

Compensated electron and hole pockets in an underdoped high- T_c superconductor

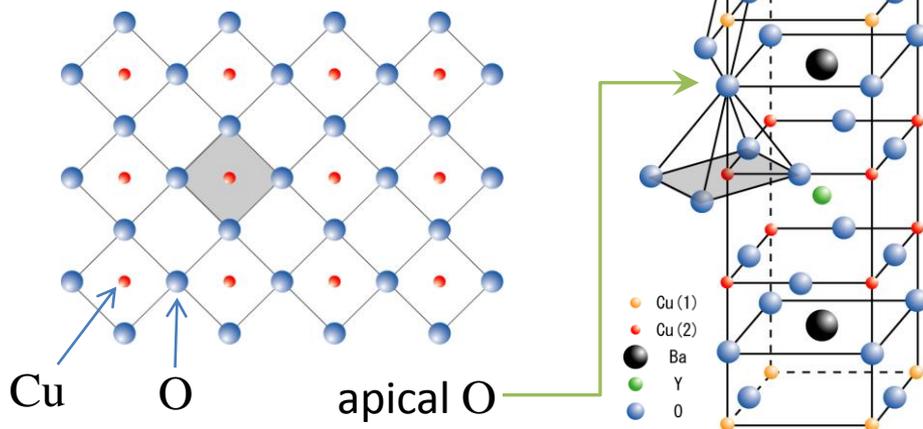
2010/07/23 Summer seminar

R. Katsumata

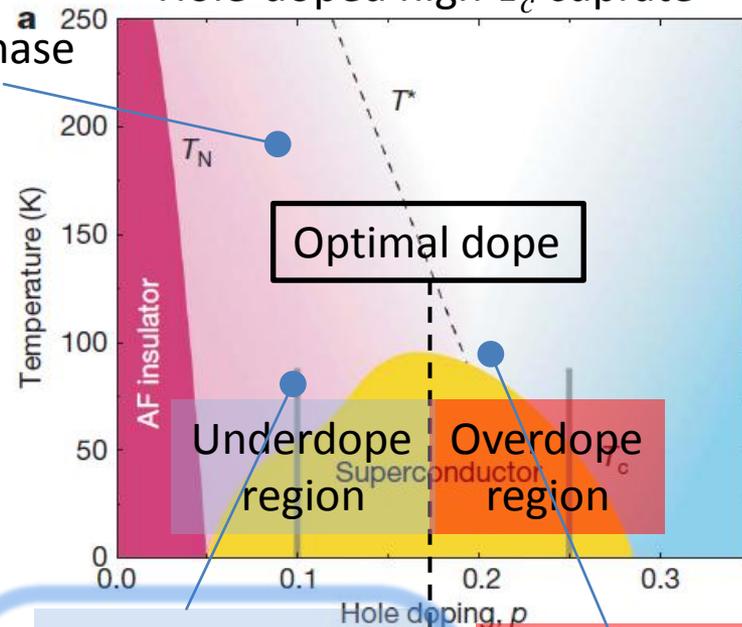
Introduction

High- T_c superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

“Stage of the S.C.”
 CuO_2 layer

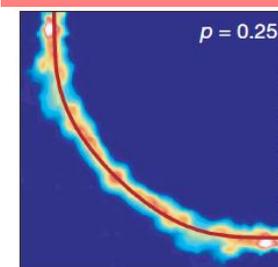
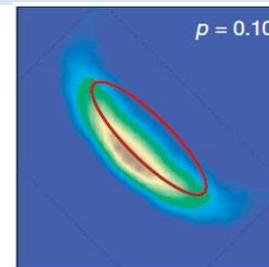


Phase diagram of
 Hole-doped high- T_c cuprate



Underdoped region

Overdoped region



Fermi arcs (\neq surface)
 (Pseudogap phase)

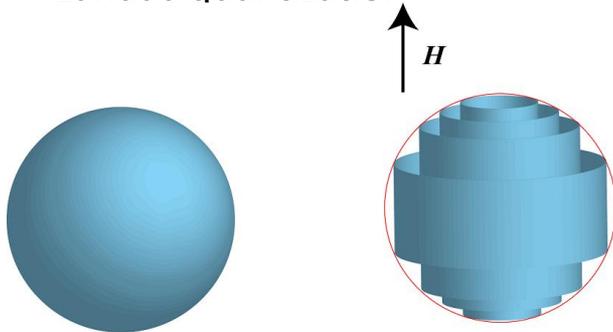
Fermi surface (F.S.)
 (normal state)

Low-lying excitations in
underdoped high- T_c cuprate
 is not clarified.

Experiment

Quantum oscillation (Q.O.) : powerful probe to study topology of F.S.

Magnetic field // c axis
 \Rightarrow Landau quantization

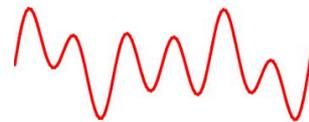
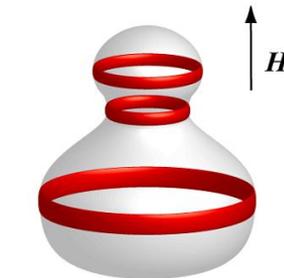


H going up, Landau level goes across Fermi level.

Conductor electrons cannot have more energy than E_f

\rightarrow Fermi level : changing periodically to $1/H$ (T⁻¹)

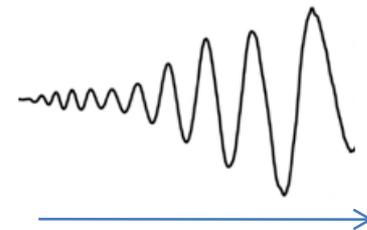
Extremal cross-sectional area of F. S. can be obtained !



