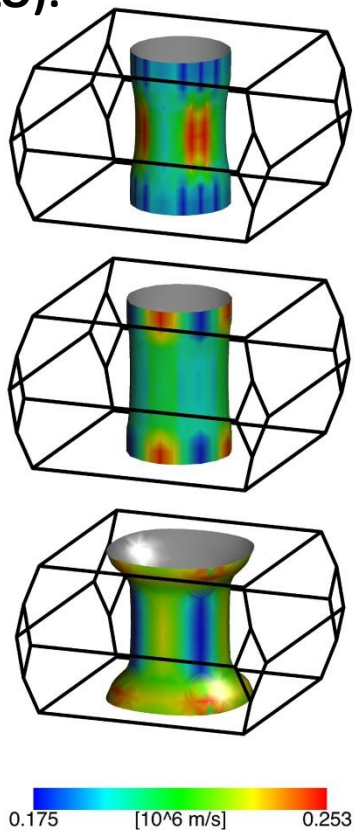
optimal doping: T_c = 34 K at high doping

ARPES: Evtushinsky (2013)



Effective model: 2 hole + 1 electron-FSS

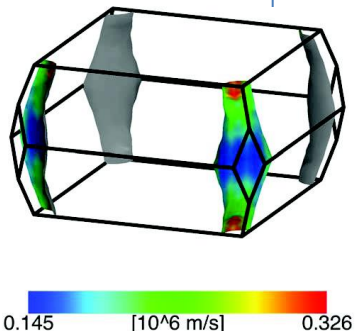
LDA(FPLO):

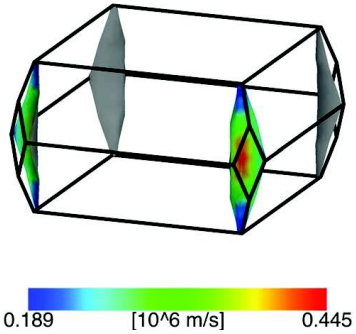


band 1

band 2

band 3





Band 44

3 hole- FSS

2 electron-FSS

$Ca_{0.32}Na_{0.68}Fe_2As_2$ – specific heat fit

3-band model for the electronic specific heat

Fitting: parameters:

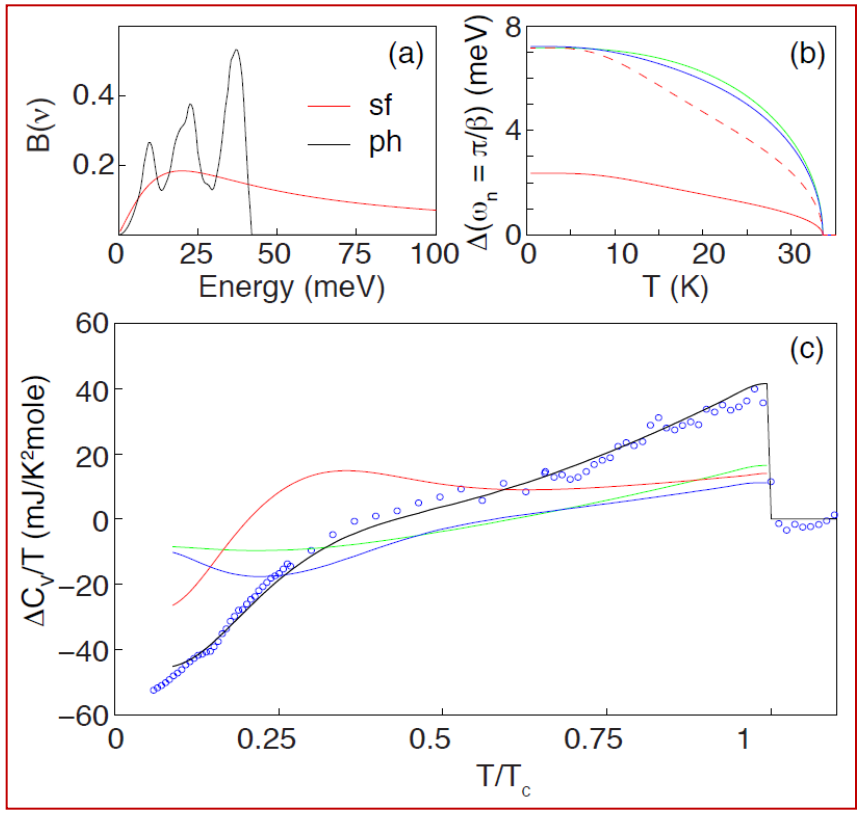
3 partial DOS

3 coupling constants:

