Interplay of multiple spin flutuation modes in the iron-based superconductors : Correspondance between momentum and real space viewpoints

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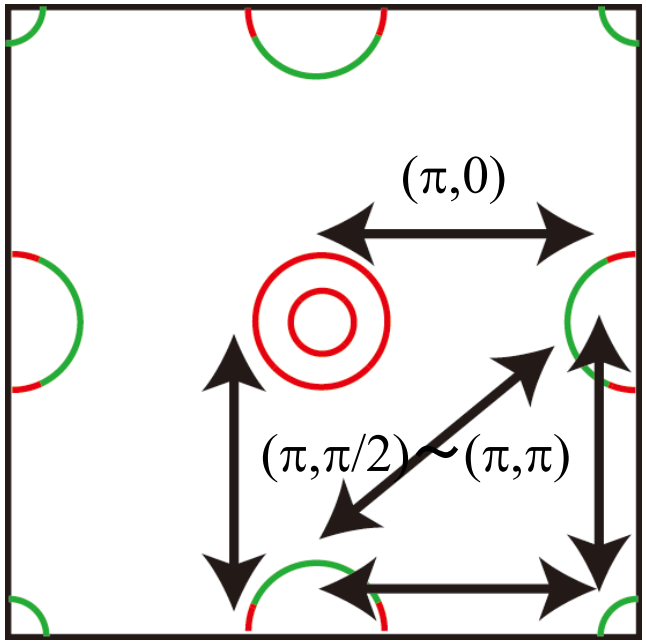
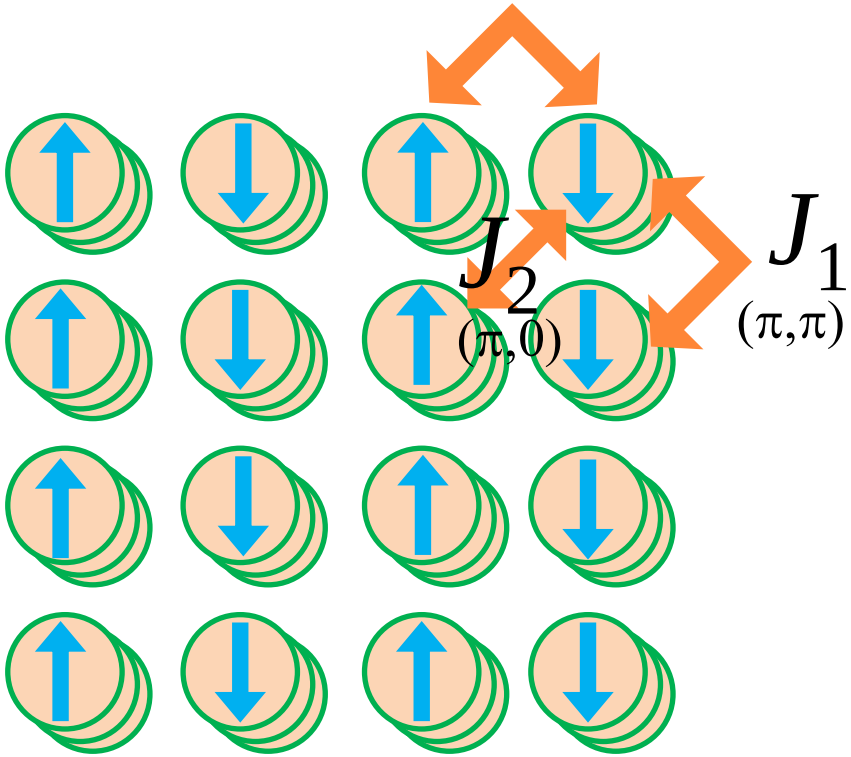
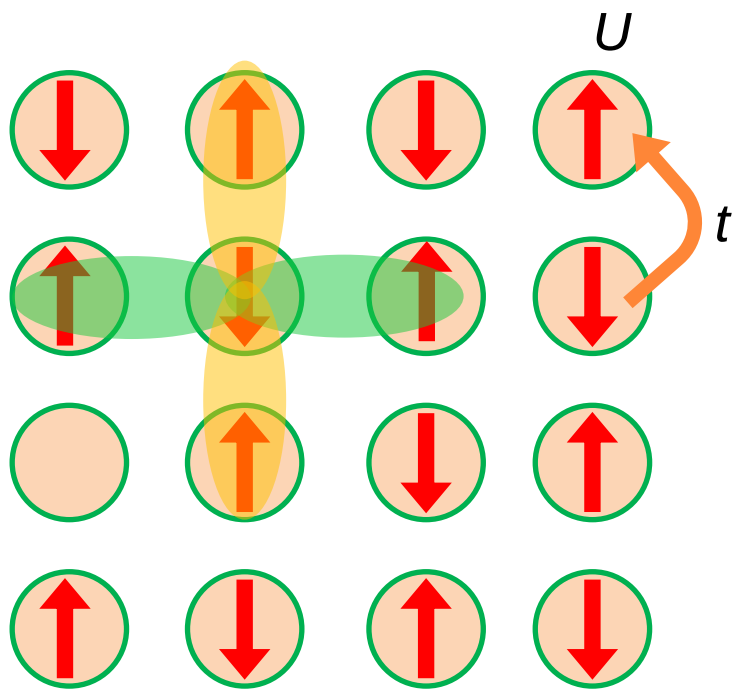
Spin correlation in iron-based SC
itinerant vs. localized, momentum vs. real space





The case of single orbital Hubbard model

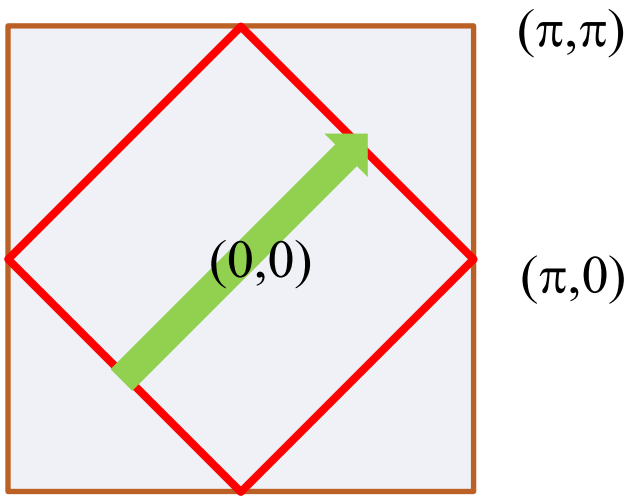
d-wave pairing

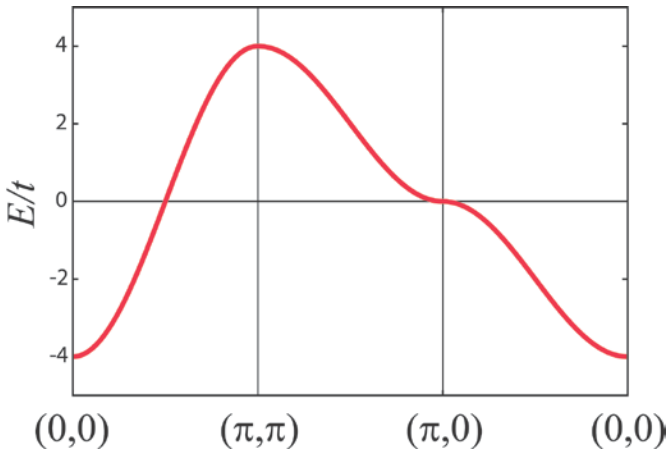


at half-filling $J\, S_i \cdot S_j$ →antiferromagnetism with q∼(π,π)

$$J = 4t^2/U$$

The case of single orbital Hubbard model

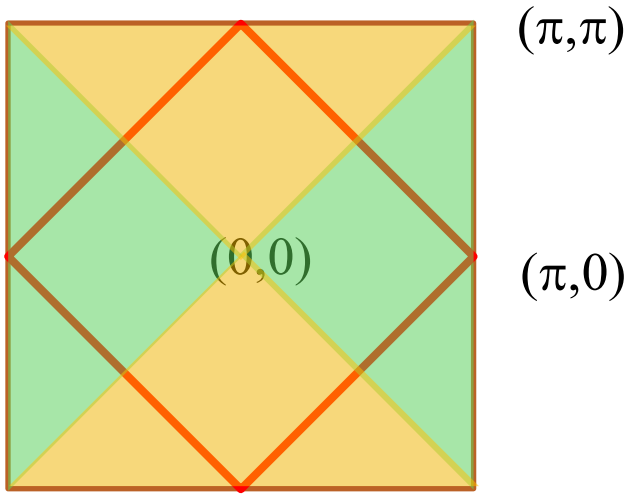




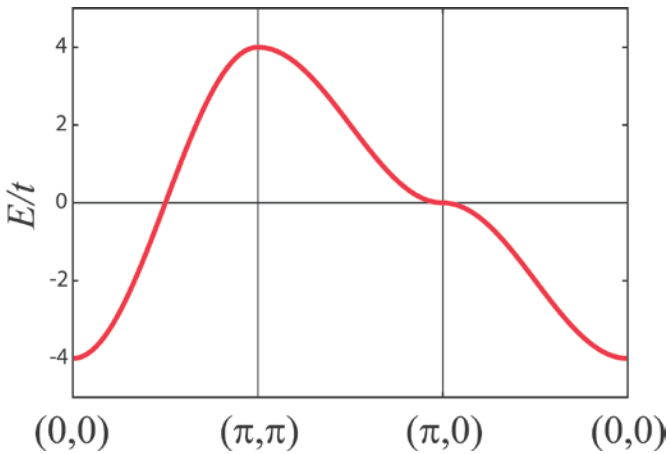
Fermi surface nesting

spin fluctuation q∼(π,π)

