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SMR. 767 - 6

MINIWORKSHOP ON STRONG CORRELATIONS
AND QUANTUM CRITICAL PHENOMENA
(4 - 22 July 1994)

WHY ARE THE CUPRATES HIGH-TC SUPERCONDUCTORS?

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These are preliminary lecture notes, intended only for distribution to participants.

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(Nagoya University)

Why are the Cuprates High-T_c Superconductors?

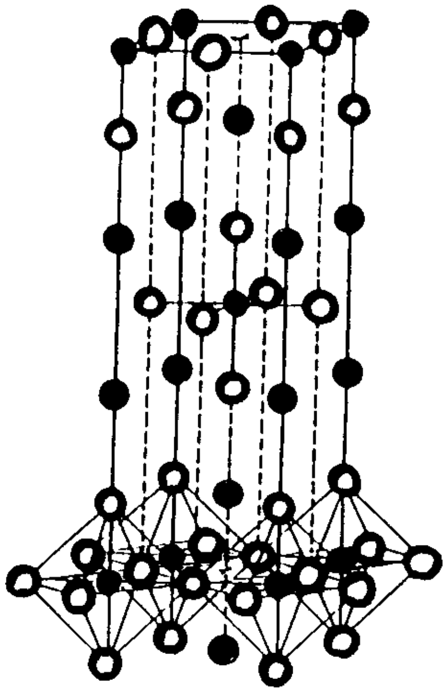
1. Crystal structure and carrier-doping.
   → stability of CuO_2 plane against doping.
   → duality of ionic and metallic properties due to 2-dimensional character.

2. Crystal structure and electronic structure.
   → strong quantum antiferromagnetic effects at $S = 1/2$ caused by charge-transfer-type electronic structure

3. Mapping onto 2-dimensional tJ model.
   → $d(x^2-y^2)$-wave pairing.

$\Downarrow$

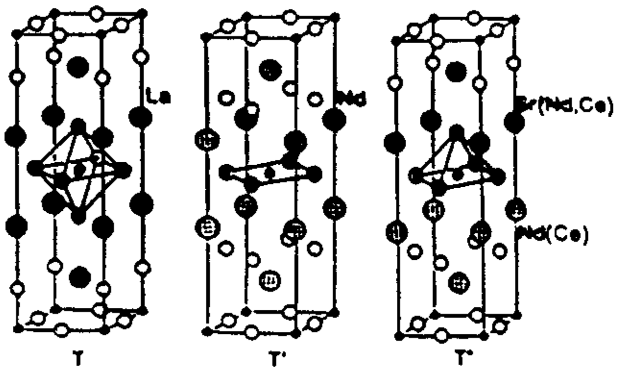
high-T_c superconductivity

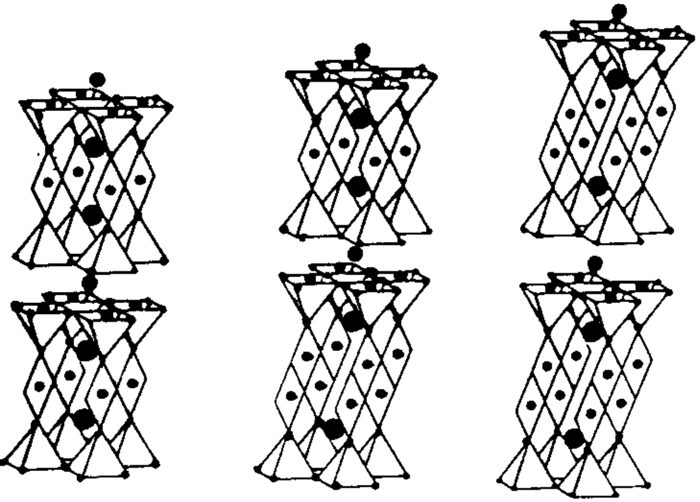


$(La^{3+}, M^{2+})_2 CuO_4$

$M = Ba, Sr, Ca$

Fig. 1 Layered perovskite structure, ● La or Ba, Sr, Ca; ●: Cu; O: O.