1 intraband (el-ph)

2 interband (el-sf)

$\lambda_{11}= \lambda_{22}= \lambda_{33} = 0.45$
$\lambda_{13}=-1,\ \lambda_{12}= -0.1, \lambda_{23}=0$
$\lambda_{tot} = 0.9$
$T_c(\lambda_{ph}=0) = 19$ K
$T_c(\lambda_{sf}=0) = 5$ K
$T_c(\lambda_{ph}+\lambda_{sf}) = 34$ K



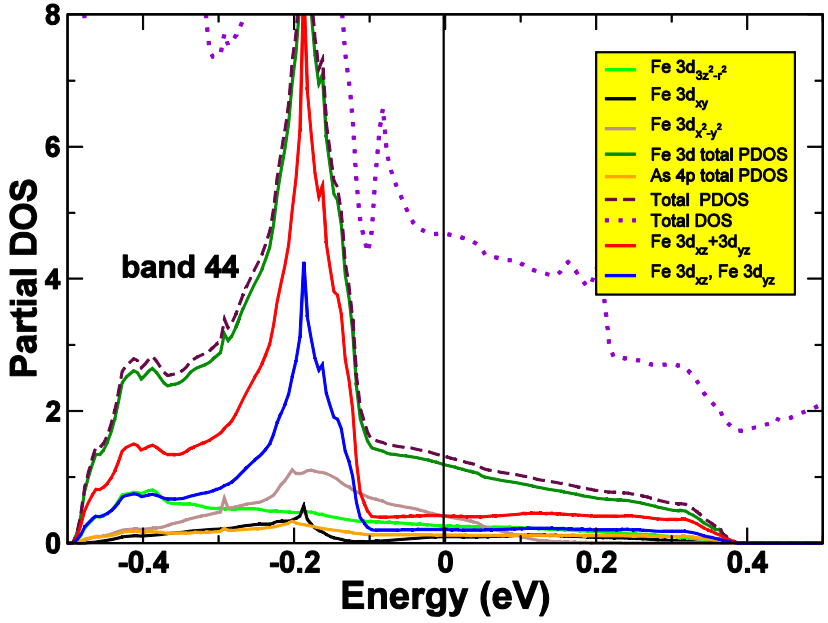
High T_c without strong coupling !

3 gaps predicted:

Δ_1=7.2 meV, Δ_2=2.3 meV, Δ_3=7.1 meV in accord with recent ARPES data (Evtushinsky 2013)

$Ca_{0.32}Na_{0.68}Fe_2As_2$ -III

Remaining problems: significant deviations in the PDOS for band 44 (2) between our fit and the LDA (FPLO) calculations by a factor of 2



one LDA-band starts to fail

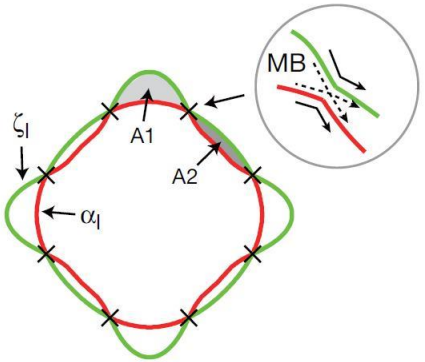
precursor of the K122 problems ?

KFe_2As_2 (K-122)

SH & LDA: large mass enhancement (me) ≈ 9 !!

Where does it come from ?

dHvA (Terashima2013): **highly nonuniform** me 2.2 – 24 !!