Onsager expression

$$F = \Delta \left(\frac{1}{B} \right) = \frac{2\pi e}{\hbar c S}$$

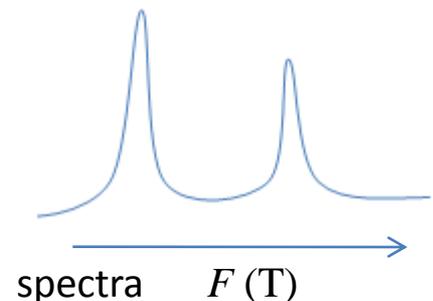
$$A_k = \frac{2\pi e}{\hbar} F$$



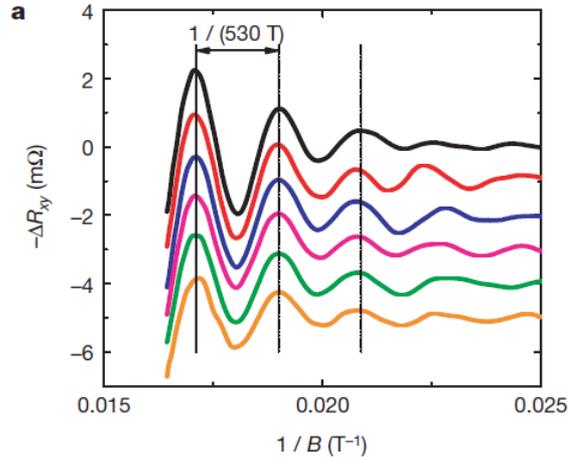
$\downarrow H$ (T)

1. x-axis translation
 $(\mu_0 H) T \rightarrow (1/\mu_0 H) T^{-1}$
 to make the graph periodic
2. Fourier translation
 wavelength (T⁻¹)
 \rightarrow frequency (T)

\downarrow



Experiment



Hall resistance of $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$

The first observation of Q.O. in underdoped high- T_c cuprate

N. Doiron-Leyraud, et al., *Nature* 447, 565 (2007)

Recent study about Q.O. in

underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

by Suchitra E. Sebastian et al. ($x = 0.56$)

Experimental remarks

- Measurement of Contactless conductivity
- Wide range in field $28 \leq \mu_0 H \leq 85$ T
- High resolution enough to identify more distinct Q.O. frequencies
- Angular dependence of out-of-plane & in-plane rotation (θ and ϕ)

Remarkable results and new interpretations I introduce from now were offered !!

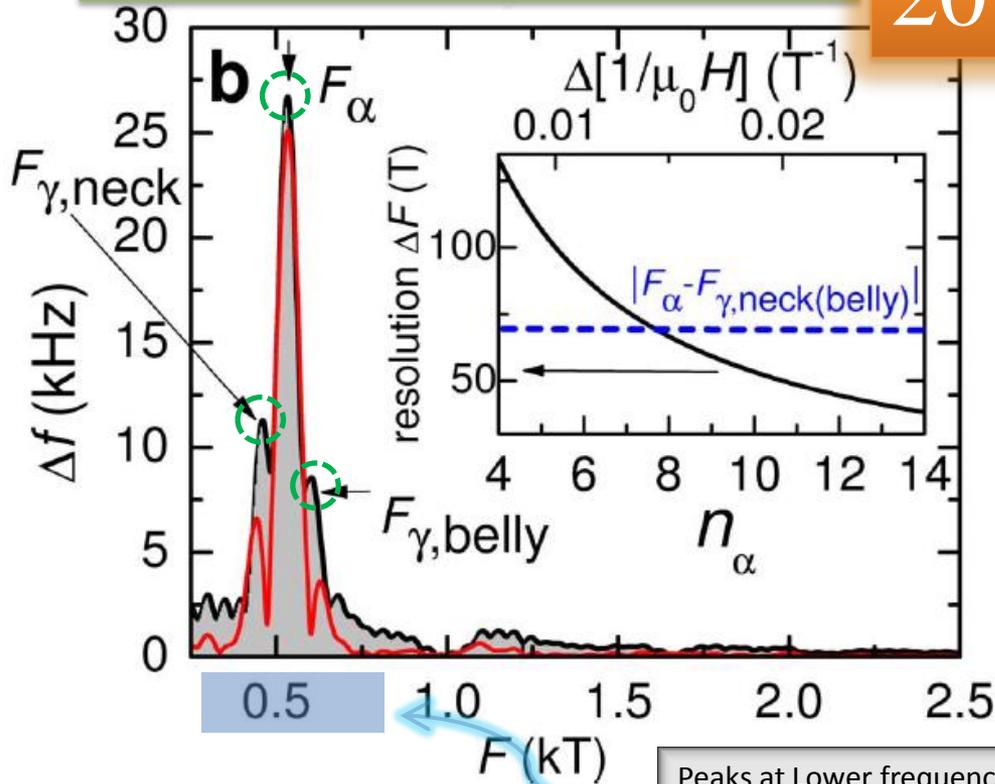
S.E. Sebastian, et al., *Nature* 454, 200 (2008)

S.E. Sebastian, et al., *PRB* 81, 214524 (2010)

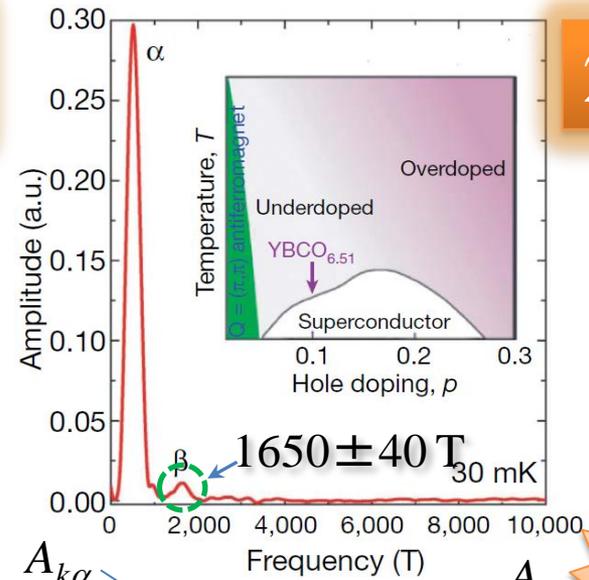
Results and analysis

What is derived from these spectra ?