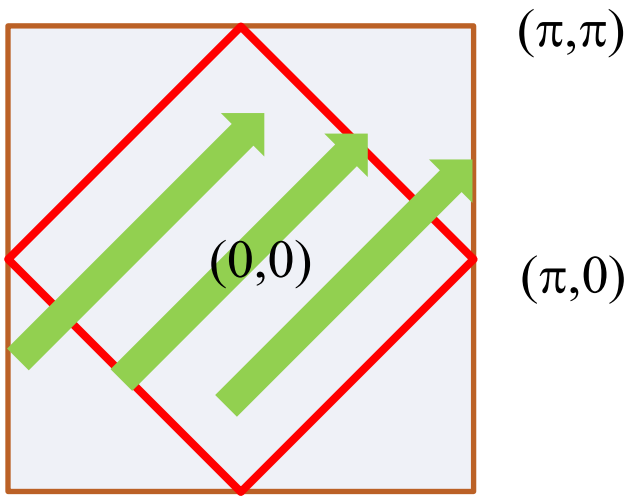
The case of single orbital Hubbard model

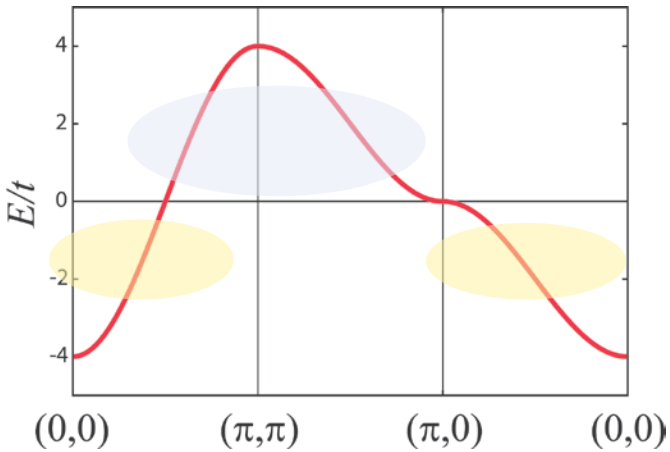


d-wave pairing



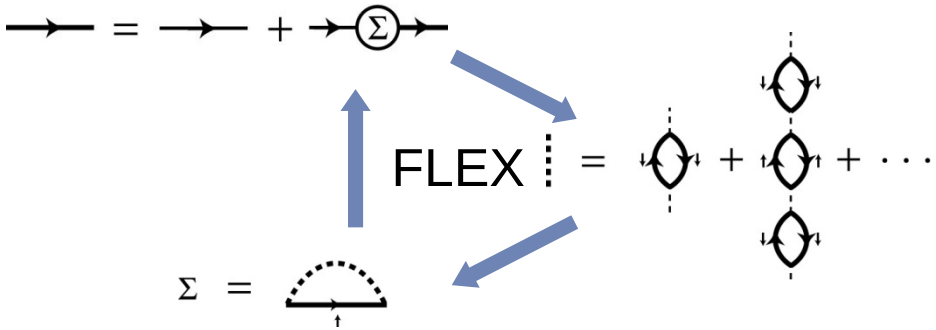
The case of single orbital Hubbard model





Fermi surface nesting

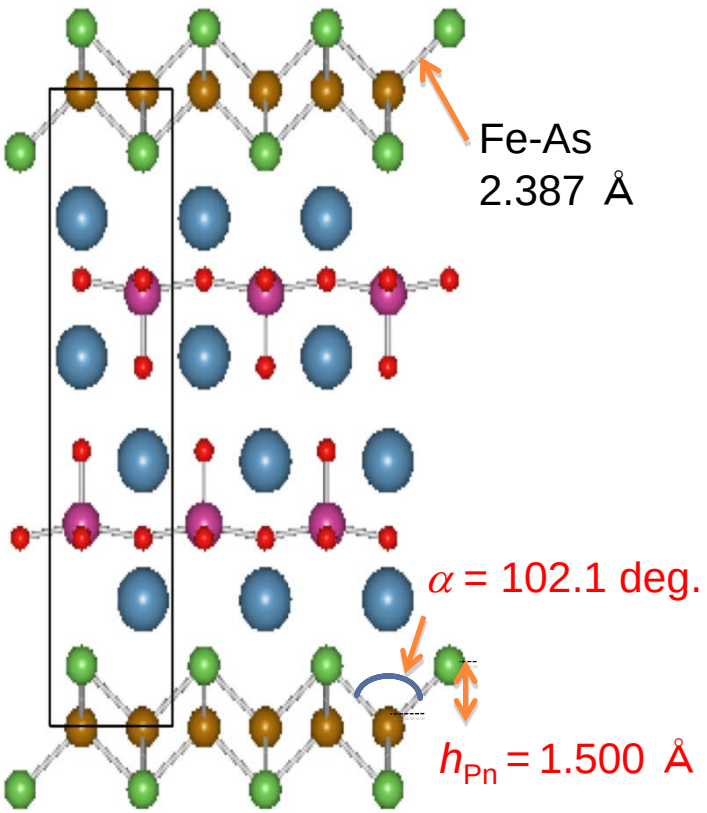
Interaction between electrons and holes away from E_F is also important
→ Important to take into account self energy corrections

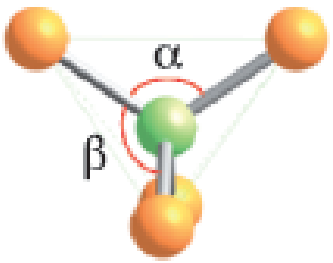


Bickers et al, 1988

Σ due to spin fluctuation

CaAl42622





$FeAs_4$-tetrahedron

a = 3.7133 Å cf. a=4.005 Å ($LaFeAsO_{1-y}$)

c = 15.404 Å

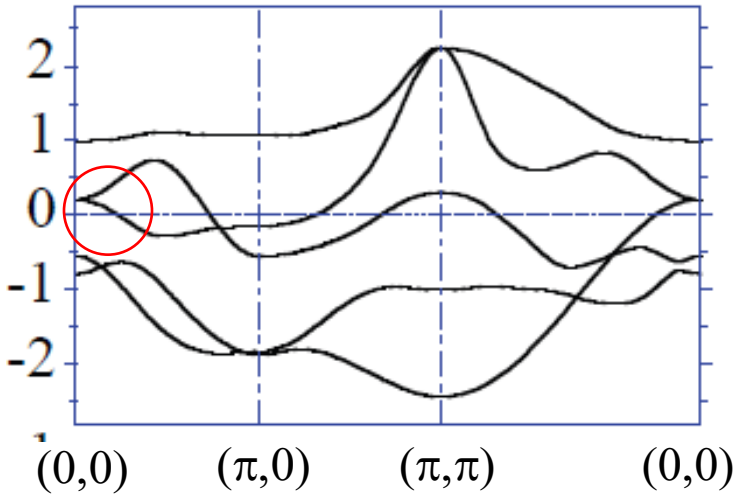
P.M.Shirage et al., Applied Physics Letters 97(2010)172506