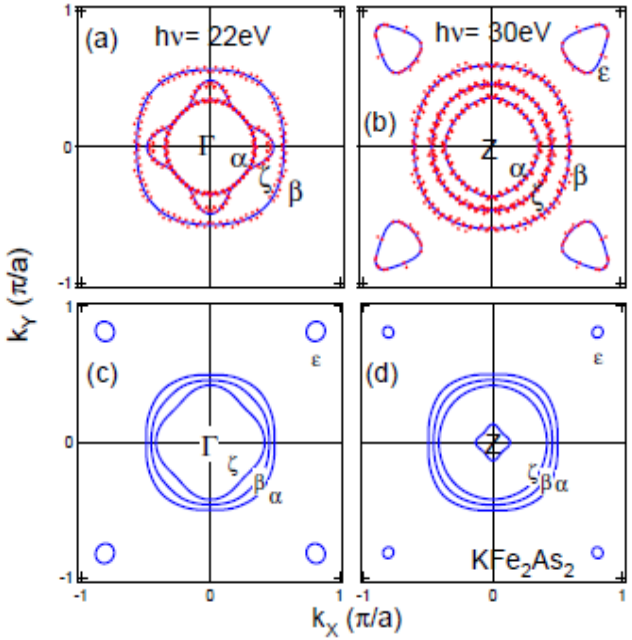


FIG. 3. (Color online) Comparison of FSs obtained by ARPES and those predicted by band-structure calculation. (a),(b) FSs determined by ARPES. k_F positions in Fig. 2 have been symmetrized in the first BZ. (c),(d) FSs given by the band-structure calculation. A small FS around the Z point comes from a three-dimensional d_{z^2} band shown in Fig.

TABLE I. Cross-sectional areas and effective masses of FSs of KFe_2As_2 determined by ARPES and dHvA experiment. The areas are expressed as a percentage of the area of the 2D BZ. m_e and m_b are the free-electron and band masses, respectively.

FS	k_z	area			m^*/m_e (m^*/m_b)		
		ARPES	dHvA	LDA	ARPES	dHvA	LDA
α	Γ	9.1	8.2	20.8	5.1 (2.0)	6.0 (2.3)	2.6
	Z	9.8	8.6	21.6	6.6 (2.3)	6.5 (2.2)	2.9
ζ	Γ	12.2	10.3	12.2	11.0 (7.9)	8.5 (6.1)	1.4
	Z	17.0	15.7	13.8	9.6 (4.0)	18 (7.5)	2.4
β	Γ	27.3		16.7	16.3 (6.3)		2.6
	Z	30.0		17.4	17.9 (6.9)		2.6
ϵ	Γ	2.1	0.86	0.11	5.6 (18.7)	6.0 (20)	0.3
	Z		1.29	0.36		7.2 (24)	0.3

LDA-problems in describing K-122

1. wrong sequence of bands near Γ
2. wrong FSS cross sections
3. Large shifts band shifts required (e.g. +0.6 eV for the $3d_{xy}$ orbitals and down shifts for the remaining orbitals to keep charge neutrality

