THE UNIVERSITY OF TOKYO

基研研究会「熱場の量子論」
31 August 2010

鉄系超伝導
Iron-based superconductor --- an overview

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My talk today

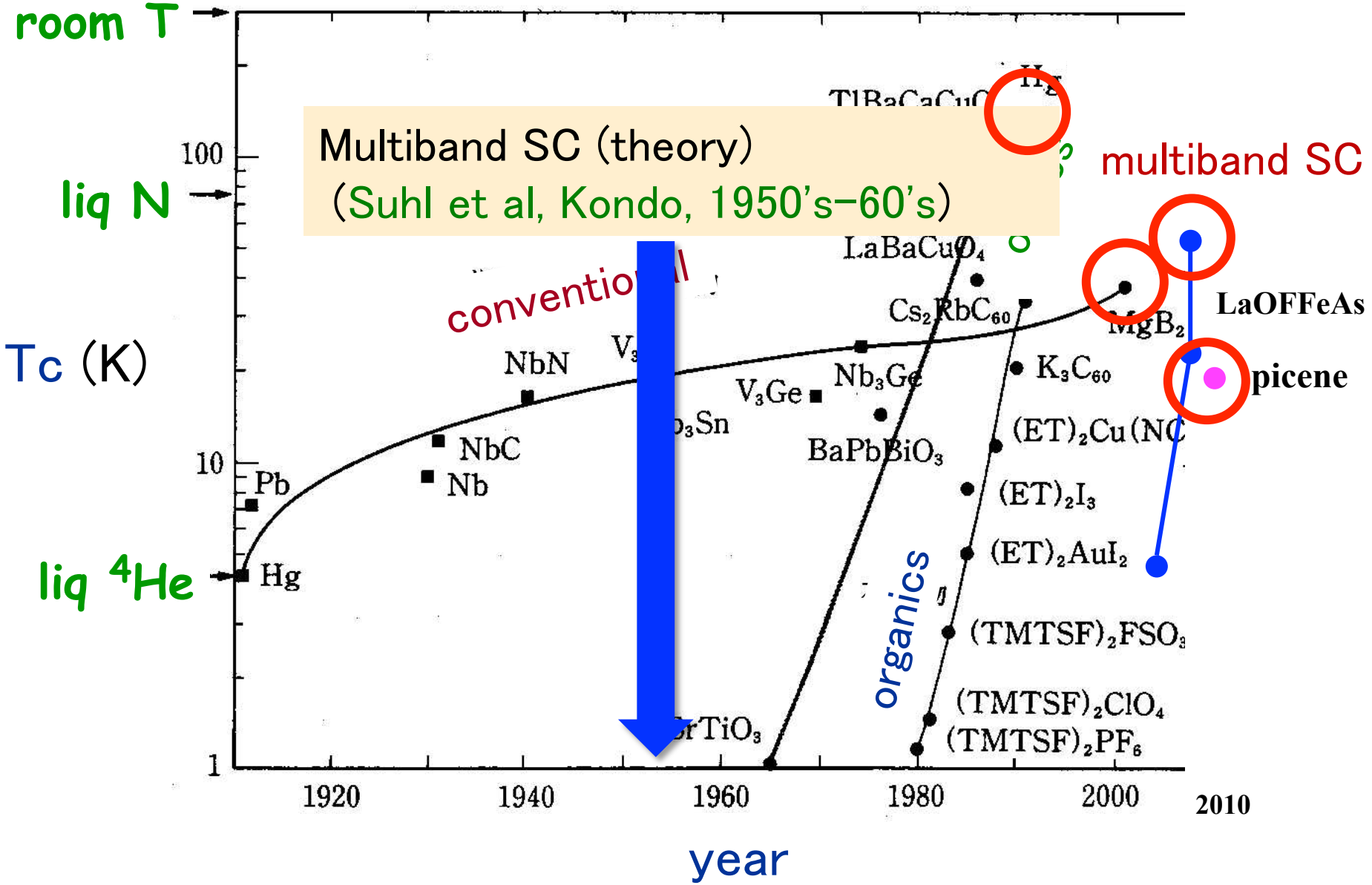
- A brief introduction for the iron-based SC
- Mechanism for s± pairing
- Material-dependence (s± ⇔ d)
- Collective (phase) modes in multiband SC

Keyword: Multiband SC

Kazuhiko Kuroki, Hidetomo Usui　Univ Electro-Commun
Ryotaro Arita　Univ Tokyo

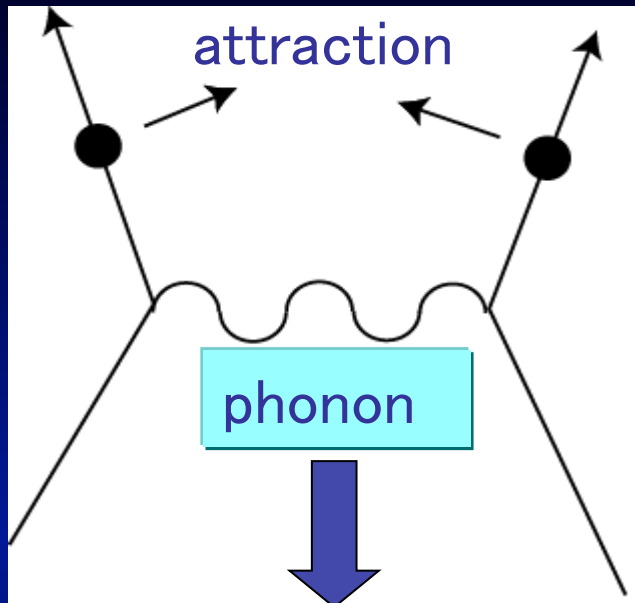
Yukihiro Ota,　Masahiko Machida　Japan Atomic Energy Agency
Tomio Koyama　Tohoku Univ

Why multiband SC ?



* phonon mechanism

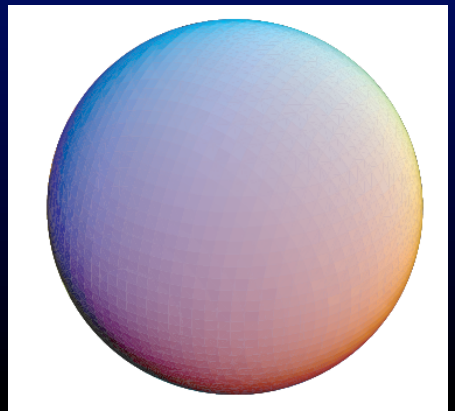
attraction



phonon

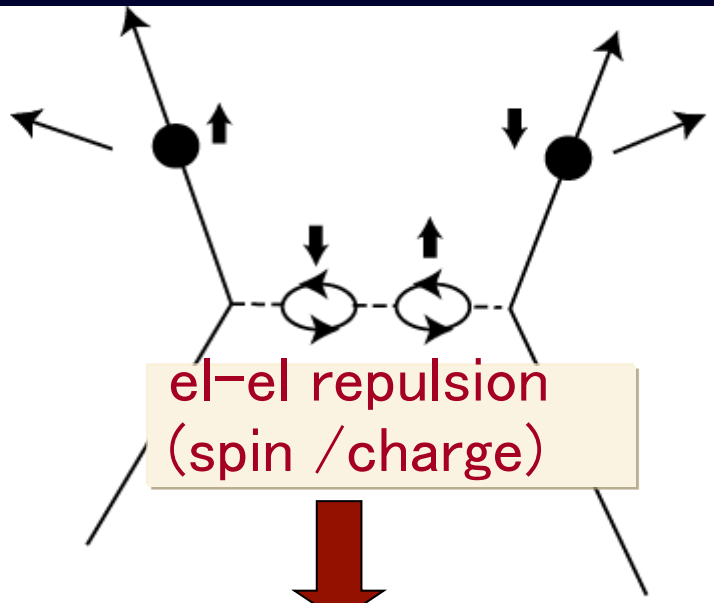
$T_c \sim 0.1\omega_D$

10K ← 100K



isotropic pairing

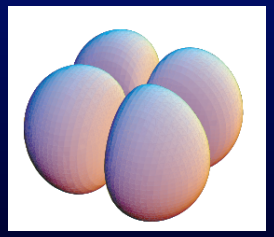
* electron mechanism



el-el repulsion (spin /charge)

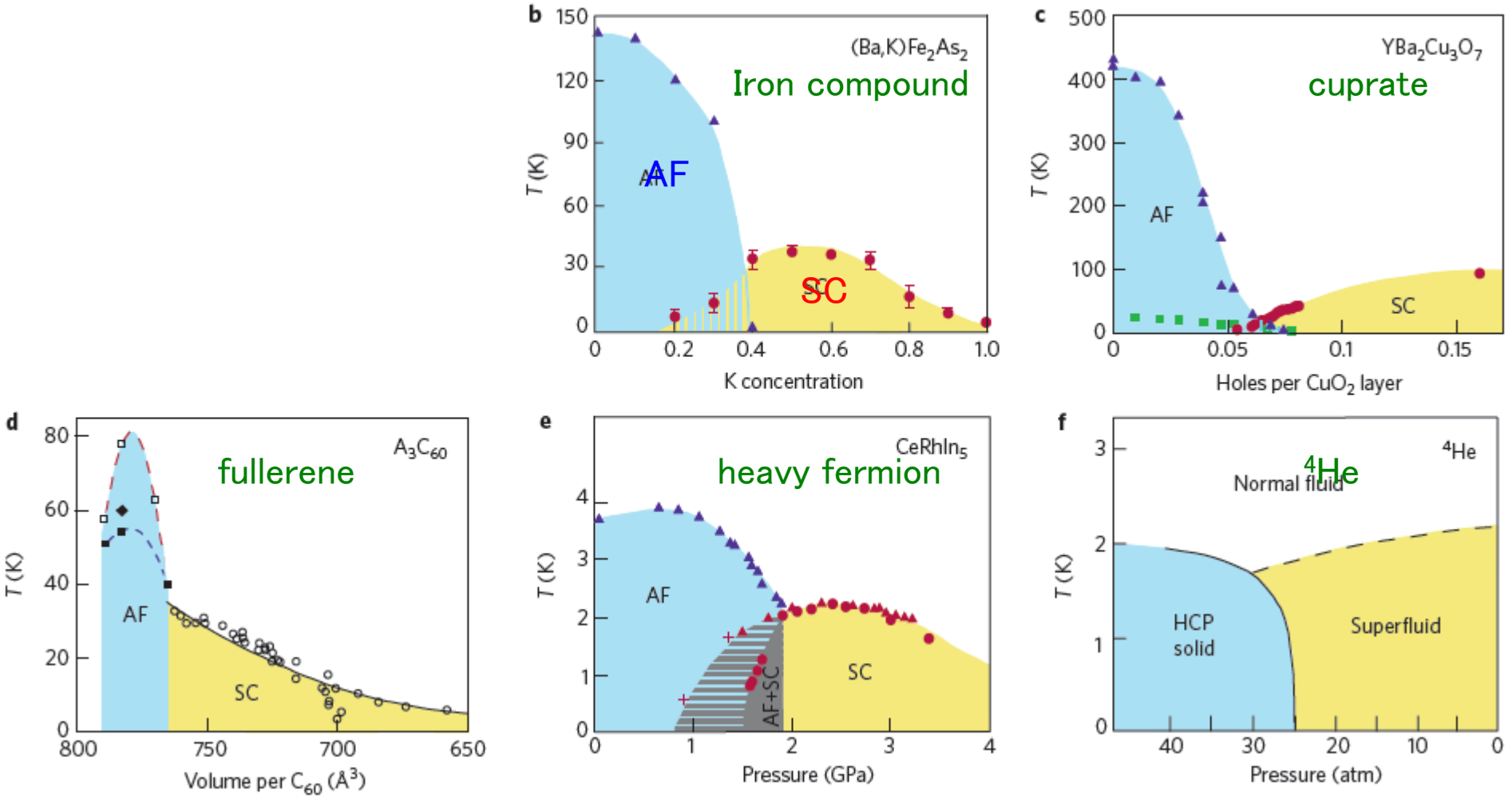
$T_c \sim 0.01t$

100K ← 10000K



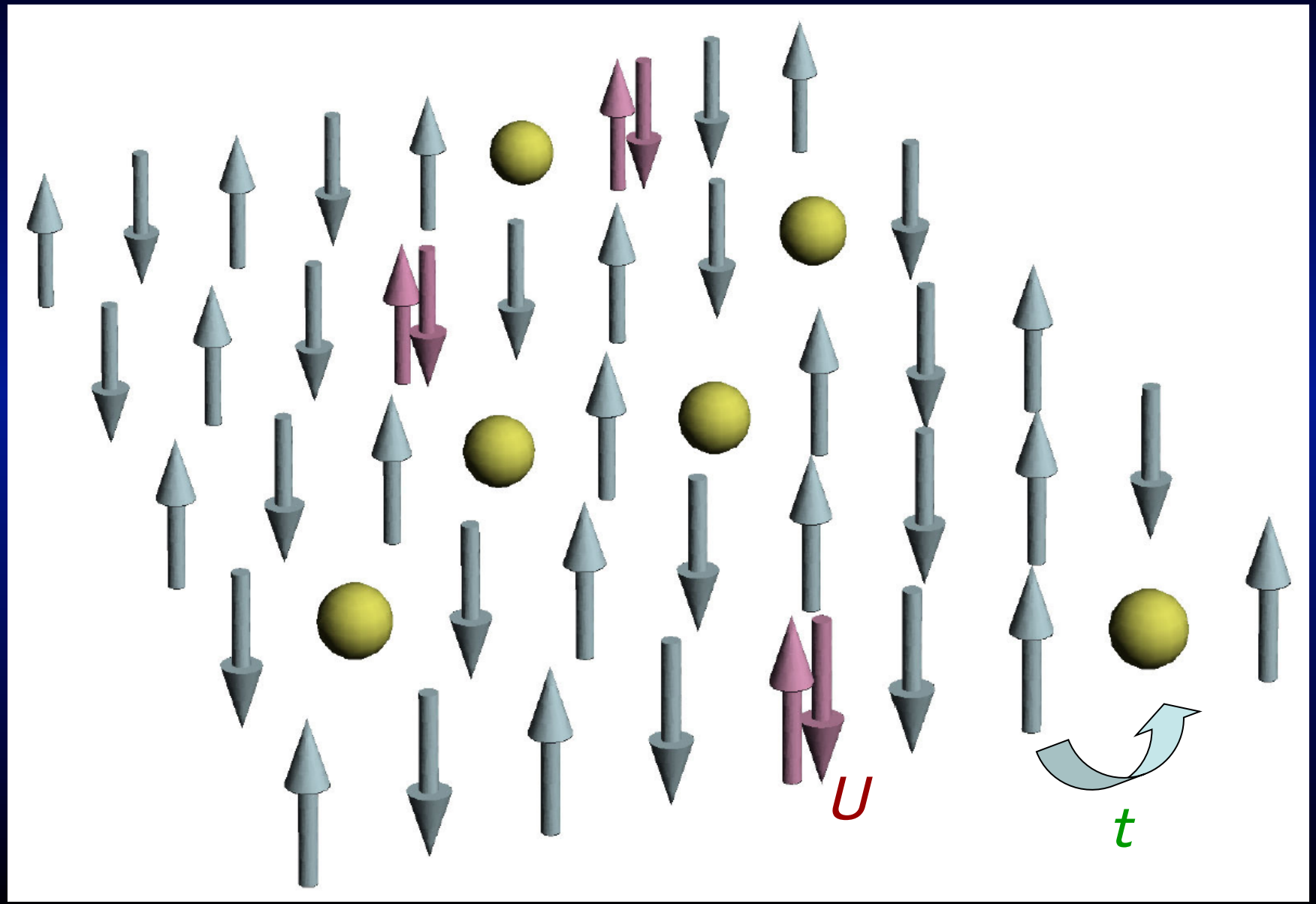
anisotropic pairing

Phase diagrams for various classes of materials



Uemura, nature mat, news&views 2009

Hubbard model (a generic model)



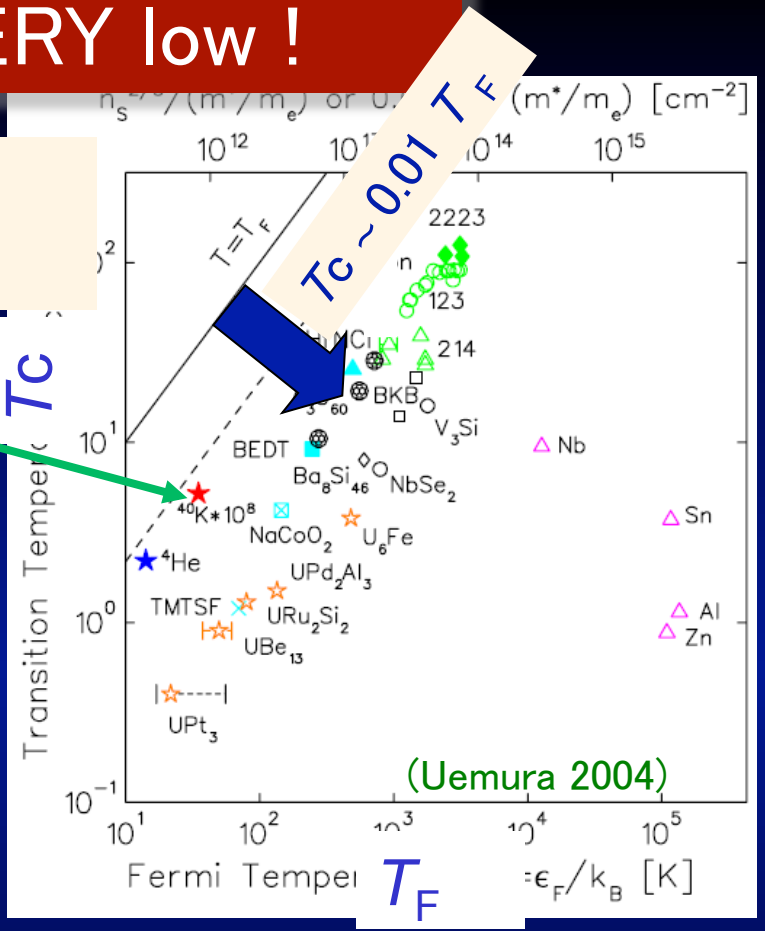
Tc ~ T_F/100 is VERY low !