smallest α and highest h_{Pn} is realized

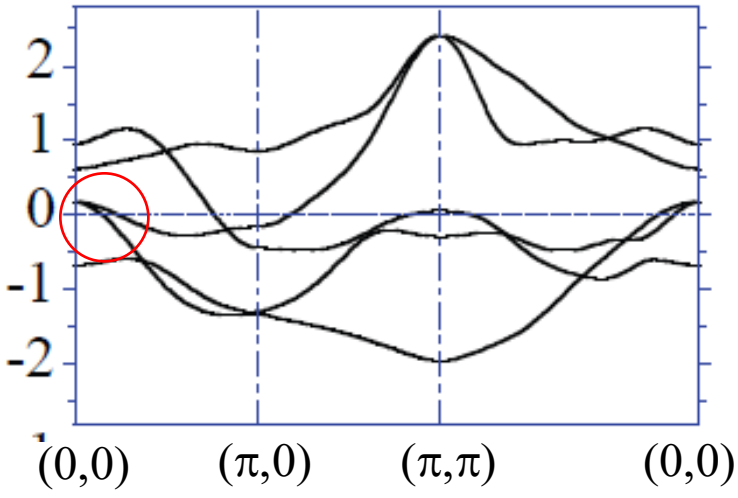
CaAl42622

T. Miyake *et al.*: J. Phys. Soc. Jpn. **79** 123713
T. Kosugi *et al.*: J. Phys. Soc. Jpn. **81** 014701

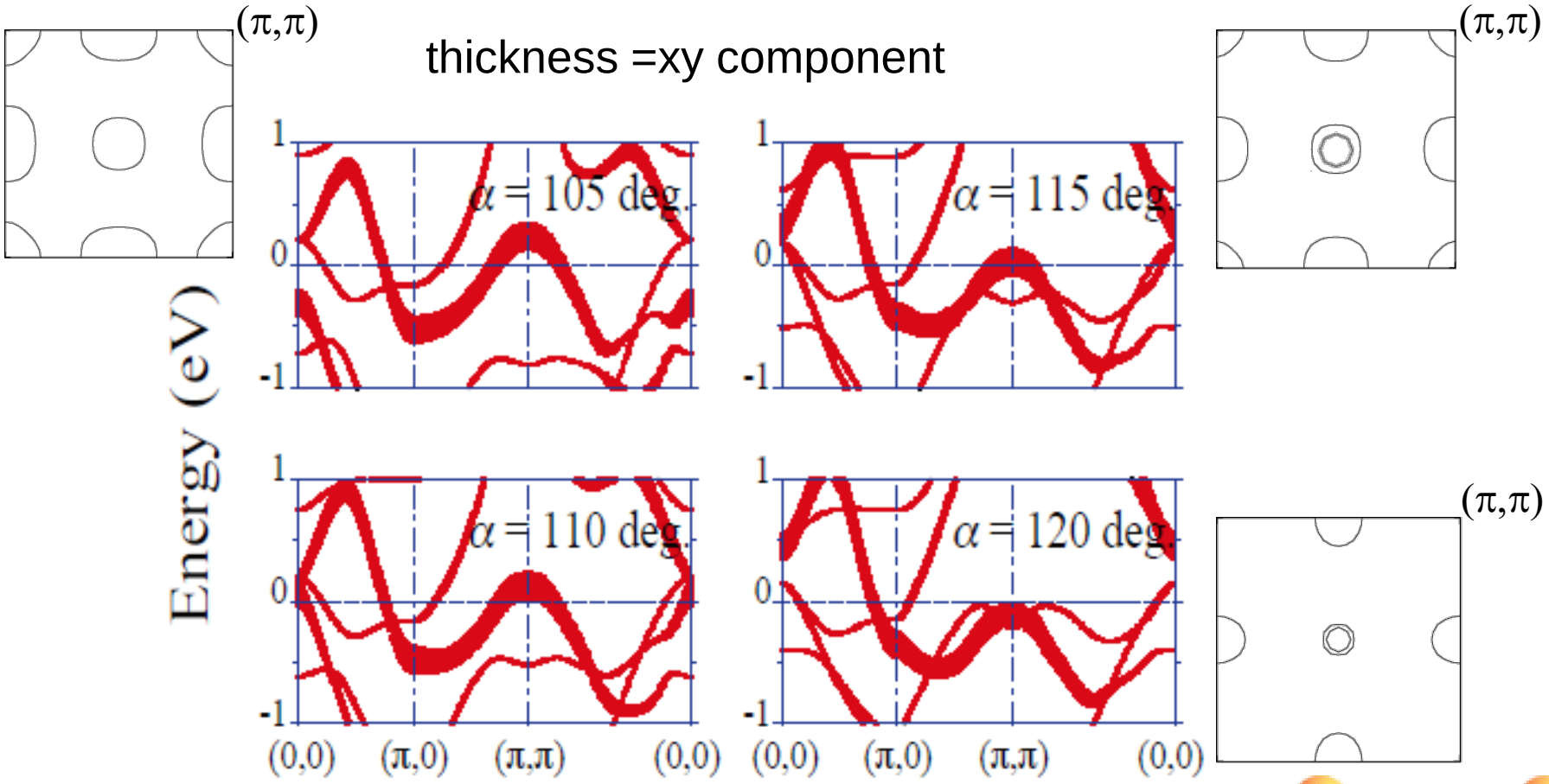
$Ca_4Al_2O_6Fe_2As_2$



LaFeAsO

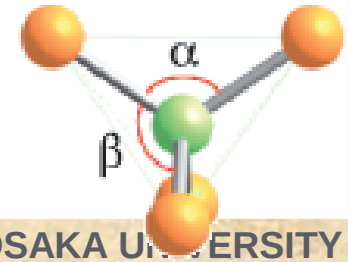


Band structure variance against bond angle



T. Miyake et al, 2010

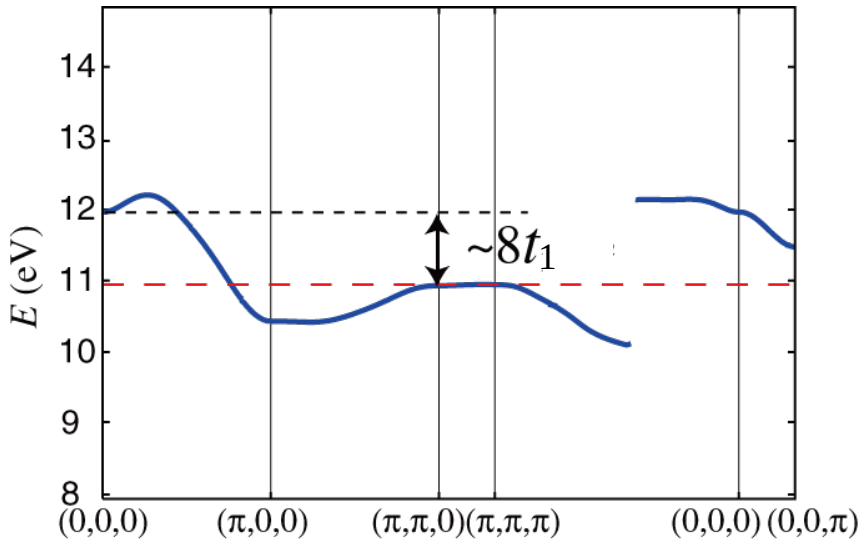
bond length = constant

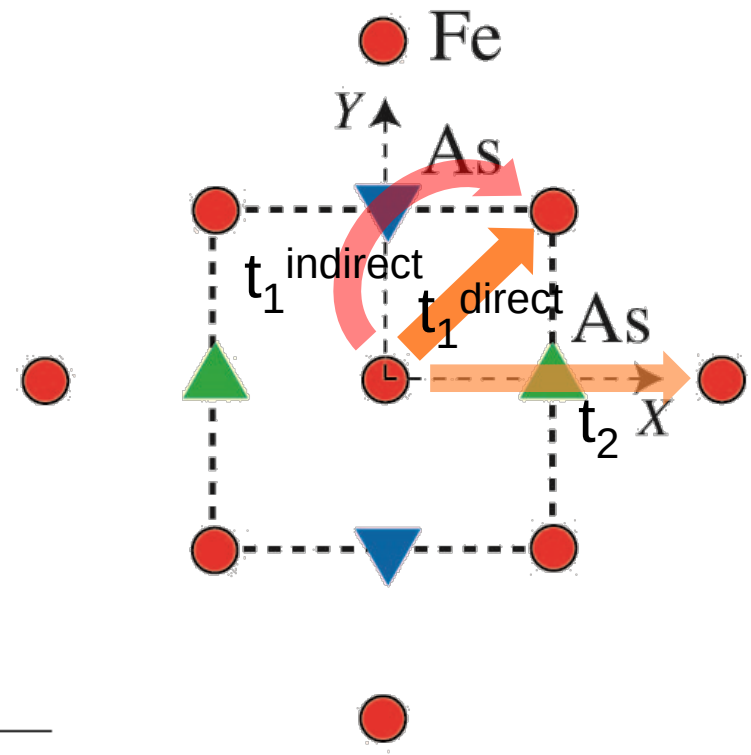


Real space hoppings

$$\varepsilon_{xy} \sim 2t_1(\cos k_x + \cos k_y) + 4t_2 \cos k_x \cos k_y$$

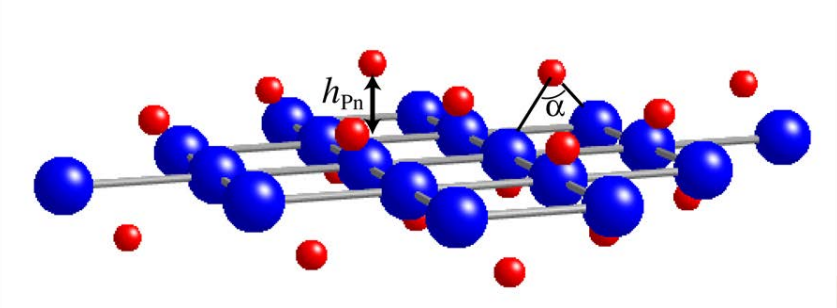
xy orbital portion of the band





	ε_{xy}	t_1	t_2
LaFeAsO	0.189	0.151 (−0.243)	0.117
$Ca_4Al_2O_6Fe_2As_2$	−0.189	−0.040 (−0.369)	0.066