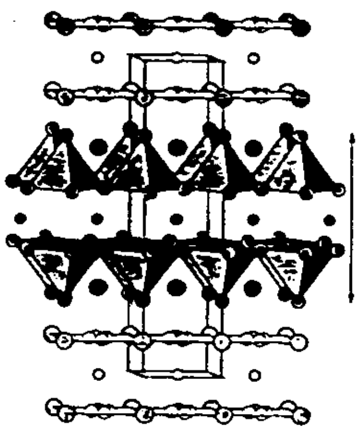


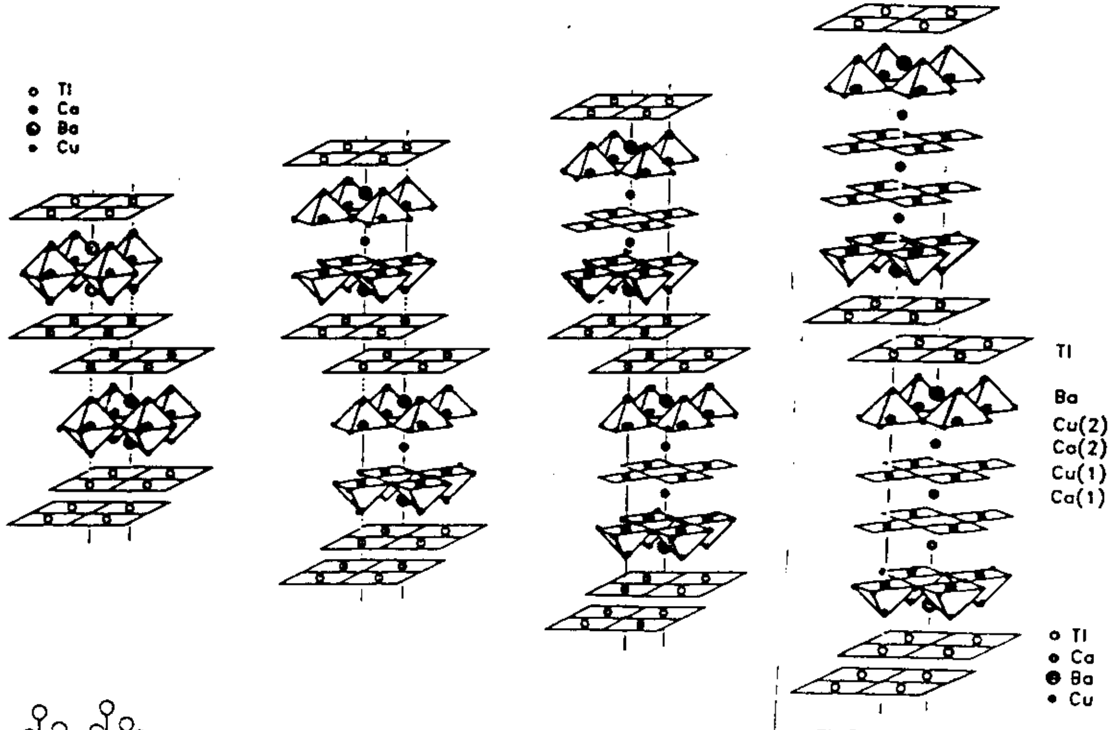
$YBa_2Cu_3O_7$

$T_c \approx 9 \circ K$

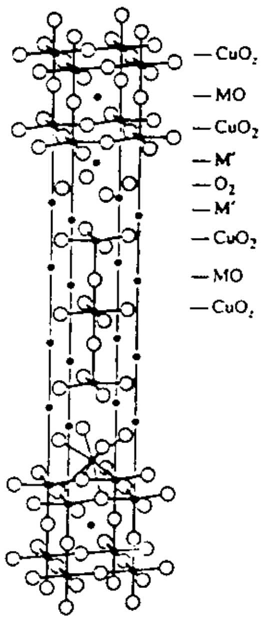
$YBa_2Cu_{3.5}O_{7.5}$

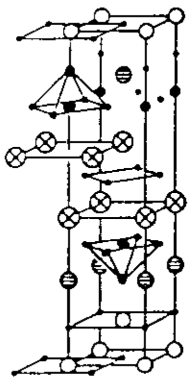
$YBa_2Cu_4O_8$





$Tl_2\,Ba_2\,Ca_3\,Cu_4\,O_{12}$





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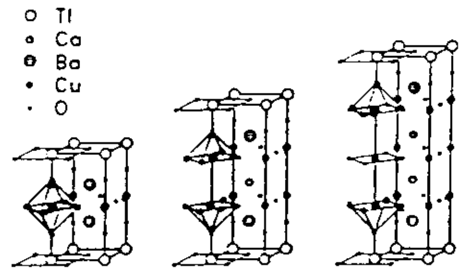
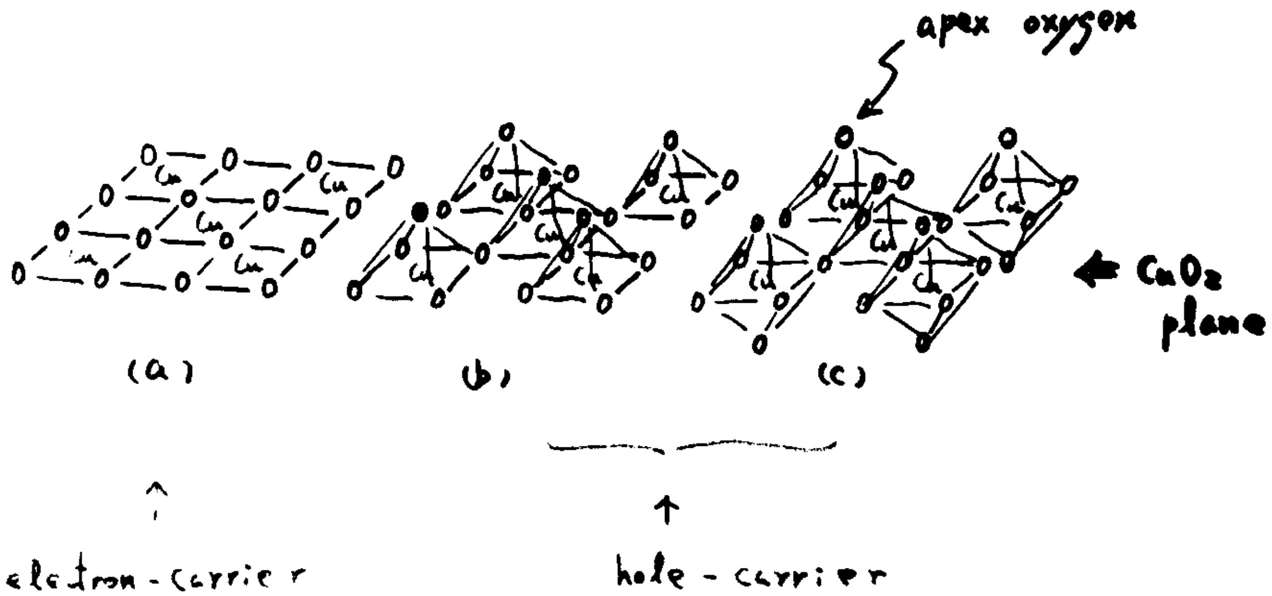


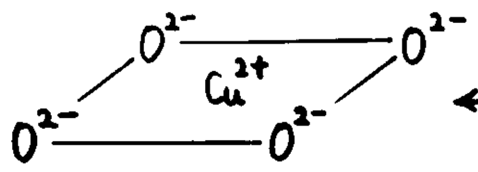
$T_c(K)$	1021	1122	1223
		65–85	100–110

3



apex oxygen
CuO_2 plane
Cu
O
(a)
(b)
(c)
electron - carrier
hole - carrier

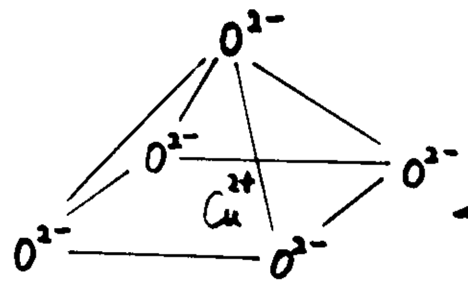
(a)



$\longleftarrow$ $-e$

electron-doping

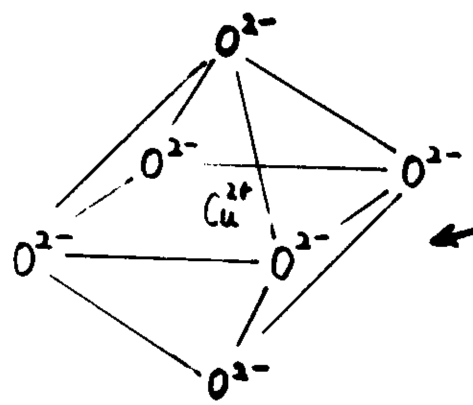
(b)



$\longleftarrow$ $+e$

hole-doping

(c)



$\longleftarrow$ $+e$

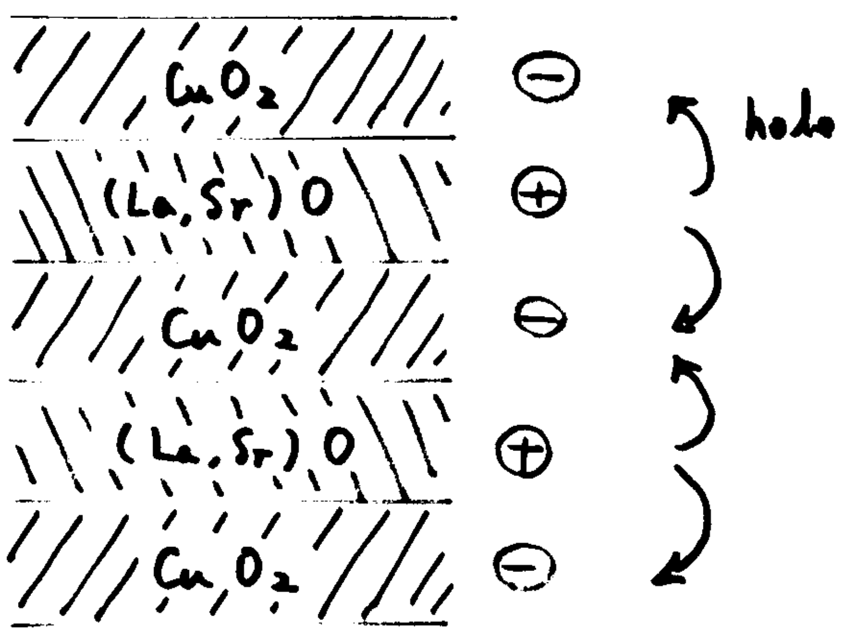
hole-doping

$\rightarrow$ Apex oxygen controls carrier-doping.

$\Downarrow$

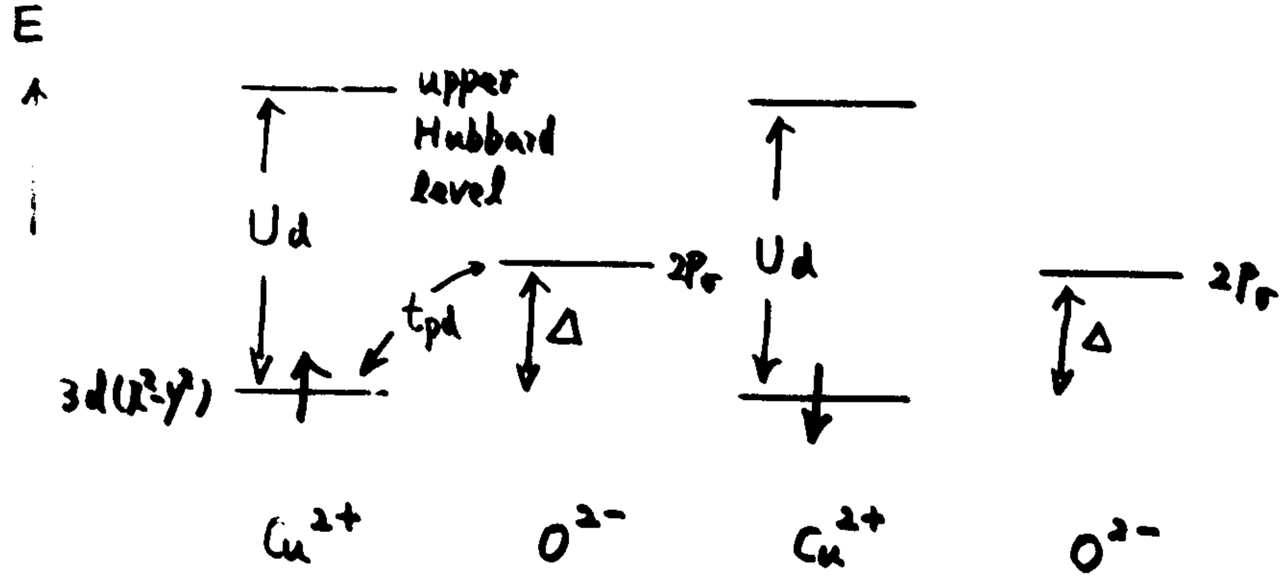
Apex oxyson may have some information for high Tc.

