Realistic Theories of Correlated Electron Materials, KITP Santa Barbara
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# Material dependence of the electronic structure of cuprates: Possible relation to $T_C$

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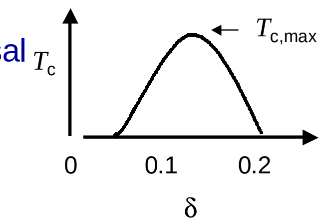
## What determines $T_C$ ?

- Answer from chemistry
- Answer from superconductivity phenomenology
- Answer from microscopic model parameters

## Answer from chemistry

apart from disorder such as Zn impurities

- Hole concentration
  - $T_c/T_{c,max}$ vs $\delta$ curve is universal



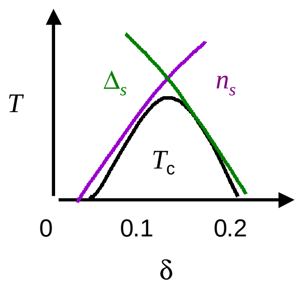

- Number of $CuO_2$ layers
  - determines $T_{c,max}$
- Crystal structure: BSCCO, YBCO, LSCO, …. •
  - especially the position of apical oxygen
  - determines $T_{c,max}$

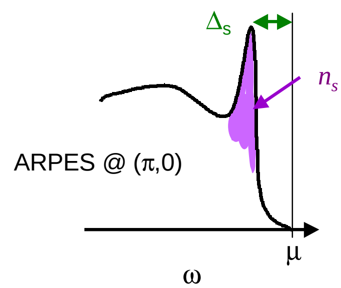
## What determines $T_C$ ?

- Answer from chemistry
- Answer from superconductivity phenomenology
- Answer from microscopic model parameters

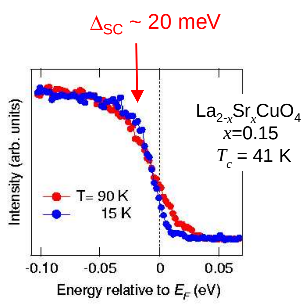
## Answer from superconductivity phenomenology

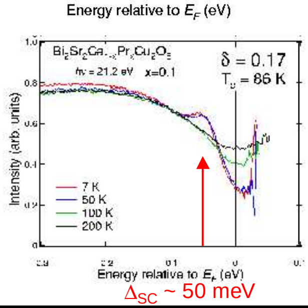
- Binding energy of a Cooper pair
  = gap magnitude $\Delta_s$
- Phase coherence between Cooper pairs
  = superfluid density $n_s$

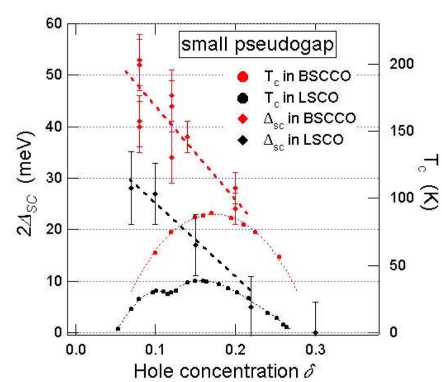



## $T_{c,max}$ vs superconducting gap, "small pseudogap"



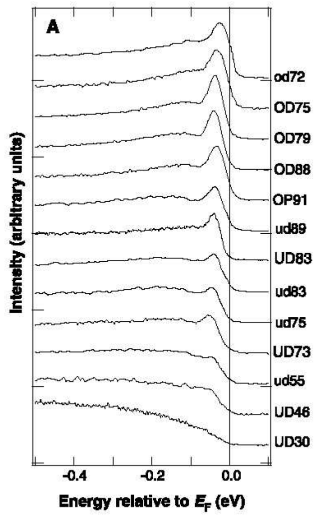



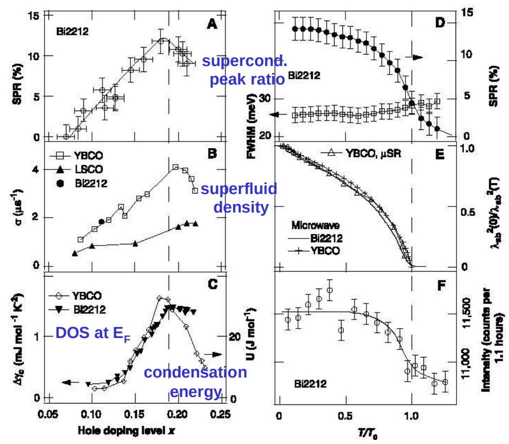




K. Tanaka et al, T. Yoshida et al.
J. M. Harris et al., PRB '96
A. Ino et al., PRB '02

Differences in the electronic structure of the CuO2 plane between different cuprate systems

