Symmetry analysis of ARPES and EELS: probing the standard model of HTSC

R. Hayn

part A: Polarization dependent ARPES of $Sr_2CuO_2Cl_2$

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part B: EELS of $Sr_2CuO_2Cl_2$ and Sr_2CuO_3

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Standard model

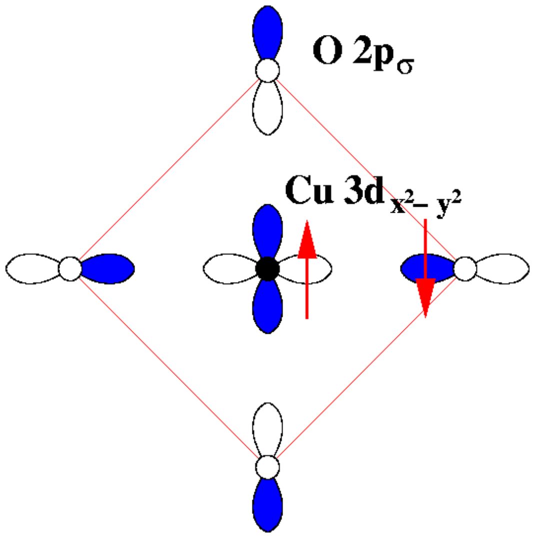
Charge transfer insulator
(Optics , PES/IPES)

Relevant orbitals : Cu 3 d_{x2-y2} O 2 p_σ
(three band Emery model)

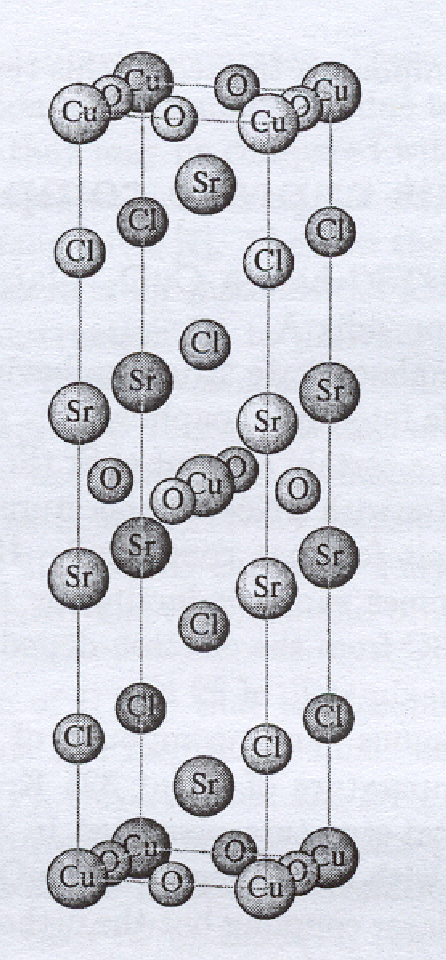
Zhang-Rice singlet

tJ - model

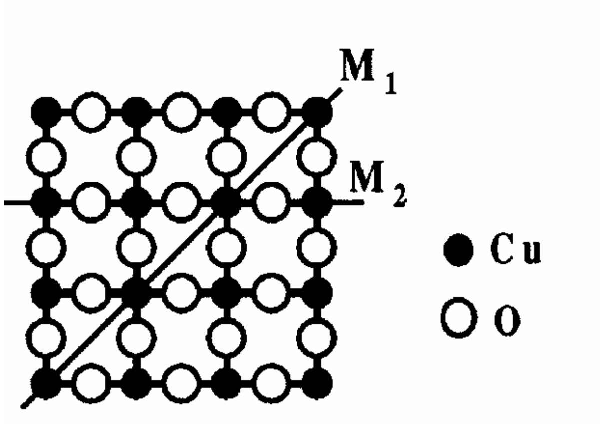
Spin fluctuations



$Sr_2CuO_2Cl_2$

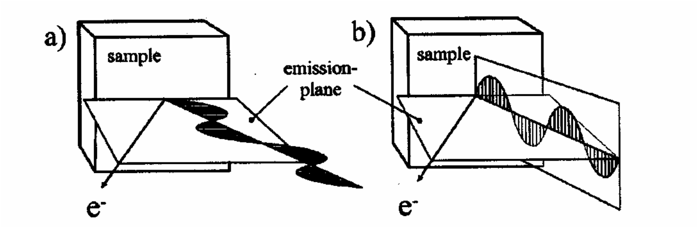


mirror planes



Polarization

parallel perpendicular



symmetric (+)
(out-of-plane)