$(La^{3+}, Sr^{2+})_2\, CuO_4$



→ CuO_2 plane is stable against doping!

→ CuO_2 plane becomes metallic and carries superconductivity.



$$J = t_{pd}^4 / \Delta^3 .$$

small Δ ← charge transfer type

↓

→ large J

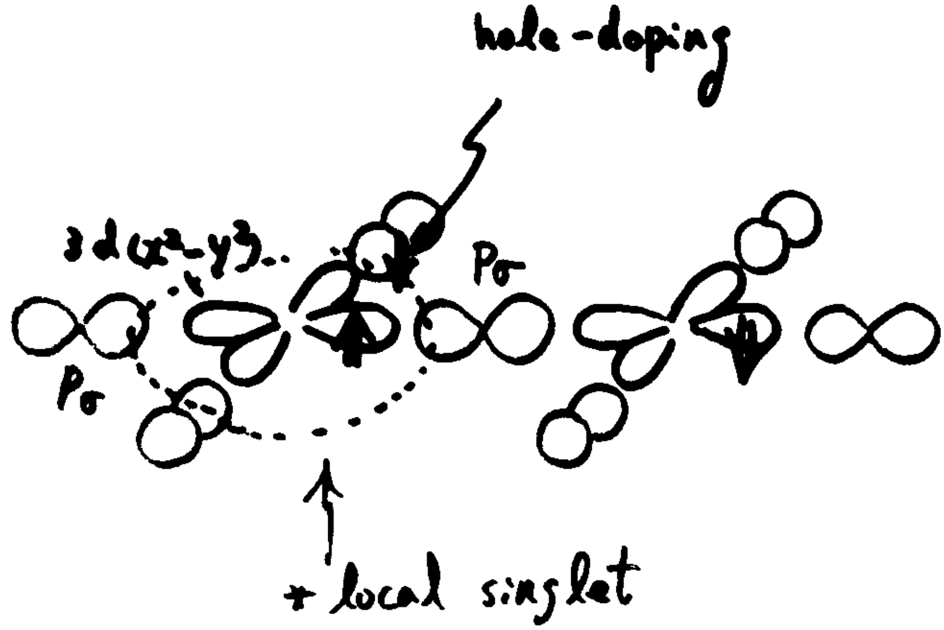
→ $S = 1/2$ in Cu^{2+} ion

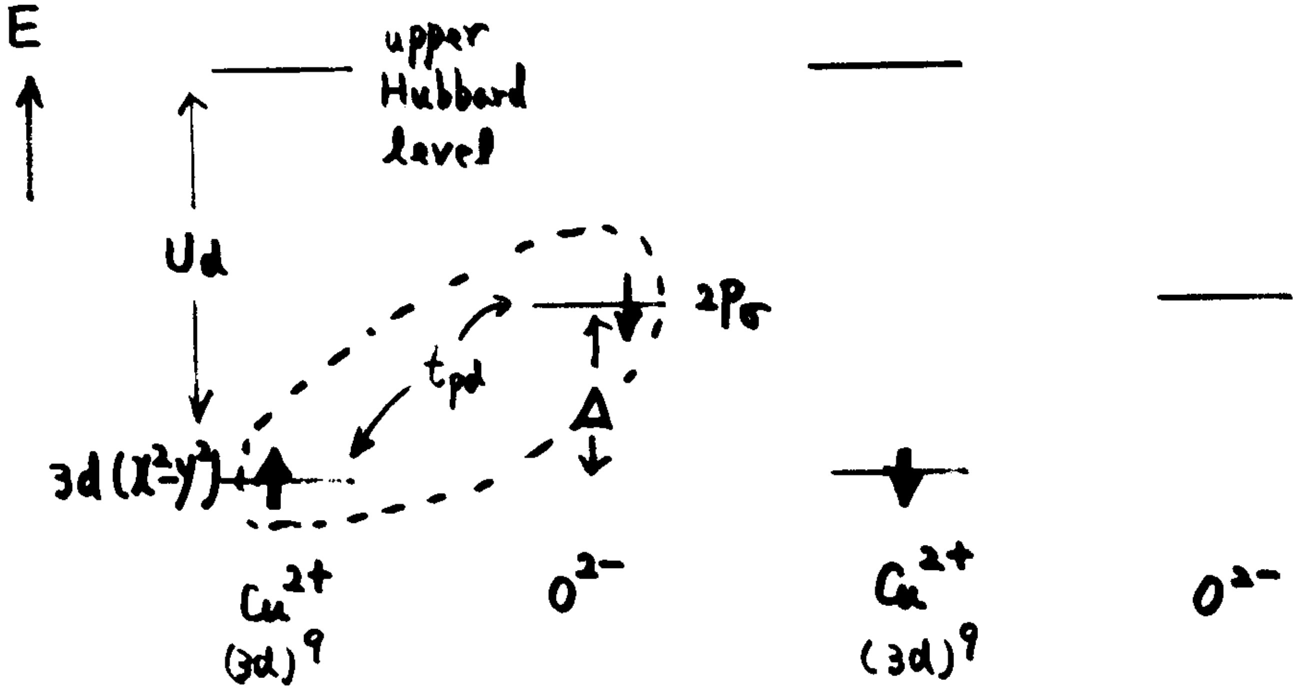
→ 2-dimension

⇓

strong quantum effects of spins !

Electronic states in CuO_2 plane :



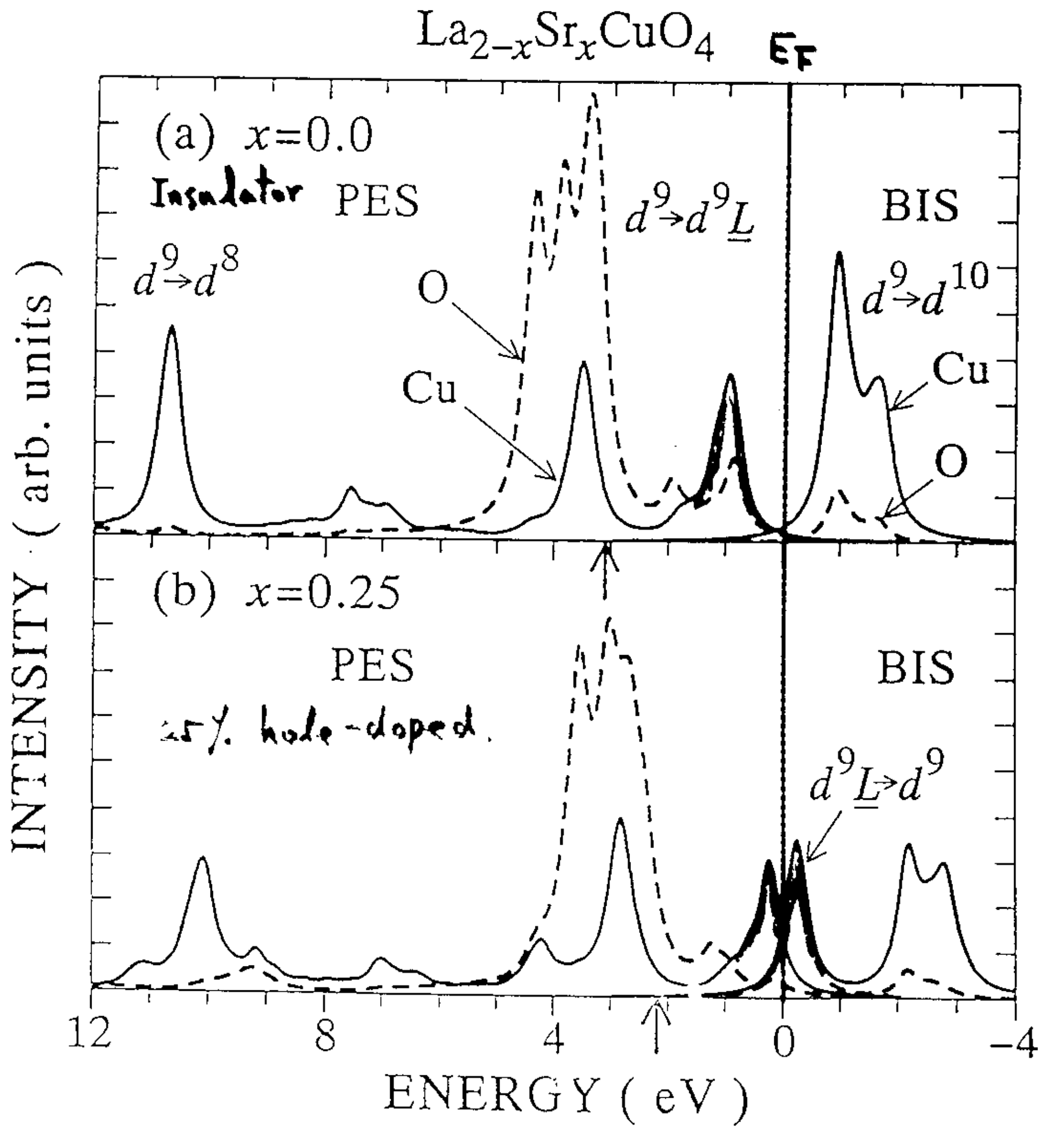


→ AF exchange interaction : $H = J\,\vec{S}_i \cdot \vec{S}_j$.