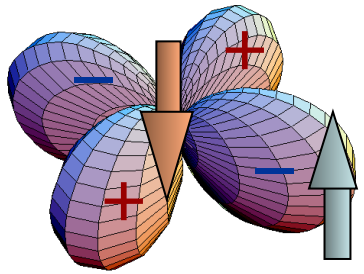
(1)Pairing int'action from el-el repulsion
= weak

Cf. Cold Fermi gas(2004)
← superfluid Tc ~ 0.1 T_F
← attractive int'action
↑ Feshbach resonance

(2) Self-energy correction
→ quasi-particles short-lived

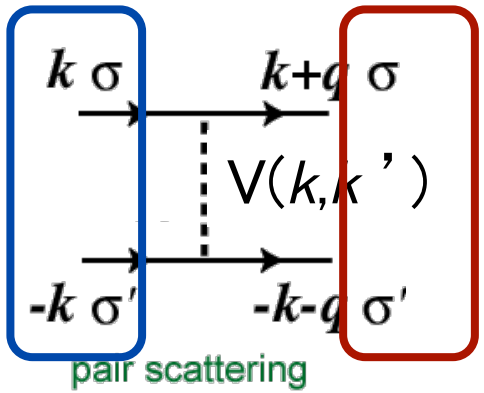
(3) Pairing from el-el repulsion
= anisotropic
(i.e., nodes in Δ_{BCS})

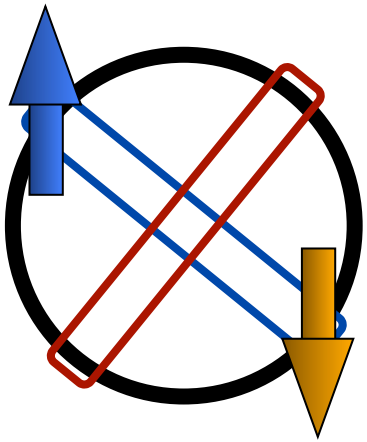




SC from repulsion: nothing strange

Attraction → isotropic SC

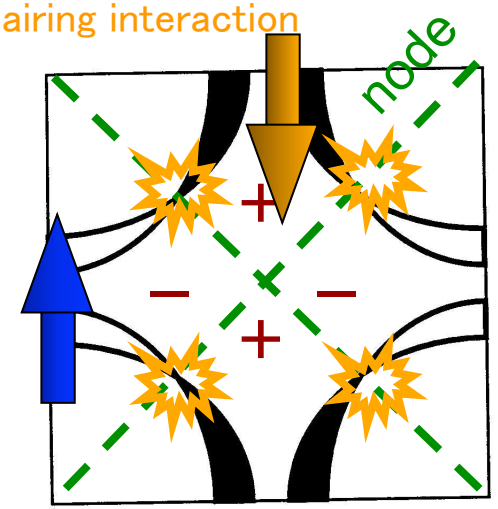




$$\Delta(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} V(\boldsymbol{k},\boldsymbol{k}') \frac{\Delta(\boldsymbol{k}')}{2E(\boldsymbol{k}')} \tanh\left(\frac{1}{2}\beta E(\boldsymbol{k}')\right)$$

Repulsion → anisotropic SC

spin–fluctuation mediated
pairing interaction

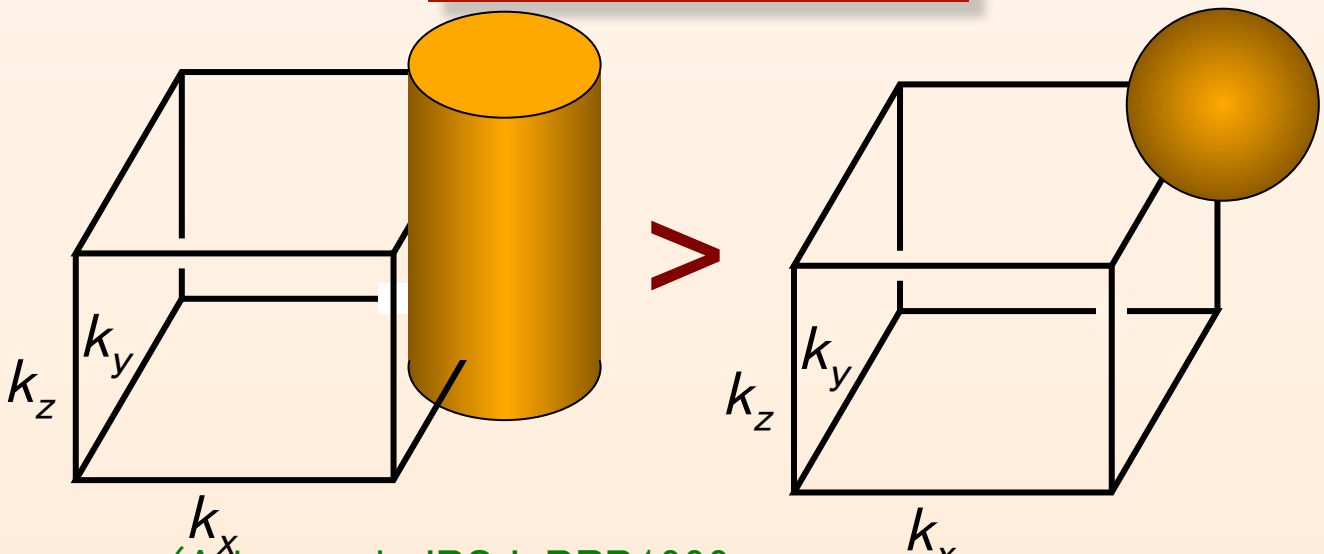


→ attraction

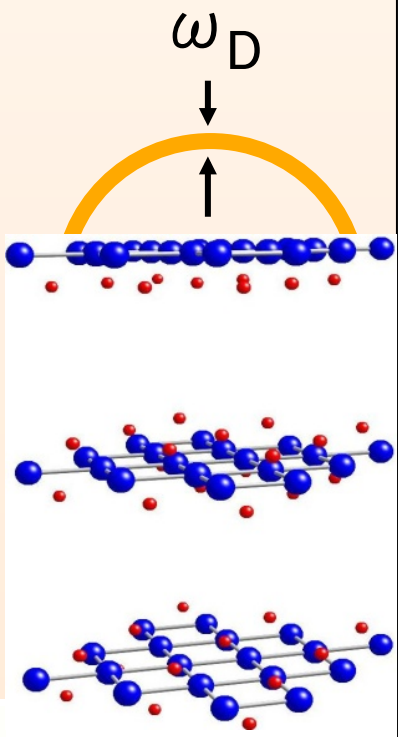
as in d wave pairing in cuprates

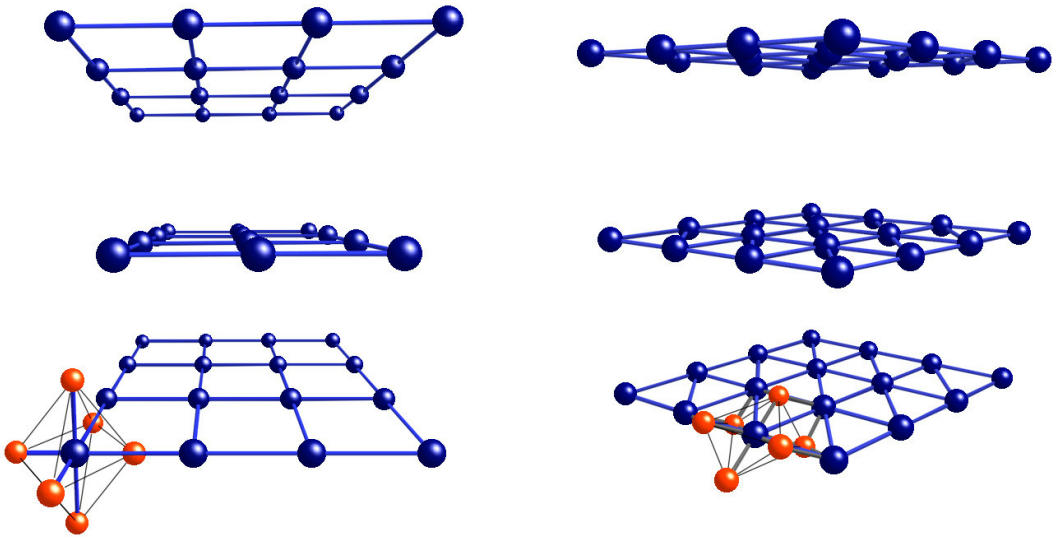
Scalapino et al,
Moriya & Ueda,
QMC: Kuroki & Aoki,
DCA: Jarrell,
VMC: Yokoyama et al, . . .

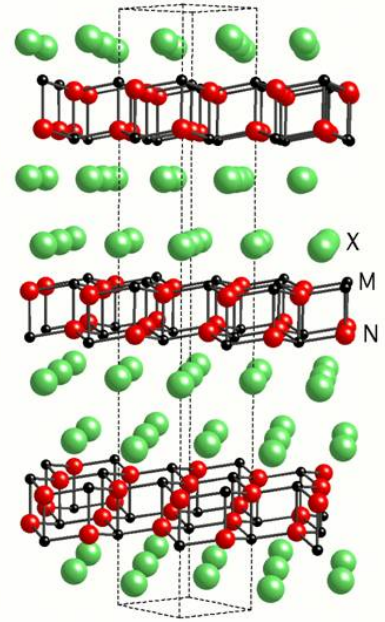
2D or 3D ?

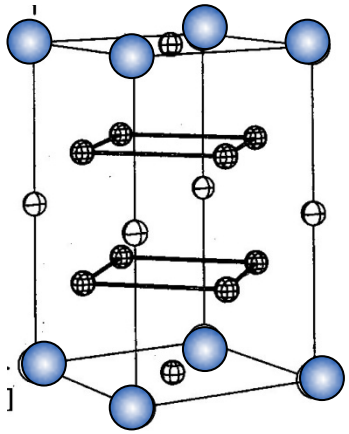


(Arita et al, JPSJ; PRB1999;
Monthoux & Lonzarich PRB 1999)









My talk today

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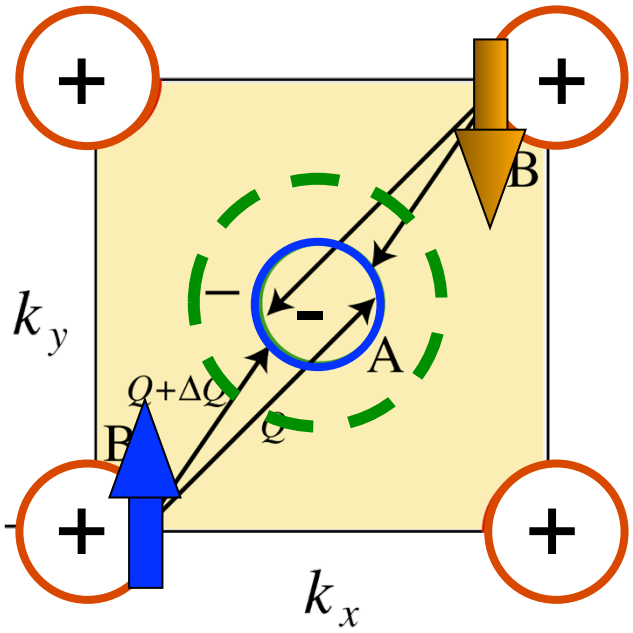
- ✔ Mechanism for s± pairing
  [Kuroki et al, PRL 101, 087004 (2008)]
- ✔ Material-dependence (s± ⇔ d)
- ✔ Collective (phase) modes in multiband SC

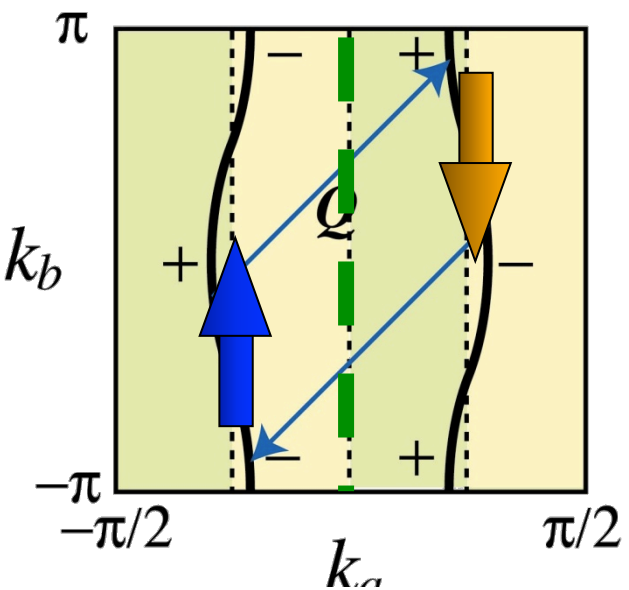
Keyword: Multiband SC

Disconnected Fermi surfaces



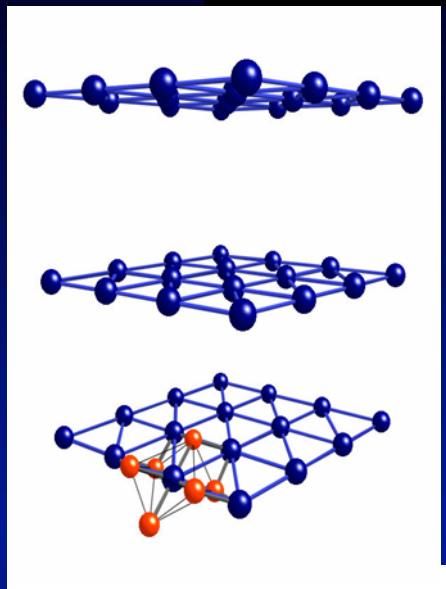
(Kuroki & Arita, 2001)

TMTSF

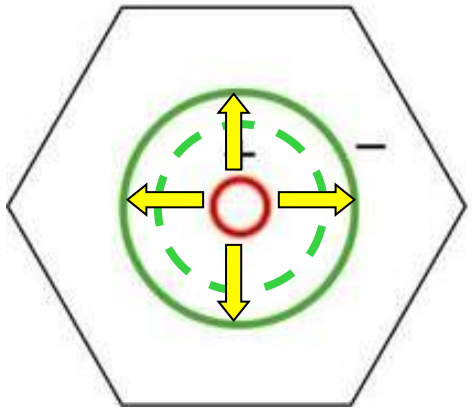


(Kuroki et al 2001; 2004)