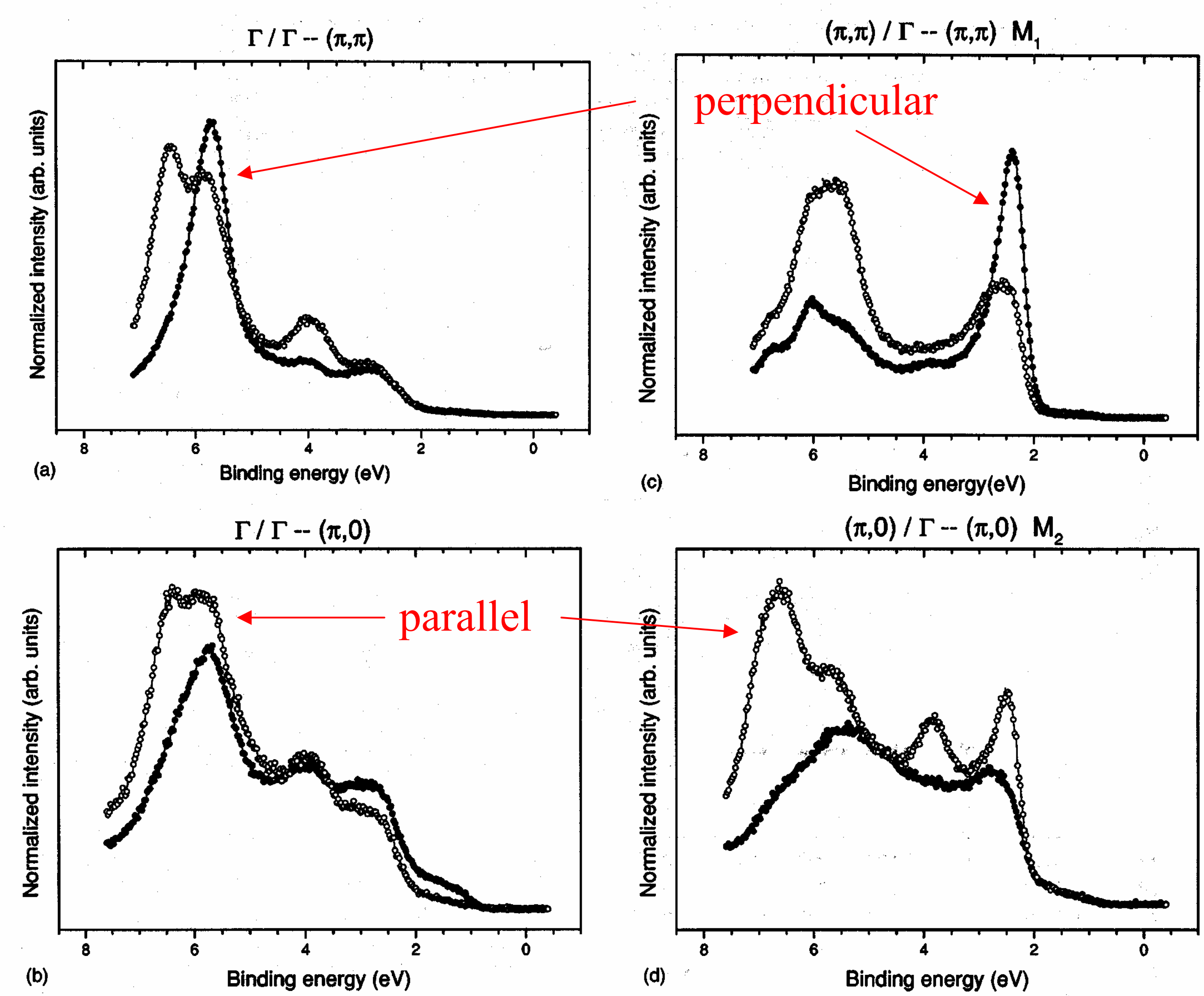
antisymmetric (-)

$$\langle \psi_i | \vec{E}\vec{r} | \psi_f \rangle = \langle + | + | + \rangle \neq 0$$

$$\langle - | - | + \rangle \neq 0$$

Spectra

35 eV
300 K



LDA+U

group theory

point (π,π) (group D_{4h})

orbitals	representation	M_1
$d_{3z^2-r^2}$ $\tilde{p}_\sigma$	A_{1g}	$+$
p_π	A_{2g}	$-$
$d_{x^2-y^2}$ p_σ	B_{1g}	$-$
d_{xy} $\tilde{p}_\pi$	B_{2g}	$+$
$d_{(x,y)z}$ p_z	E_g	o