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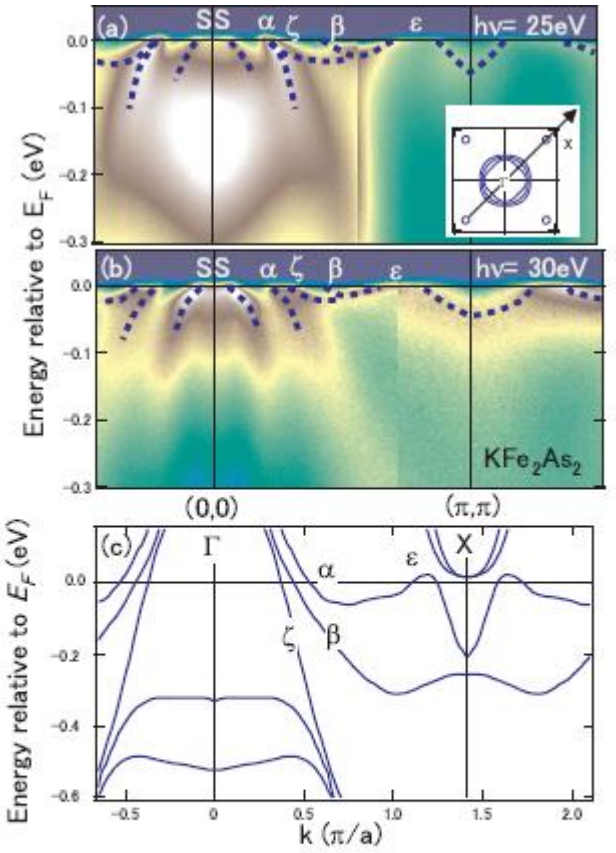
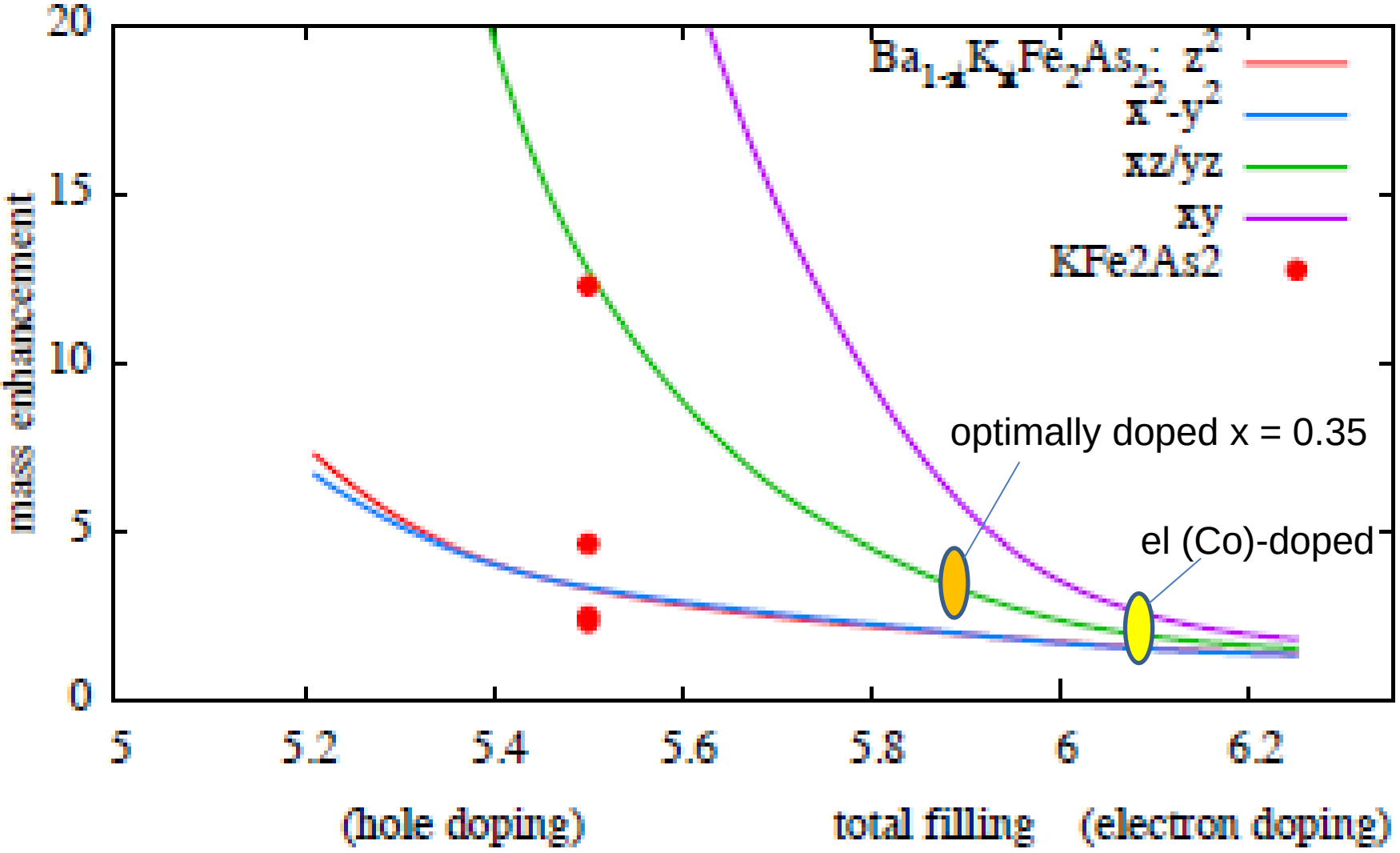


FIG. 1. Band dispersions of KFe_2As_2 in the zone diagonal direction. (a),(b) ARPES spectra taken at hν= 25eV and 30eV, respectively, corresponding to k_z=6.5 and 7.0 ($2\pi/c$). SS denotes surface states. (c) Band dispersions predicted by band-structure calculation.

Selected Mottness and its consequences for the orbital dependent high-energy mass enhancement



Approaching the Mott-transition at n_{el}= 5 (Fe^{+3}), the mass start to **diverge**