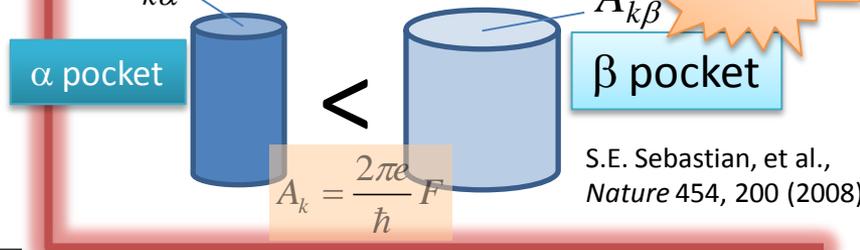
2010



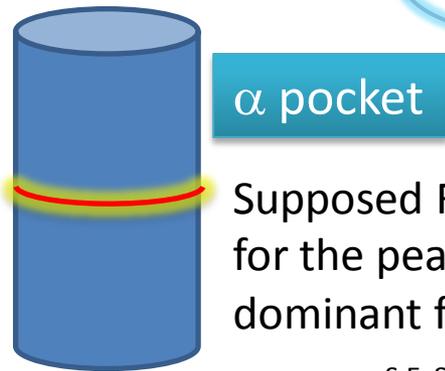
2008



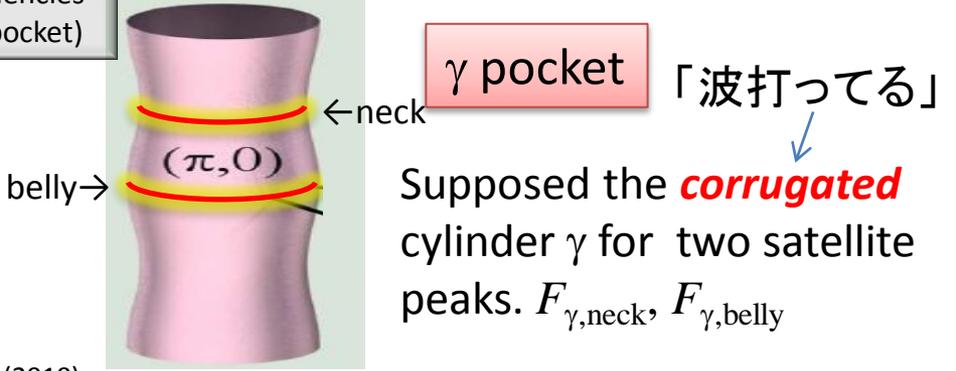
New!!



S.E. Sebastian, et al., Nature 454, 200 (2008)



Peaks at Lower frequencies meaning small F.S. (pocket)



S.E. Sebastian, et al., PRB 81, 214524 (2010)

Results and analysis

Analysis by Fourier translation

Fitting !

$$\Delta f = \sum_{i=\alpha,\gamma} \Delta f_{i,0} R_T R_D J_0 \left(\frac{2\pi \Delta F_{i,\theta}}{\mu_0 H \cos \theta} \right) \cos \left(\frac{2\pi F_i}{\mu_0 H} \right)$$

↑
amplitude

$$F_{i,(neck,belly)} \cos \theta = F_i \pm \Delta F_{i,\theta}$$

↑
Effect of
depth of corrugation
of sheet i , angle θ

Temperature Damping factor

$$R_T = (2\pi^2 k_B m_i^* T / e \hbar \mu_0 H) / \sinh(2\pi^2 k_B m_i^* T / e \hbar \mu_0 H)$$

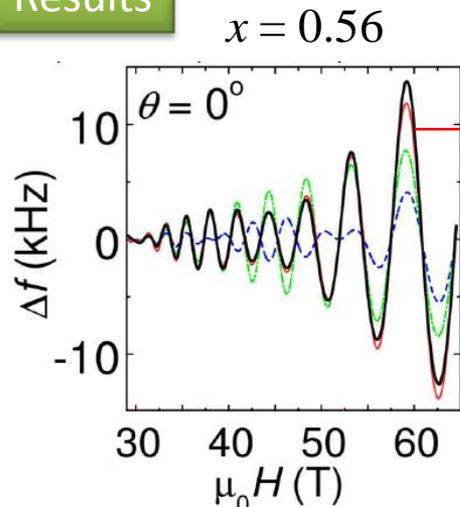
Dingle Damping factor

$$R_D = \exp\left(\frac{-\Gamma_i}{\mu_0 H}\right)$$

Γ_i : damping constant

J_0 : Bessel function (phase smearing)

Results



Red one

α pocket

$$F_{\alpha,0} = 531 \pm 2 \text{ T}, \Delta F_{\alpha,0} \leq 11 \text{ T}$$

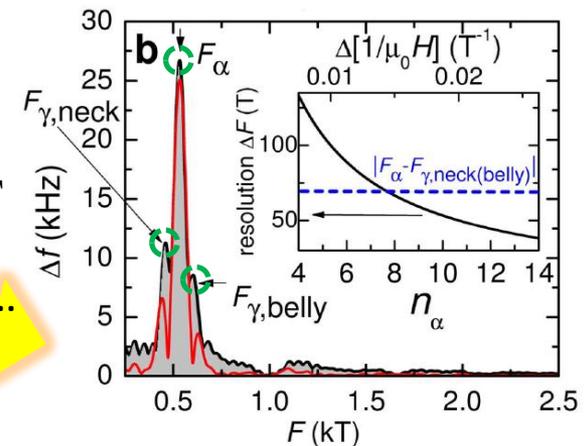
γ pocket

$$F_{\gamma,0} = 532 \pm 2 \text{ T}, \Delta F_{\gamma,0} = 72 \pm 11 \text{ T}$$

Corresponding to...

Reasonable results !

and we can subtract the dominant α component.



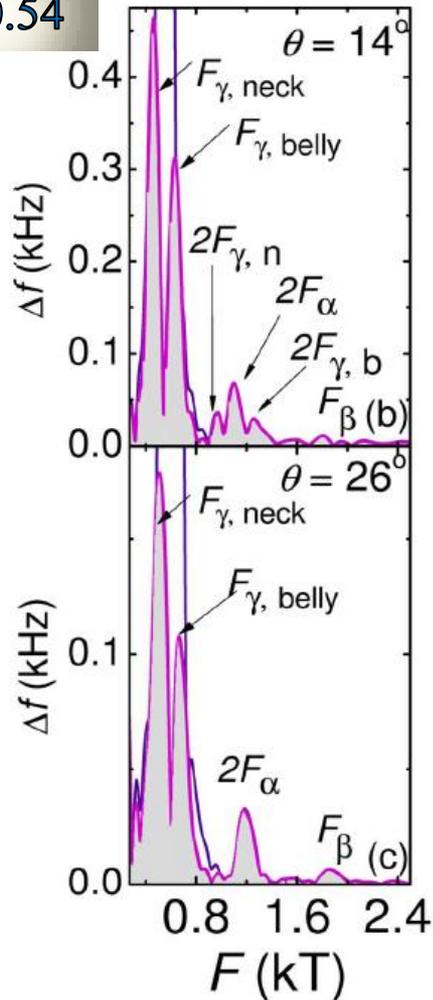
$$F_\alpha = 531 \pm 2 \text{ T}$$

$$F_{\gamma,neck} = 460 \pm 4 \text{ T}, F_{\gamma,belly} = 604 \pm 4 \text{ T}$$