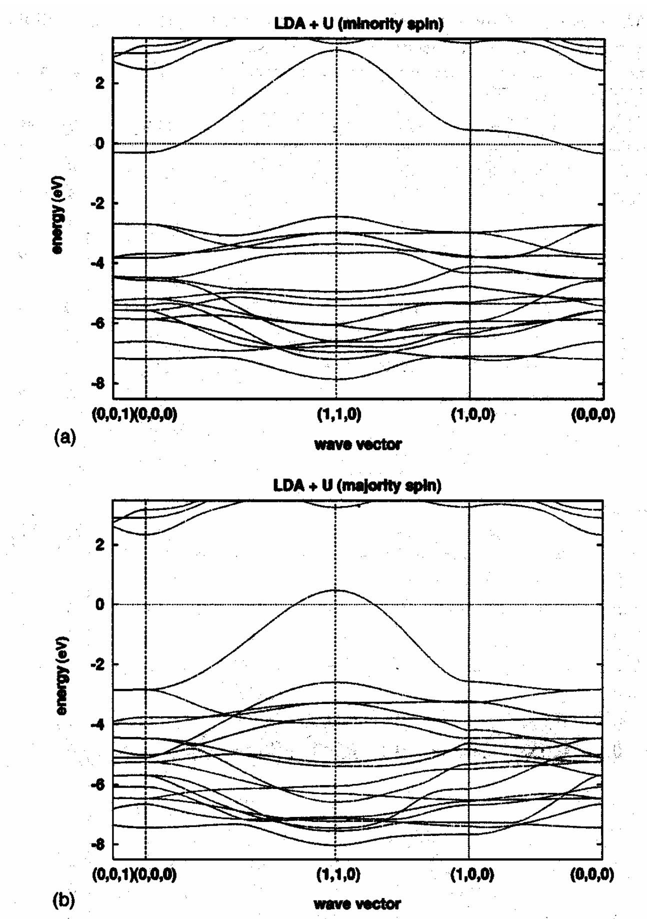
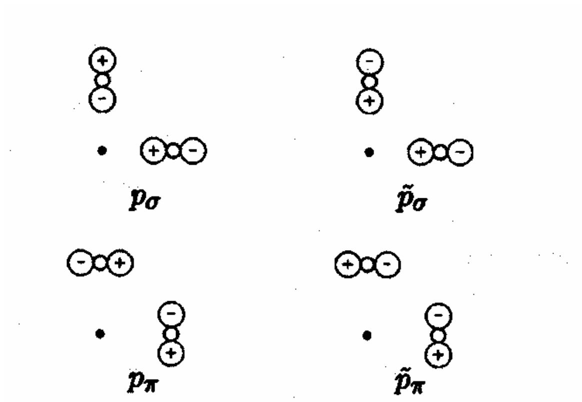
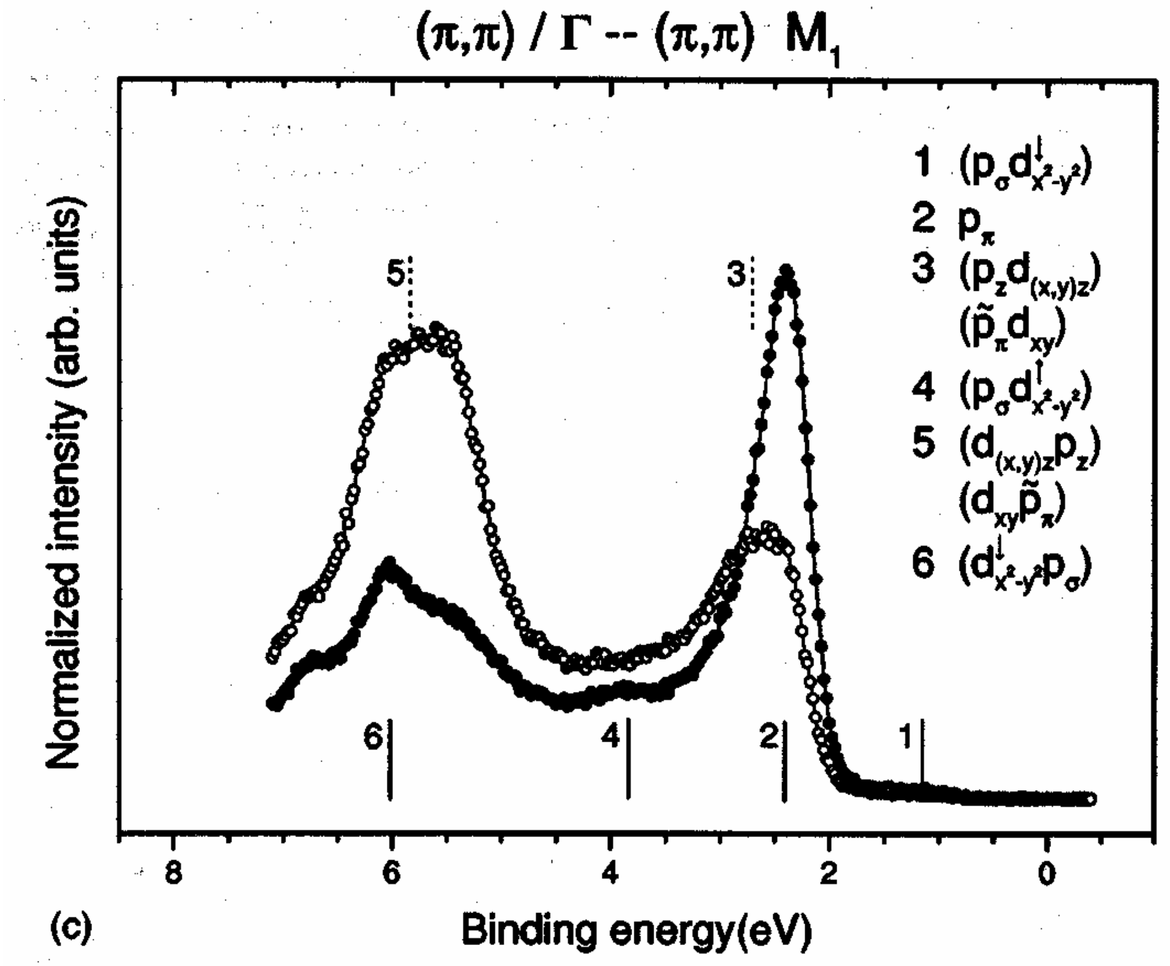


FIG. 5. LDA+U band structure: (a) minority spin (↑); (b) majority spin (↓).