$J = t_{pd}^4 / \Delta^3$ $\quad (S = 1/2)$

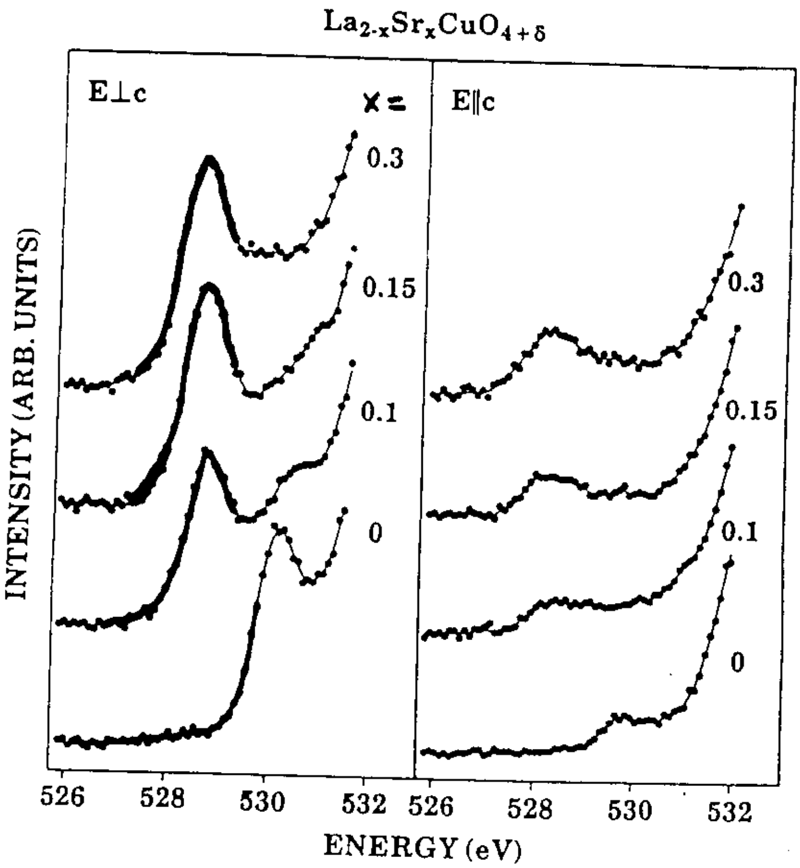
$$\left.\begin{array}{l} U_d \sim 8\,\mathrm{eV} \\ \Delta \sim 2\text{-}3\,\mathrm{eV} \\ t_{pd} \sim 1\,\mathrm{eV}. \end{array}\right\} \Rightarrow J \sim 0.1\,\mathrm{eV}$$

One-particle spectral-density of Cu 3d (x^2-y^2) and O 2p$_\sigma$ (exact diagonalization of Cu_4O_{13} cluster)



Ingap state near E_F

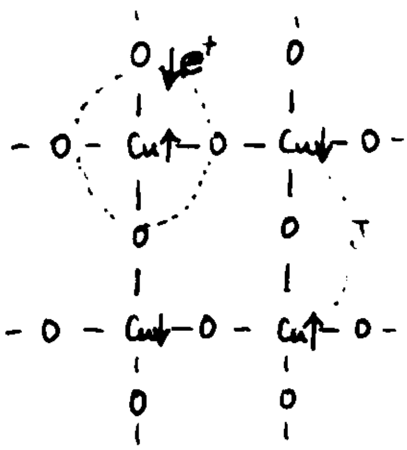
(S.M. Y. Ohta. T. Tohyama : Springer 106, 29 ('92))



Polarization dependent X ray absorption spectroscopy on O1s edge:

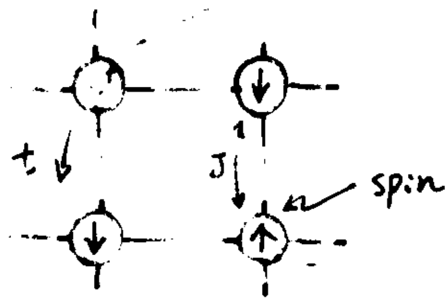
E. Pellegrin et al. (preprint.)

Hole-doped case.



J : antiferromagnetic exchange

$\Downarrow$ – charge locked in local singlet



$\rightarrow$ t - J model :

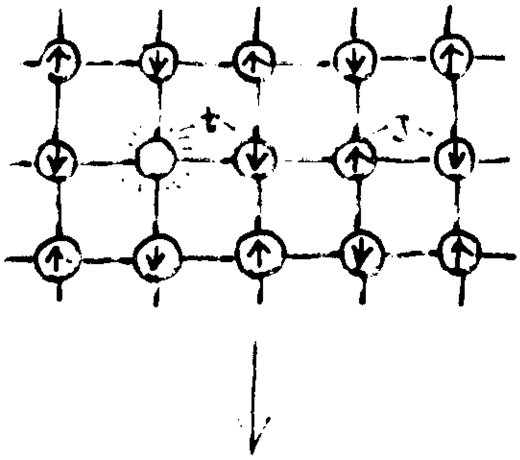
$$H = -t \sum_{\substack{\langle ij \rangle \\ \sigma}} \tilde{c}^{+}_{i\sigma} \tilde{c}_{j\sigma} + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j .$$

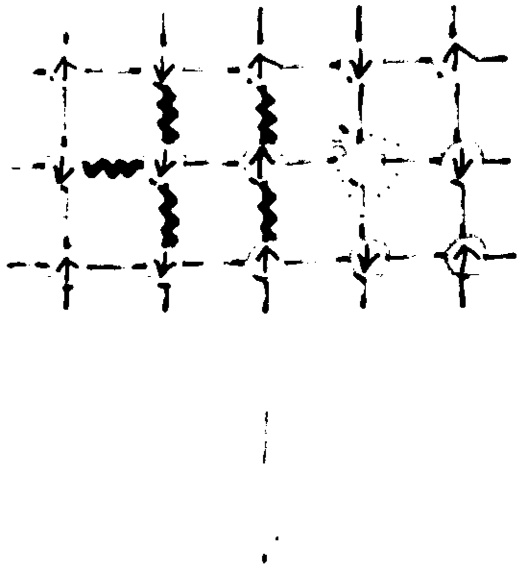
$\uparrow$ antiferromagnetic exchange between Cu spins

$$\left.\begin{array}{l} t \simeq 0.25\ \mathrm{eV} \\ J \simeq 0.1\ \mathrm{eV} \end{array}\right\} \text{ in } La_2CuO_4 \ : \ \frac{J}{t} \simeq 0.4$$

{ strong coupling between spin and charge.

• Motion of a hole in an antiferromagnet :

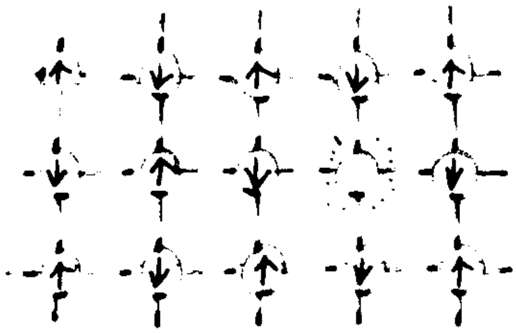




string of wrong spins.

[illegible]

quantum effect of spins



[illegible]

[illegible] and quantum spin fluctuation.

* What is a relevant model ?

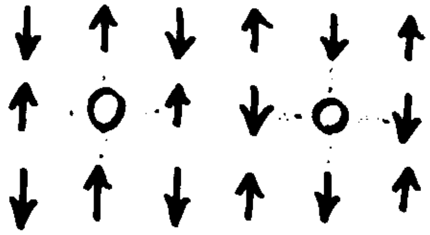
tJ model in the 2D square lattice.

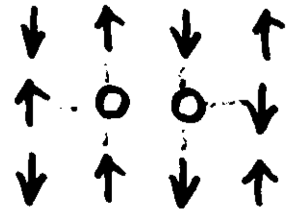
$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} \tilde{c}_{i\sigma}^{+} \tilde{c}_{j\sigma} + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j .$$

→ one of the simplest models for CuO_2 plane.