Results and analysis

Analysis by Yamaji's expression

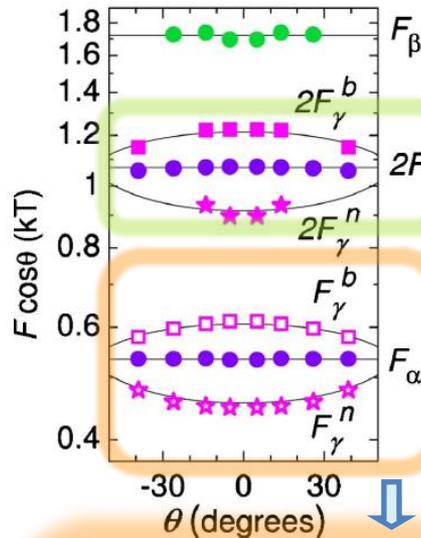
$x = 0.54$



γ (neck+belly) and β components after subtracting α

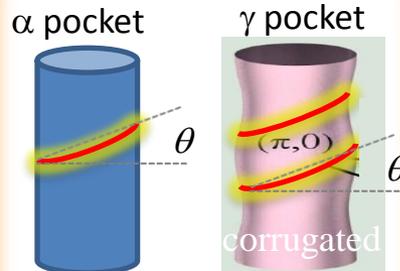
S.E. Sebastian, et al., PRB 81, 214524 (2010)

Angular dependence (about θ)



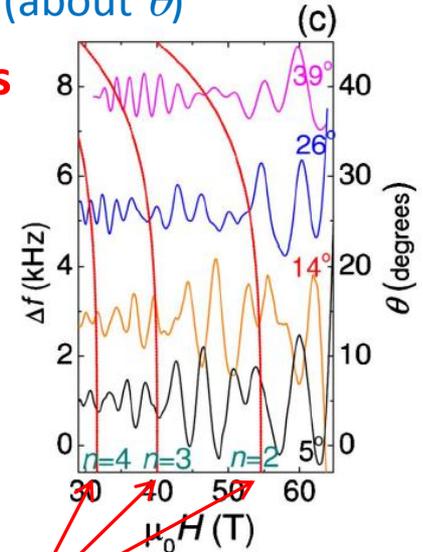
Harmonics are also observed!!

Similarly sized



Onsager expression

$$F = \Delta \left(\frac{1}{B} \right) = \frac{2\pi e}{\hbar c S}$$



Fitting

Detecting locations of **nodes** in oscillation component of γ (neck+belly)

$$\mu_0 H_n \cos \theta = \frac{8\Delta F_{\gamma,\theta}}{4n+3}$$

n : number of node
 $H_{n,i}$: the field at n th node

Yamaji's expression

$$\Delta F_{i,\theta} = \Delta F_{i,0} J_0(k_{\parallel} c \tan \theta)$$

Results and analysis

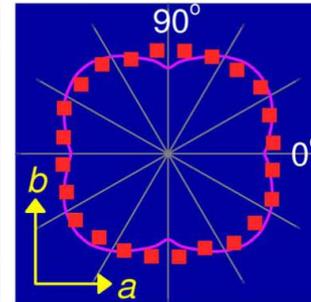
Angular dependence of In-layer rotation (ϕ)

α pocket : independent on ϕ
because of less corrugation
periodic in $1 / \mu_0 H \cos \theta$

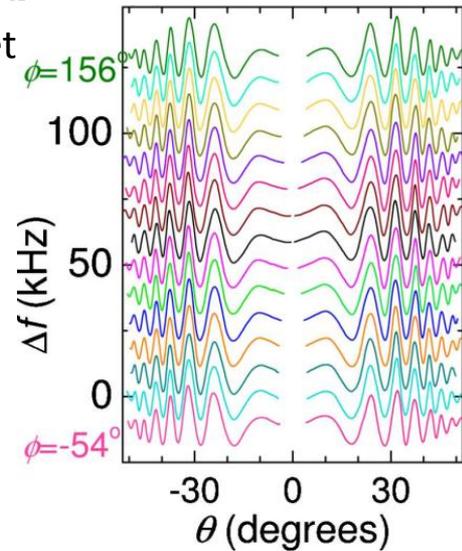
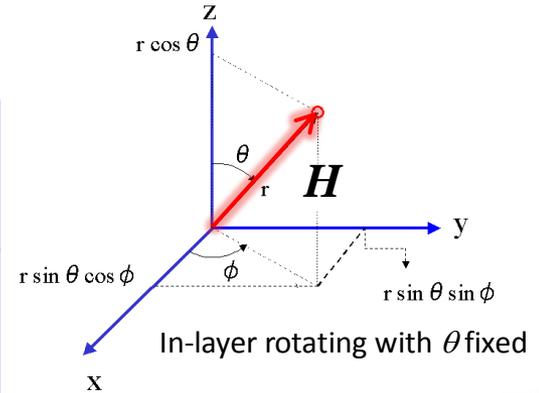
The topology of γ pocket

Consistent with numerous
F.S. reconstruction models

$k_{||}/k_F$



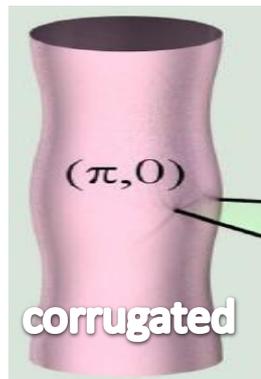
In-layer dispersion in γ pocket



α pocket

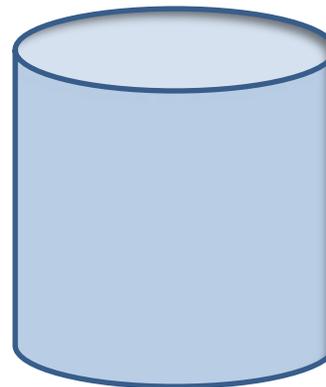


γ pocket



New!!