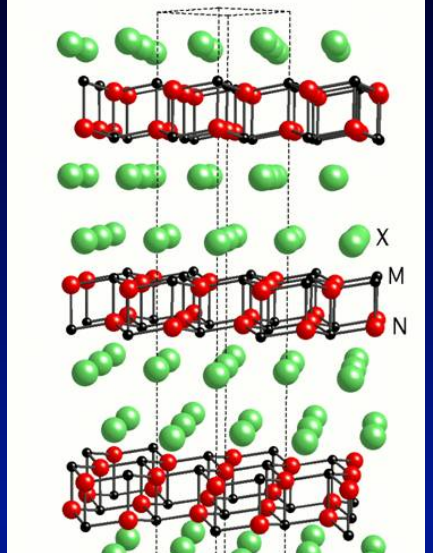
Disconnected Fermi surfaces in real materials



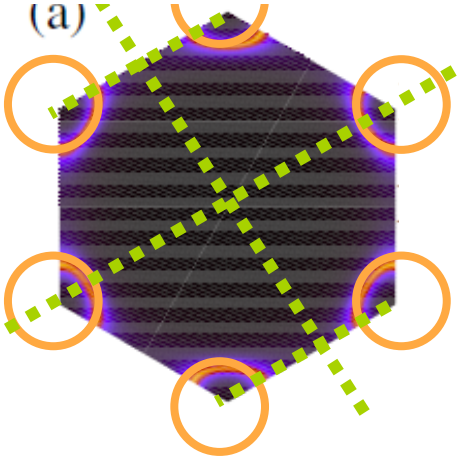
Co compound



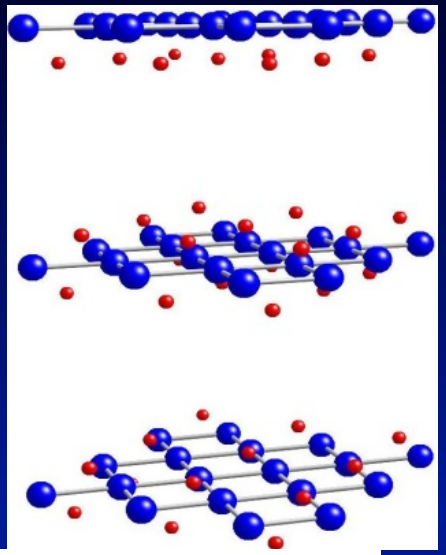
Kuroki et al, JPSJ(06); PRL(07); JPSJ(07)



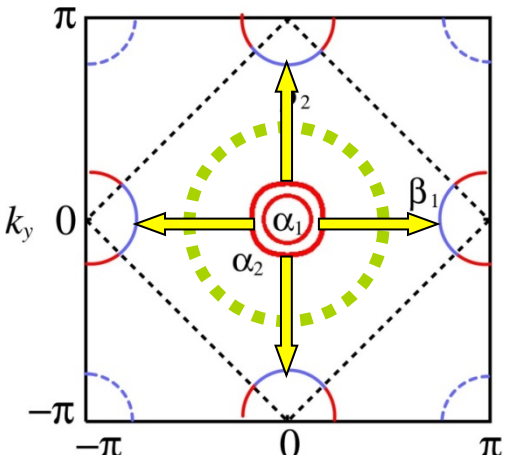
Hf nitrides



Kuroki, to appear in Proc LT 25; arXiv0902.3695



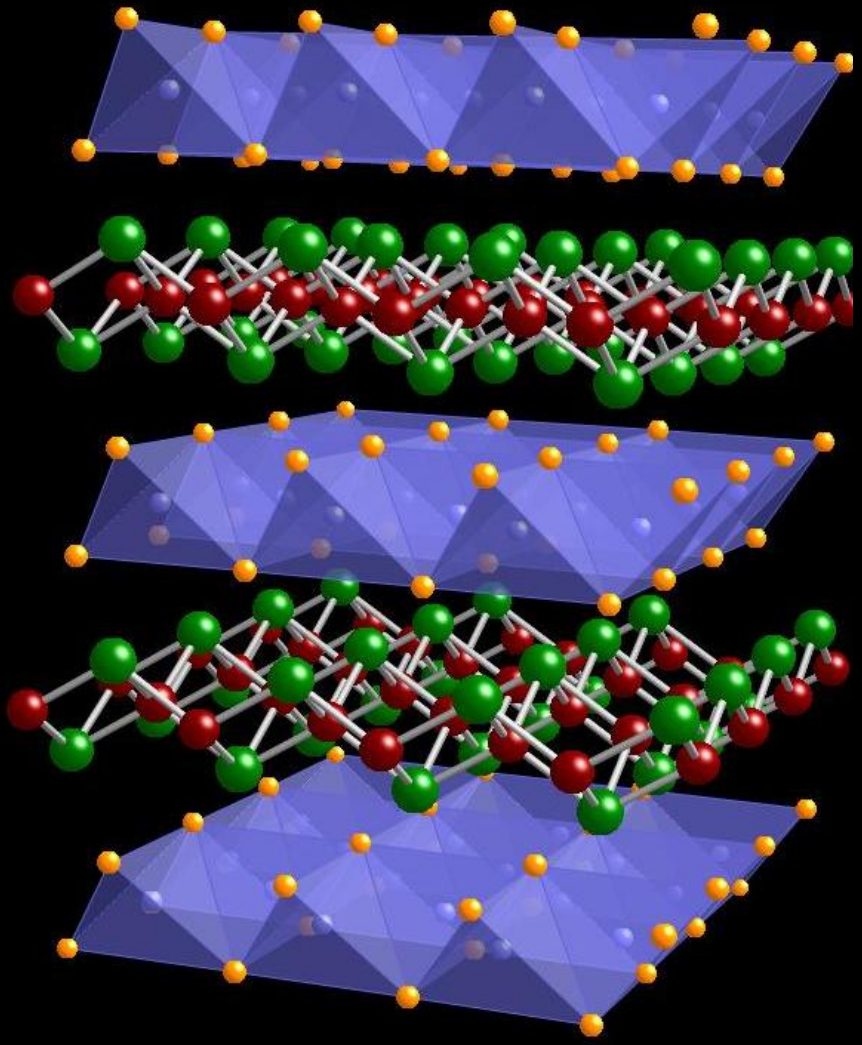
Fe compound



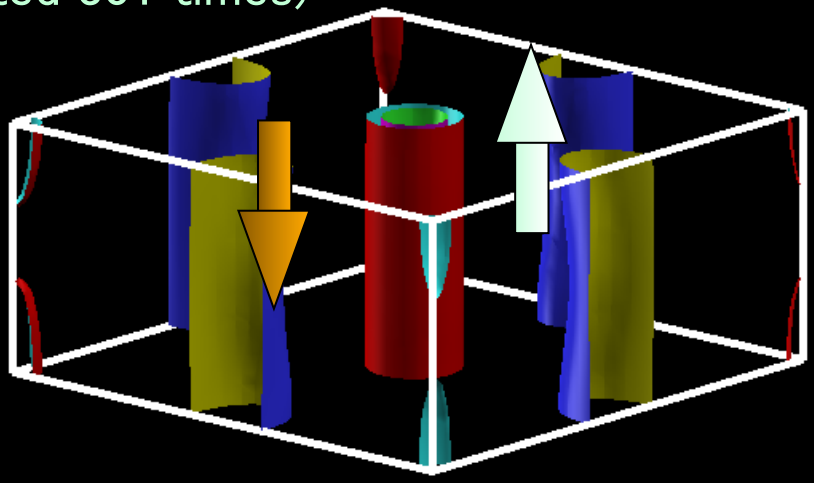
Kuroki et al, PRL(08)

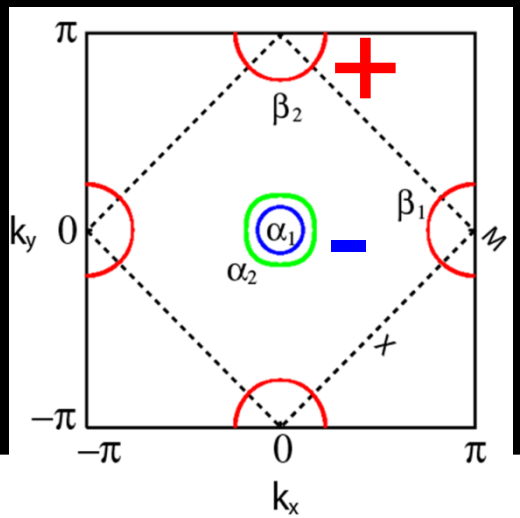
Fe-compound

Kamihara et al, JACS 130, 3296 (2008)



Kuroki et al, PRL 101, 087004 (2008)
(cited 301 times)





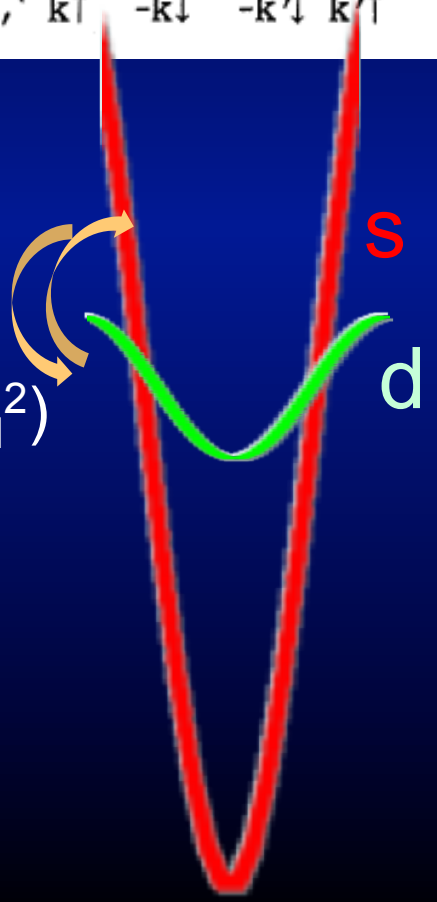
Suhl–Kondo mechanism

(Suhl et al 1959; Kondo 1963)

$$H = \sum_{k\sigma} \epsilon_{ks} c_{k\sigma}^{*} c_{k\sigma} + \sum_{k\sigma} \epsilon_{kd} d_{k\sigma}^{*} d_{k\sigma} - \sum_{kk'} V_{ss} c_{k\uparrow}^{*} c_{-k\downarrow}^{*} c_{-k'\downarrow} c_{k'\uparrow} - V_{dd} \sum_{kk'} d_{k\uparrow}^{*} d_{-k\downarrow}^{*} d_{-k'\downarrow} d_{k'\uparrow}$$

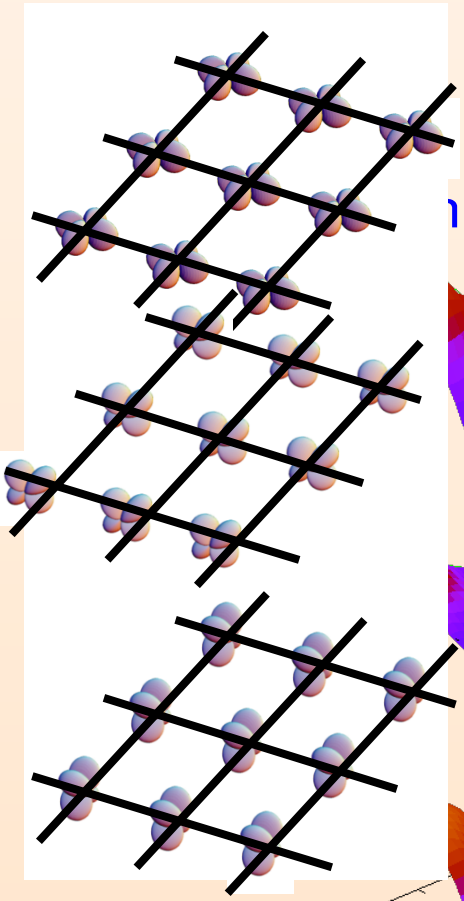
$$- V_{sd} \sum_{kk'} (c_{k\uparrow}^{*} c_{-k\downarrow}^{*} d_{-k'\downarrow} d_{k'\uparrow} + d_{k\uparrow}^{*} d_{-k\downarrow}^{*} c_{-k'\downarrow} c_{k'\uparrow})$$