Assignement



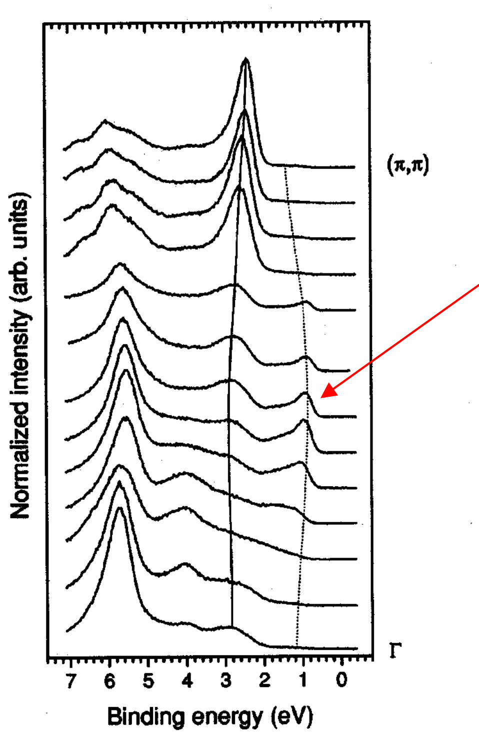
Comparison

point (π,π)

orbitals	LDA + U	Exp.
$\left(p_\sigma d^{\downarrow}_{x^2-y^2}\right)(ZRS)$	0.65	-1.2
p_π	-2.43	-2.4
$\left(p_z d_{(x,y)z}\right)$	-2.98	-2.7
$\left(\tilde{p}_\pi d_{xy}\right)$	-3.35	-2.7
$\left(p_\sigma d^{\uparrow}_{x^2-y^2}\right)(ZRT)$	-4.94	-3.8
$\left(d_{((x,y)z)} p_z\right)$	-6.62	-5.8

orbitals	LDA
$\left(d_{x^2-y^2} p_\sigma\right)$	2.32
$\left(d_{xy} \tilde{p}_\pi\right)$	-1.33
$\left(d_{(x,y)z} p_z\right)$	-1.58
$\left(d_{3z^2-r^2} \tilde{p}_\sigma\right)$	-1.87
p_π	-2.12

Zhang-Rice singlet dispersion



t t' t'' J model with ab-initio like parameters

life time – phonons : Rösch/Gunnarson Sawatzky, Shen

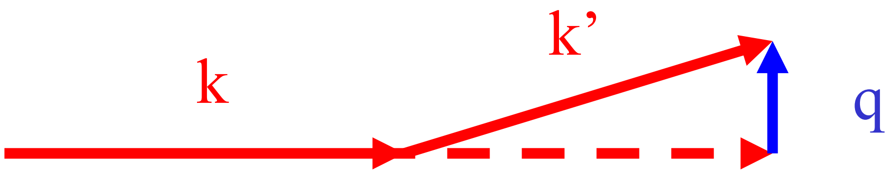
perpendicular polarization

no peak with parallel polarization

Conclusion – part A

- Assignement of all peaks by LDA+U (LDA does not work)
- First electron removal state of main valence band at (π,π) is p_π orbital (confirms Pothuizen et al)
- ZRS is best visible at $(\pi/2,\pi/2)$ and has lower binding energy

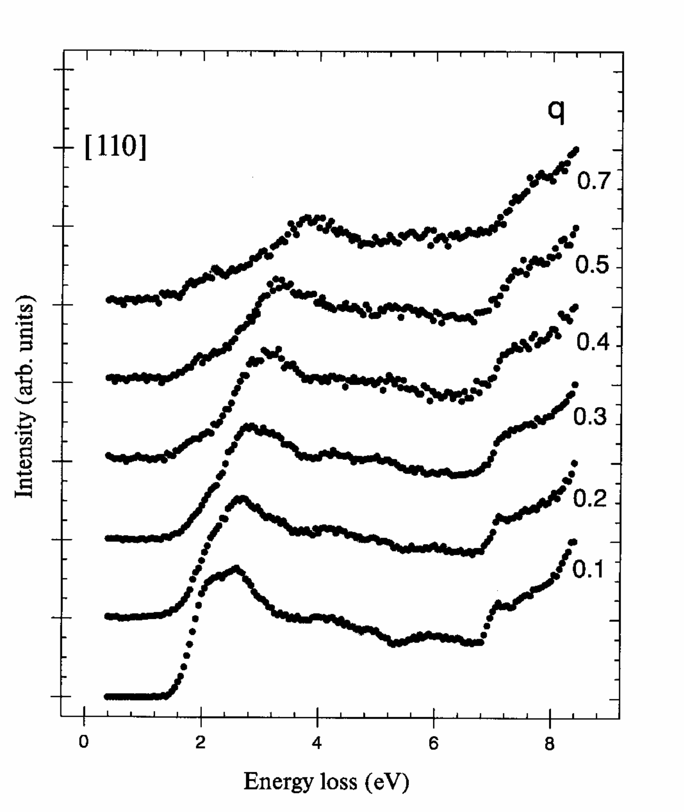
$E_{lectron}$ E_{nergy} L_{loss} $S_{pectroscopy}$