β pocket



Similar size

Discussion

In-layer dispersion ($\mathbf{k} = (k_x, k_y)$) Cu $d_{x^2-y^2}$ like band

$$\varepsilon(\mathbf{k}) = -4t \left[u(\mathbf{k}) + 2r \frac{v(\mathbf{k})^2}{1 - 2ru(\mathbf{k})} \right]$$

$$u(\mathbf{k}) \equiv \frac{1}{2}(\cos k_x + \cos k_y)$$

$$v(\mathbf{k}) \equiv \frac{1}{2}(\cos k_x - \cos k_y)$$

STEP1

Tightbinding model

If r is small...

$$\varepsilon(\mathbf{k}) = \text{const.} - 2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y),$$

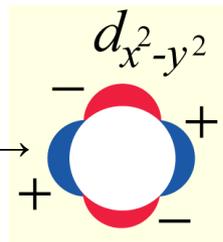
Hopping to next neighbor $t' = rt$
third neighbor $t'' = rt/2$

STEP2

Considering interlayer hopping... ↙ axial orbital

t_c : 4-fold rotation symmetry ← gap function $\Delta(\mathbf{k})$ →

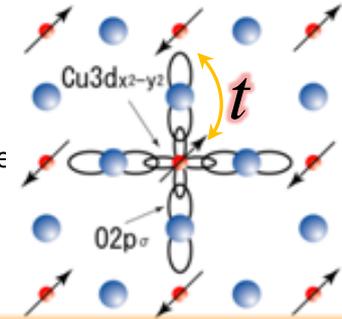
$r \rightarrow r + (t_c^0/t) \cos k_z$ k_z : interlayer dispersion



For $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ ($x \sim 0.5$), $t \sim 400 \text{ meV}$

t_c^0 causes to r vary $0.28 \sim 0.32$

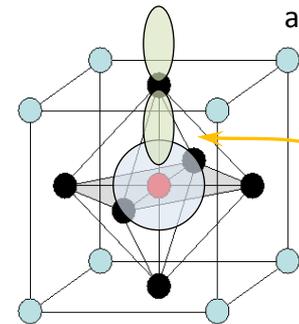
Perturbation in $r(\mathbf{k})$



t : the nearest neighbor (in-layer hopping integrals)

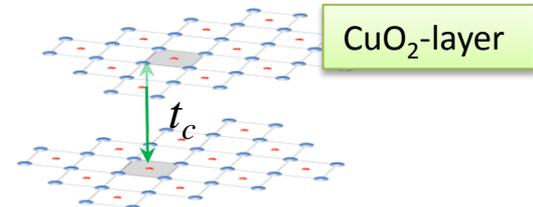
axial orbital: Hybrid of mostly Cu 4s and apical O $2p_z$

r : the range parameter of in-layer hopping via **axial orbital**



● : Cu ● : O

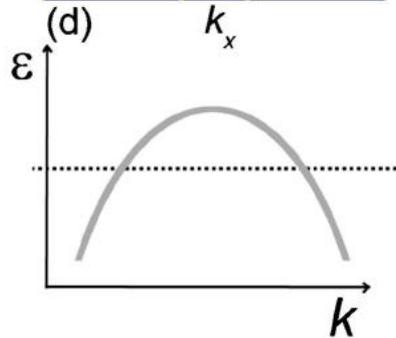
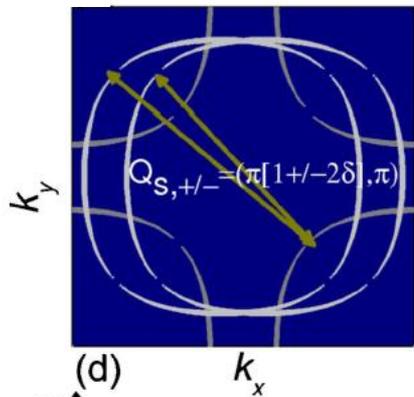
t_c : interlayer hopping integrals



Discussion

r perturbation $\rightarrow k_z$ dispersion \rightarrow Corrugation of pockets

Same symmetry in k_z (thickness of lines) and gap Δ ... \rightarrow Nodal point $(\pi/2, \pi/2) : \Delta = 0, k_z \sim \text{min}$
Antinodal point $(0, \pi) : \Delta \sim \text{max}, k_z \sim \text{max}$



Unreconstructed F. S. & band structure

Reconstruction \rightarrow

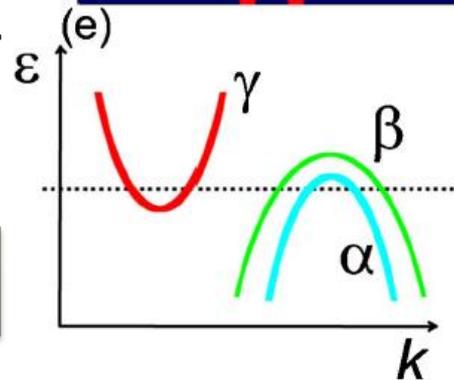
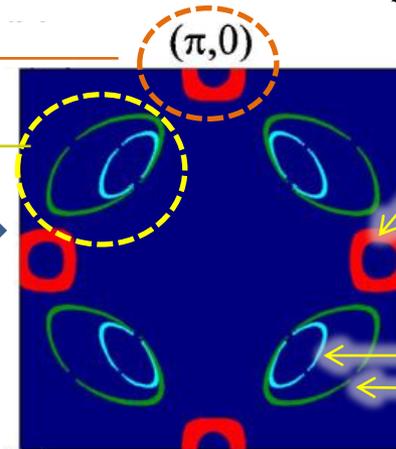
Translational symmetry-breaking order

by incommensurate vector

$$Q_{s,\pm} = (\pi[1 \pm 2\delta], \pi)$$

Order parameter : Δ_s

First instability



Reconstructed F. S. & band structure

Large k_z = corrugated γ pocket ?

Small k_z = less corrugated α, β pocket ?

Discussion

What kind of order reconstructs F.S. ?