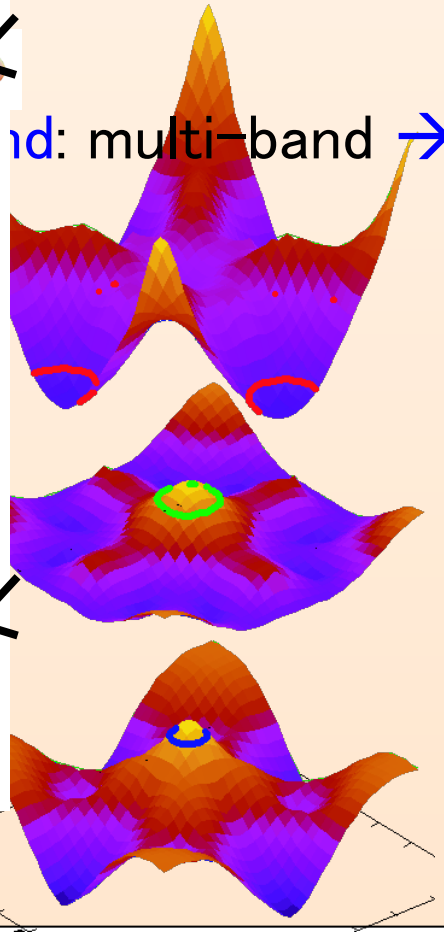
Tc enhanced ~ $O(V_{sd}^{2})$



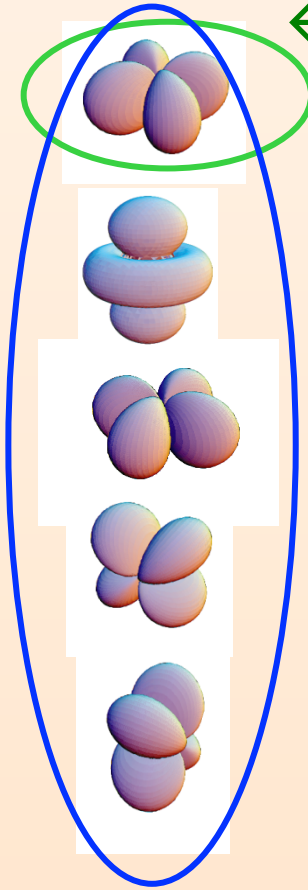
single-band vs multi-band

4	Ti $3d^2$	V $3d^3$			Fe $3d^6$	Co $3d^7$	Ni $3d^8$	Cu $3d^{10}$

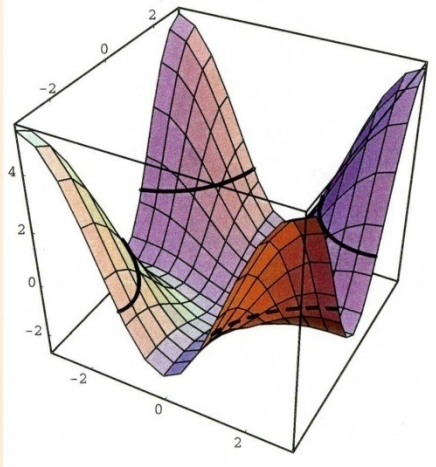




d: multi-band →

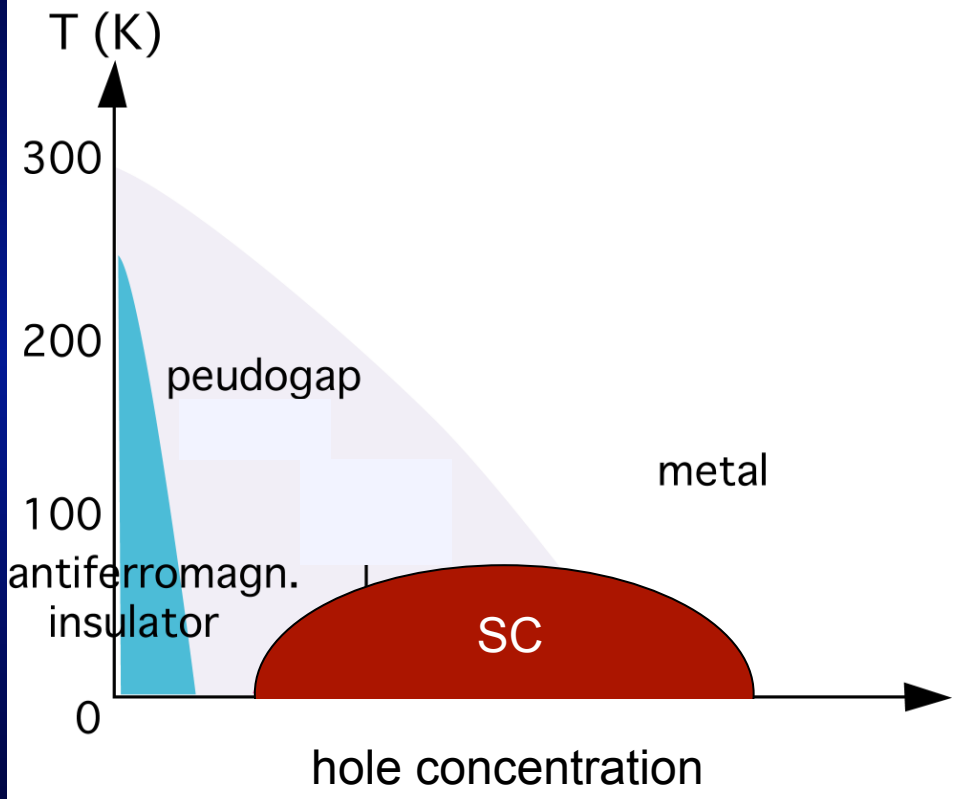


← Cuprate:
nearly half-filled one-band

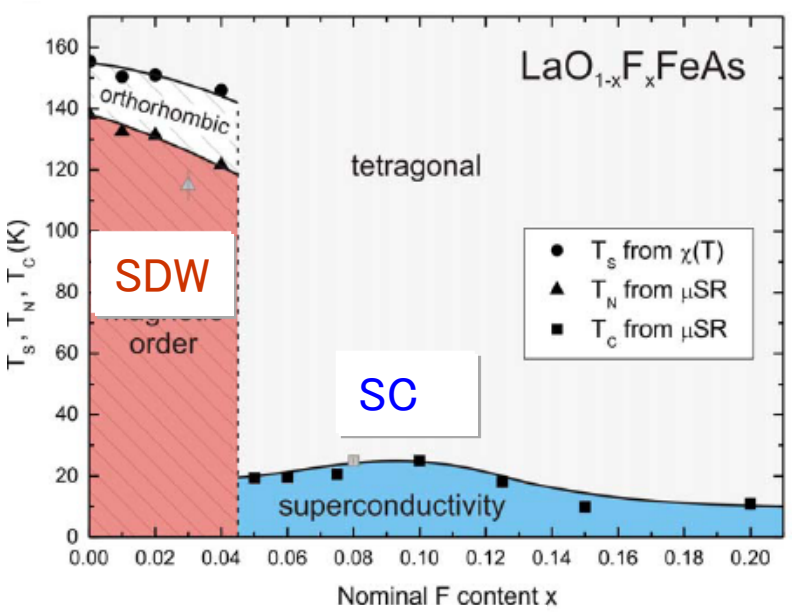


Phase diagram

High-Tc



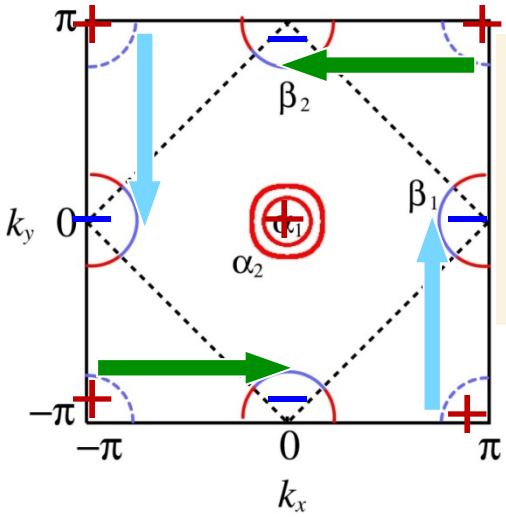
Iron-based



(Luetkens et al, 2008)

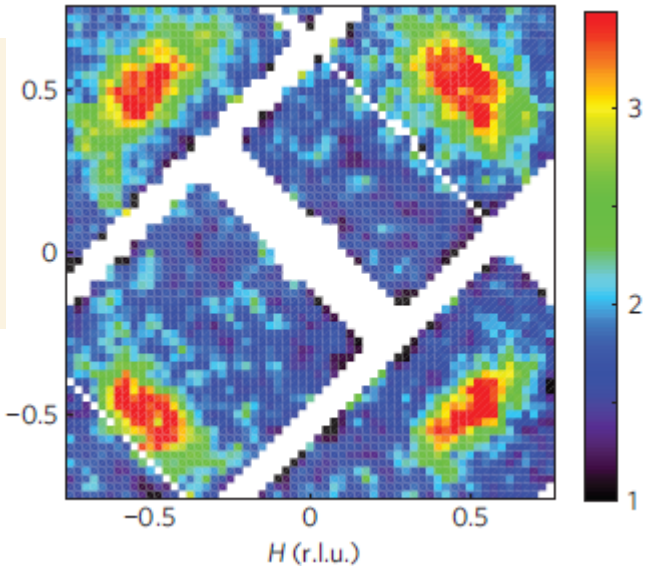
Susceptibilities: 5-band RPA result

5-band RPA
(Kuroki et al, PRL 2008)

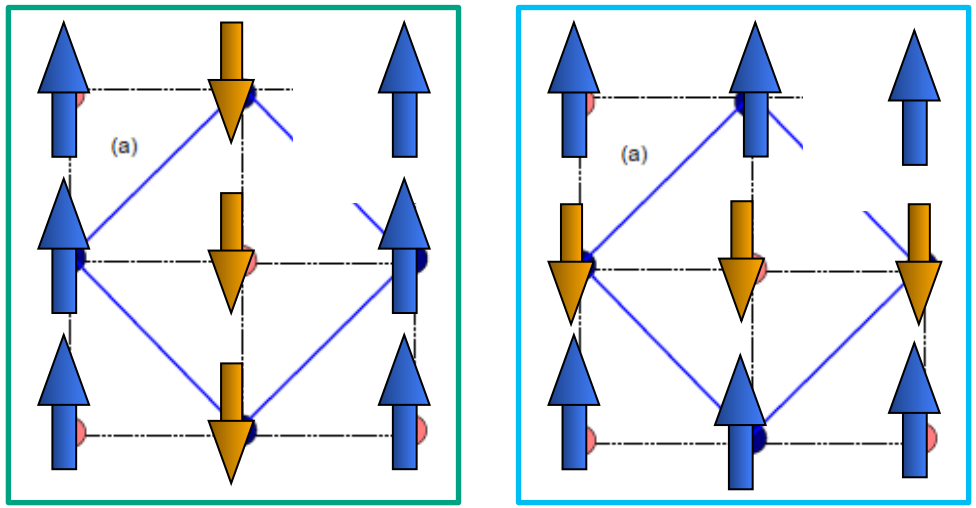


Spin-fluct mediated s± pairing

Inelastic neutron scattering
(Lumsden et al, nature phys 2010)



colinear SDW



Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

$$\mathcal{H}_0 = \sum_{ij}\sum_{\mu\nu}\sum_{\sigma} t_{ij}^{\mu\nu} c_{i\mu\sigma}^{\dagger} c_{j\nu\sigma} + \sum_{i\mu\sigma} \epsilon_{\mu} n_{i\mu\sigma}$$

i, j: site、m,n: orbitals

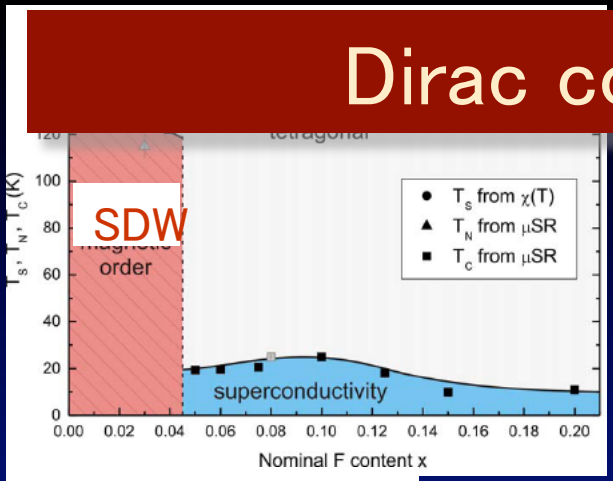
$$\mathcal{H}_1 = \sum_{i} \left[U \sum_{\mu} n_{i\mu\uparrow} n_{i\mu\downarrow} + U' \sum_{\mu>\nu} n_{i\mu} n_{i\nu} + J \sum_{\mu\neq\nu} \boldsymbol{S}_{i\mu} \cdot \boldsymbol{S}_{i\nu} + J' \sum_{\mu\neq\nu} c_{i\mu\uparrow}^{\dagger} c_{i\mu\downarrow}^{\dagger} c_{i\nu\downarrow} c_{i\nu\uparrow} \right]$$

intraorbital *U* interorbital *U*' Hund's *J* pair hopping *J*'

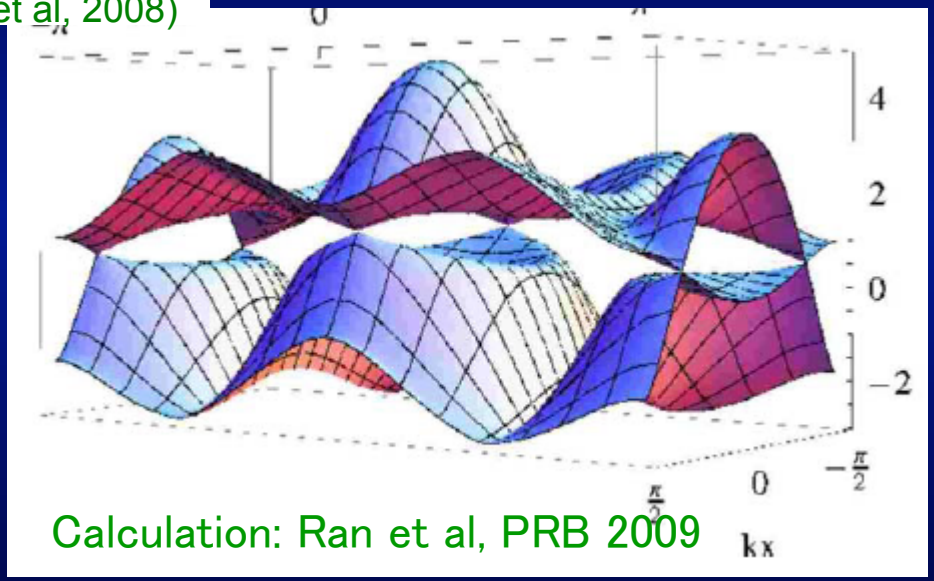
U,U',J, J' in general depends on orbital

Evaluation from first principles: Nakamura et al, JPSJ **77** (2008) 093711;
Anisimov et al, JPCM **21** 075602 (2009);
Miyake et al, JPSJ **77** Suppl.C 99 (2008)

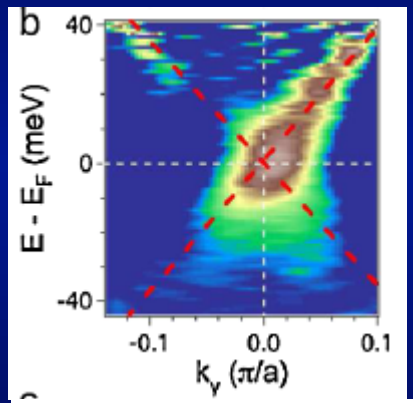
Dirac cones in the iron-based SC



(Luetkens et al, 2008)



Calculation: Ran et al, PRB 2009



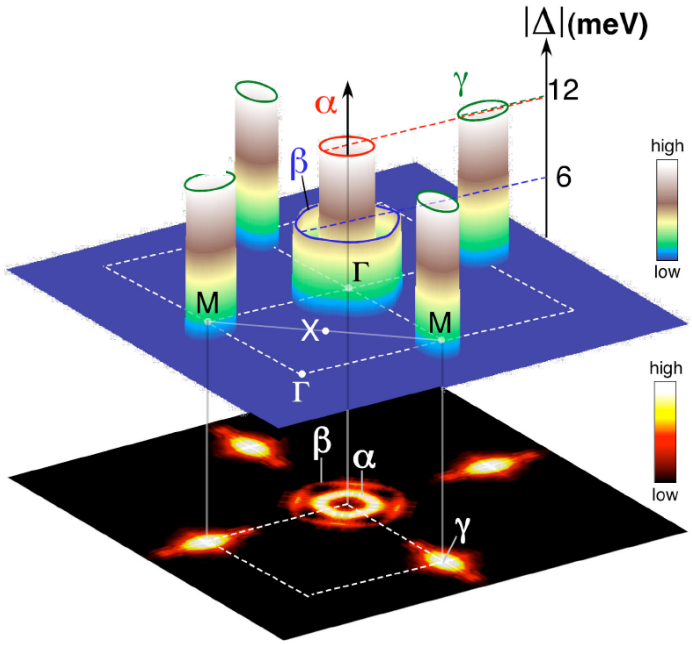
ARPES: Richard et al, PRL 2010

Experimental evidence for multiband nature

- ✔ Quasiparticle excitations (penetration depth, thermal conductivity)
- ✔ ARPES
- ✔ NMR

...

ARPES



(BaK)Fe_2As_2: Ding et al, EPL 83, 47001 (2008)

JPS 2010 March meeting
Symposium "Pairing symmetry in the iron-based SC"

✔ Shibauchi: Penetration depth, thermal cond
→ consistent with full gap, while P-compound has a node

✔ Shimojima: ARPES
→ 122 has full gap, but factors other than spin fluctuation may be relevant

✔ Hanaguri: Fourier transform STM
→ s±

✔Mukuda: NMR
→ various powers in T observed for T_1 below T_c

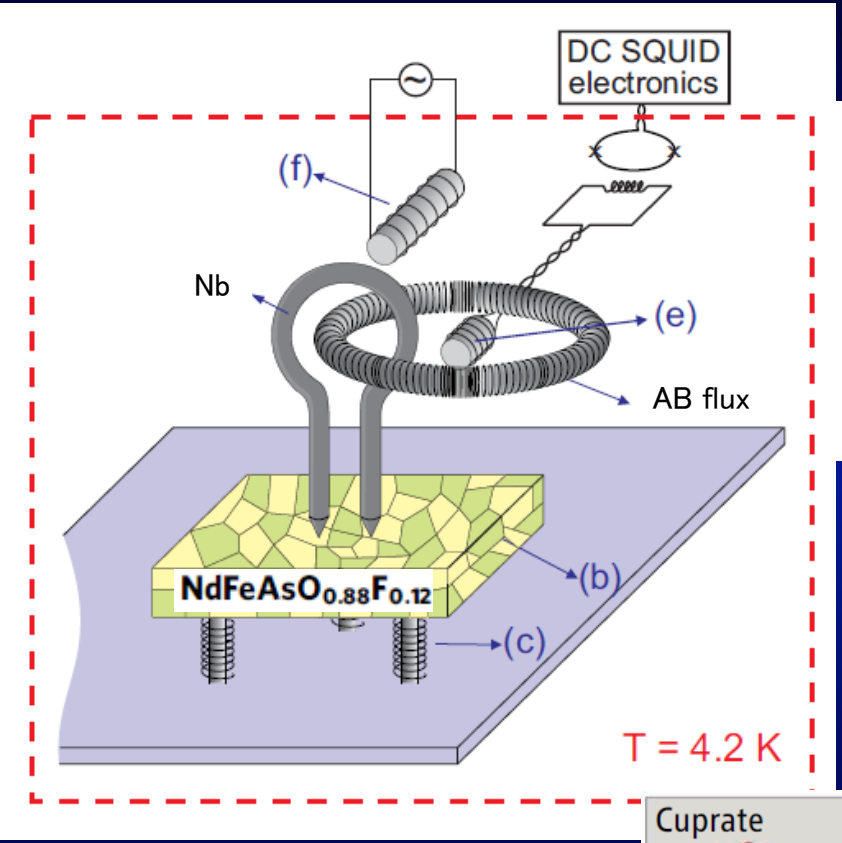
✔ Sato: neutron scattering
→ magnetic excitations, resonance peak