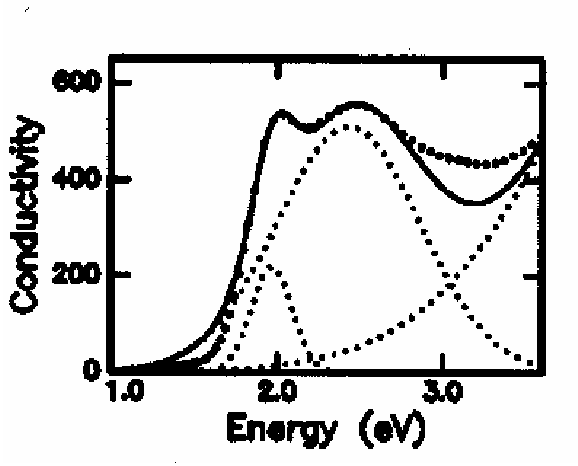
$$I \propto \frac{1}{q^2} \left| \left\langle \psi_{exc} \left| e^{i\vec{q}\vec{r}} \right| \psi_{GS} \right\rangle \right|^2 \propto \frac{1}{q^2} \left| \left\langle \psi_{exc} \left| \vec{q}\vec{r} \right| \psi_{GS} \right\rangle \right|^2$$

dipole matrix element

EELS of $Sr_2CuO_2Cl_2$

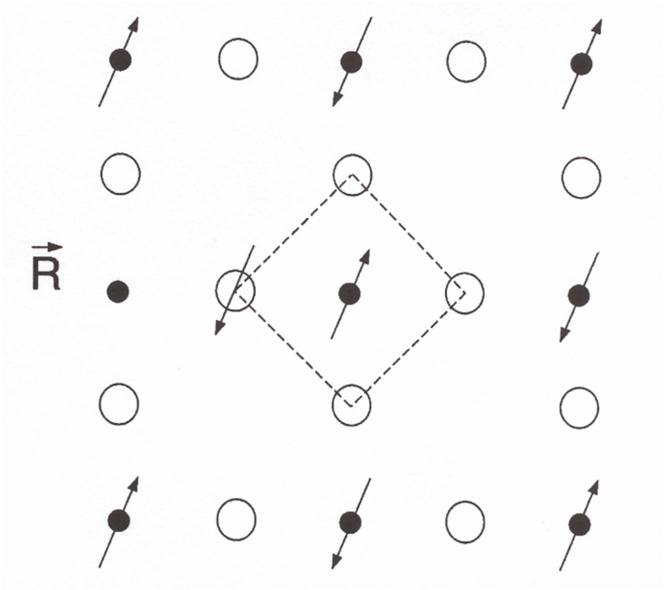


optical conductivity
(Choi et al)