Translational symmetry-breaking order

Incommensurate vector

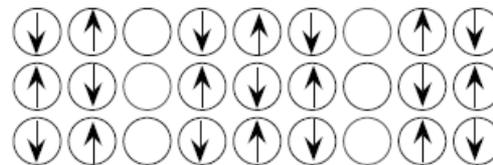
$$Q_{s,\pm} = (\pi[1 \pm 2\delta], \pi)$$

Order parameter : Δ_s

(1) **Stripe** structure

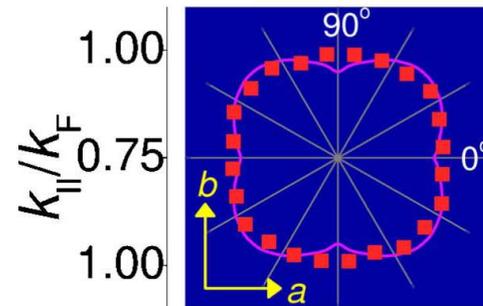
Typically $\delta = 1/8$

stripe SDW



Charge stripe
(antiphase domain wall)

A. J. Mills, et al., PRB 76, 220503 (2007)



S.E. Sebastian, et al., PRB 81, 214524 (2010)

(2) **Helical** structure ← considered now

Typically $\delta = 1/16$

helical SDW

or DDW $\Delta_{\mathbf{k}} = i2\Delta_{\text{DDW}}(\cos k_x - \cos k_y)$

Adjusting $\Delta_s = 0.625t$ yields ($p \sim 0.117$)

- three pockets of size (within 2%)
- carrier type
- corrugation depth
- shape

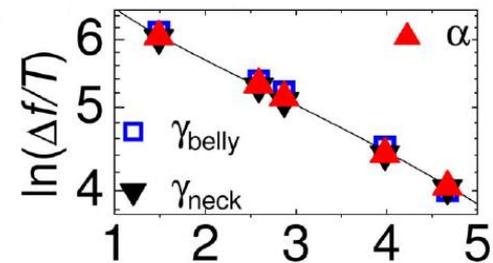
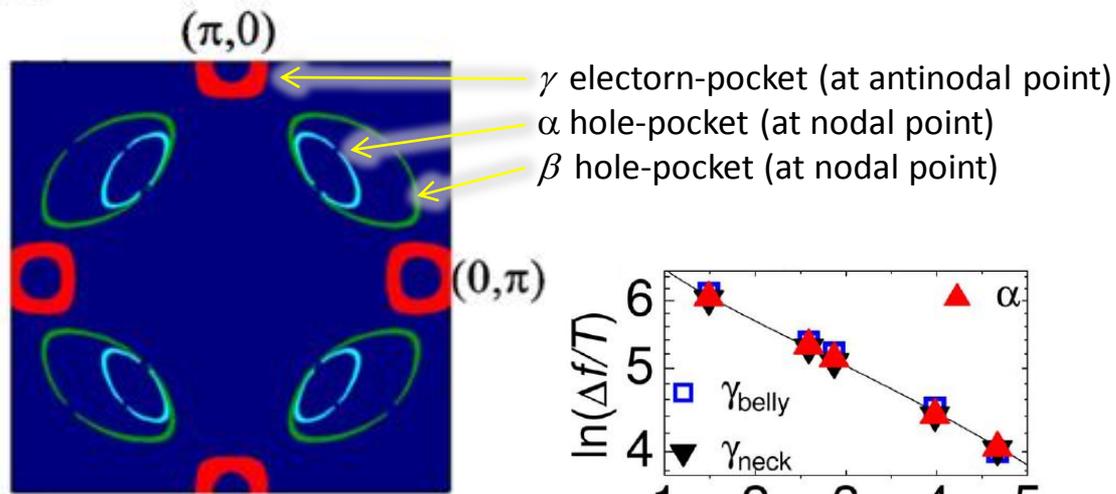
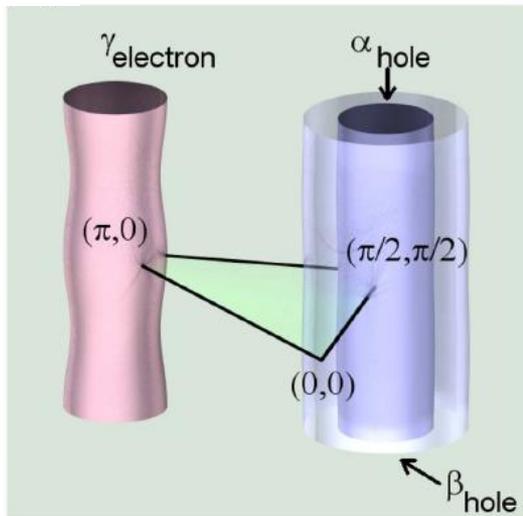
(observed $t \sim 100\text{meV}$)

consistent with results !

「しま模様」

「らせん状」

Discussion



Compensated two pockets

α hole-pocket
 γ electron-pocket

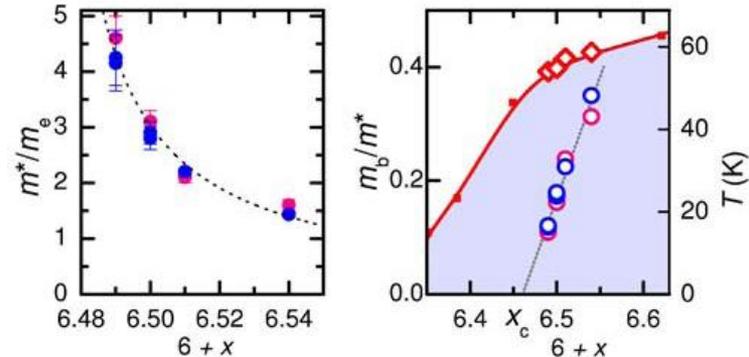
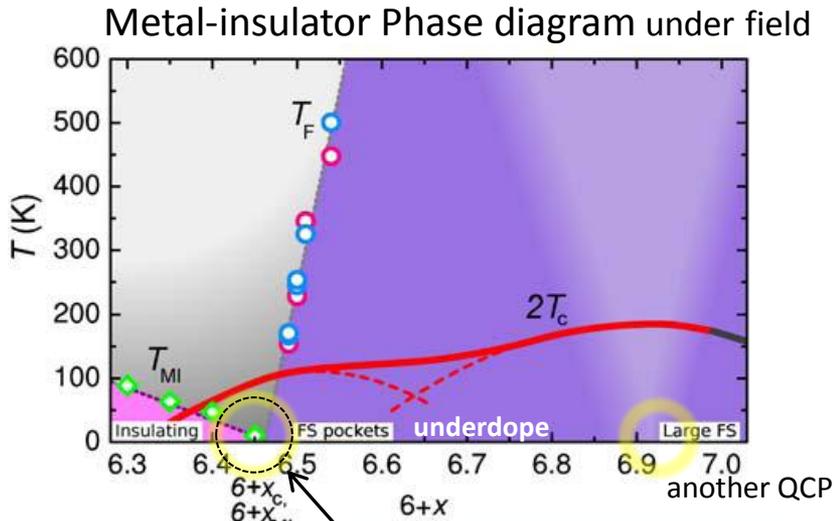
occupying 1.91 ± 0.01 % of B.Z.
 (for example, $x=0.56$)