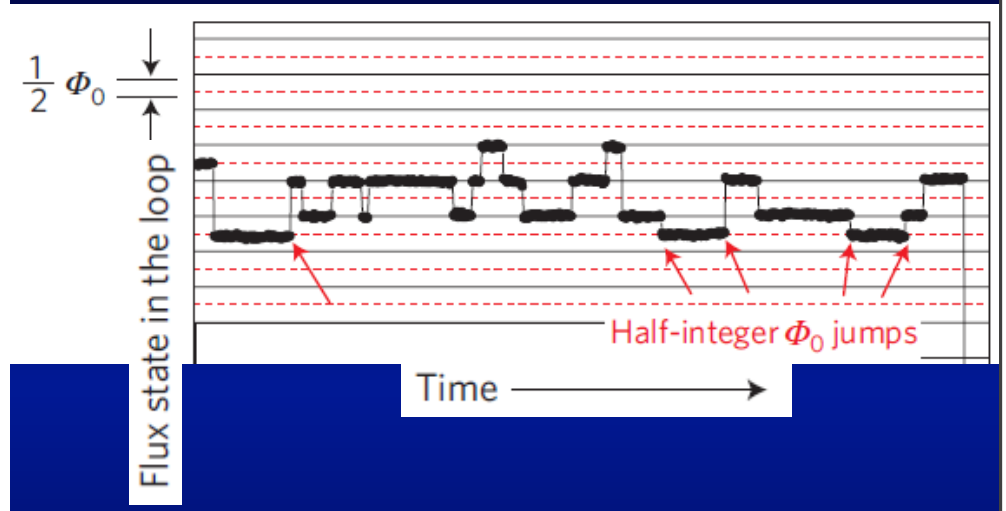
✔ Iketa: 1st principles calc for multiorbits, impurity potential
→ s±

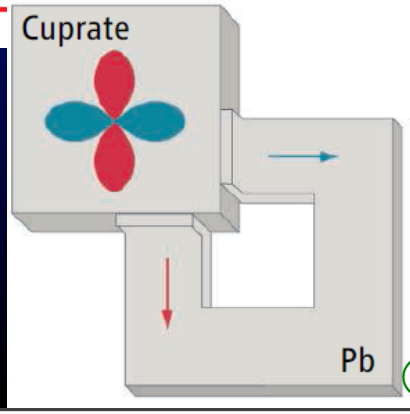
✔ Onari: : Theory for impurity effect, resonance peak
→ s++, orbital fluctuation mechanism

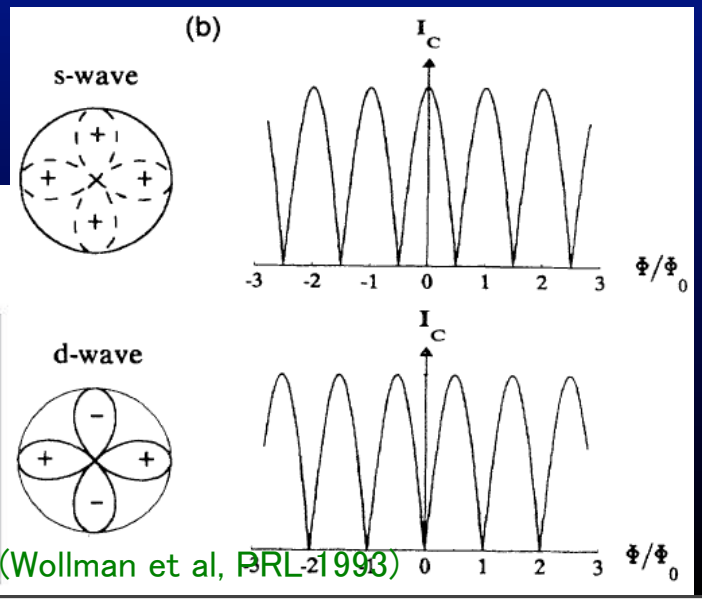
Phase-sensitive measurement (1)

(Chen et al, nature physics 2010)





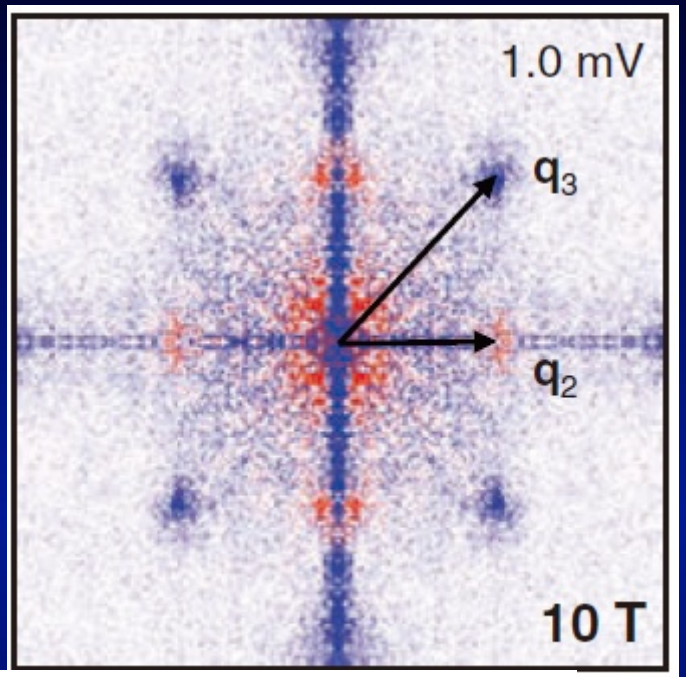




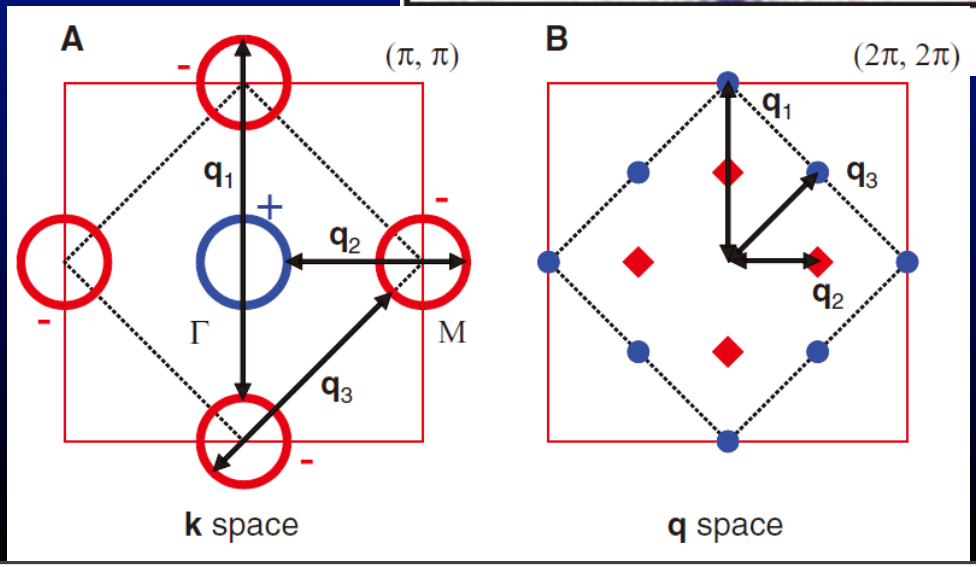
(Wollman et al, PRL 1993)

Phase-sensitive measurement (2)

——— Fourier-transform STM spectroscopy



(Hanaguri et al, Science 2010)

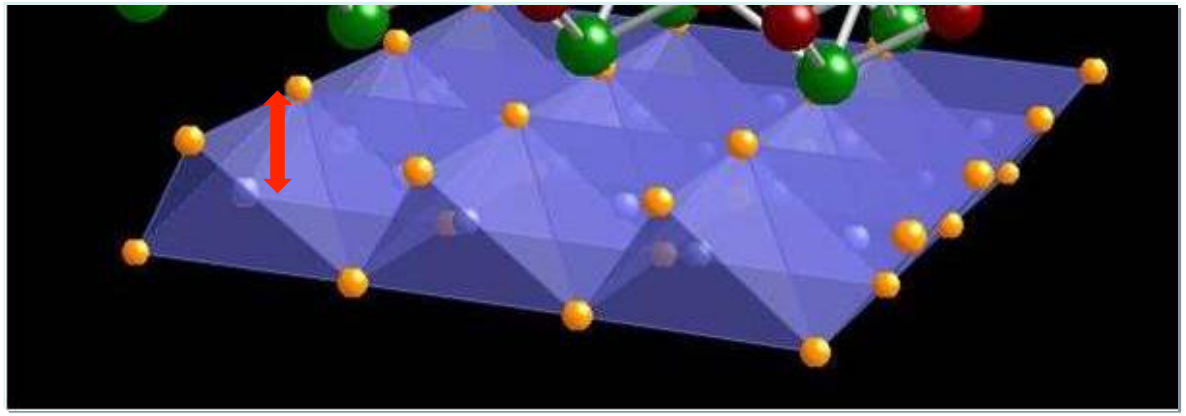


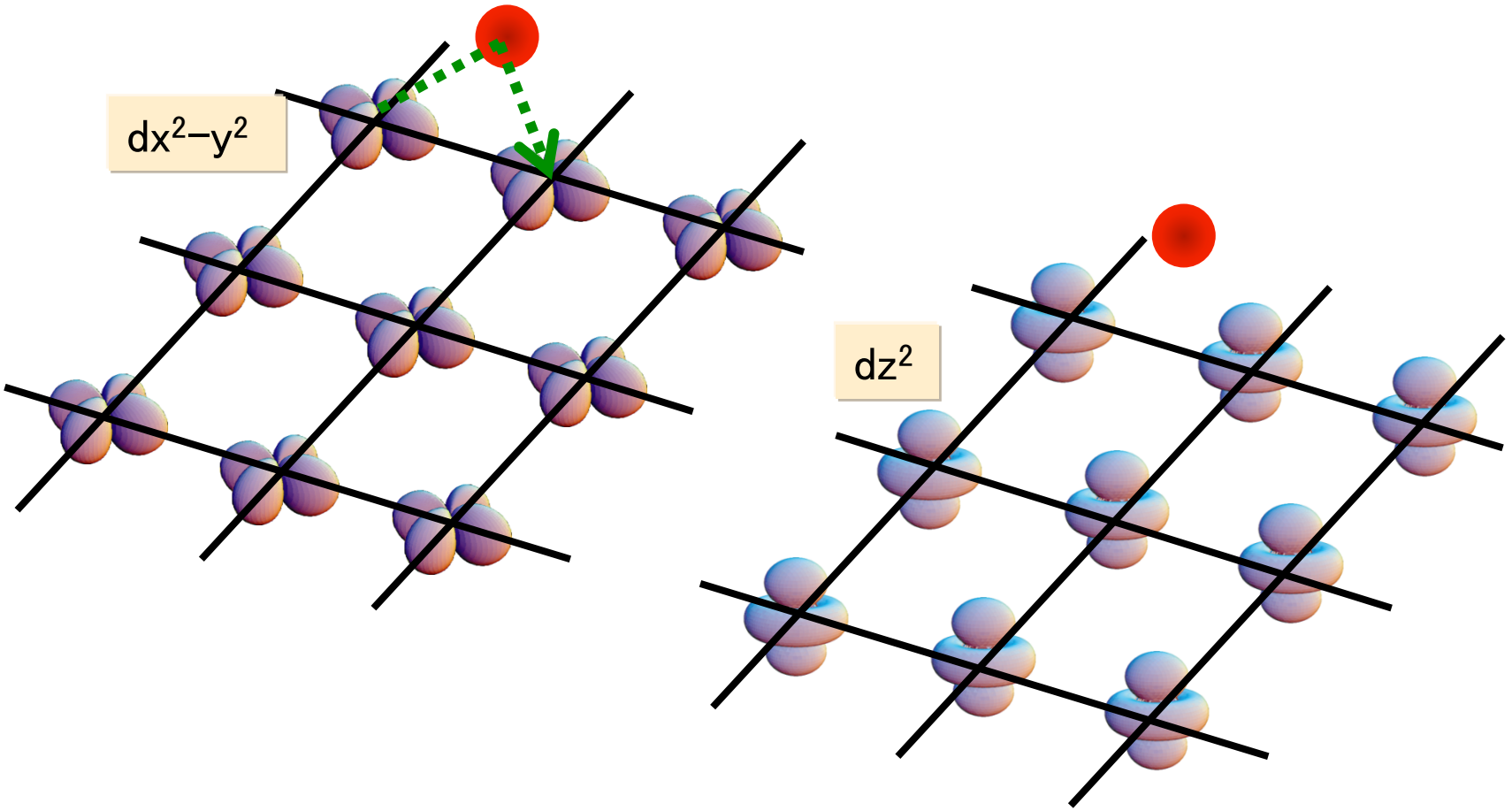
My talk today

- ✔ A brief introduction for the iron-based SC
- ✔ Mechanism for s± pairing
- ✔ Material-dependence (s± ⇔ d)
  [Kuroki et al, PRB **79**, 224511 (2009)]
- ✔ Collective (phase) modes in multiband SC

Keyword: Multiband SC

NdFeAsO h = 1.38 Å
LaFeAsO h = 1.32 Å
LaFePO h = 1.14 Å





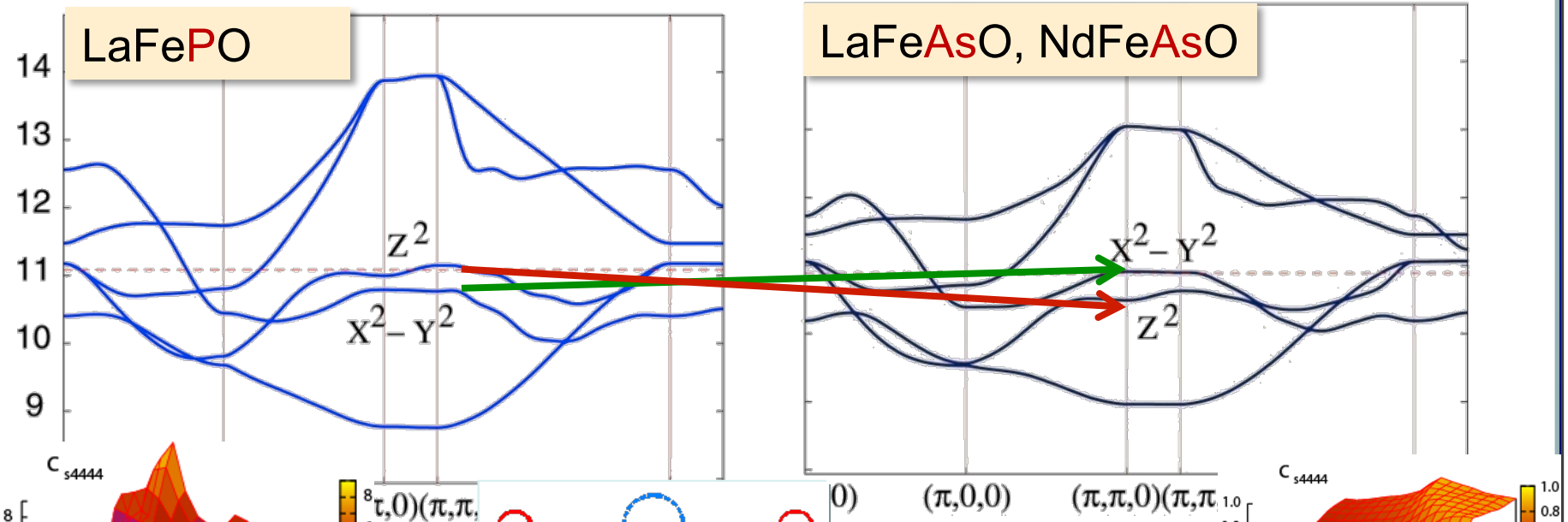
Multibands modified

(Kuroki et al, PRB 2009)