→ one of the simplest models for superconductivity in the strongly correlated regime.

- Pairing interaction in tJ model :



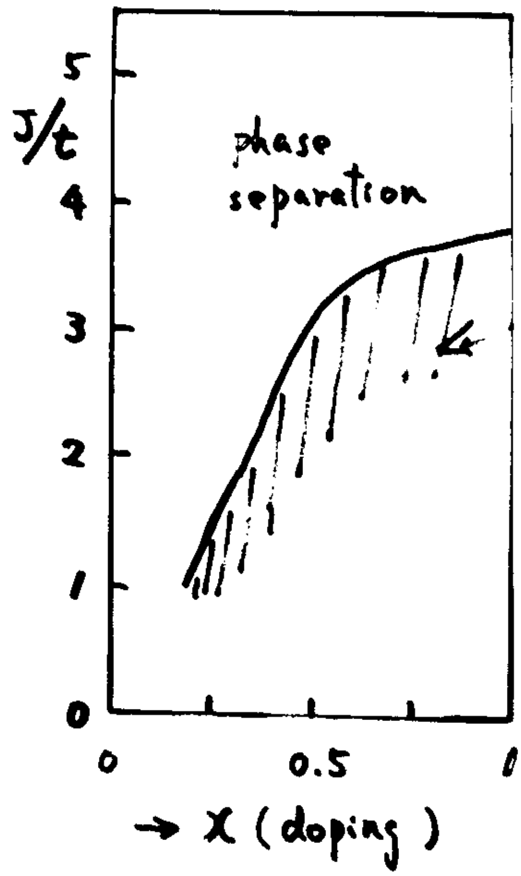


+4J +4J +7J

$\downarrow$

attractive interaction.

- phase diagram in square lattice :



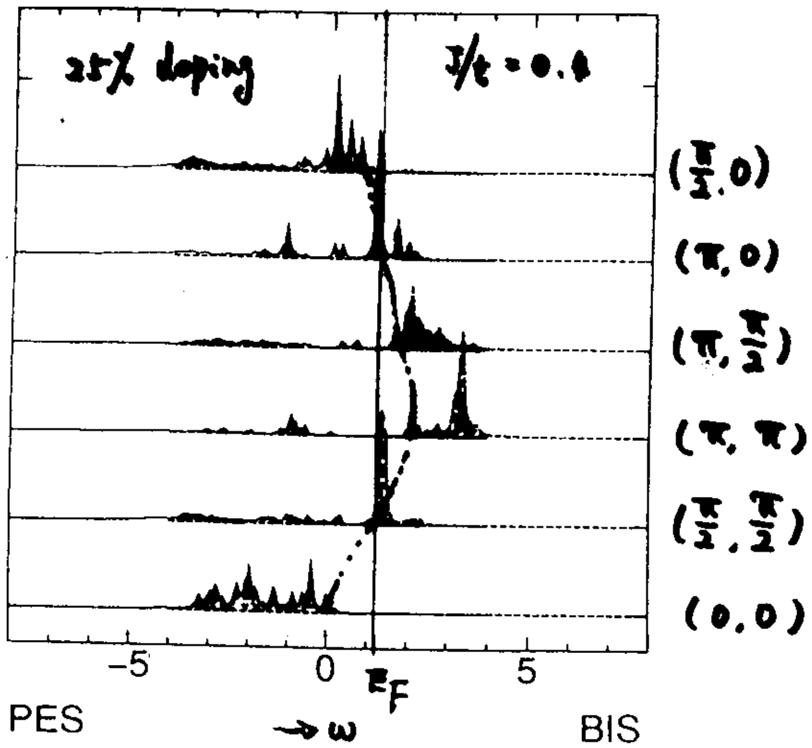
super. $(d(x^2-y^2))$

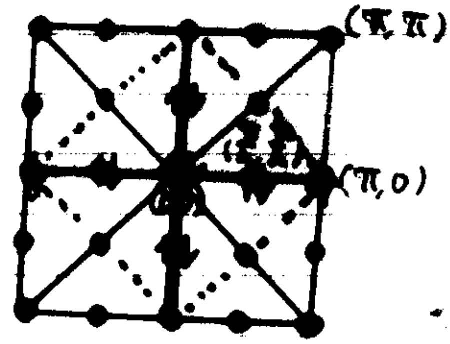
E. Dagotto and J. Riera :
Phys. Rev. Lett. 70 ('93) 682.

* One particle spectral-density in tJ model :

(exact diagonalization in 16 site cluster)

16site4hole,J=0.4,t=−1



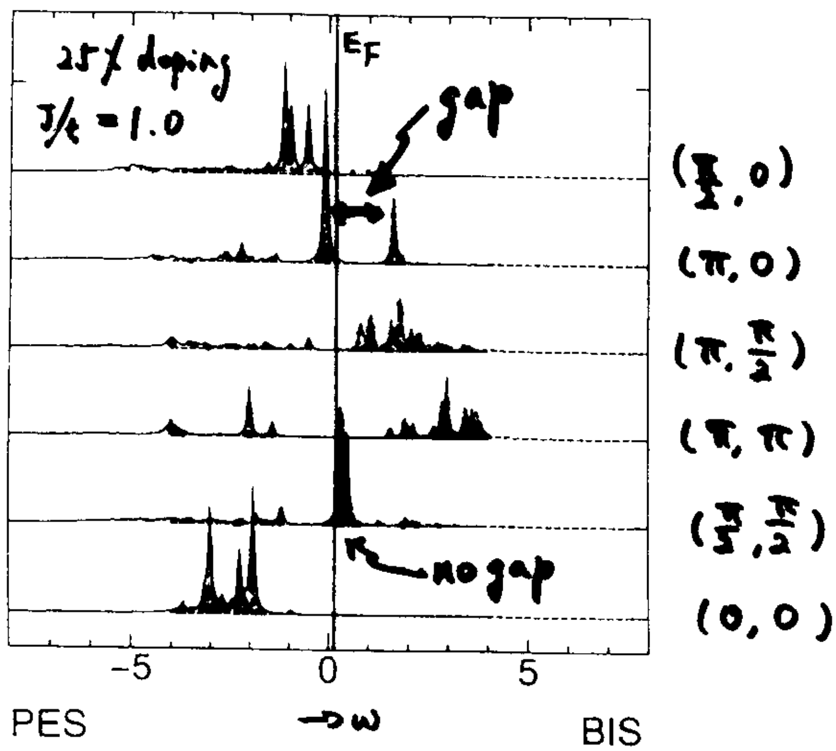


$$\Delta_k^d = \Delta_0 (\cos k_x - \cos k_y)$$

d-wave super.
(x^2-y^2)

(25% doping
$|J/t| = 1.0$)

