Optical conductivity in one-dimensional Mott insulator Sr_2CuO_3

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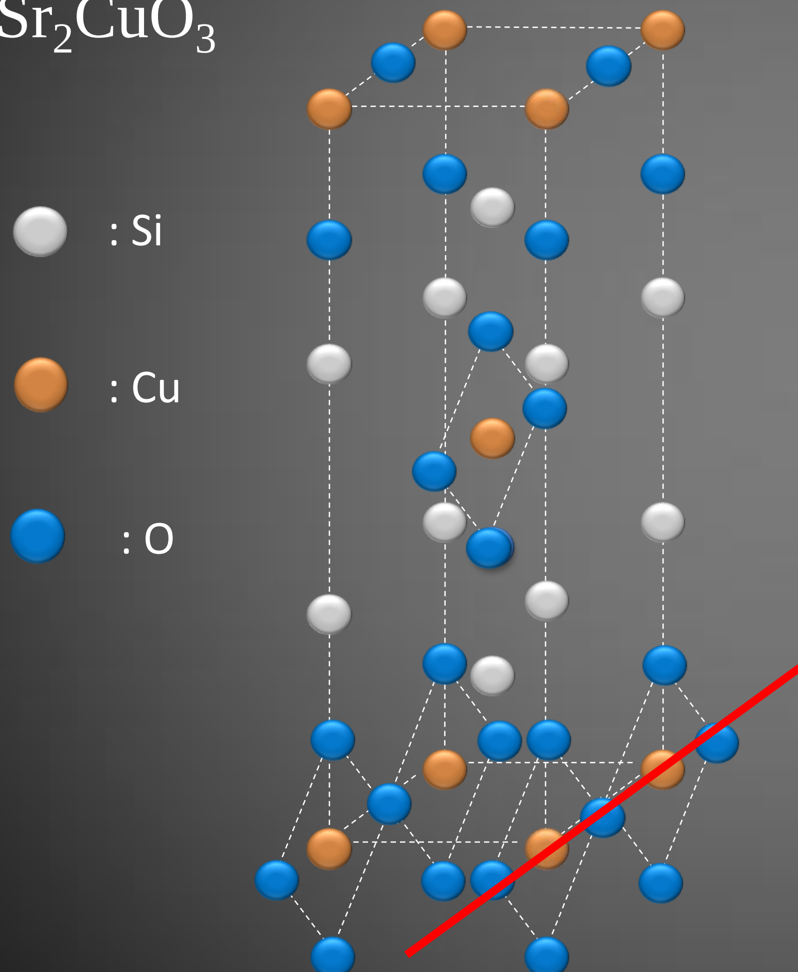
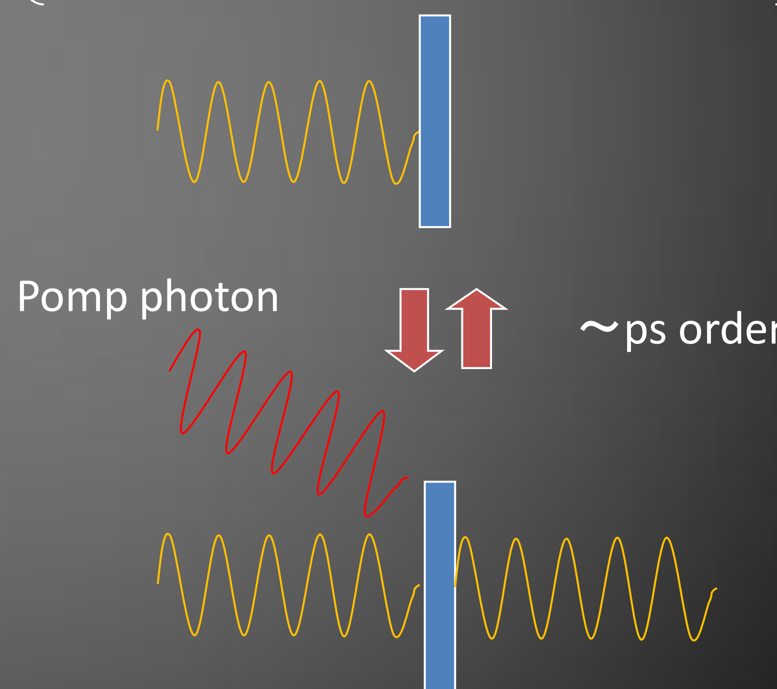
Introduction

Sr_2CuO_3



Optical response

- Giant non-linear optical response
- Ultra fast relaxation time



New optical switching device!