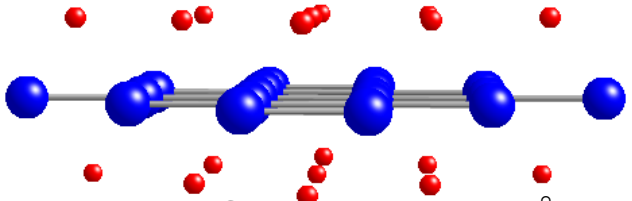
pnictogen height

z_{As}=0.630 (h_{As}= 1.14)

z_{As}=0.658 (h_{As}= 1.38)



Multiple nesting vectors compete

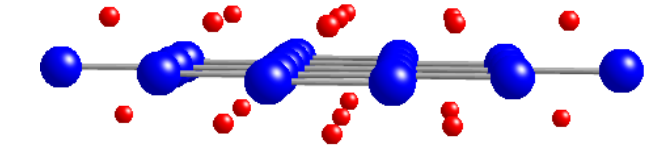


NdFeAsO h = 1.38 Å

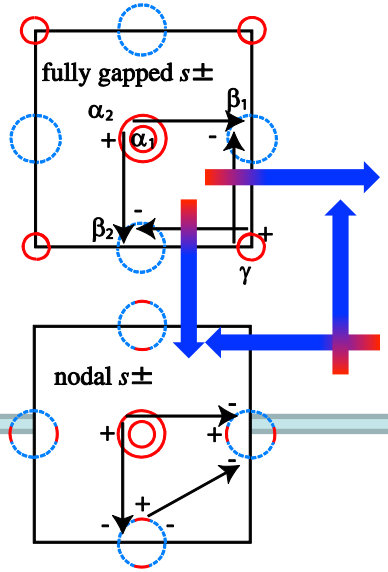
LaFeAsO h = 1.32 Å

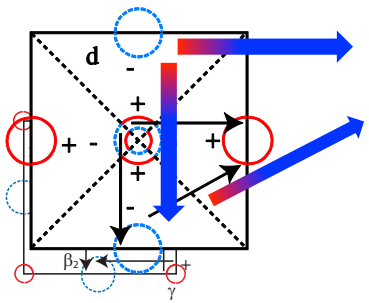
Pnictogen height as a "switch"

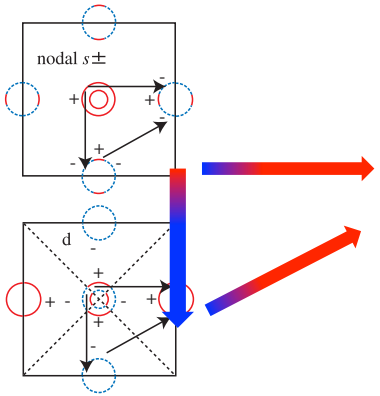
Height matters



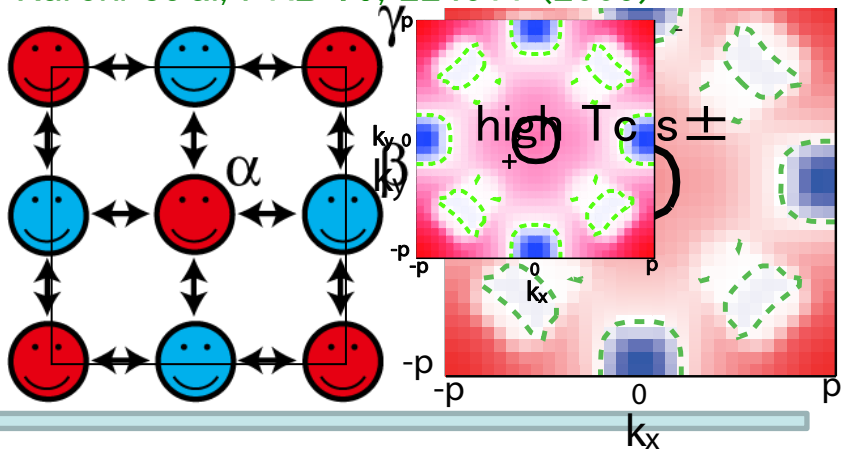
LaFePO h = 1.14 Å



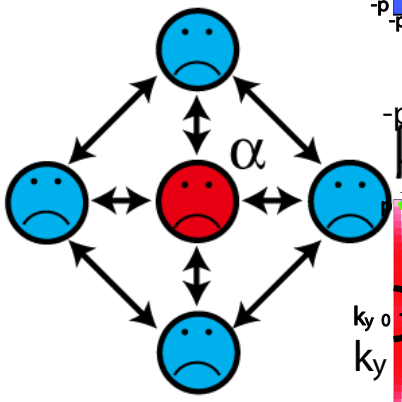


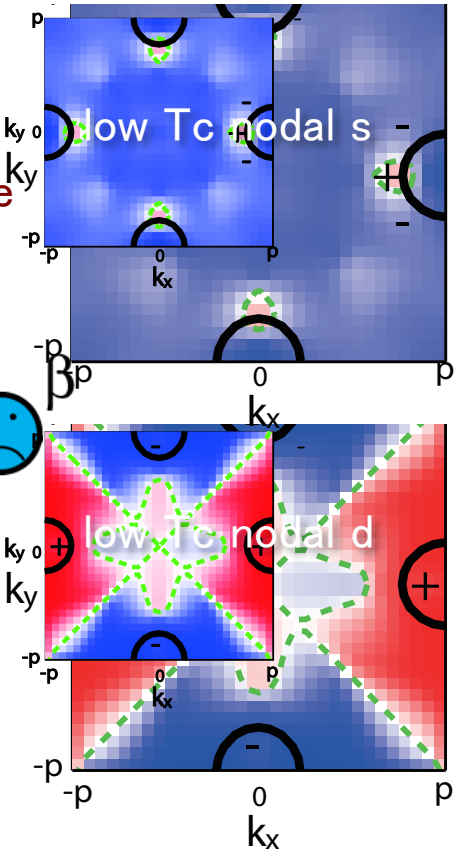


Kuroki et al, PRB **79**, 224511 (2009)



"Frustration" in momentum space





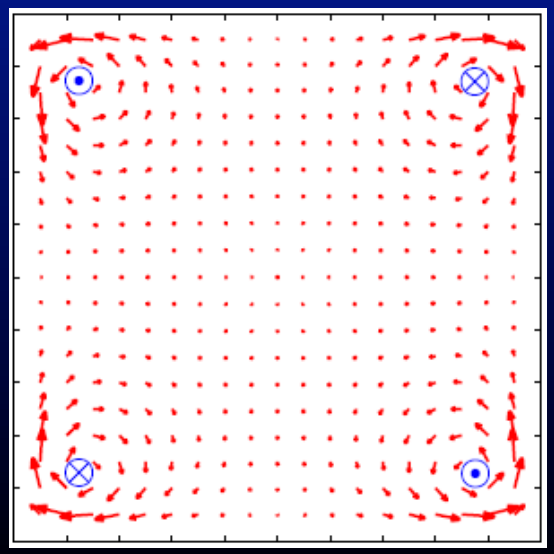
Multiband systems

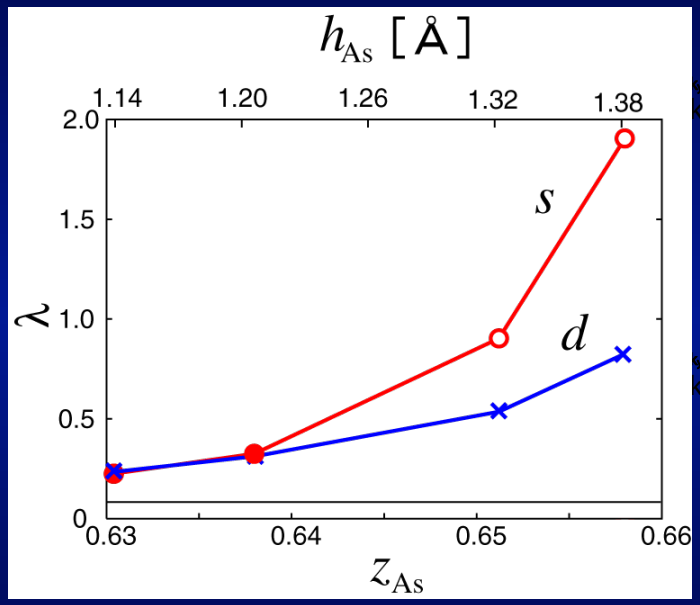
→ various pairings when materials / p are tuned

Degeneracy point

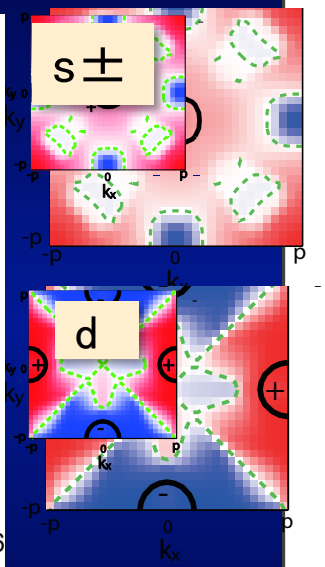
→ s+id？

(S.C. Zhang's group, PRL 2009)





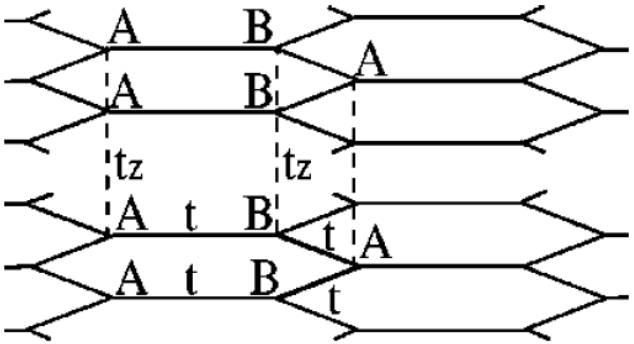
(Kuroki et al, PRB 2009)

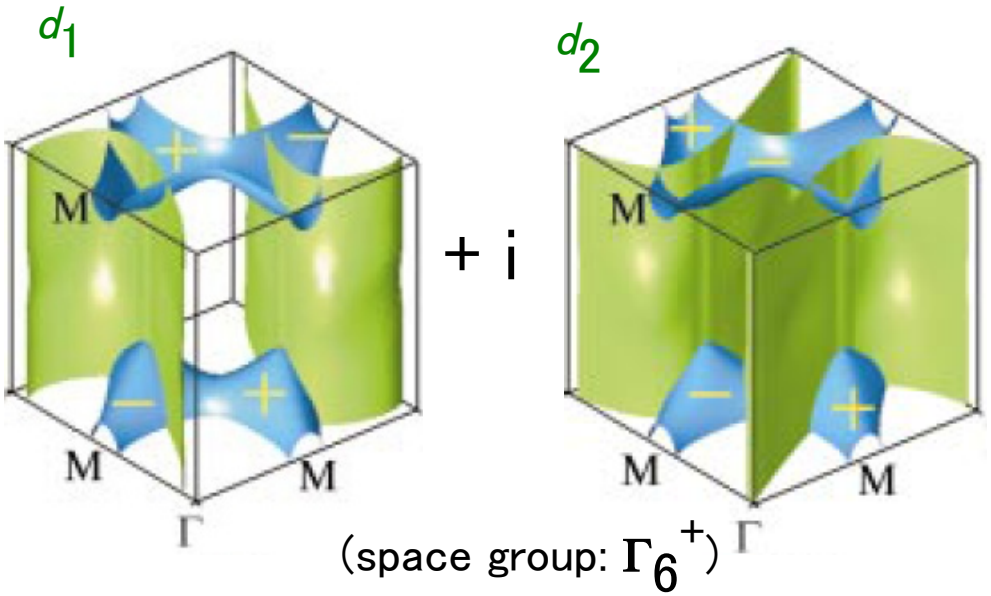


When T-broken pairing can occur?

When the space group has a two-dimensional rep:
as in

- $p + ip$ for triplet SC
- $p + ip$ for graphene (Uchoa et al, PRL 2007)
- $d + id$ for singlet SC (Onari *et al*, PRB 2002)





(space group: Γ_6^+)

My talk today

- ✔ A brief introduction for the iron-based SC
- ✔ Mechanism for s± pairing
- ✔ Material-dependence (s± ⇔ d)
- ✔ Collective (phase) modes in multiband SC

  [Ota et al, arXiv:1008.3212]

  Keyword: Multiband SC

Collective excitation modes in SC

Collective mode in one-band SC

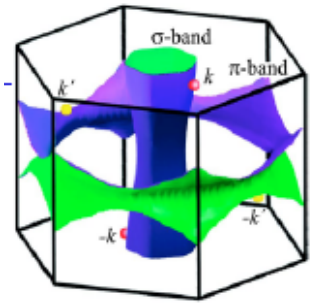
Phase modes (Bogoliubov 1959, Anderson 1958, Nambu 1960)
= massless Nambu-Goldstone mode for neutral SC
→ massive for real (charged) SC (Anderson-Higgs mechanism 1963)
as observed in $NbSe_2$(Raman: Sooryakumar & Klein 1980, Littlewood & Varma 1981)

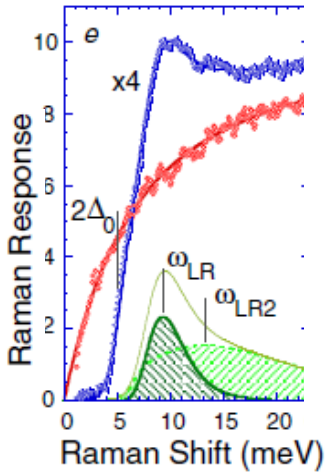
Collective modes in two-band SC

Out-of-phase (countersuperflow) mode (massive, Leggett 1966)

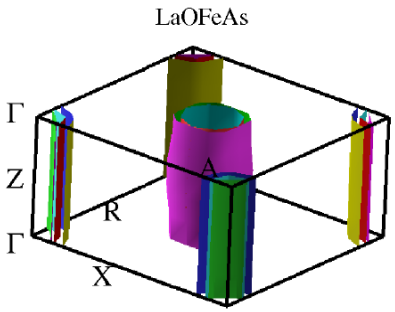
Two-band SC

Leggett mode observed in MgB_2 (Blumberg et al 2007)





Three-band SC



* Iron-compound

* Cold atoms on optical lattices
  with multiple hyperfine states

Question: 3-band ≠ 2-band
in terms of the collective modes ?

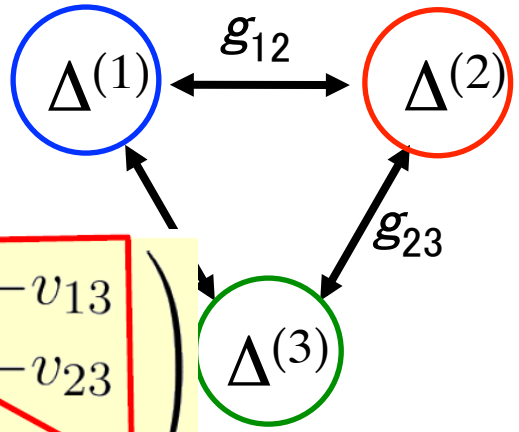
Yes, more than one collective Leggett modes emerge
in 3-band SC
← large difference in mass when
multiple (internal) Josephson currents subtract

(Ota et al, arXiv:1008.3212)

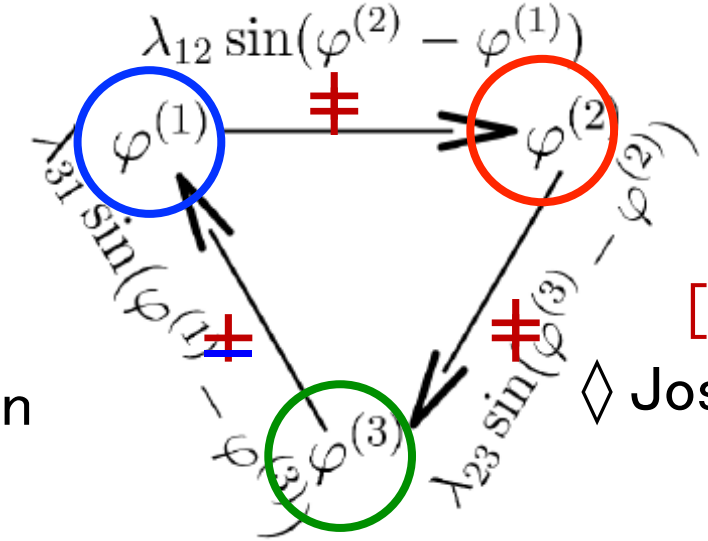
Question here: 3-band = 2-band
in terms of the collective modes ?