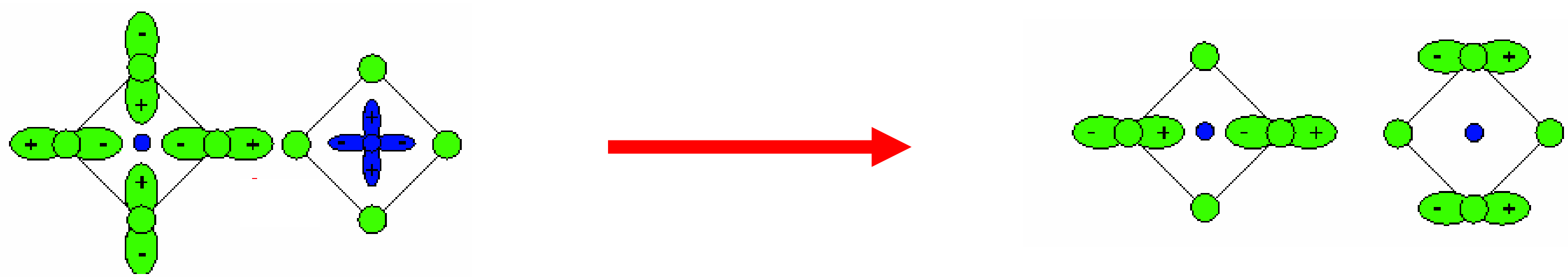


Zhang and Ng

large exciton dispersion in the standard model



One center excitons



b_{1g}^{b} $\quad$ $e_u(\sigma)$ $\quad$ $e_u(\pi)$

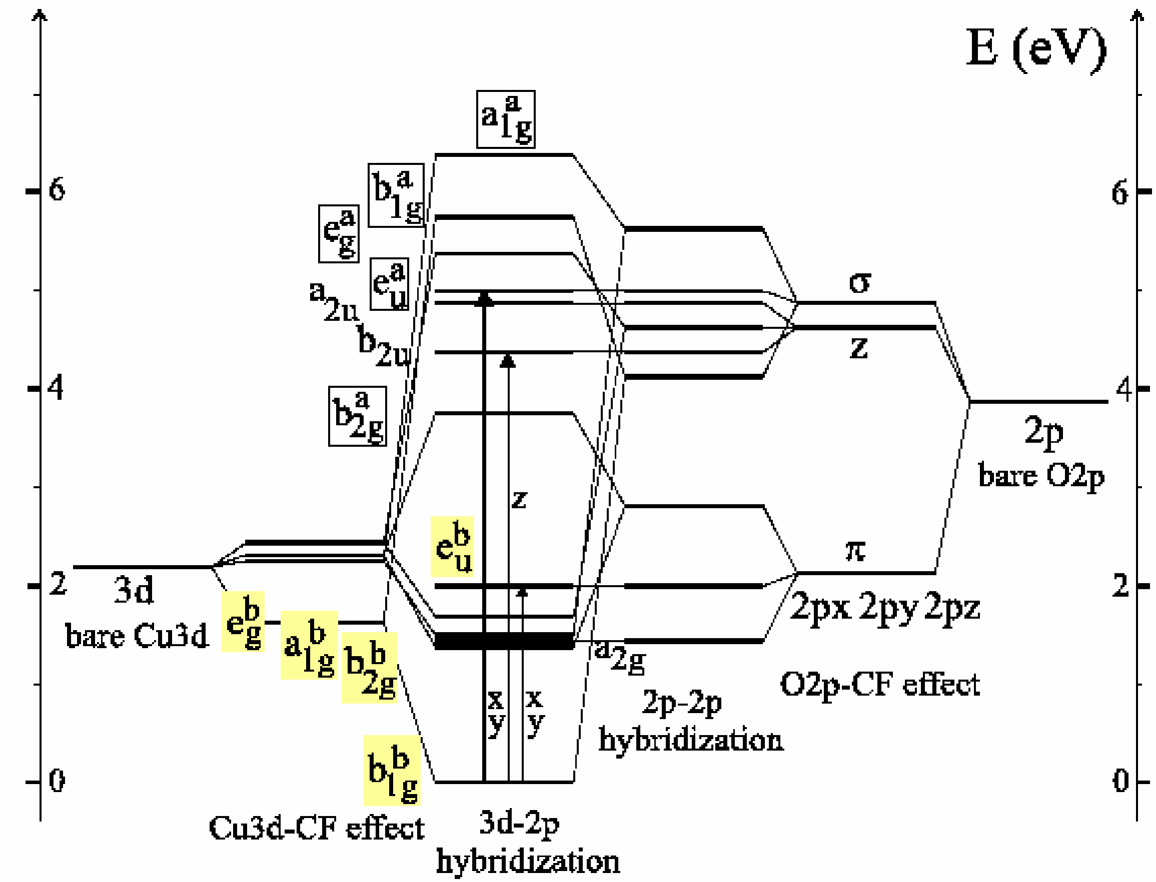
$$\left|e_u(x)\right\rangle = \cos\alpha\ \left|e_u(\pi)\right\rangle + \sin\alpha\ \left|e_u(\sigma)\right\rangle$$

(dipole allowed)

$$\left\langle \psi_{exc} \left| e^{i\vec{q}\vec{r}} \right| \psi_{GS} \right\rangle = \left\langle e_u(x) \left| e^{i\vec{q}\vec{r}} \right| b_{1g}^{b} \right\rangle \propto \sin\frac{q_x a}{2} \propto q_x$$

Cluster diagonalization

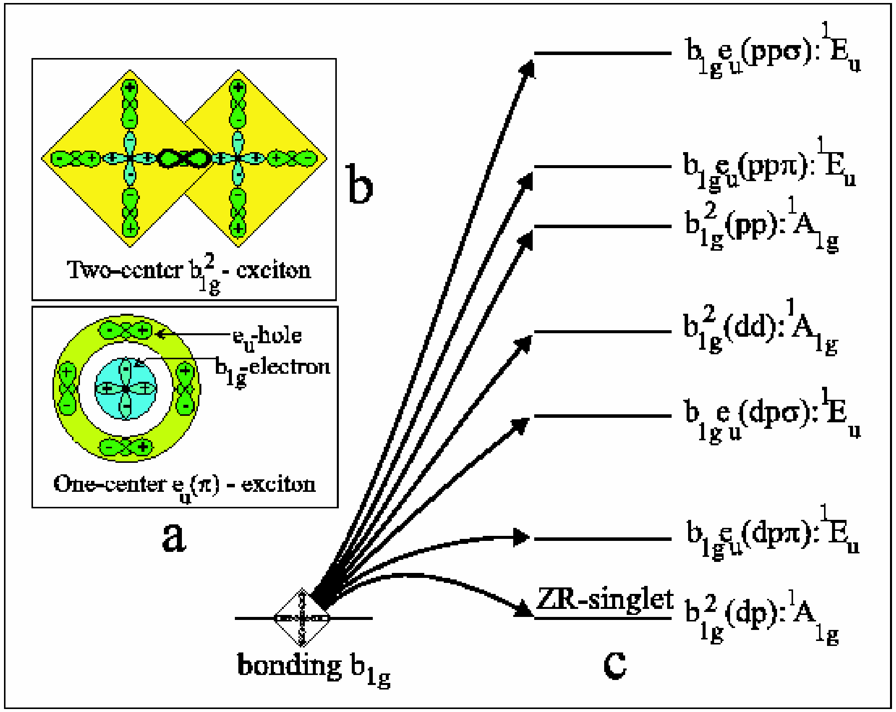
(standard parameters for cuprates, one plaquette)