Optical excited state of one-dimensional Mott insulator

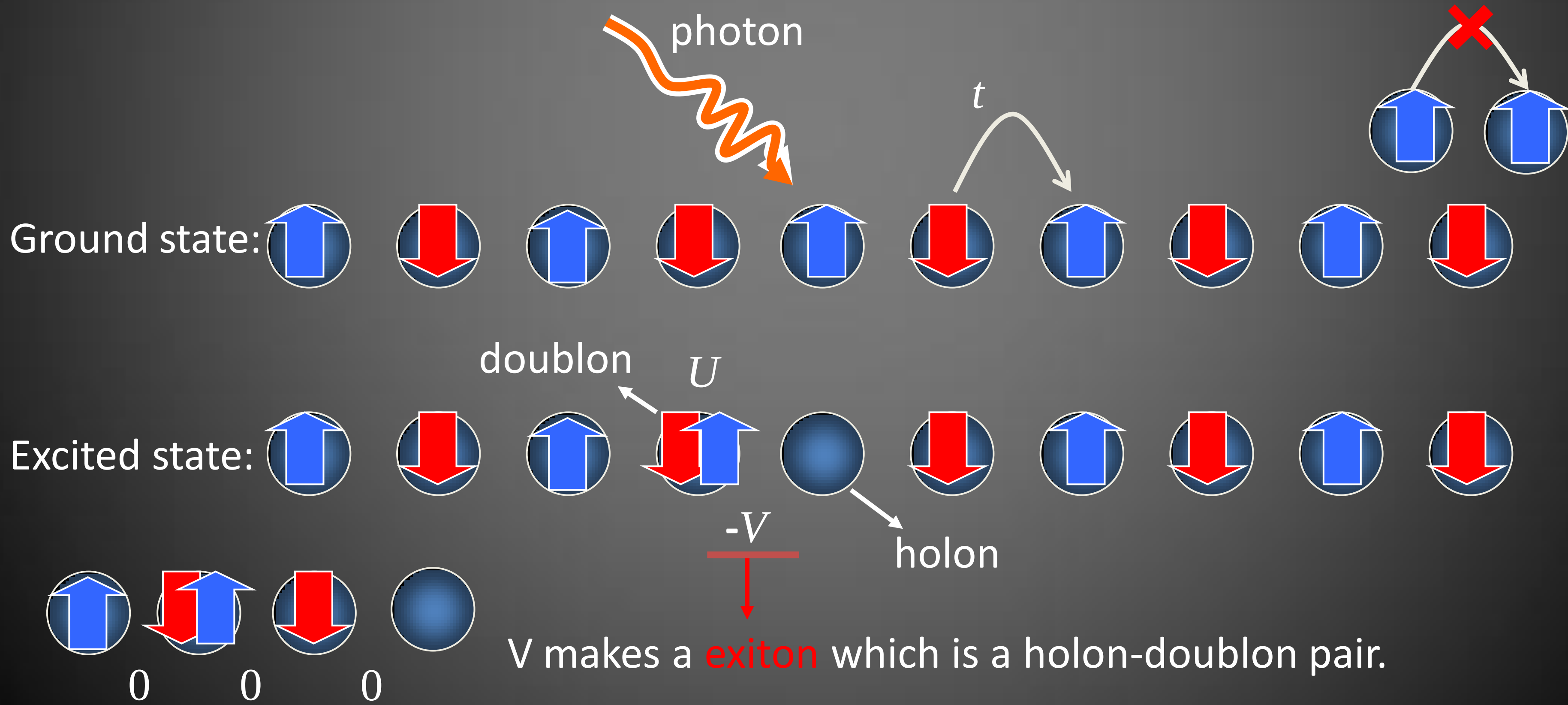
Extended Hubbard model

$$H_{ex-hubbard} = -t\sum_{i,\sigma}(c^{\dagger}_{i+1,\sigma}c_{i,\sigma} + h.c.) + U\sum_{i} n_{i,\downarrow}n_{i,\uparrow} + V\sum_{i}(n_i - 1)(n_{i+1} - 1)$$