Miyake et al, 2011



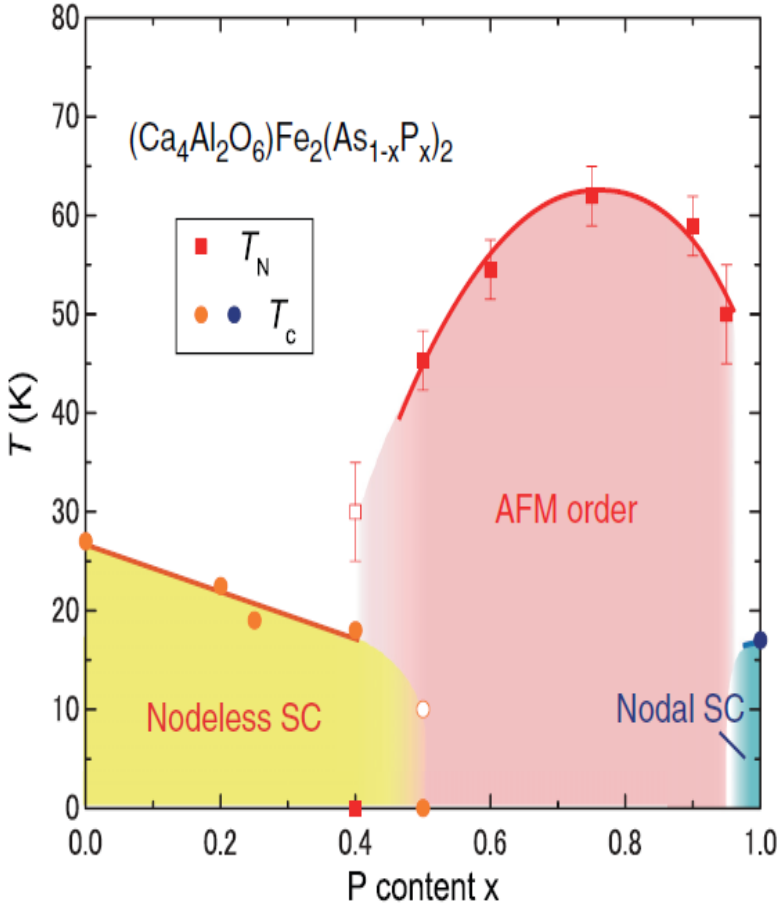
$t_1 = t_1^{direct} + t_1^{indirect}$

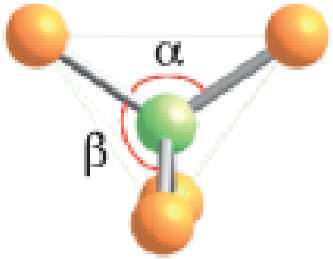
for smaller bond angle

$t_1^{direct} < 0$ ↗

$t_1^{indirect} > 0$ ↘

CaAl42622 phase diagram





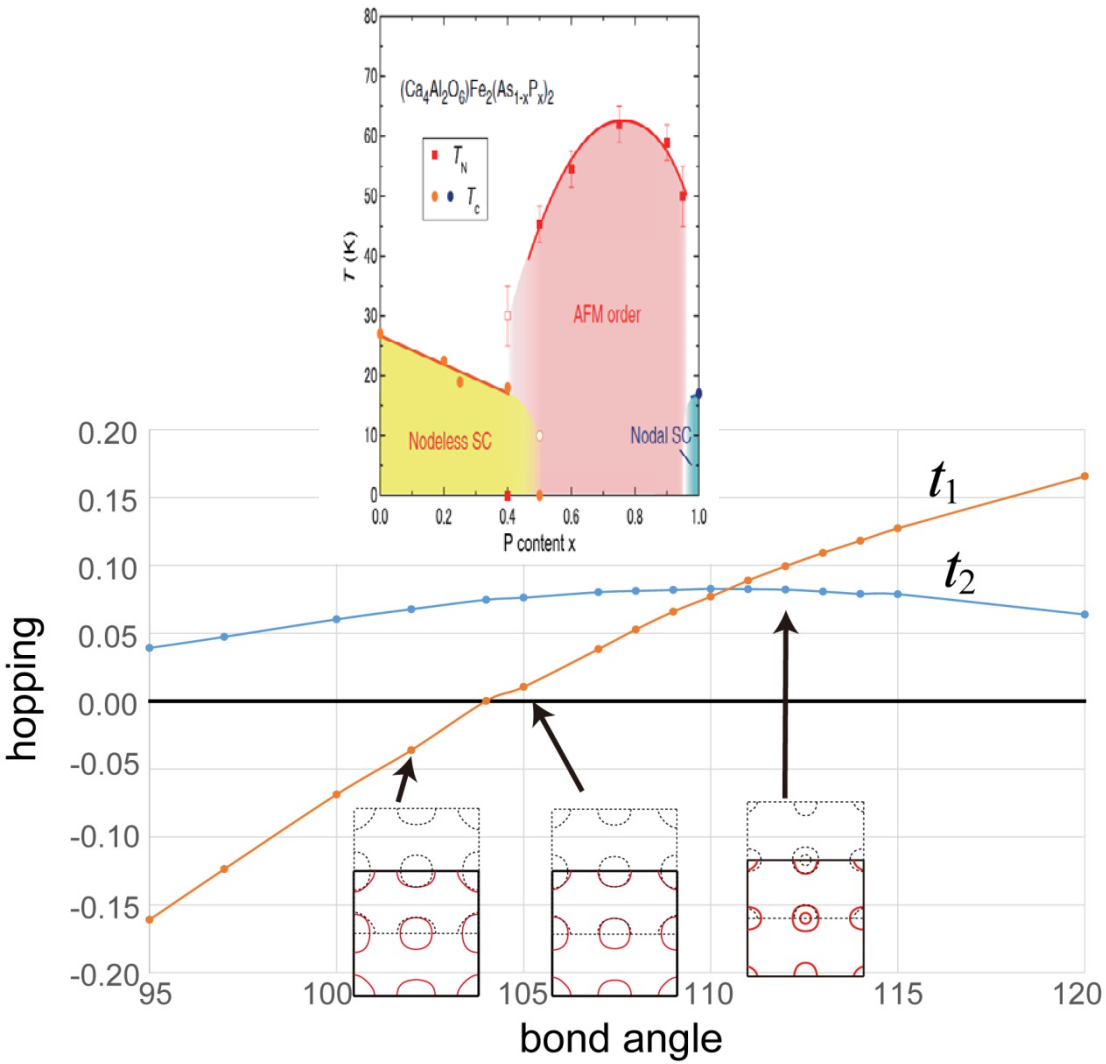
$FeAs_4$-tetrahedron

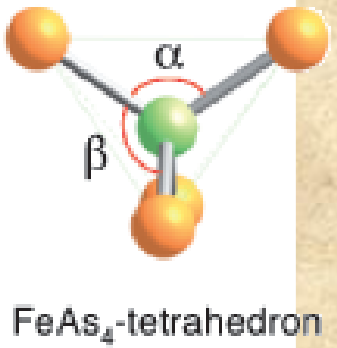
102° ⟷ 109°

α

Kinouchi, Mukuda et al, 2012

CaAl42622 phase diagram

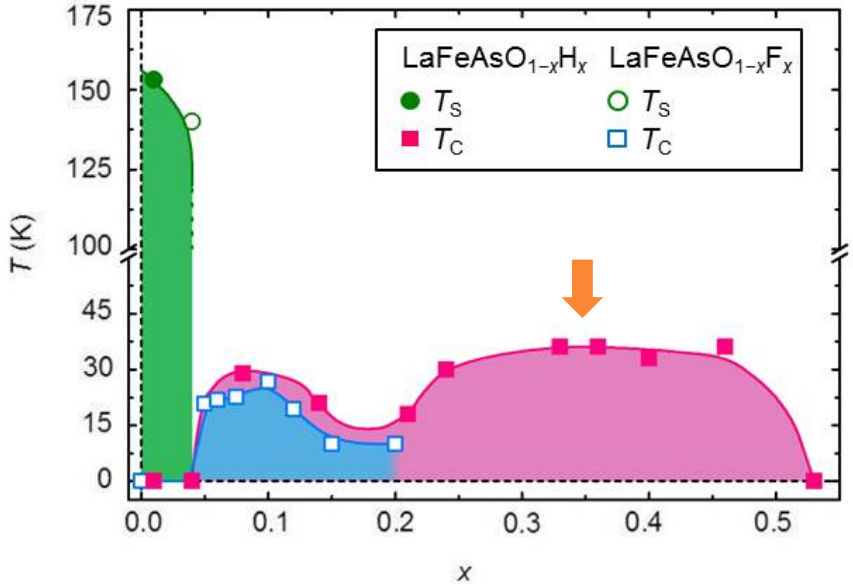




$t_1 \sim 0$(→"$J_1 \sim 0$") and good nesting roughly coincides
→AF sandwiched between SC