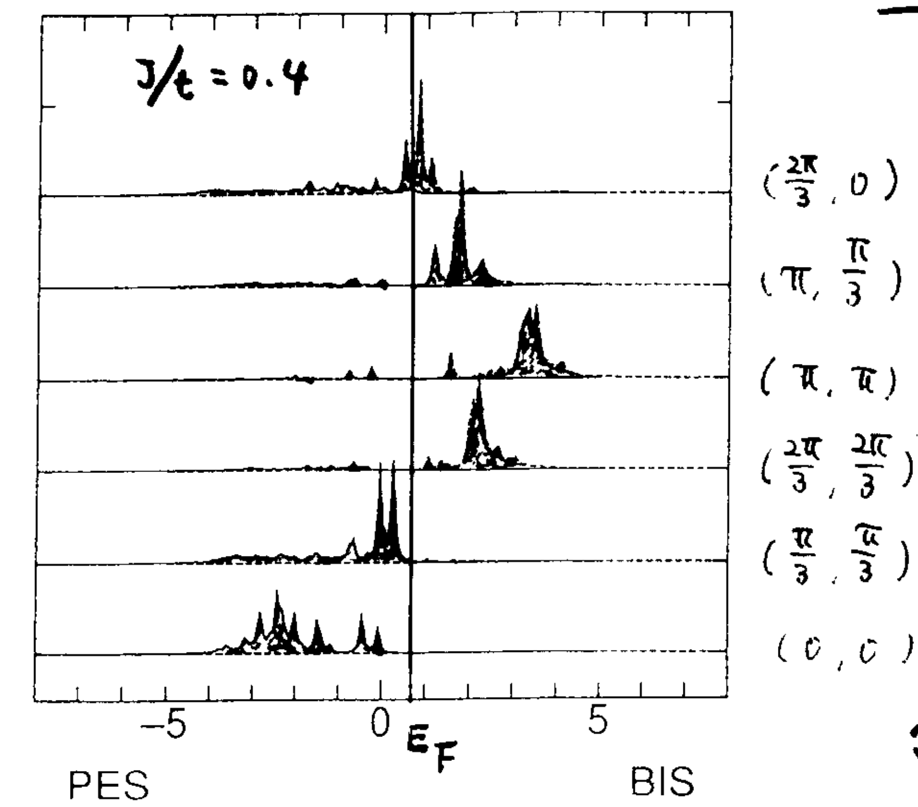
16site4hole,J=1.0,t=−1

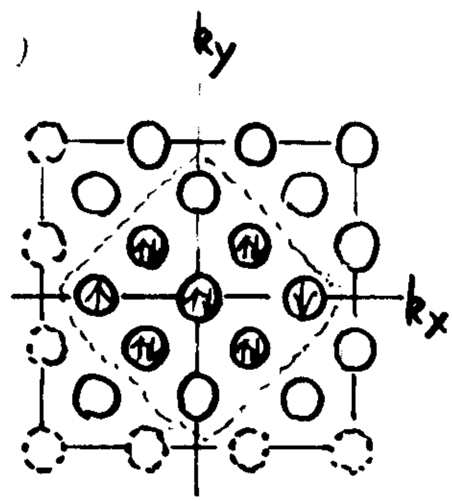


(Y. Ohta, T. Shimozato, SM)

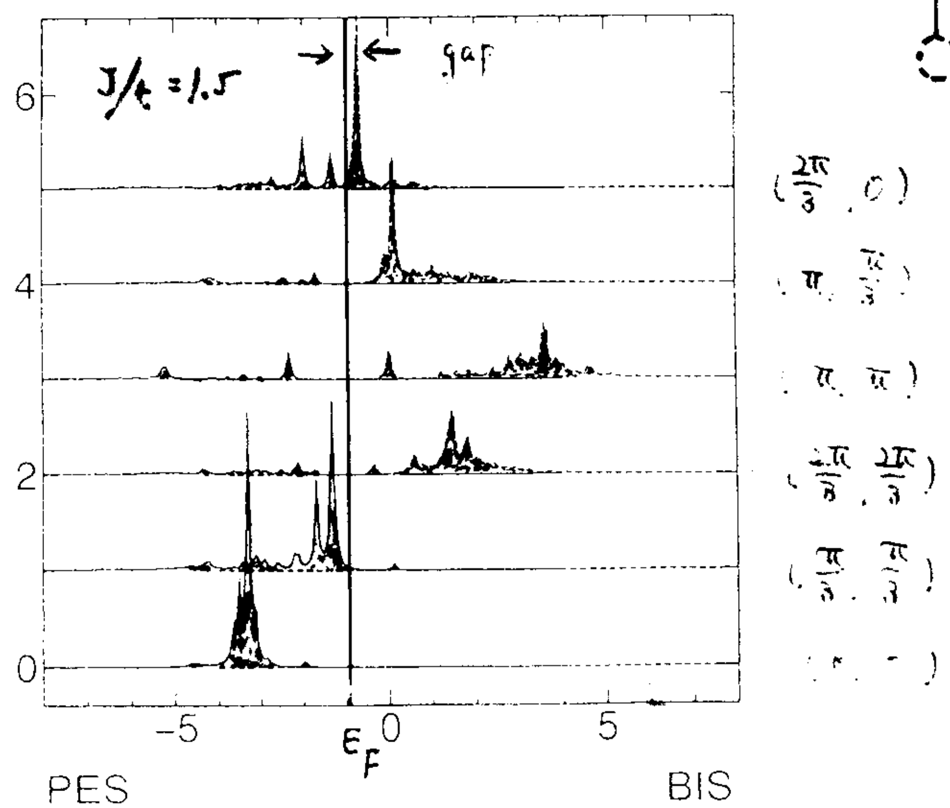
33% doping

18 site 6 hole J=0.4t



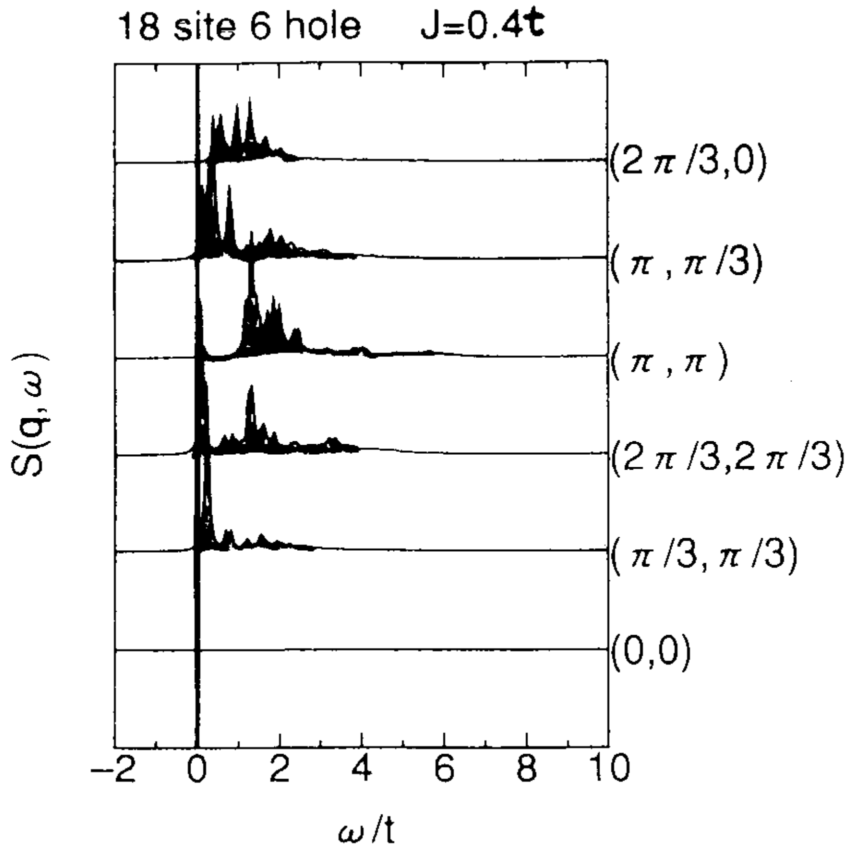


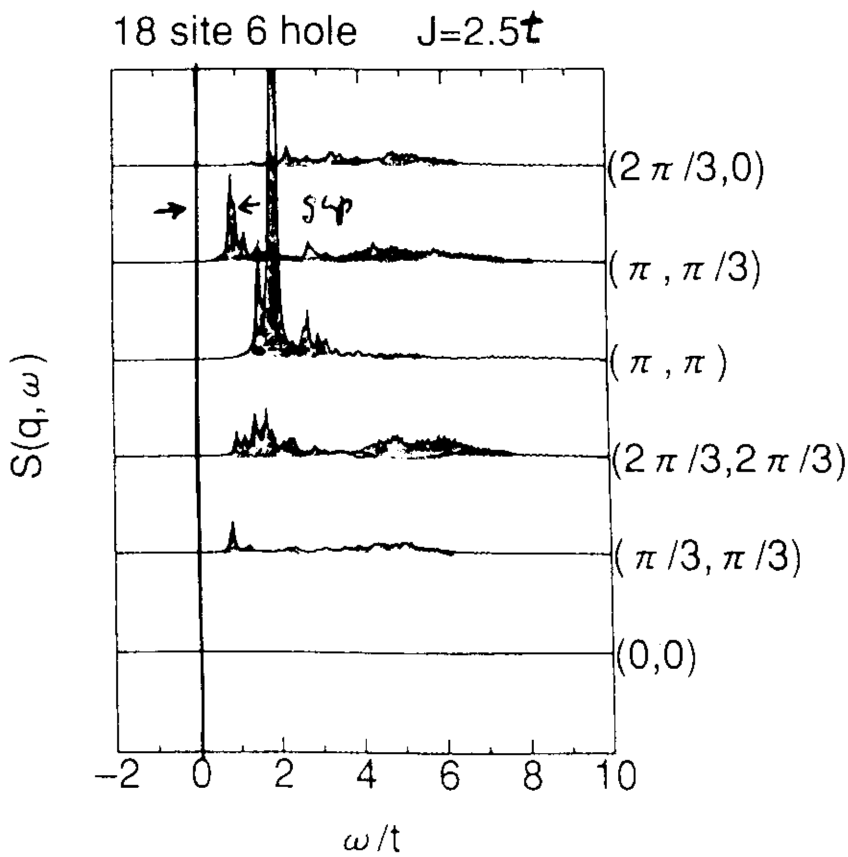
18site6hole,J=1.5,t=+1



Spin excitation spectra

33% doping.





spin gap in all directions ?