(Ota et al, 2010)

$$\hat{\mathcal{H}}_{\rm pair} = -\sum_{i,j} g_{ij} \underbrace{\hat{\psi}_{\uparrow}^{(i)\dagger} \hat{\psi}_{\downarrow}^{(i)\dagger}}_{i\text{th band}} \underbrace{\hat{\psi}_{\downarrow}^{(j)} \hat{\psi}_{\uparrow}^{(j)}}_{j\text{th band}}$$



$$\boldsymbol{g} = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{12} & g_{22} & g_{23} \\ g_{13} & g_{23} & g_{33} \end{pmatrix} \Rightarrow \boldsymbol{g}^{-1} = \begin{pmatrix} v_{11} & -v_{12} & -v_{13} \\ -v_{12} & v_{22} & -v_{23} \\ -v_{13} & -v_{23} & v_{33} \end{pmatrix}$$



even / odd
← $(\boldsymbol{g}^{-1})_{ij}$

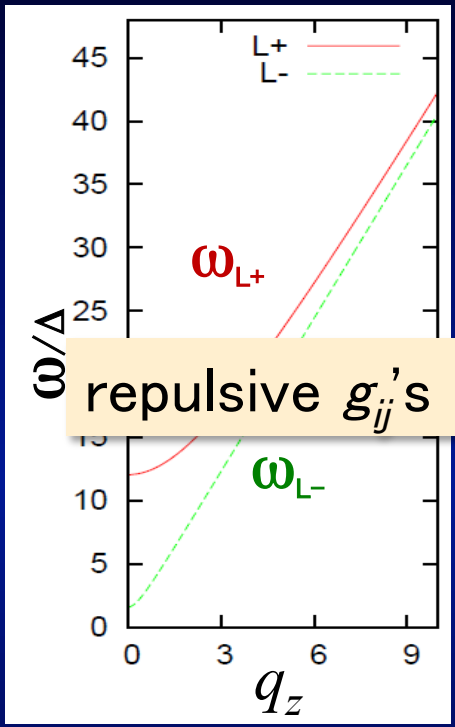
[class "even"]
→ internal Josephson c's add

[class "odd"]
◊ Josephson c's subtract

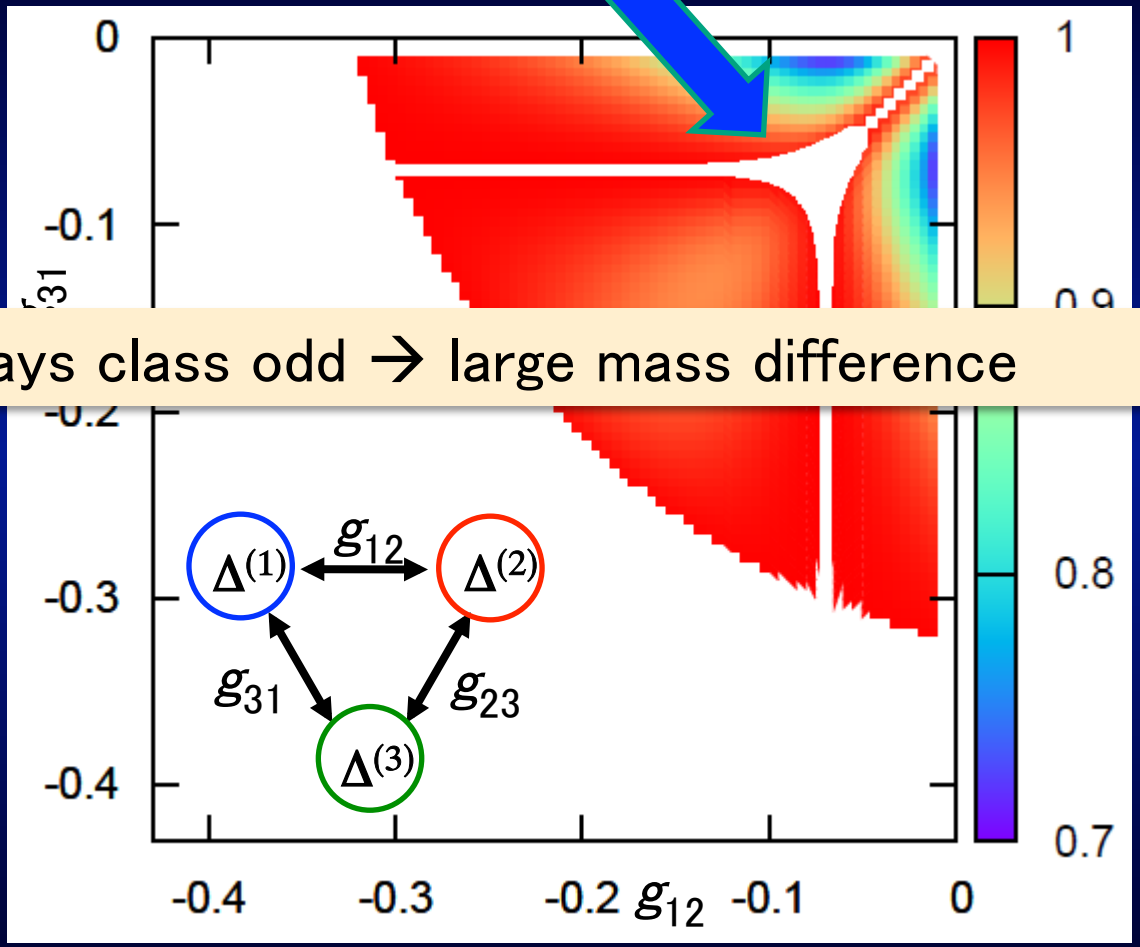
When the pairing interactions g_{ij} are varied

(Ota et al, arXiv1008.3212)

multiple Leggett modes



mass difference



repulsive g_{ij}'s → always class odd → large mass difference

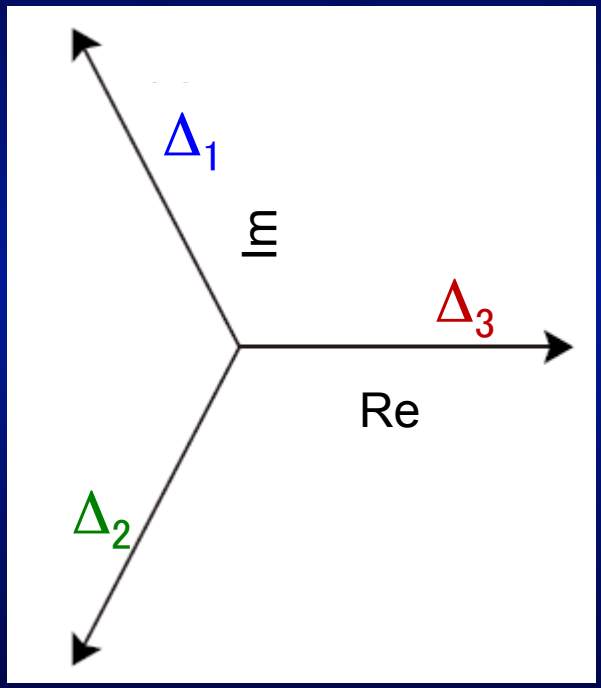
$$\begin{bmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{bmatrix} \begin{bmatrix} |d\rangle \\ |s\rangle \\ |b\rangle \end{bmatrix} = \begin{bmatrix} |d'\rangle \\ |s'\rangle \\ |b'\rangle \end{bmatrix}$$

g_{23}=−0.07

"Frustration" in the three-band SC
→ complex (T-reversal broken) Δ

(Stanev & Tesanovic, PRB 2010)

when $|g_{12}| \sim |g_{23}| \sim |g_{31}|$



Summary and outlook

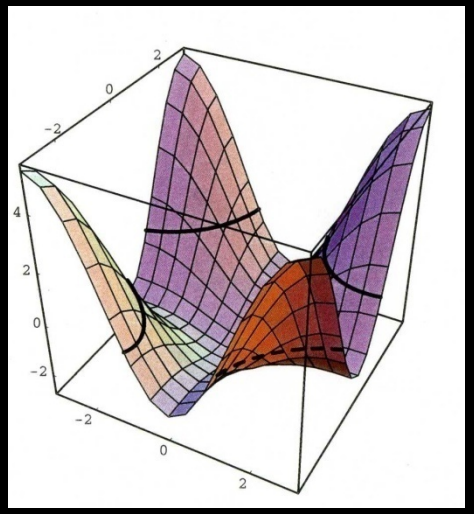
✔ Iron-based SC --- a prototype multiband SC
various possibilities incl. various pairings
✔ Collective phase mode in 3-band

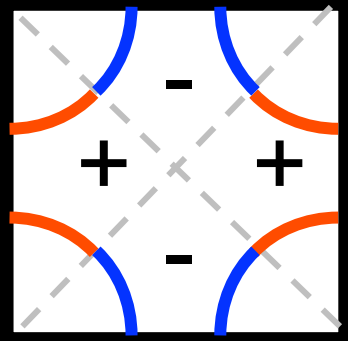
Multiband SC → rich prospects

Other multiband SC's ?

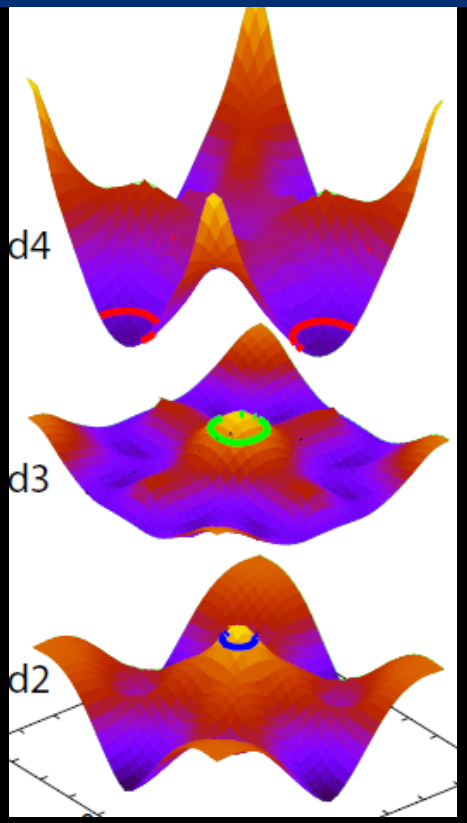
✔ Even the cuprate has to be viewed as multiband

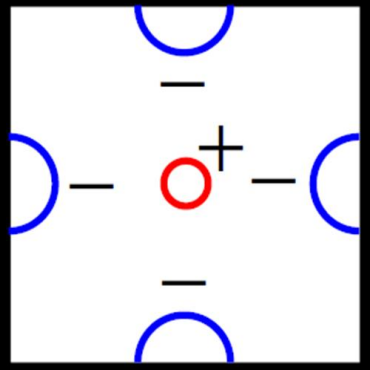
Cuprates: single-band





Iron-based: multi-band





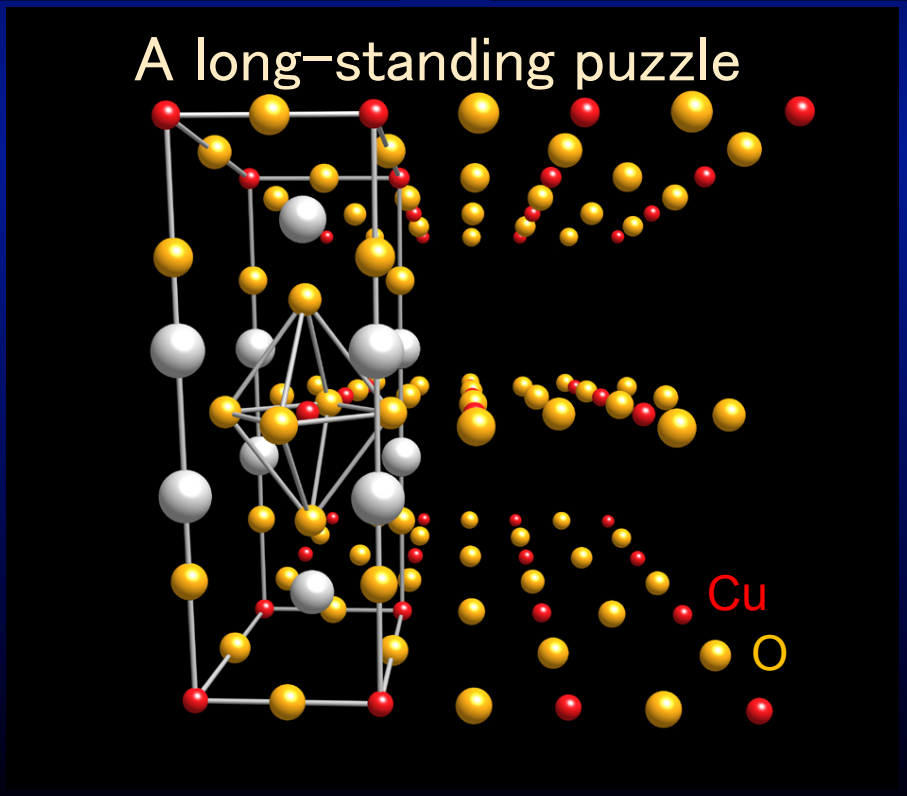
Cuprates: still a lot of puzzles

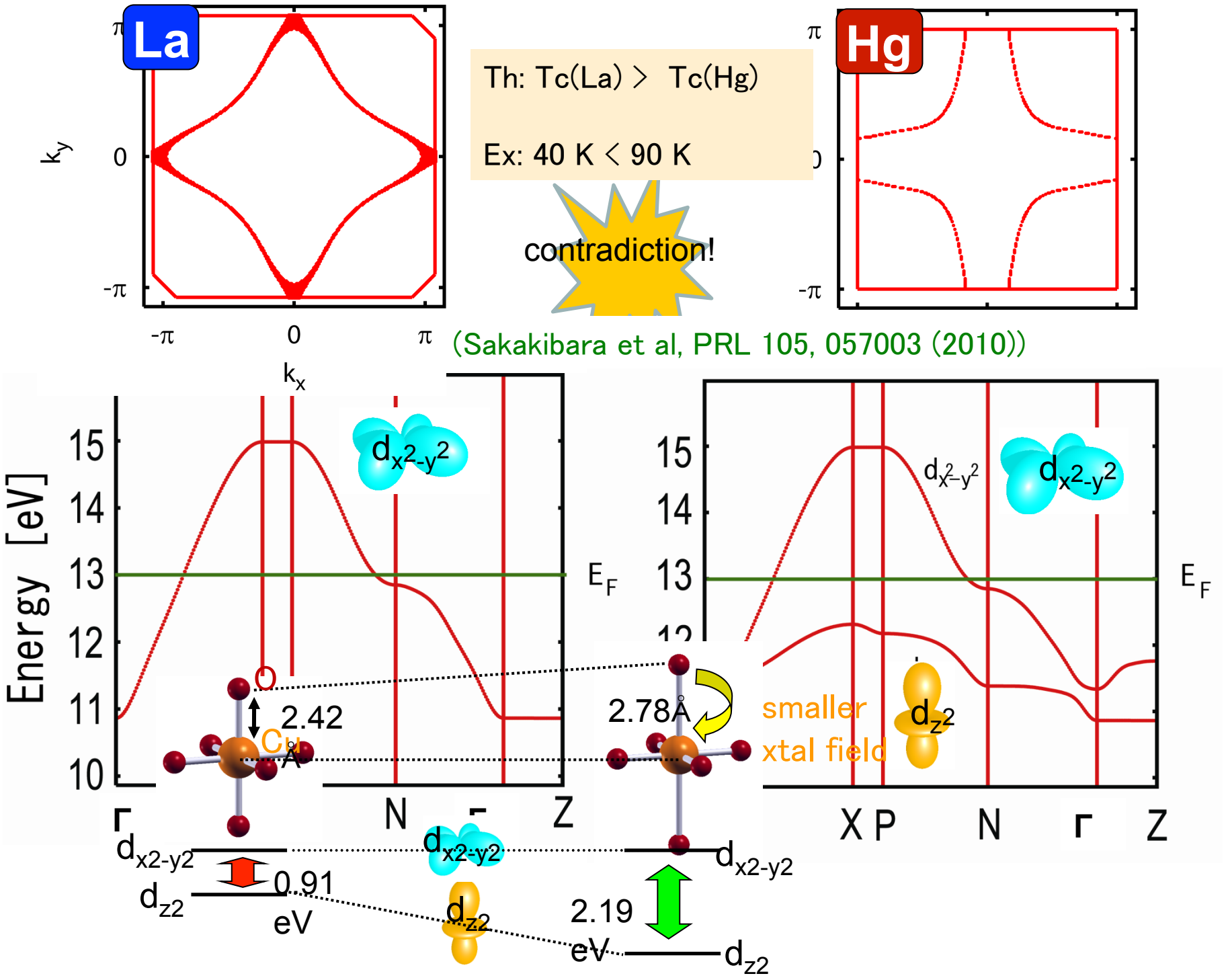
Various classes of cuprates

single-layered (simplest possible)