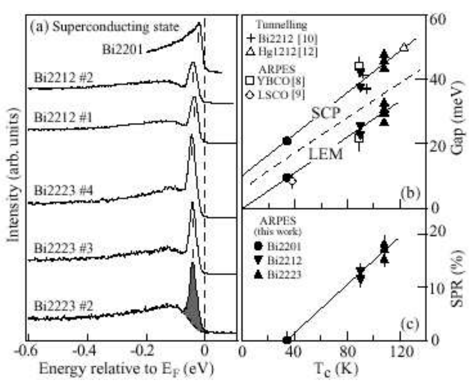
## Peak at $k \sim (\pi, 0)$ and superfluid density in $Bi_2Sr_2CaCu_2O_{8+\delta}$

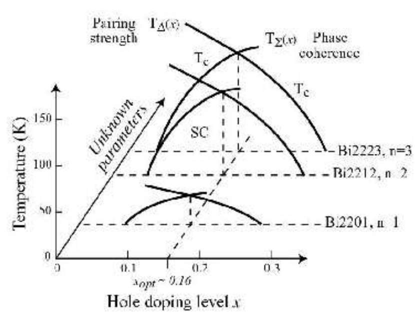



D. L. Feng et al., Science '00

## Gap magnitude and phase coherence in single-, double- and triple-layer BSCCO




Smaller bilayer splitting

- Both pairing strength and phase coherence is important for high Tc
- Interlayer tunneling is irrelevant to high Tc

D.L. Feng et al., PRL '02

## What determines $T_C$ ?

- Answer from chemistry
- Answer from superconductivity phenomenology
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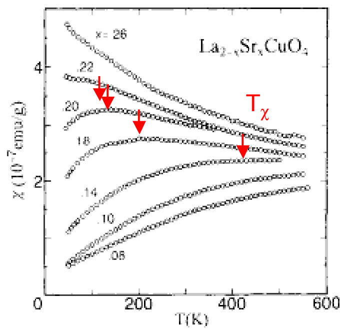
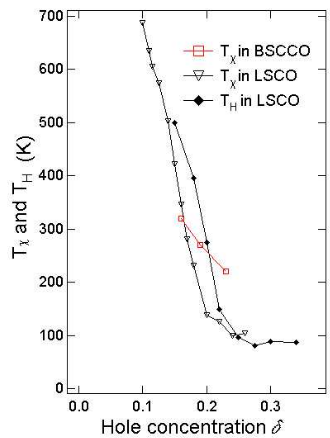
## Answer from microscopic models

Hubbard ($U$-$t$, $U$-$t$-$t'$, ...) model, $t$-$J$ ($t$-$t'$-$t''$-$J$,…) model, ...

- $U$ ~ 3 eV, $t$ ~ 0.3 eV and $J$ ~ 0.1 eV are common.
- $t'$ , $t''$, .. are different.
- We have to answer the questions of:
  - How does crystal structure influence $t'$ ?
  - How does $t'$, $t''$ influence $\Delta_s$ and $n_s$ ?

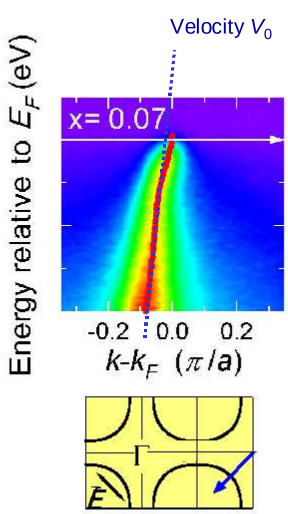
## Common *J* - from magnetic susceptibility