t : electron hopping

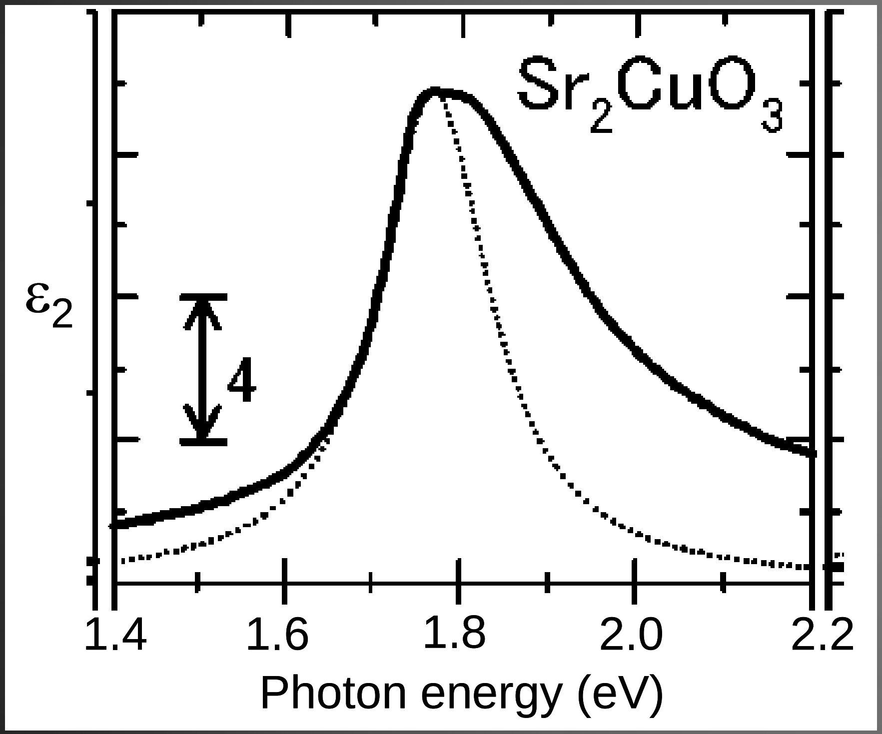
U : onsite coulomb interaction

V : coulomb interaction between electrons at nearest neighbor sites



Experimental data

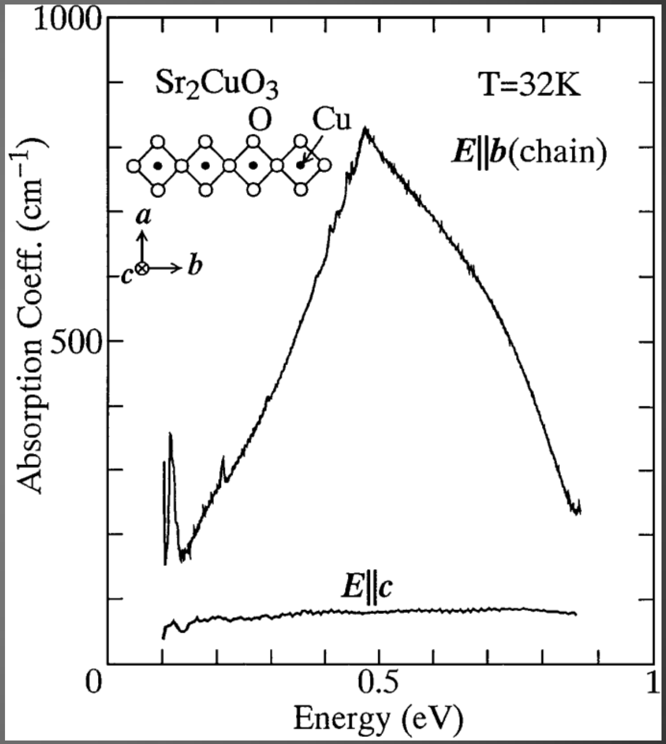
Carge transfer excitation



M. Ono *et al*, Phys. Rev. B. **70**, 085101 (2004)

exiton＋continues states＋phonon

spin excitation



H. Suzuura *et al*, Phys. Rev. Lett. **76**, 2579 (1996)

Phonon assisted spin excitation

Electron-phonon interaction is important!

Motivation

we would like to describe the one-dimensional electron system of Sr_2CuO_3 to understand this optical response.

- model: Hubbard-Holstein model
- method: Dynamical Density Matrix Renormalization Group (Dynamical DMRG) + Regulated Polynomial Expansion (RPE)

•Hubbard-Holstein model

Hamiltonian:

$$H = H_{ex-hubbard} + H_{phonon} + H_{el-ph}$$

$$H_{ex-hubbard} = -t\sum_{i,\sigma}(c^{\dagger}_{i+1,\sigma}c_{i,\sigma} + h.c.) + U\sum_{i} n_{i,\downarrow}n_{i,\uparrow} + V\sum_{i}(n_i - 1)(n_{i+1} - 1)$$

$$H_{phonon} = \omega_0 \sum_{i} b^{\dagger}_{i+1/2} b_{i+1/2}$$

Employing Einstein phonon

$$H_{el-ph} = -g\sum_{i}(b^{\dagger}_{i+1/2} + b_{i+1/2})(n_i - n_{i+1})$$

Holstein-type electron phonon interaction

- Dynamical current-current correlation function

$$\chi_j(\omega) = \frac{1}{\pi N_s} \mathrm{Im} \langle 0 | j^\dagger \frac{1}{\omega - H - \varepsilon_0 - i\gamma} j \; | 0 \rangle$$