Rather different high-energy (?) band renormalizations

Terashima2013

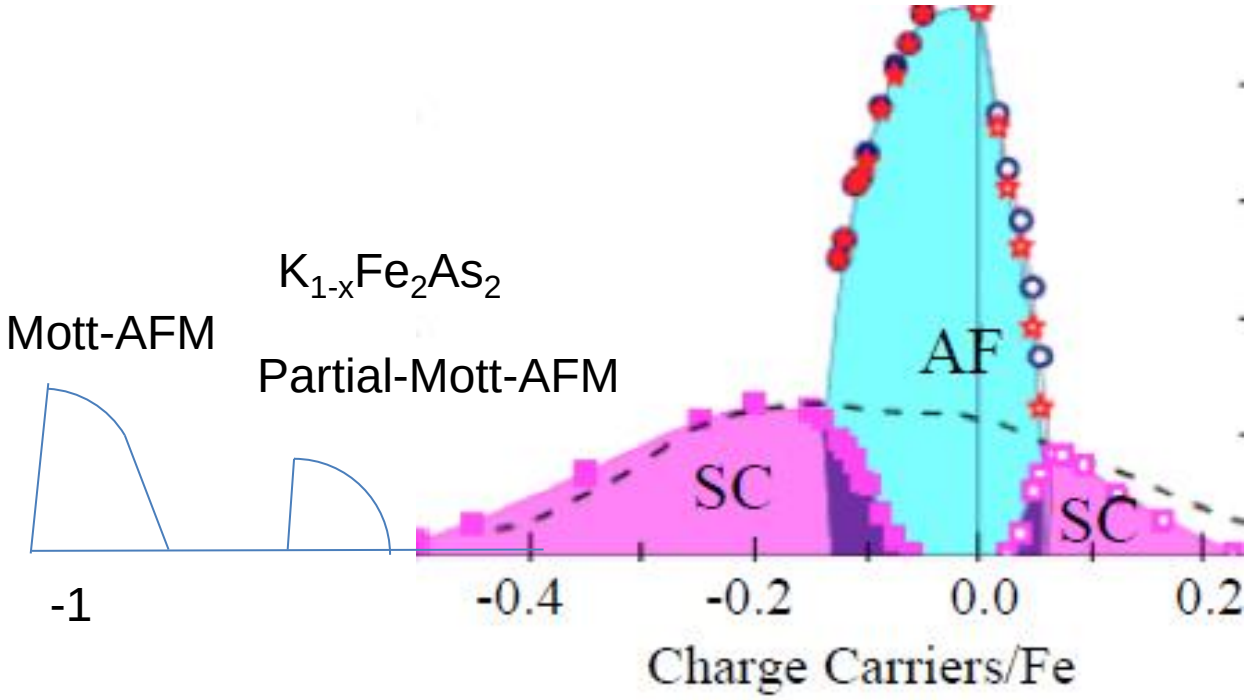
FSS	γ_i [mJ/mol K^2]	me (dHvA)	me (ARPES)
propeller ε	**4 x 9.6 = 38.4**	**20 - 24**	18.7 **20.3**
inner cylinder α –	9.1	2.3 5	2 4.05
square ζ d_{x2-y2}	**27.6**	**7.9 5**	**6.1 4.05**
rounded big square β d_{xy}	**19.2**	**6.3 -6.9**	6.6
Total	**94**		

η_{CH} = **2.54**
like for other weakly correlated pnictides

η_{CH} = **3.35**
like for more correlated pnictides

From Eliashberg-analysis $\lambda_{tot,b}$ = 0.97, λ_{sf} =0.6, λ_{ph} = 0.17

Possible phase diagram



Avci et al. PRB 85, 184507 (2012)

Remarks on other pnictides

LiFeAs : $s_{\pm}$ - wave, T_c=18 K, $\lambda_{tot,\,b} \approx 0.6$, $\lambda_{el\text{-}ph} \approx 0.2$

no strong coupling ! From fitting the el-specific heat & quasi- particle interference

Optimally doped $(Ba,K)Fe_2As_2$: from LDA + spec. heat data (Popovic, 2011) we have:

$$(1+\lambda_{el\text{-}b})\eta_{CH} \approx 5 \quad \rightarrow \lambda_{el\text{-}b} \leq 1 \div 1.5 \text{ , if } \eta_{CH} \approx 2 \div 2.5$$

No room left for high-energy renormalizations !

Electron (Co) doped Ba-122:

$(1+\lambda_{el\text{-}b})\eta_{CH} \approx 2 \div 3$

one way out: a pseudo-gap ???

In some of these systems pseudo-gap like features have been observed!

Summary & Outlook

1. Three Fe-pnictide SC (1111, 122, 111) can be well described by the multiband $s_{\pm}$-Eliashberg-theory at intermediate coupling strength
2. High-energy mass renormalization is always important!

   Strong constraint for the strong el-boson coupling
3. Approaching the overdoped hole region, different high-energy renormalizations for different bands – special role of Fe 3 d_{xy}- orbitals
4. K122 multiband ***d***-wave model proposed

1. **What about the Rb-122 and Cs-122? Mott transition for a single band ?**
2. **More studies of disorder effects includung magnetic impurities are necessary**
3. **What about the real high-T_c (45- 56 K) superconductors, selenides and tellurides?**

Selected Mottness