La_2CuO_4: Tc ~ 40K **$HgBa_2CuO_4$: Tc ~ 90K**

A long-standing puzzle

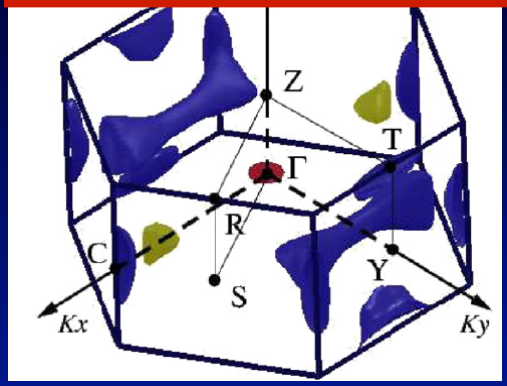



La
Hg
Th: Tc(La) > Tc(Hg)
Ex: 40 K < 90 K
contradiction!
(Sakakibara et al, PRL 105, 057003 (2010))
k_y
k_x
π
0
-π
Energy [eV]
15
14
13
12
11
10
E_F
$d_{x^2-y^2}$
O
Cu
2.42 Å
2.78Å
smaller
xtal field
d_{z^2}
Γ
N
Z
X
P
d_{x2-y2}
d_{z2}
0.91 eV
2.19 eV

Outlook (1): diverse multiband SC's

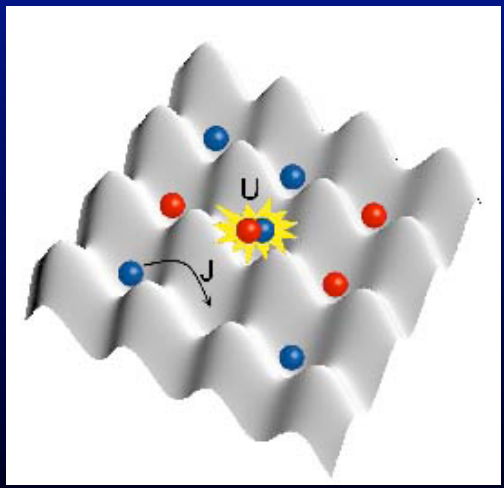
* Molecular solids tend to be multiband

Metallic H at 414 GPa

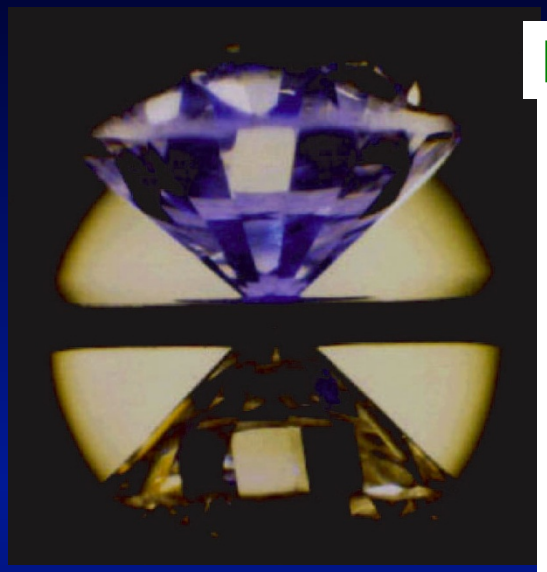


(Gross et al, 2009)

* Cold atoms
(different hyperfine states
on optical lattices)

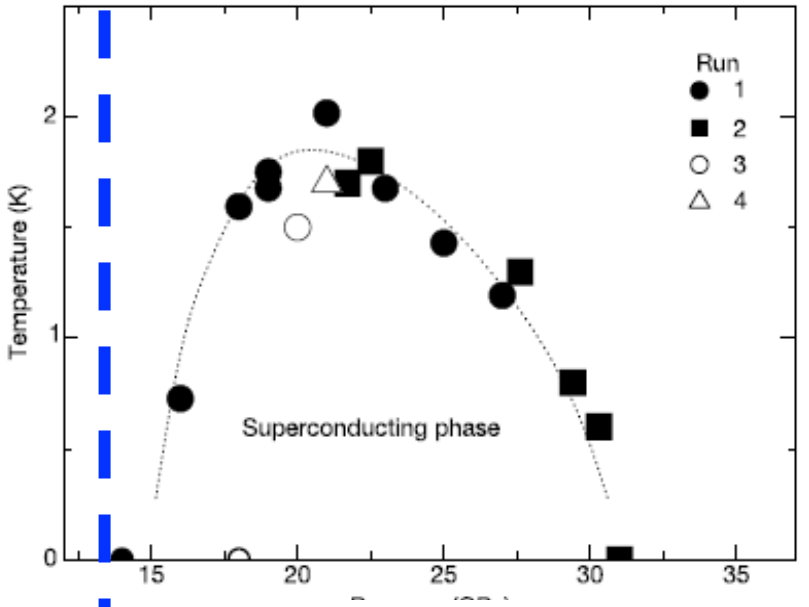


SC in elemental Fe under p

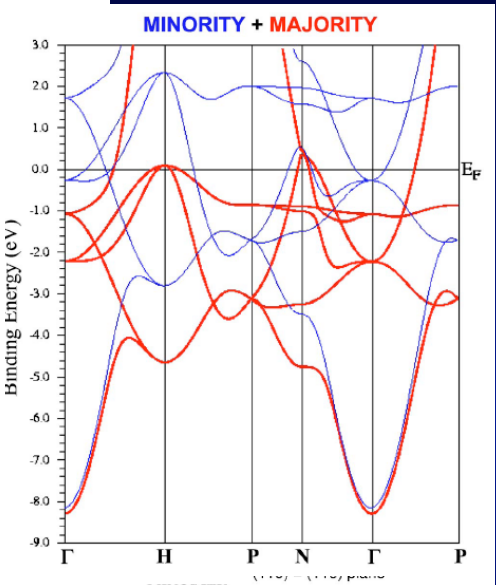


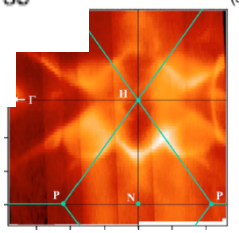
http://www.physics.nmsu.edu

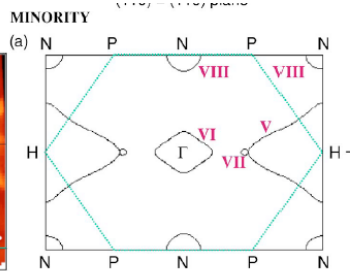
[Shimizu et al, Nature 412, 316 (2001)]

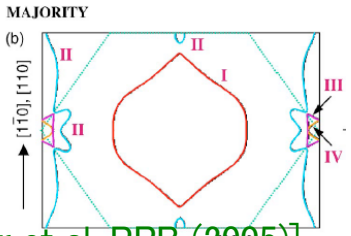


bcc(magnetic) hcp(nonmagnetic, SC)









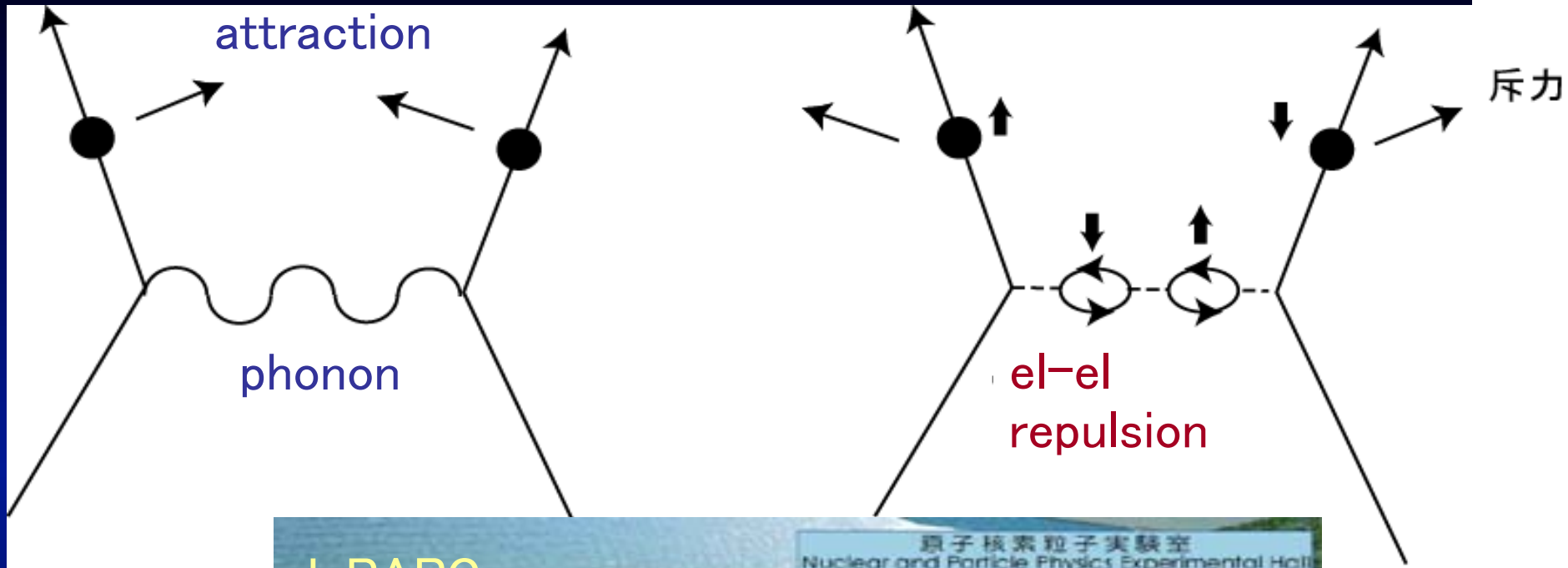
[Schafer et al, PRB (2005)]

Theories:

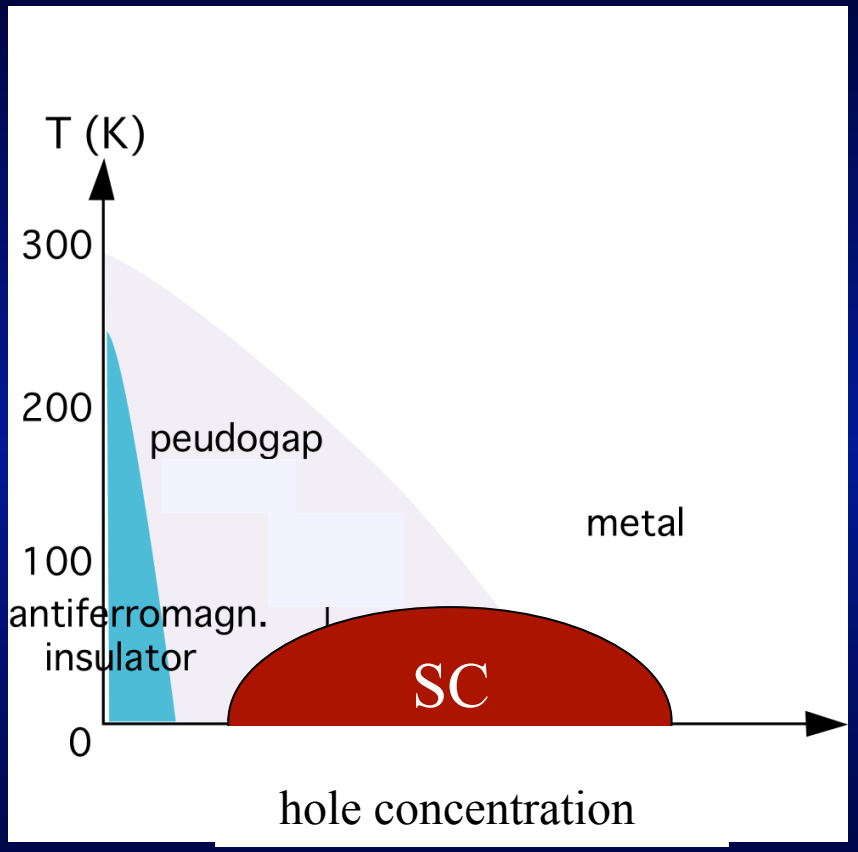
el-ph cannot explain Tc [Suzuki et al, 2002;
Mazin et al, PRB 2002],

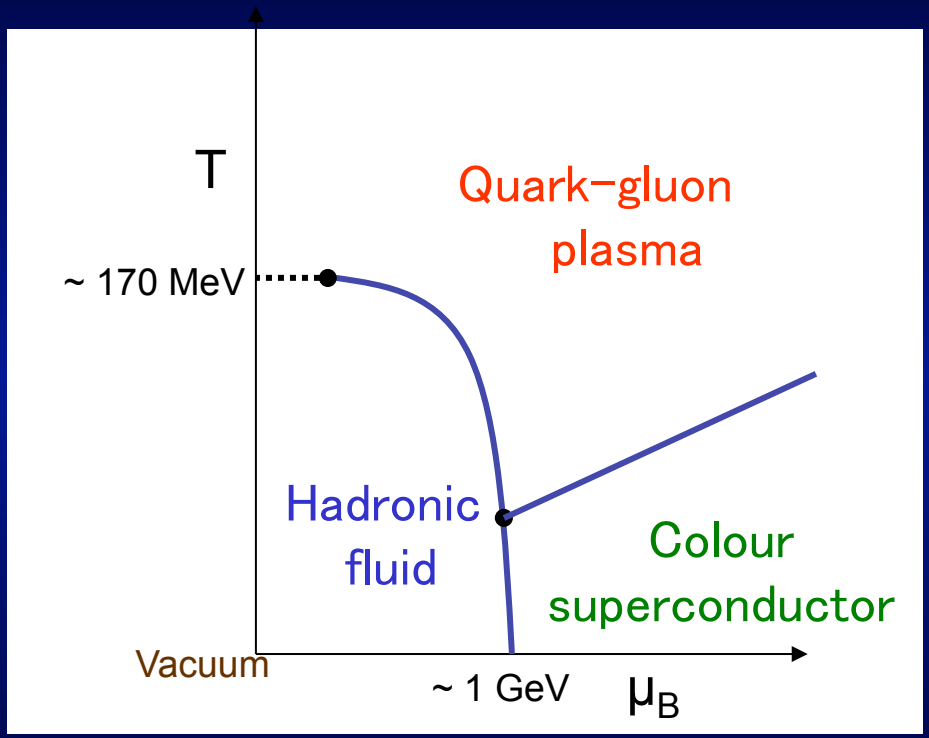
→ spin fluctuations have to be considered

To actually look at the interactions



Outlook (2): Colour SC in hadron physics





Spin–fluct mediated,
Multi–band SC,
. . .

Gluon,
various SC phases,
. . .

Differences in SC in solid-state vs hadron phys

	solid-state	hadron phys
Energy scale	~ 10 meV	~ 100 MeV
Length scale	1 ~ 10^3 nm	1 ~ 10 fm
Particles involved	e's with anisotropic FS	relativistic quarks with isotr FS
Interaction	e-e, e-phonon	gluon-mediated long-range
Tc	Tc ~ 0.01 ε_F	Tc ~ 0.1 ε_F
Internal deg	spin, orbit	colour, flavour, spin
Order of phase tr	weakly 1st ← fl of EM	1st ← thermal fl of gluons