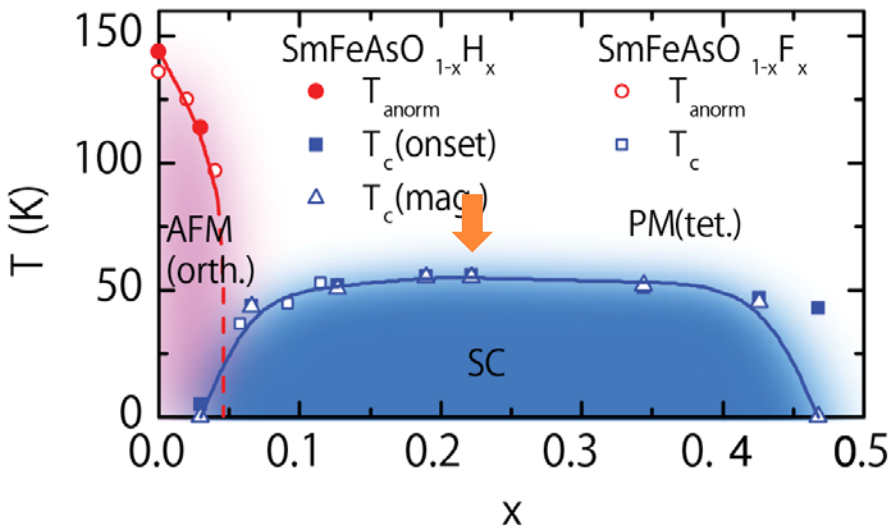
Heavily electron-doped 1111 Iron-based SC

La



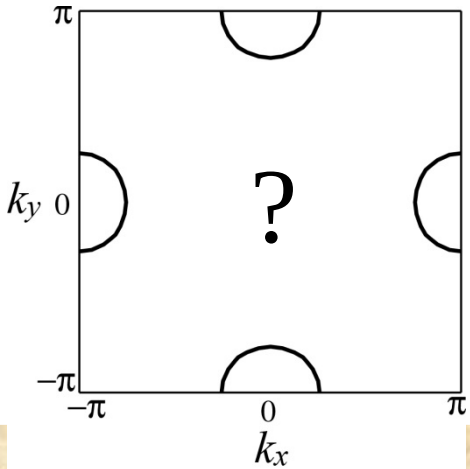
Iimura *et al*. ,Nat. Comm. **3** 943 (2012)

Sm



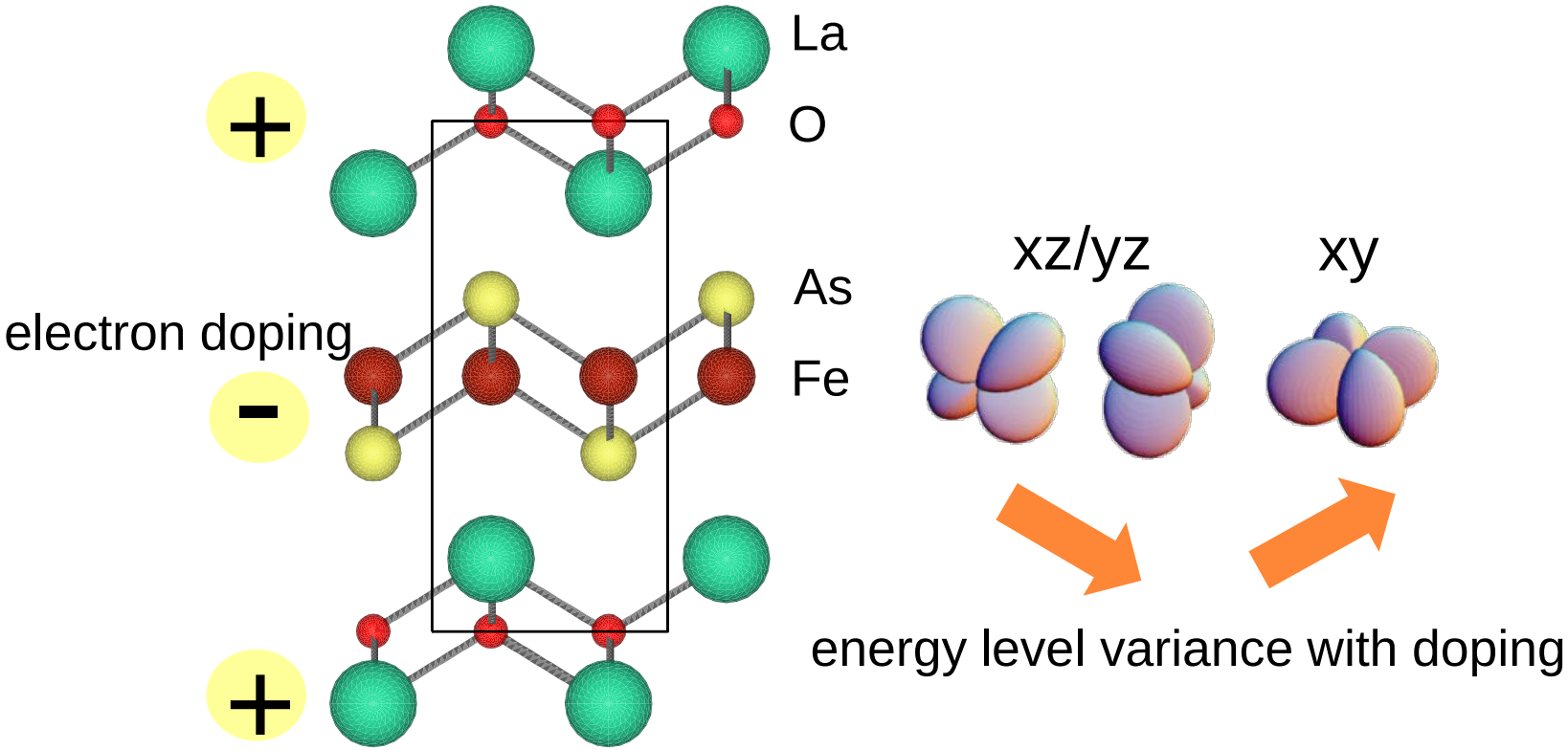
T. Hanna *et al.*, Phys. Rev. B **84** 024521 (2011)

maximum Tc is obtained
In the heavily doped regime



In the rigid band picture,
the hole Fermi surface disappears in the
highly electron doped regime

Effect of doping on the band structure (I) : energy level



consider the band variation by doping adopting virtual crystal approx
=average potential of different atoms

.

Model construction

for each doping rate,
first principles band structure → 5 orbital tightbinding model

VASP , experimentally determined bond angle

wannier90

+

Multiorbital FLEX

Bickers et al,, H.Ikeda et al

Dyson eq.

Green's function in orbital representation: $G(k)$

irreducible susceptibility: $\hat{\chi}^0_{l_1 l_2, l_3 l_4}(q) = -\frac{T}{N}\sum_k G_{l_1 l_3}(k+q) G_{l_4 l_2}(k)$

l_i : orbital indices

spin susceptibility:

$$\hat{\chi}^s(q) = \frac{\hat{\chi}^0(q)}{1 - \hat{S}^0 \hat{\chi}^0(q)}$$

charge (orbital) susceptibility:

$$\hat{\chi}^c(q) = \frac{\hat{\chi}^0(q)}{1 + \hat{C}^0 \hat{\chi}^0(q)}$$

self energy-$\Sigma^R(\omega=0)$

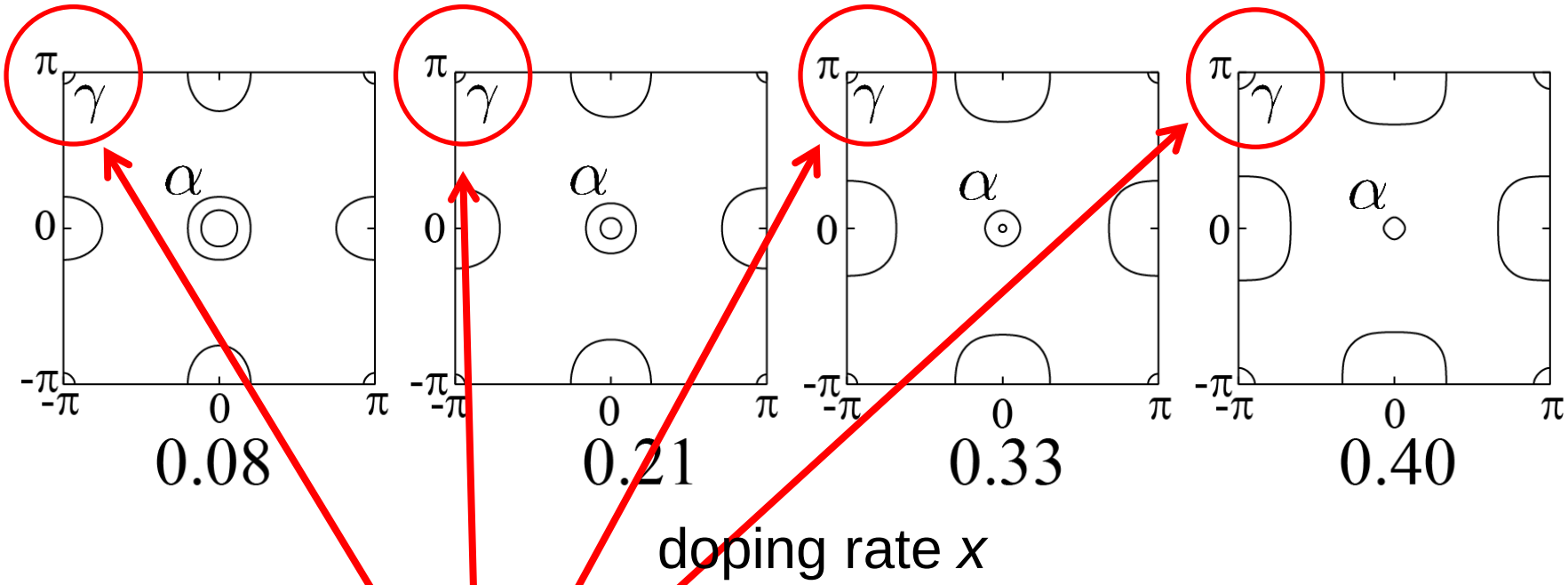
fluctuation mediated
pairing interaction (mainly spin)

linearized Eliashberg eq:

$$\lambda \Delta_{l_1 l_4}(k) = -\frac{T}{N}\sum_q \sum_{l_2 l_3 l_5 l_6} \hat{V}^{s(t)}_{l_1 l_2, l_3 l_4}(q) G_{l_2 l_5}(k-q) \Delta_{l_5 l_6}(k-q) G_{l_3 l_6}(q-k)$$

$\lambda(T)=1$ at $T=T_c$, λ at a fixed temperature used as a qualitative measure of T_c

Fermi surface of the 5 orbital model of La1111



(0,0) *xz/yz*: disappears by doping

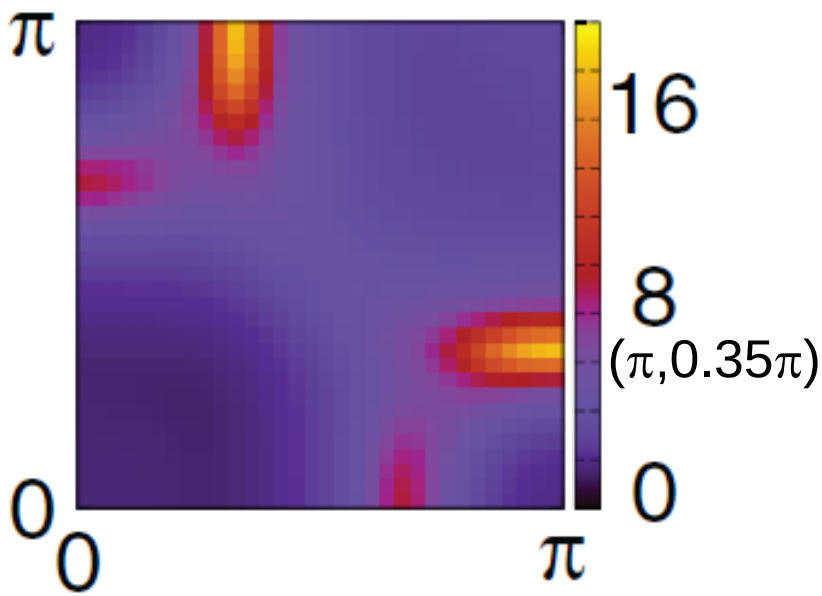
(π,π) $xy=X^2-Y^2$: nearly unchanged by doping

Still, nesting becomes worse by doping

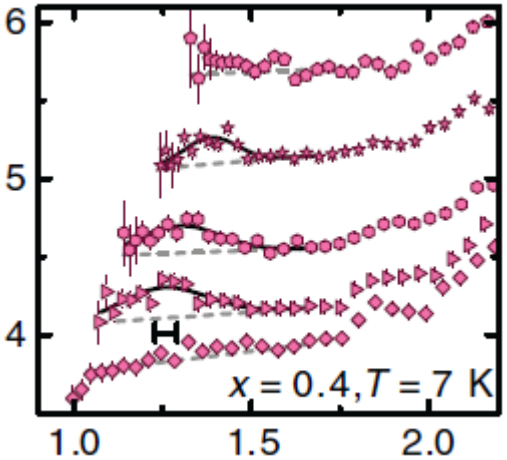
Incommensurate spin fluctuations

x=0.4

spin susceptibility



Inelastic neutron scattering



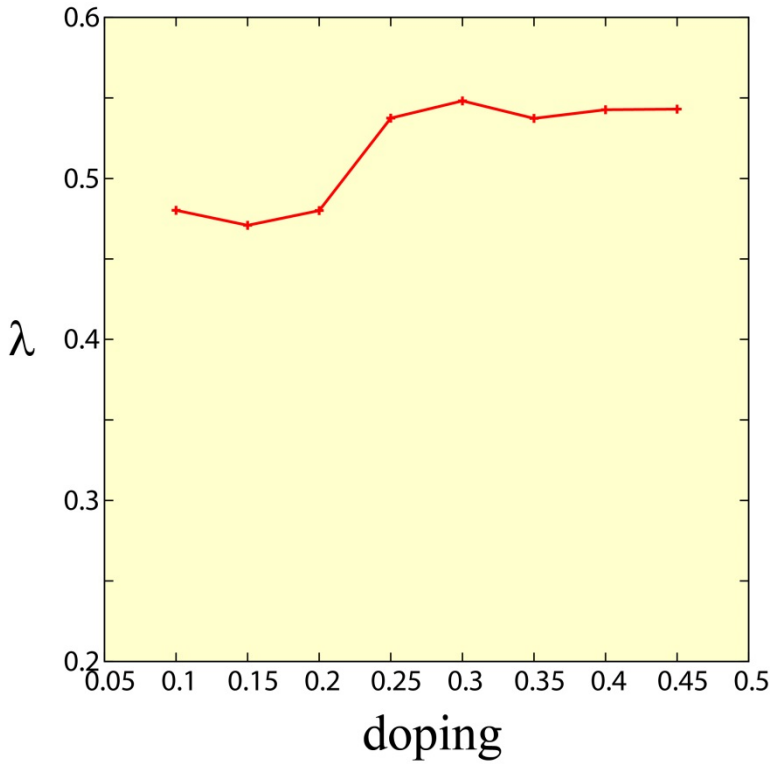
Q~1.26 Å $^{-1}$=(π,0.35π)

Iimura et al, 2013

also indications of magnetic ordering around x～0.45-0.5

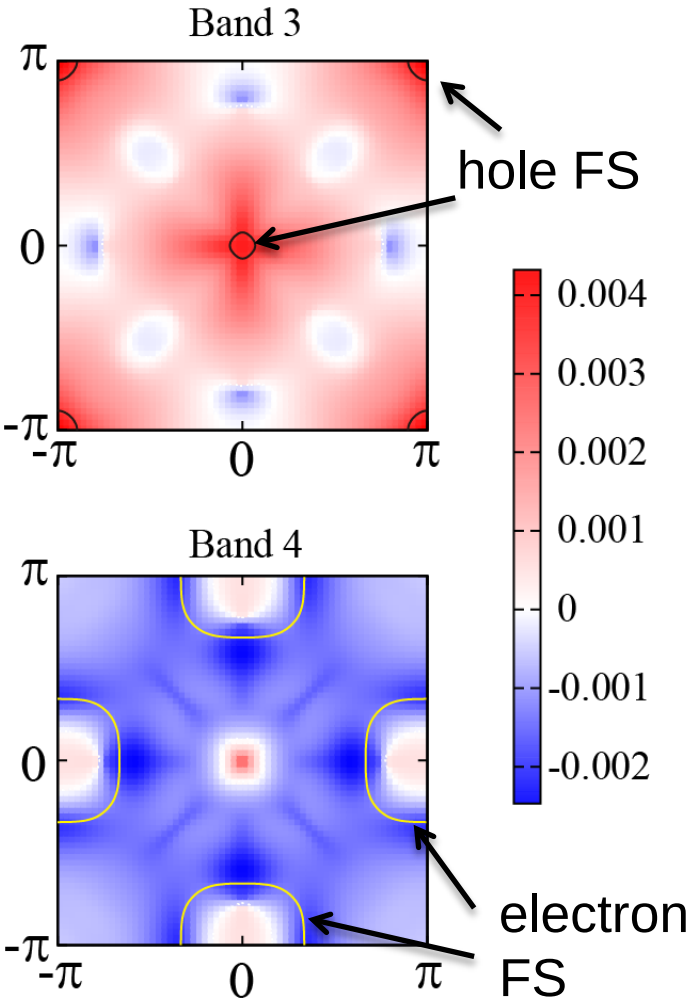
Doping dependence of Eliashberg eq. eigenvalue