• Anomalous Green's function :

$$F(k,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,\langle \Psi_0^{N+2} | \tilde{c}_{k\uparrow}^{+} \frac{1}{\omega + i\eta - H + E_0} \tilde{c}_{-k\downarrow}^{+} | \Psi_0^{N} \rangle .$$

In BCS theory ,

$$c_{k\uparrow}^{+} = u_k \gamma_{k\uparrow}^{+} + v_k \gamma_{-k\downarrow} ,$$

(Bogoliubov quasi-particle)

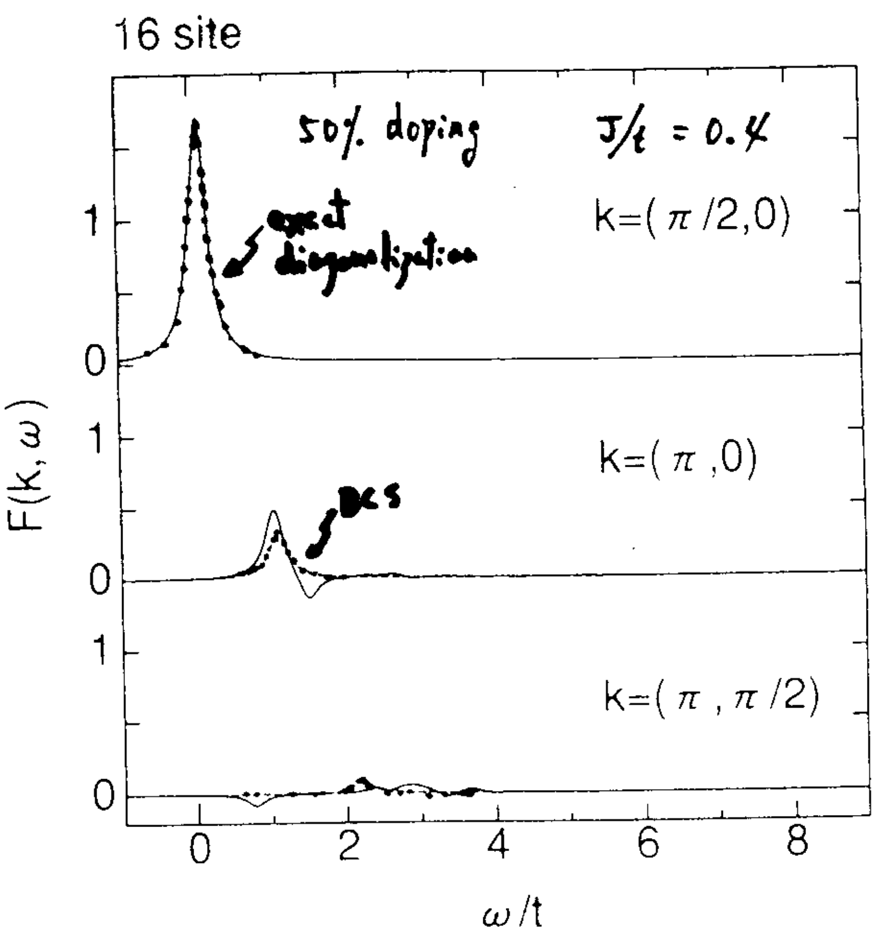
and , thus .

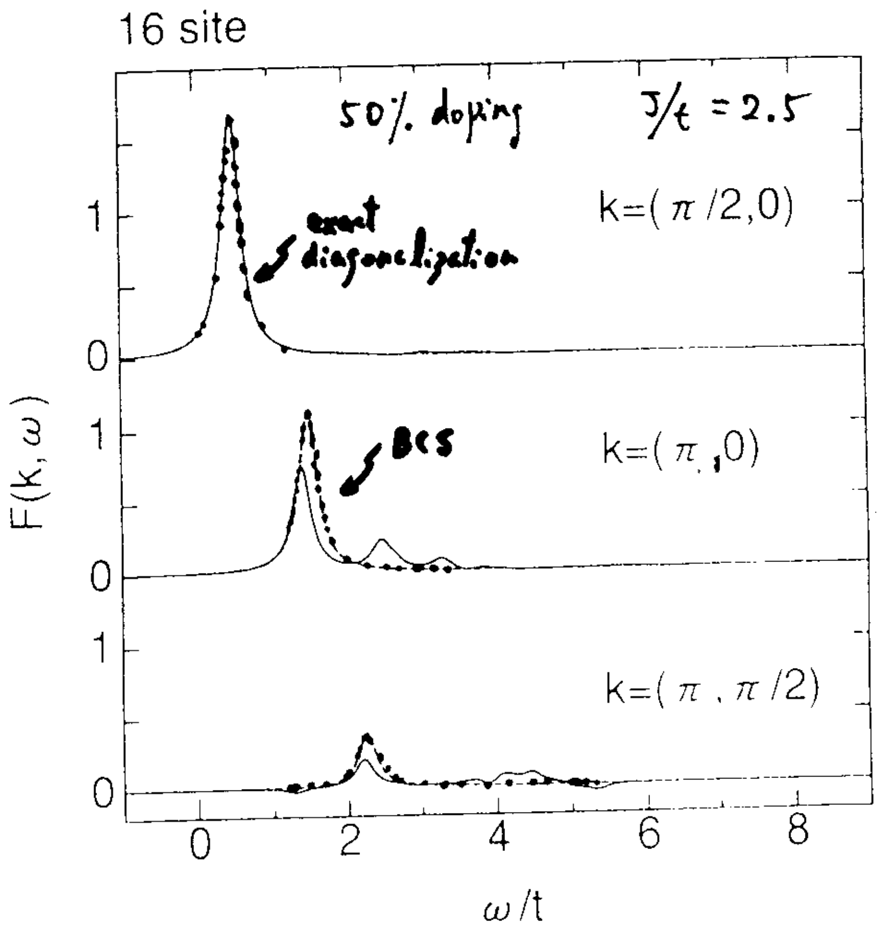
$$F(k,\omega) = -\frac{1}{\pi}\, u_k v_k \,\mathrm{Im}\, \langle BCS | \gamma_{-k\downarrow} \frac{1}{\omega + i\eta - H + E_0} \gamma_{-k\downarrow}^{+} | BCS \rangle$$

$$= \frac{\Delta_k}{2 E_k^{BCS}}\, \delta(\omega - E_k^{BCS}) .$$

$$\begin{cases} E_k^{BCS} = \sqrt{\xi_k^2 + \Delta_k^2} , \\ \xi_k = -2 t_{eff} (\cos k_x + \cos k_y) - \mu . \end{cases}$$

$$\Delta_k = \Delta_d (\cos k_x - \cos k_y).$$

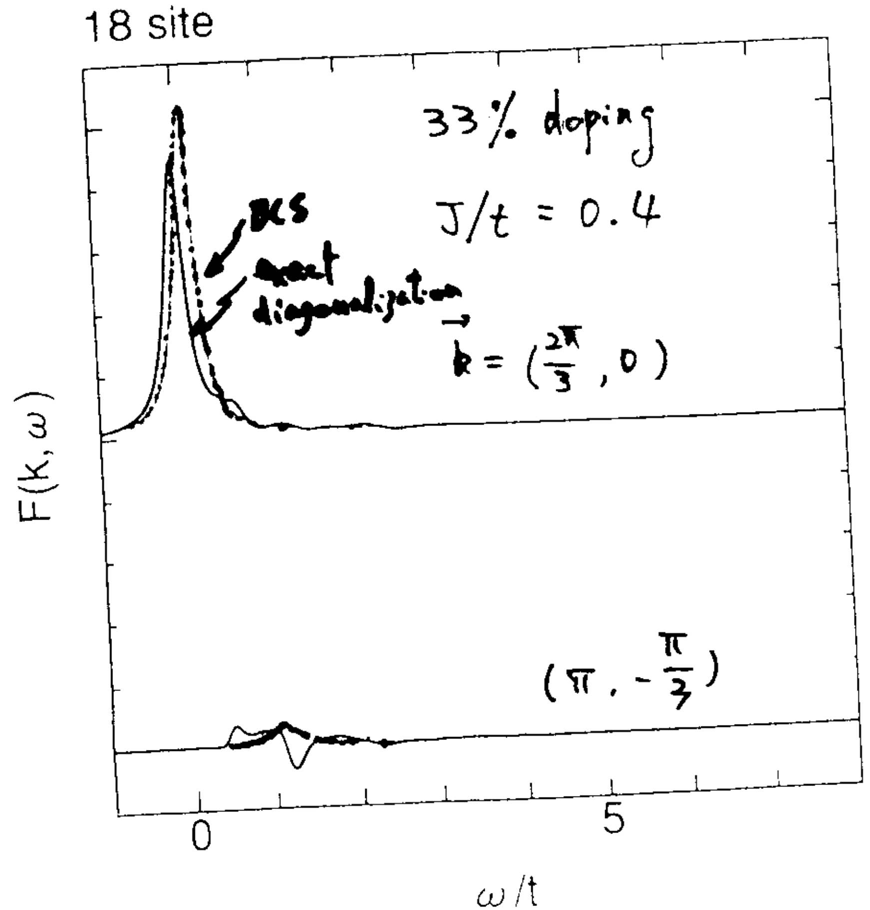

16 site
50% doping
J/t = 0.4
exact diagonalization
BCS
k=(π /2,0)
k=(π ,0)
k=(π , π /2)
F(k, ω)
ω /t