$$m_{\alpha}^* \approx m_{\gamma}^* \approx 1.6m_e$$

β pocket acts as a reservoir of charge carriers,
 satisfying Luttinger count in the SDW state.

Discussion

Excitonic insulator instability



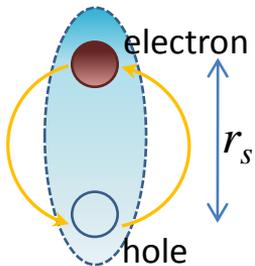
Observed divergence of effective mass

$x_c = 0.46$

metal-insulator QCP ?

S.E. Sebastian, et al., Proc. Natl.Acad. Sci. U.S.A. **107**, 6175 2010

Exciton : electron-hole pair (boson)



Analogy to hydrogen atom

Binding energy $Ry^* \sim 430 \text{ meV}$

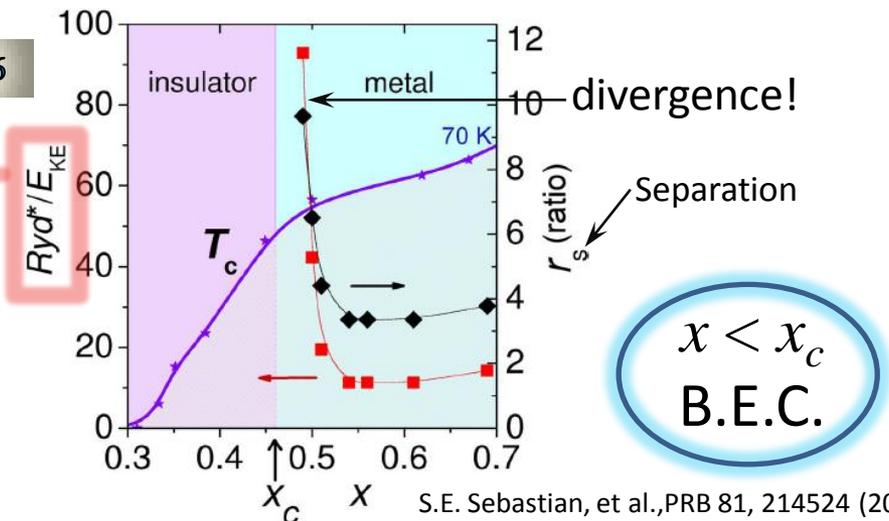
effective "Rydberg"

Individual kinetic energy $E_{KE} \sim 37 \text{ meV}$

$$Ry^* = \frac{\mu}{m_e} \frac{1}{\epsilon^2} Ry \quad E_{ke} = \frac{e\hbar F}{m^*}$$

$$a^* = \epsilon \frac{m_e}{\mu} a_0 \quad r_s \approx \frac{1}{a^*} \sqrt{\frac{1}{\pi n}}$$

$x = 0.56$



divergence!

Separation

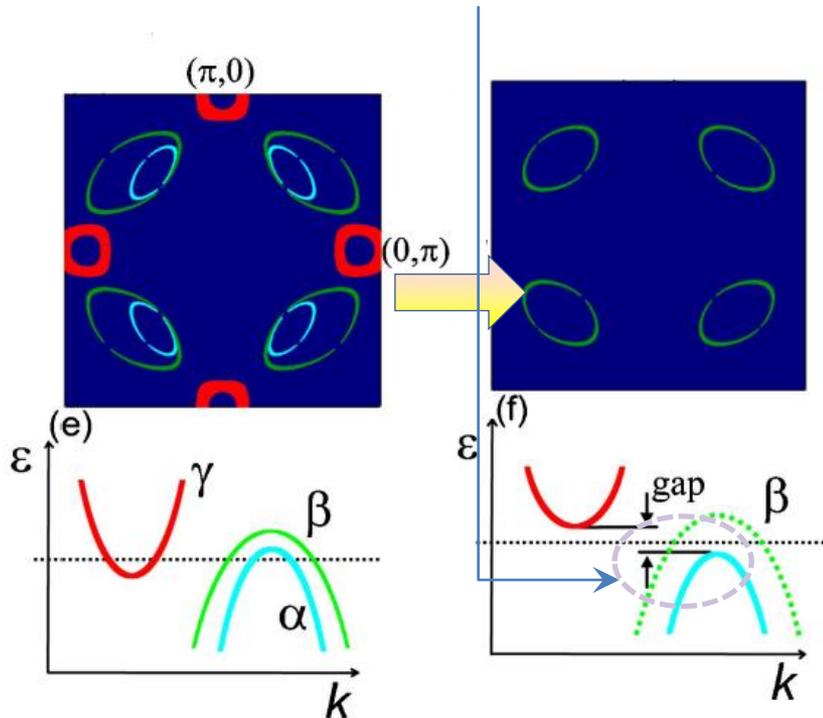
$x < x_c$
B.E.C.

S.E. Sebastian, et al., PRB 81, 214524 (2010)

Discussion

Secondary instability ~Destruction of compensated pockets ~

Gap due to excitonic insulator instability ($x < x_c$)



Observed F.S.
(and band)

F.S. after secondary
reconstruction



Accompanying **charge order**

“stripelike”

by $\mathbf{Q}_C = 2\mathbf{Q}_s = (\pm 4\delta\pi, 0)$

- Phonon broading
- superlattice

- spin order
- magnetic excitation

(This order can accompany SDW.)