Two center excitons

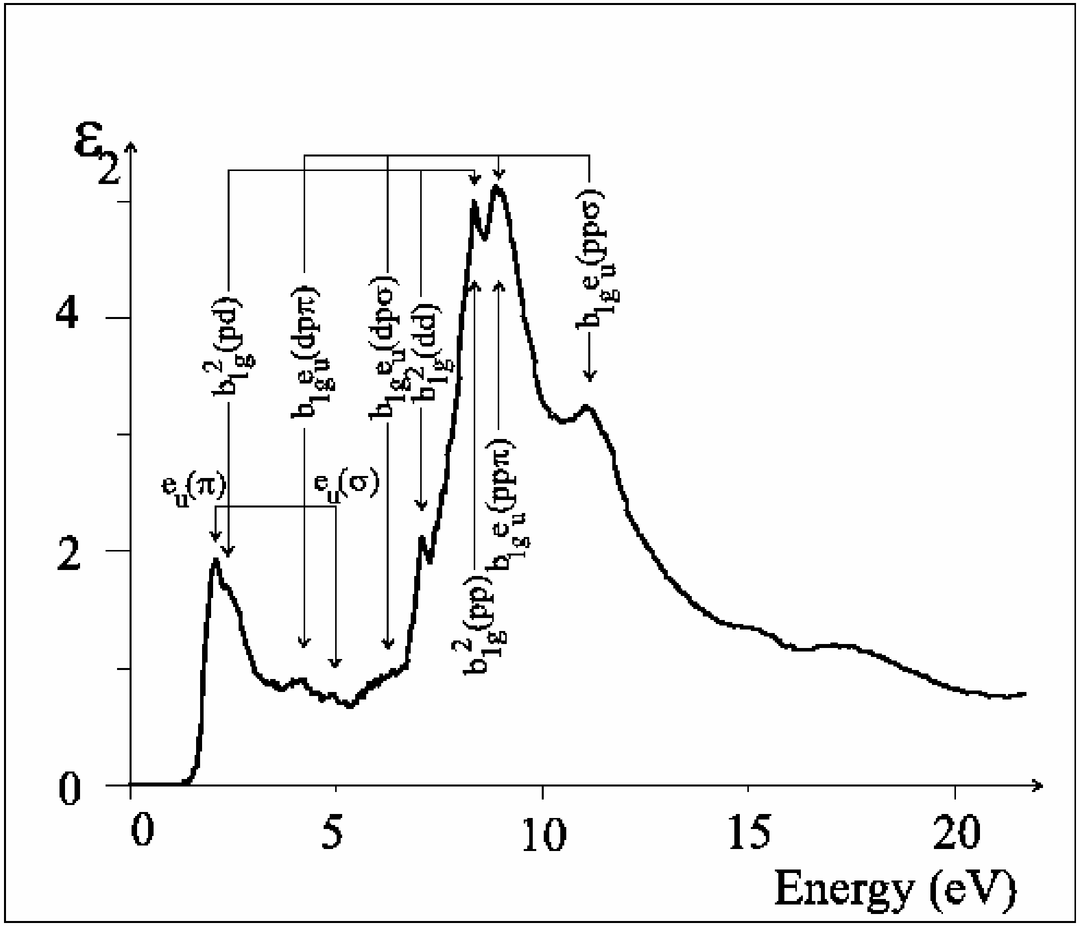
$$CuO_4^{6-} + CuO_4^{6-} \rightarrow CuO_4^{7-} + CuO_4^{5-}$$

$(d^{10}p^6)$ (two holes)