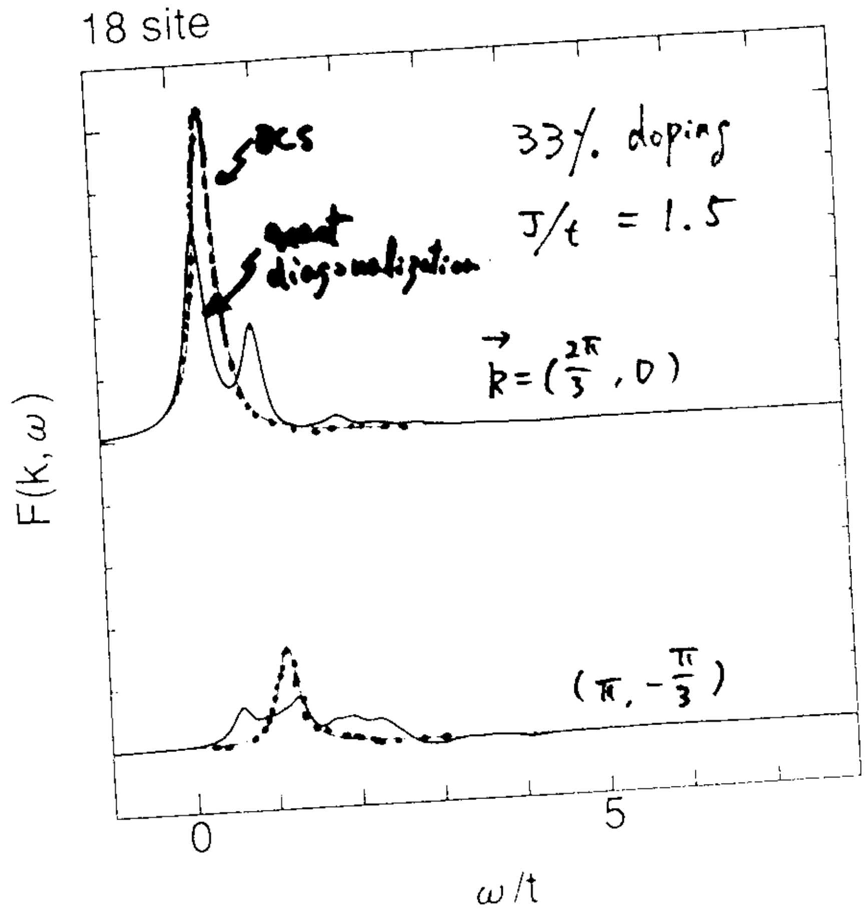

16 site
50% doping
J/t = 2.5
exact diagonalization
BCS
k=(π /2,0)
k=(π ,0)
k=(π , π /2)
F(k, ω)
ω /t

1a

$$\Delta_k = \Delta_d (\cos k_x - \cos k_y) .$$

$$E_k^{BCS^2} = [-2t_{eff} (\cos k_x + \cos k_y) - \mu]^2 + \Delta_k^2 .$$





$\Delta_d = 0.05$.

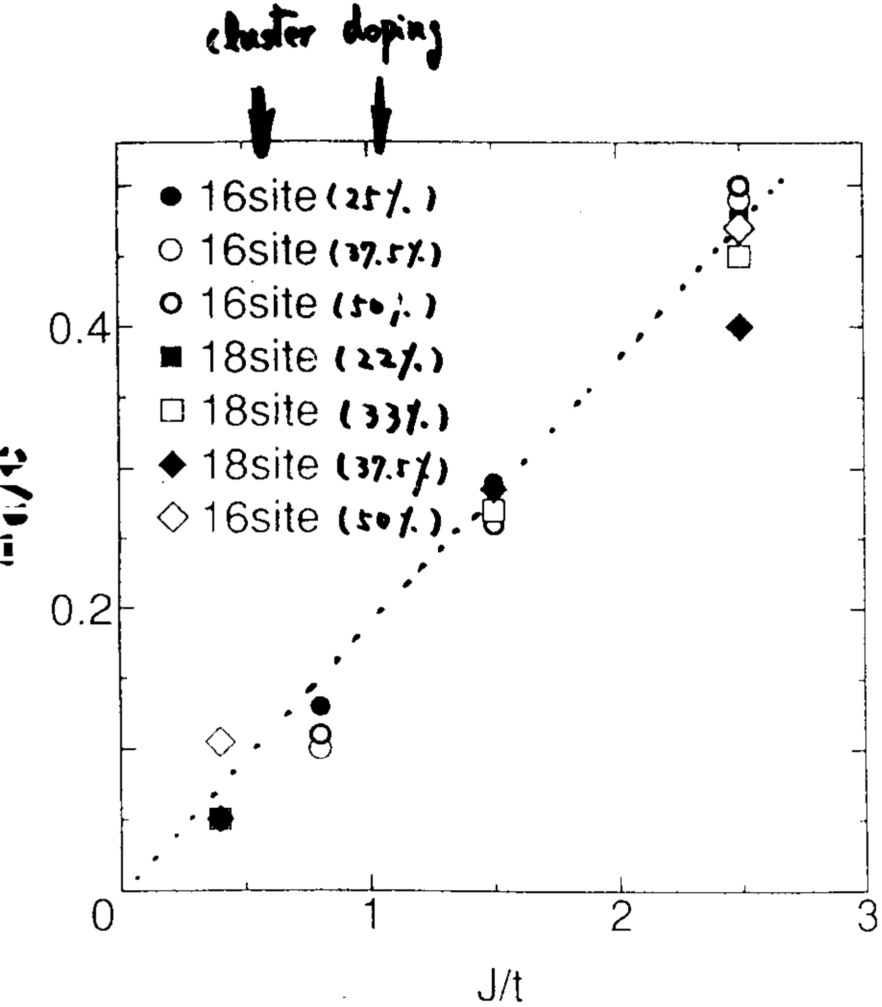
$t_{eff} = 0.45$

$\mu = -0.45$ in units of t.

$\Delta_d = 0.27$

$t_{eff} = 0.45$

$\mu = -0.45$ in units of t.



$$\Delta_k = \Delta_d (\cos k_x - \cos k_y).$$

$$\Delta_d / t \approx 0.2 \, J/t$$

16site F(k, ω)

doping	J	Δ_d	μ	t_{eff}
25%	0.8	0.13	0.00	0.55
	1.5	0.29		
	2.5	0.48		
37.5%	0.8	0.10	-1.10	0.55
	1.5	0.26		
	2.5	0.49		
50%	0.8	0.11	1.10	0.55
	1.5	0.25		
	2.5	0.50		

18site F(k, ω)

doping	J	Δ_d	μ	t_{eff}
22%	0.4	0.05	0.15	0.45
	1.5	0.27		
33%	0.4	0.05	0.45	0.45
	1.5	0.27		
	2.5	0.45		

F(k, k', ω)

doping	J	Δ_d	μ	t_{eff}
(18site) 33%	0.4	0.05	-0.45	0.45
	1.5	0.285		
	2.5	0.40		
(16site) 50%	0.4	0.105	1.10	0.55
	2.5	0.47		

In summary :

→ Cuprates are ionic metals with layered structure.

→ Cuprates are charge transfer type (not Mott-Hubbard type)

$\Downarrow$

large antiferromagnetic exchange J.

$S = 1/2$ in 2-dimension

$\Downarrow$

strong quantum effects of spins

→ Cuprates are mapped onto tJ model.

$\Downarrow$

$d(x^2-y^2)$-wave pairing with $\Delta_k = \Delta_d(\cos k_x - \cos k_y)$.

$\Delta d \simeq 0.2 J$.

$\Downarrow$

High T_c superconductivity.

In conclusion,

The cuprates are unique.

It seems not possible to obtain the conditions for high-T_c in the othe compounds.

But ... ,