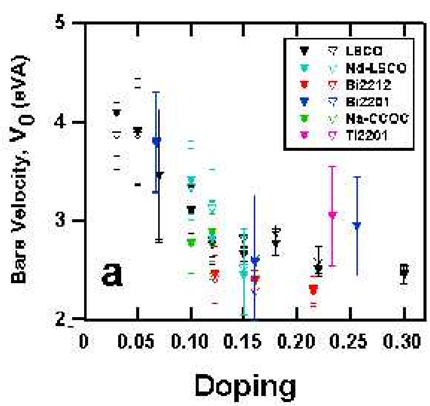




T. Nakano et al. PRB '94
M. Oda et al., Physica C '97
H.Y. Hwang et al, PRL '94

## Common *J* - from nodal quasi-particle velocity




Band width along (0,0)-(π,π) ∝ $V_0$ ∝ $J$
F.C. Zhang et al.: J. Supercond. Sci. Tech. '88




T. Yoshida et al.

X. J. Zhou et al.

## Answer from microscopic models

Hubbard ($U$-$t$, $U$-$t$-$t'$, ...) model, $t$-$J$ ($t$-$t'$-$t''$-$J$,…) model, ...

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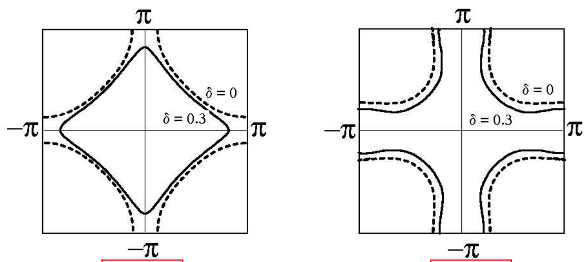
- $t'$ , $t''$, .. are different.
- We have to answer the questions of:
  - How does crystal structure influence $t'$ ?
  - How does $t'$ influence $\Delta_s$ and $n_s$ ?

## Indication of different $t'$

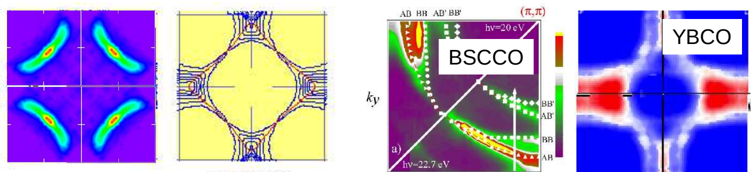
- Fermi surface
- ($\pi$,0)-($\pi$/2, $\pi$/2) energy difference in parent insulators
- Magnitude of chemical potential shift
- ($\pi$,0) flat band position
  = magnitude of "large pseudogap"

## Fermi surface shape




LSCO t'/t = -0.12, t''/t = 0.08 BSCCO t'/t = -0.34, t''/t = 0.23

T.Tohyama and S. Maekawa




x=0.05 x= 0.22

T. Yoshida et al., PRB '00.

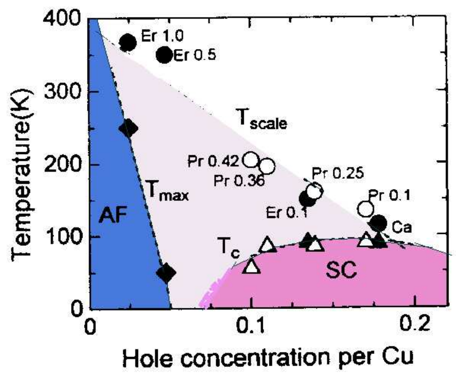
D. Feng et al., PRL '01, D. Lu, PRL '01

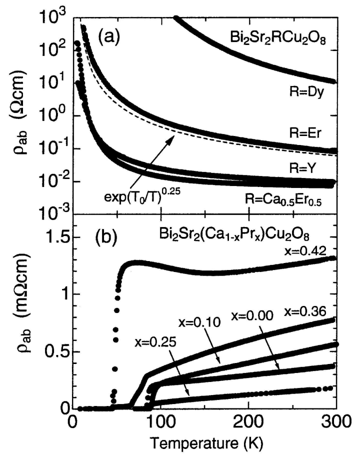
## Indication of different *t'*

- Fermi surface
- (π,0)-(π/2, π/2) energy difference in parent insulators
- Magnitude of chemical potential shift
- (π,0) flat band position
  = magnitude of "large pseudogap"

Differences in the electronic structure of the CuO2 plane between different cuprate systems