Sm1111 T=0.005, U=1.2 eV



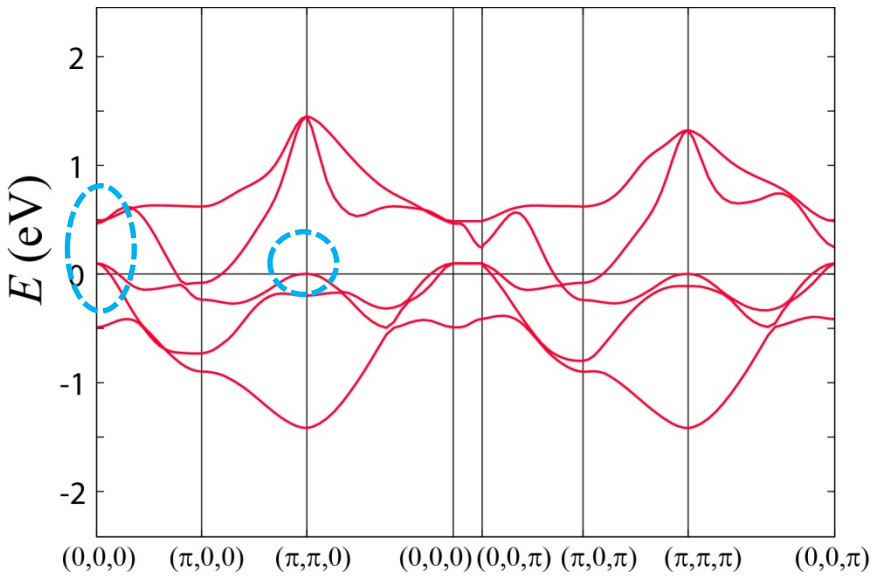
eigenvalue for SC

Suzuki, KK et al, in preparation

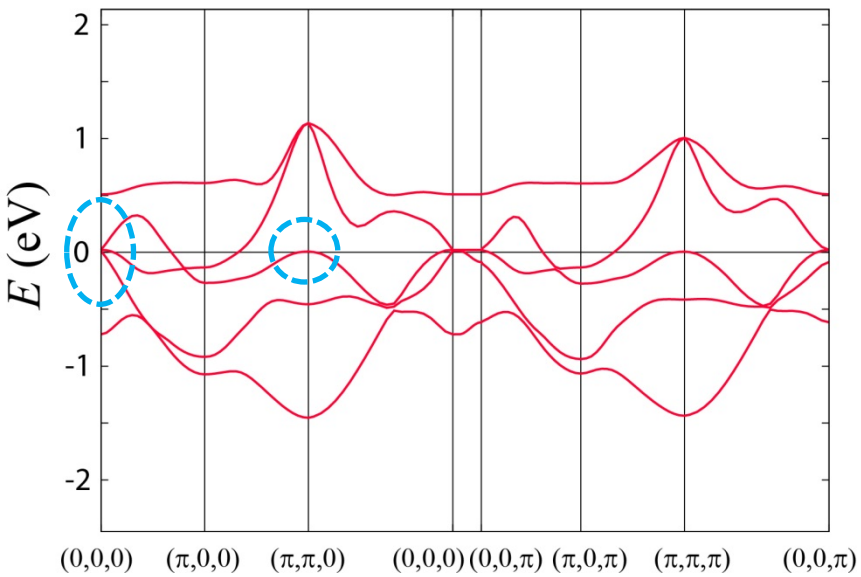


SC gap function at x=0.40

Doping dependence of band structure

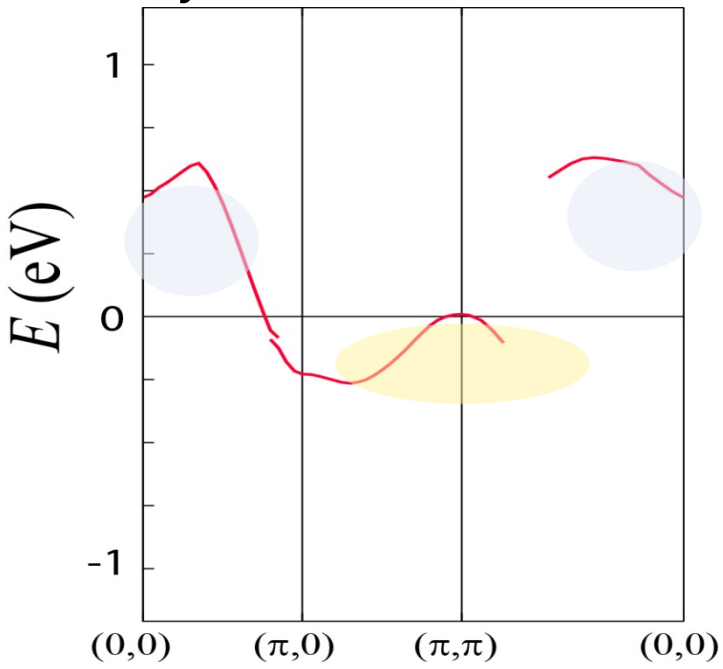


x=0.05

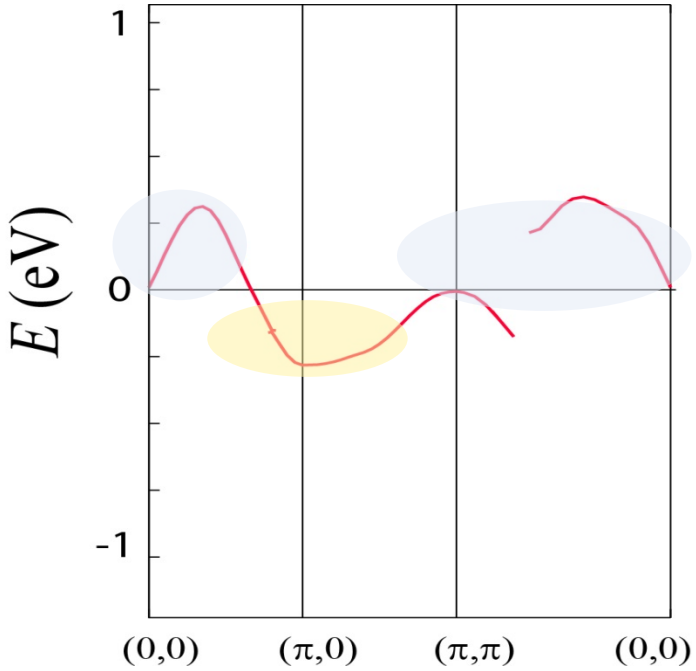


x=0.35

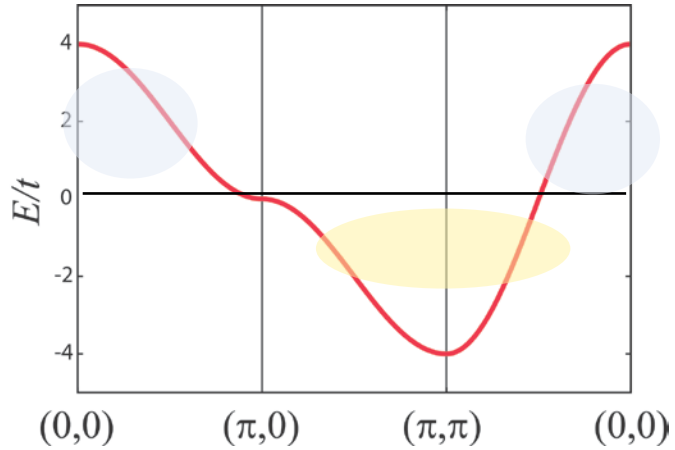
xy band, x=0.05



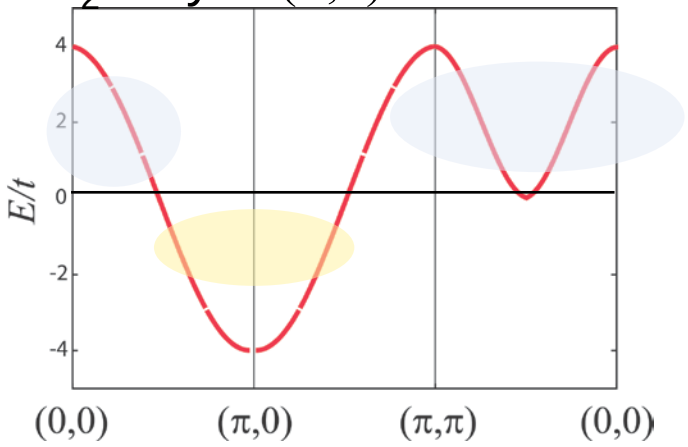
xy band, x=0.35



t_1 only→(π,π) fluctuations



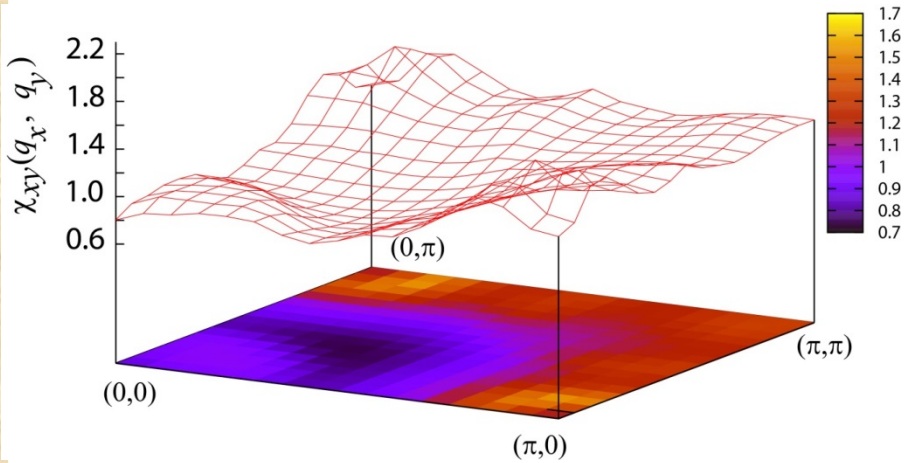
t_2 only→ (π,0) fluctuations



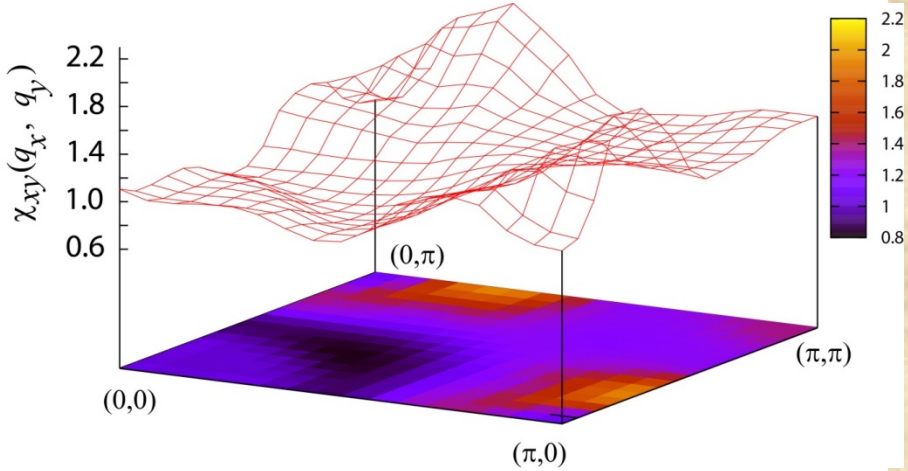
Doping dependence of orbital diagonal spin sus.

Sm1111

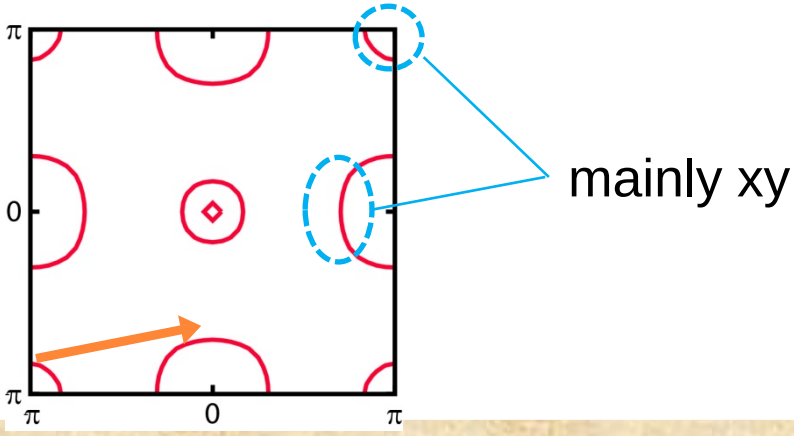
x=0.2