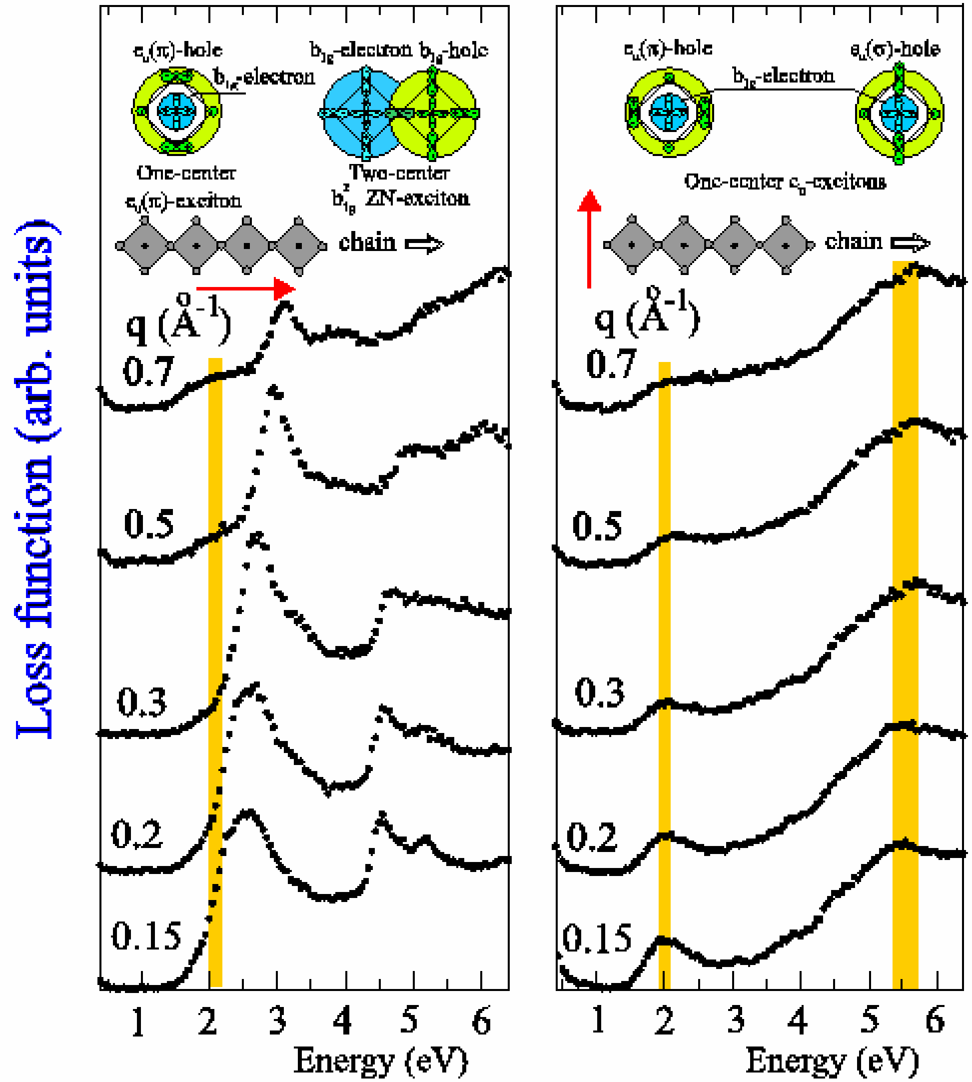
$$\left|b_{1g}^2(dp)\right\rangle = 0.95\left|pd\right\rangle - 0.25\left|dd\right\rangle - 0.19\left|pp\right\rangle$$

Assignement of peaks



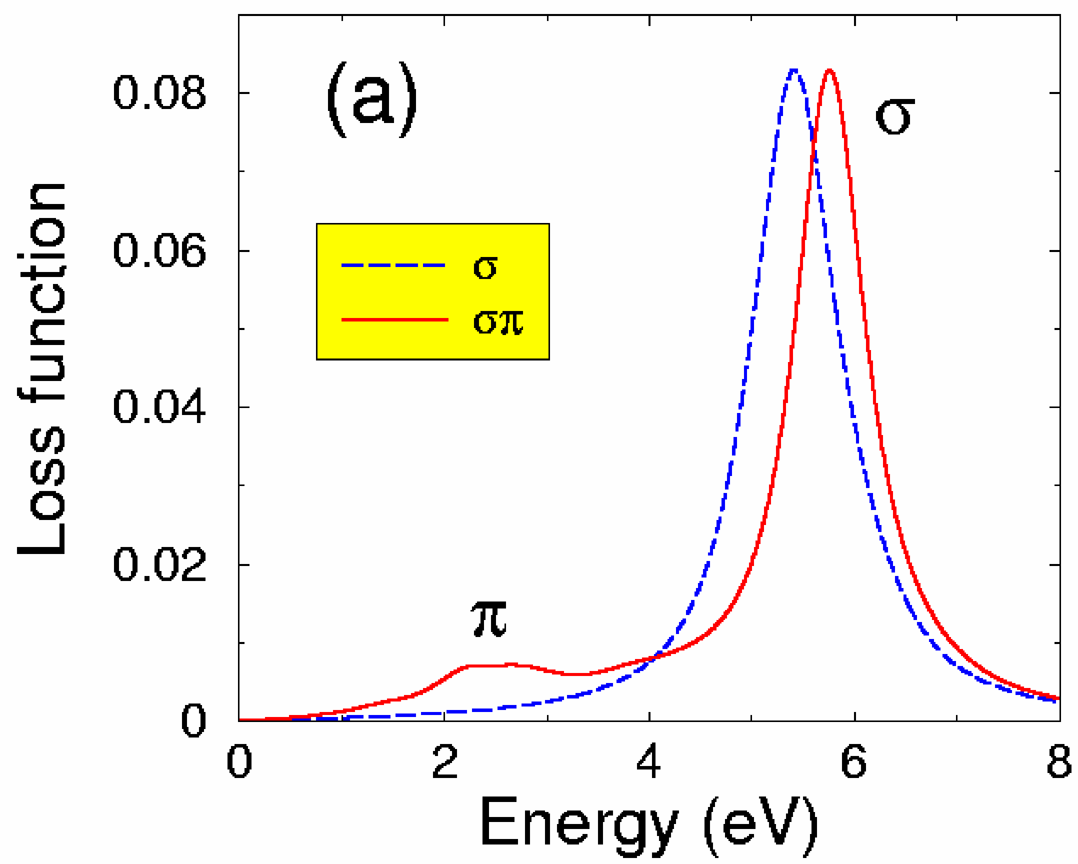
Excitons in 1D

Sr_2CuO_3



exact diagonalization

(transversal response for q=0, 4 plaquettes)



Conclusion – part B

- The CT gap in insulating parent cuprates is determined by nearly degenerate one-center, localized excitons (with oxygen p_π orbitals) and the two-center ZRS exciton.