## Lightly-doped Bi2212 and parent insulator

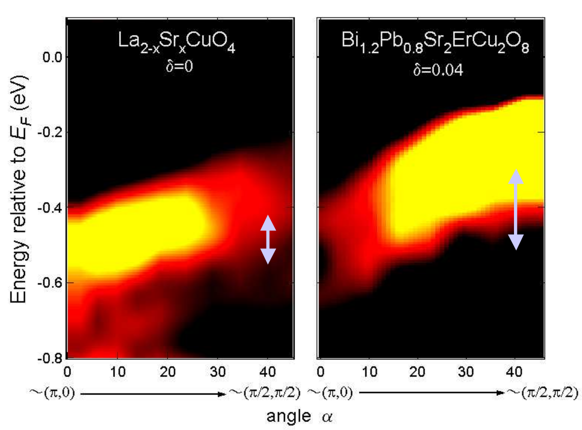


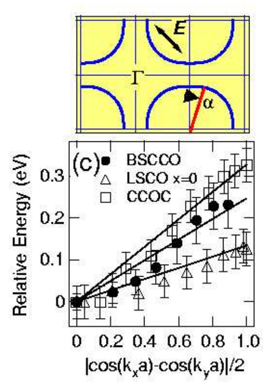




Hole content, $T_N$ from thermopower

T. Takemura et al. J. Phys. Cond. Mat. '00
T. Kitajima et al., J. Phys. Cond. Mat. '00

## Dispersion along underlying "Fermi surface" in insulator



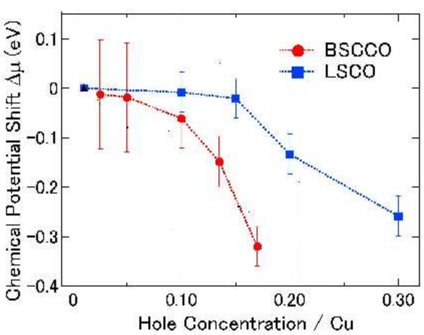

$E(\pi/2,\pi/2) - E(\pi,0) \propto |t'|$

## Indication of different *t'*

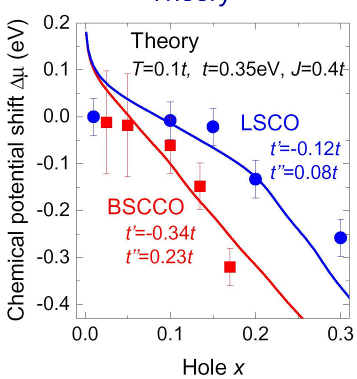
- Fermi surface
- (π,0)-(π/2, π/2) energy difference in parent insulators
- Magnitude of chemical potential shift
- (π,0) flat band position
  = magnitude of "large pseudogap"

## Magnitude of chemical potential shift

Experiment




Theory



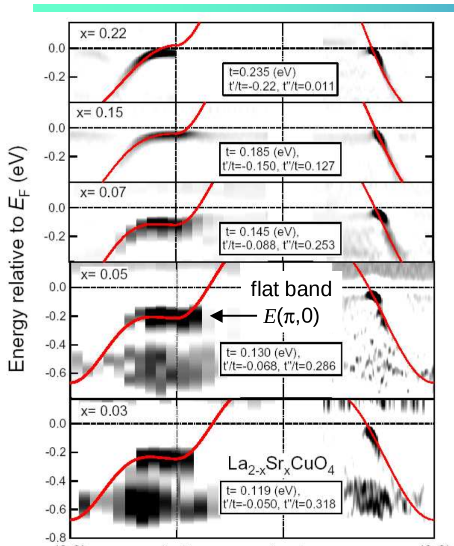

A. Ino et al., PRL '97
N. Harima et al. cond-mat/02

T. Tohyama, S. Maekawa, cond-mat/02

## Indication of different *t'*

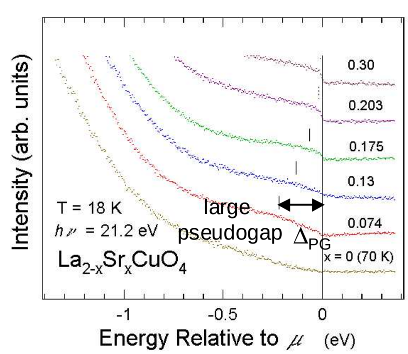
- Fermi surface
- (π,0)-(π/2, π/2) energy difference in parent insulators
- Magnitude of chemical potential shift
- (π,0) flat band position
  = magnitude of "large pseudogap"