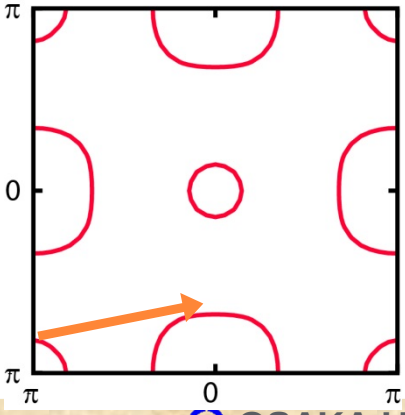
x=0.3



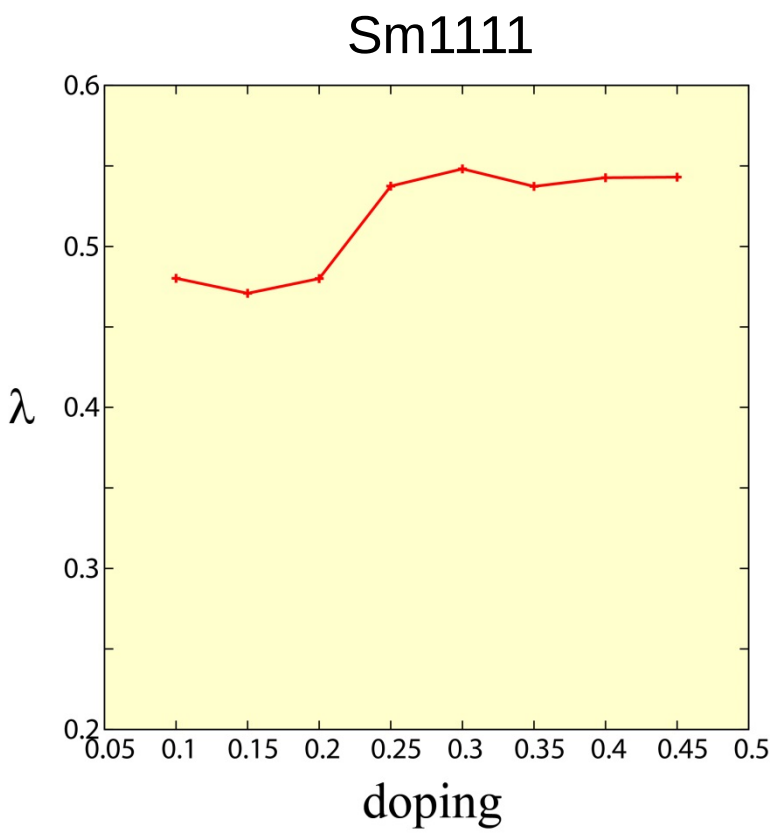
t_2/t_1=1.16

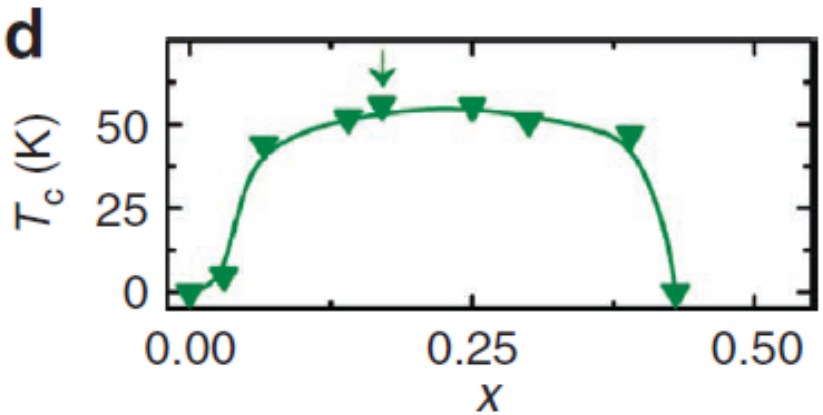


t_2/t_1=1.67



Doping dependence of Eliashberg eq. eigenvalue





Iimura *et al*. ,Nat. Comm. **3** 943 (2012)

eigenvalue for SC

Suzuki, KK et al, in preparation

Conclusions

- strong bond angle dependence of the hopping integral t_1 within the xy orbital

- In addition to the FS topology, the entire band shape roughly characterized by t_2/t_1 affects the wave vector dependence of the spin correlation

- $|t_1| < t_2$ is more favorable for spin fluctuations $\sim(\pi,0) > \sim(\pi,\pi)$ and hence s+– SC
  → correspondance to J_1-J_2 picture