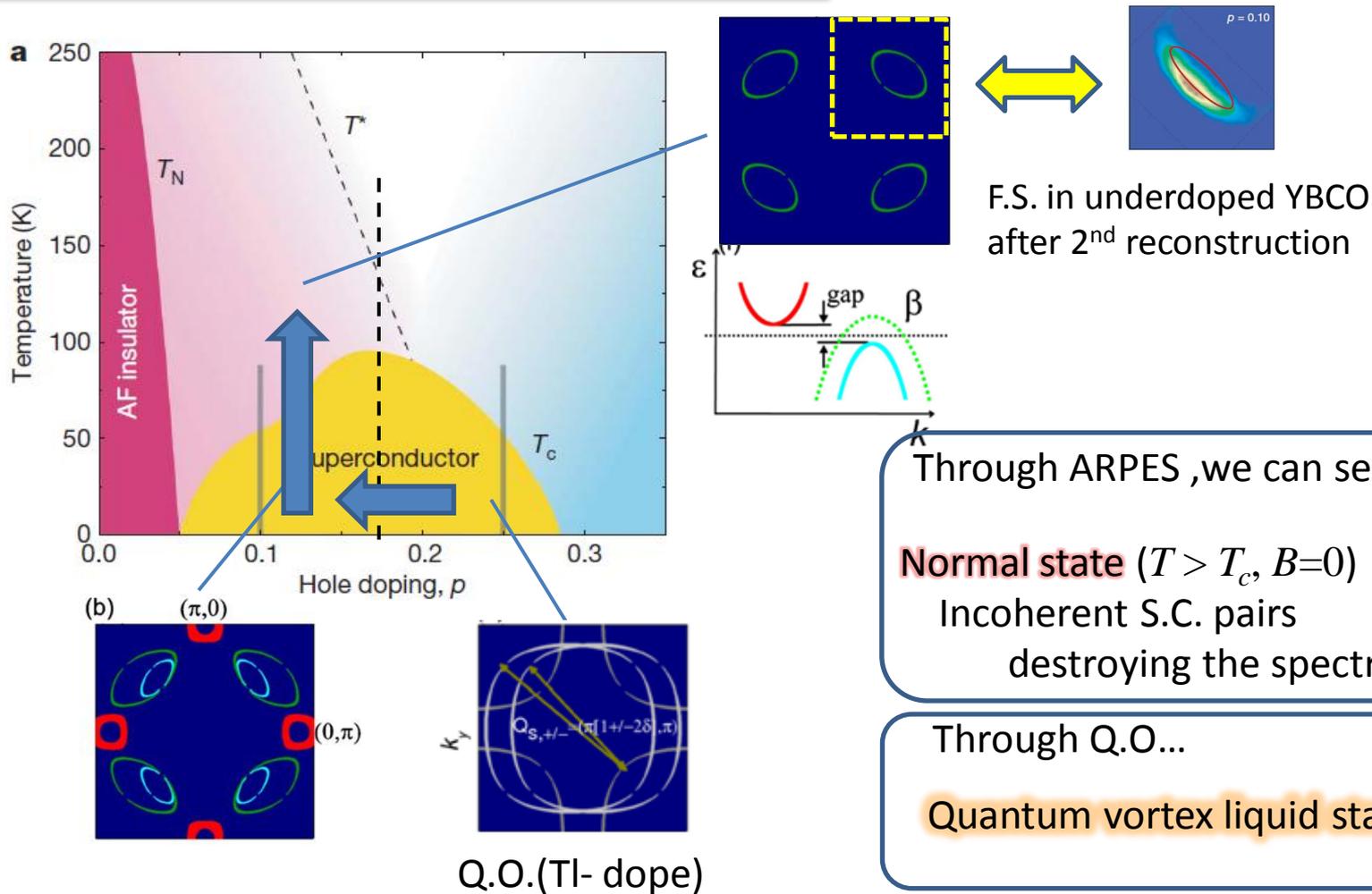
Additional new couplings

$\epsilon_{\mathbf{k}+n\mathbf{Q}_s}$ & $\epsilon_{\mathbf{k}+(n\pm 2)\mathbf{Q}_s}$

**Destruction of pockets
OR
Creation open F.S. sheets**

Discussion

Reconciliation with ARPES experiments



N. Doiron-Leyraud, et al., *Nature* 447, 565 (2007)

S.E. Sebastian, et al., *PRB* 81, 214524 (2010)

Summary

High-resolution Quantum Oscillation measurements

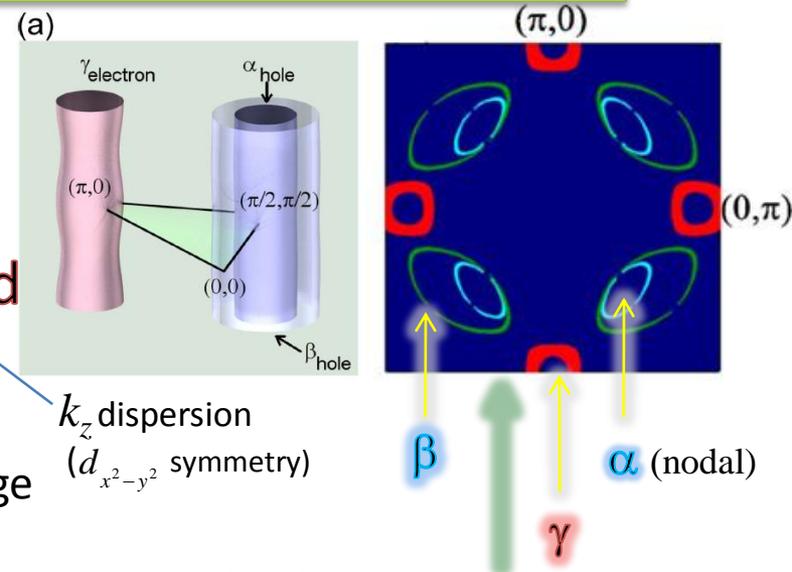
Small hole-pocket : α ← cylindrical

Large hole-pocket : β ← cylindrical

Small electron-pocket : γ ← corrugated

α , γ : Compensated by each other

- Equal volume & mass
- Opposite charge



k_z dispersion
($d_{x^2-y^2}$ symmetry)

- Helical density wave model is consistent with these results.

Translational symmetry-breaking order !

- Secondary F.S. instability by ...

- excitonic insulator ? : QCP
- stripelike charge order