## (π, 0) flat band and "large pseudogap"




tight-binding fit T. Yoshida et al., PRB '01

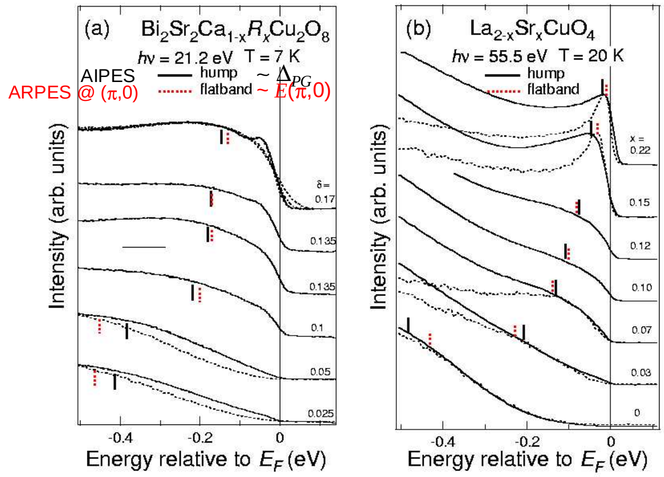
Angle-integrated photoemission spectra




A. Ino et al., PRL '98

Differences in the electronic structure of the CuO2 plane between different cuprate systems

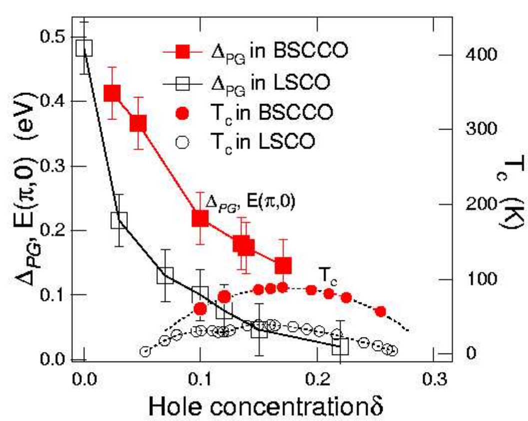
## (π,0) flat band position ~ “large pseudogap”




$E(\pi,0) \propto |t'|$ (C. Kim et al, PRL ‘98)

K. Tanaka et al.

## $T_{c,\max}$ vs “large pseudogap”




$T_{c,\max}$ scales with $\Delta_{PG}$ ~ $E(\pi,0)$ and therefore with $|t'|$ ?

## Answer from microscopic models

Hubbard (*U-t*, *U-t-t’*, ...) model, *t-J* (*t-t’-t”-J*,…) model, ...

- $U$ ~ 3 eV, $t$ ~ 0.3 eV and $J$ ~ 0.1 eV are common.
- $t’$ , $t’’$, .. are different.
- We have to answer the questions of:
  - How does crystal structure influence $t’$ ?
  - How does $t’$ influence $\Delta_s$ and $n_s$ ?

## How does crystal structure influence $t’$ ?

shorter Cu-apical O distance

→ influence of $d_{3z2-r2}$, $p_z$ orbitals

→ reduction of $|t’|$

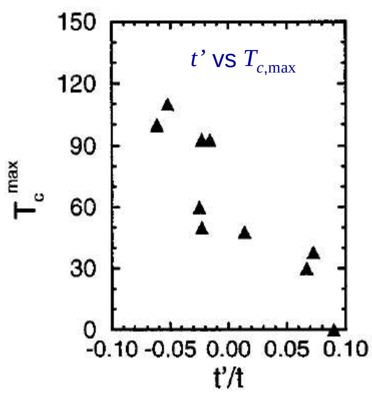



FIG. 9. Maximum critical temperature $T_c^{max}$ vs $t'/t$ for various superconducting cuprates. Compounds included are $La_2SrCu_2O_6$ ($T_c^{max}$=0 K), $La_{1.85}Ba_{0.15}CuO_4$ ($T_c^{max}$=30 K), $La_{1.85}Sr_{0.15}CuO_4$ ($T_c^{max}$=38 K), $(Ba_{0.67}Eu_{0.33})_2$ $(Eu_{0.67}Ce_{0.33})_2$ $Cu_3$ $O_{8.78}$ ($T_c^{max}$=48 K), $Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{6.11}$ ($T_c^{max}$=50 K), $YBa_2Cu_3O_{6.5}$ ($T_c^{max}$=60 K), $YBa_2Cu_3O_7$ ($T_c^{max}$=93 K), $Bi_2Sr_2Ca_{0.9}Y_{0.1}Cu_2O_{8.24}$ ($T_c^{max}$=93 K), $TlBa_2CaCu_2O_7$ ($T_c^{max}$=100 K), $Pb_{0.5}Tl_{0.5}Sr_2CaCu_2O_7$ ($T_c^{max}$=110 K).

R. Raimondi, J.H. Jefferson and L.F. Feiner, PRB ‘96

(calculation of Tc based on VHS scenario: E. Dagotto et al, PRL ‘95)

Differences in the electronic structure of the CuO2 plane between different cuprate systems

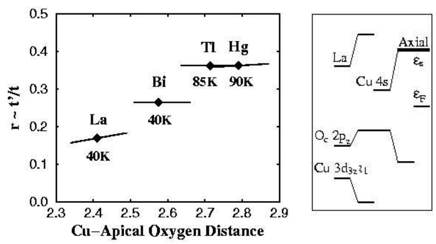
## How does crystal structure influence *t'* ?

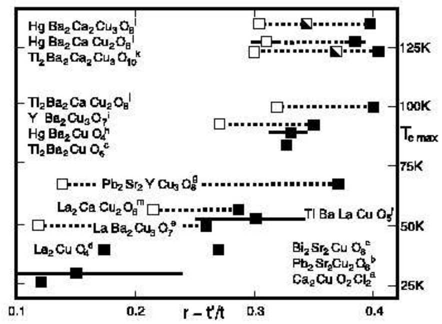
shorter Cu-apical O distance

→ pushes up Cu 4*s* orbitals

→ reduction of |*t'*|

$t'$ vs $T_{c,\max}$




E. Pavarini et al. PRL '01

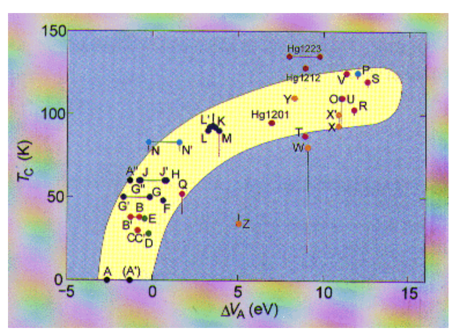
## Madelung potential difference vs $T_{c,\max}$

shorter Cu-apical O distance

→ holes move to apical O

→ destabilize Zhang-Rice singlet

$\Delta V_A$ vs $T_{c,\max}$




apical O ← holes → planar O

$\Delta V_A$ : Madelung potential difference between apical O and planer O

Y. Ohta, T. Tohyama and S. Maekawa, PRB '91

## Answer from microscopic models

Hubbard (*U*-*t*, *U*-*t*-*t'*, ...) model, *t*-*J* (*t*-*t'*-*t"*-*J*,…) model, ...

- *U* ~ 3 eV, *t* ~ 0.3 eV and *J* ~ 0.1 eV are common.
- *t'* , *t''*, .. are different.
- We have to answer the questions of:
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  - How does *t'* influence $\Delta_s$ and $n_s$ ?

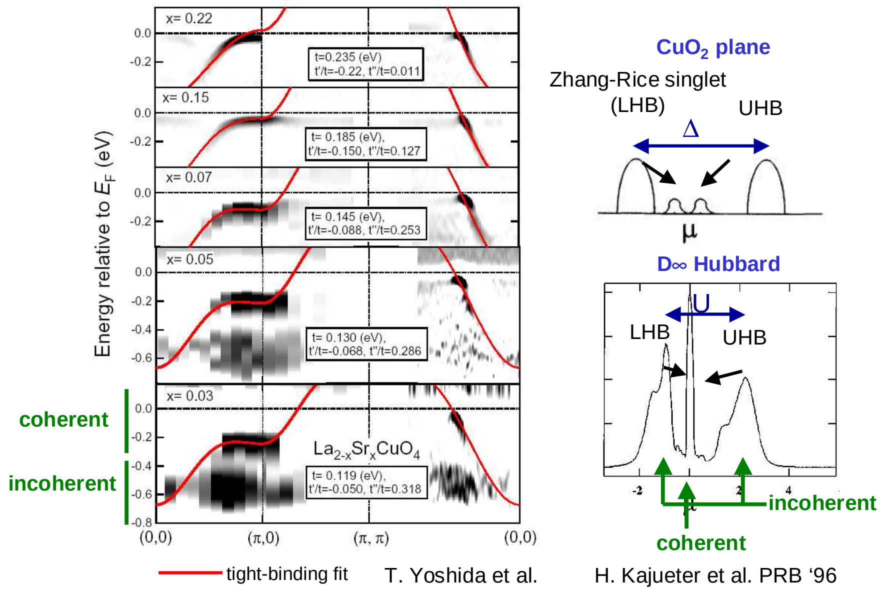
## How does *t'* influence $\Delta_S$ and $n_S$ ?

- $\Delta_s \sim \langle\omega\rangle \exp(-1/N(E_F)V)$
  - $N(E_F) \propto 1/|t'|$ in one-electron picture.
  - However, if $N(E_F)$ ~ QP spectral weight at ~ $E_F$ , $N(E_F)$ and hence $T_c$ may increase with $|t'|$.
- $n_S$
  - Then it is likely that $n_S$ ~ QP spectral weight at ~ $E_F$. So $n_S$ will increase with $|t'|$.
- large $|t'|$ → stripe formation is suppressed

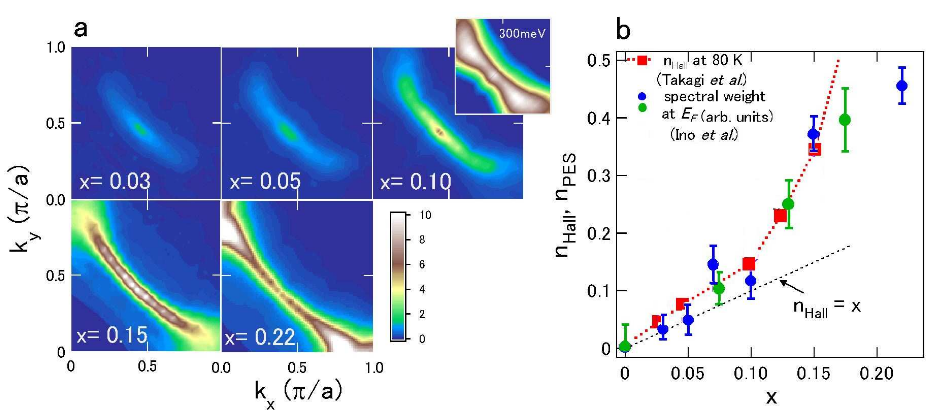
(e.g., M. Fleck et al, PRL '98)

Differences in the electronic structure of the CuO2 plane between different cuprate systems

## Spectral weight transfer between coherent and incoherent parts



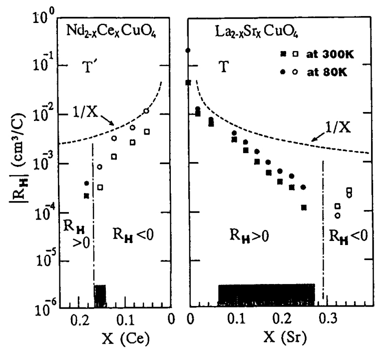

## Carrier number ≈ Spectral weight at $E_F$ ?



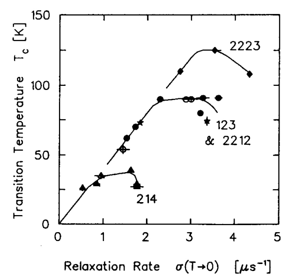

T. Yoshida et al., cond-mat/02

## $n \sim x$ behavior in underdoped cuprates

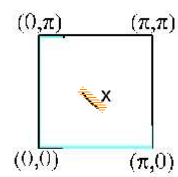
Hall effect: $n = 1/eR_H \propto x$




Superfluid density $\rho_s/m \propto x$




$\rho_s/m$




"Drude weight" in optical conductivity $\propto x$

S. Uchida, Y. Tokura, H. Takagi,... '89
Y.J. Uemura et al., PRL '89

## Conclusion

- Different $t'$ values rather than $J$ characterize different HTCS systems with different $T_{c,\max}$
  - Fermi surface
  - ($\pi$,0) flat band = large pseudogap
  - chemical potential shift
  - QP spectral weight