$$\left(\hat{H} | 0 \rangle \equiv \varepsilon_0 | 0 \rangle, \quad j \equiv it \sum_i (c_{i+1}^\dagger c_i + H.c.) \right)$$

$$\chi_j(\omega) / \omega \propto (\text{optical conductivity})$$

Method

- Dynamical DMRG method

Multi target →

$$| \, 0 \, \rangle, \qquad j | \, 0 \, \rangle, \qquad \text{and} \qquad \frac{1}{\omega - \hat{H} + \langle E \rangle - i\gamma} j | \, 0 \, \rangle$$

- Regulated Polynomial expansion using Legendre polynomial

$$\lim_{\gamma \to 0} \frac{1}{\omega - H - \varepsilon_0 - i\gamma} = \lim_{L \to \infty} \sum_{l=0}^{L} \left[2Q_l(\omega - \varepsilon_0) + i\pi P_l(\omega - \varepsilon_0) \right] \langle P_l(H) \rangle_\sigma$$

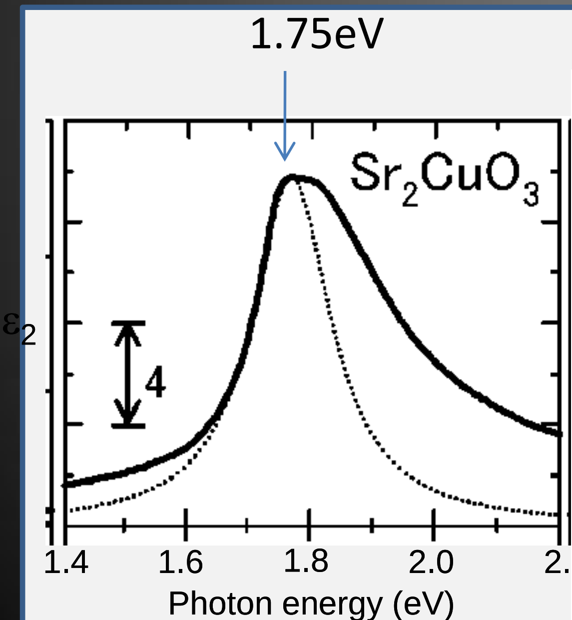
Regulated polynomial: $\langle P_l(\hat{H}_s) \rangle_\sigma \equiv \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-1}^{1} e^{-(x' - \hat{H}_s)^2 / 2\sigma^2} P_l(x') dx'$ $\quad (\sigma = 2\pi / L)$

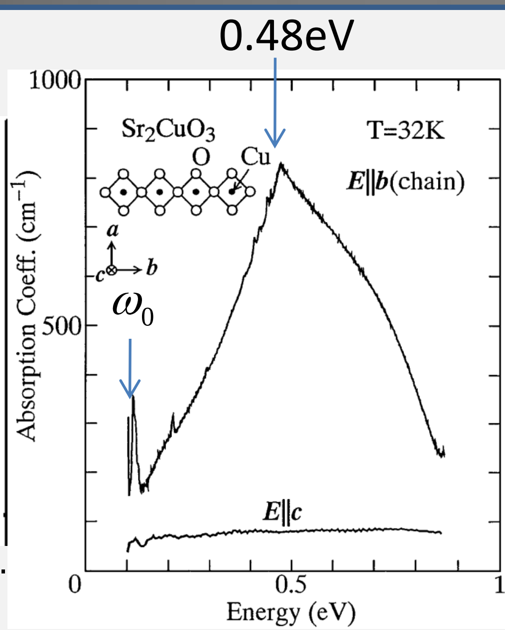
Parameters

$$H = H_{ex-hubbard} + H_{phonon} + H_{el-ph}$$

$$H_{ex-hubbard} = -t\sum_{i,\sigma}(c^{\dagger}_{i+1,\sigma}c_{i,\sigma} + h.c.) + U\sum_{i} n_{i,\downarrow}n_{i,\uparrow} + V\sum_{i}(n_i - 1)(n_{i+1} - 1)$$

$$H_{phonon} = \omega_0\sum_{i} b^{\dagger}_{i+1/2}b_{i+1/2}, \quad H_{el-ph} = -g\sum_{i}(b^{\dagger}_{i+1/2} + b_{i+1/2})(n_i - n_{i+1})$$





$t = 0.41\text{eV}$

$U = 3.3\text{eV}$

$V = 0.82\text{eV}$

$V = 2t$

$J \sim 4t^2/(U - V)$

$= 0.282\text{eV}$

$J \approx 0.26\text{eV}$

(expariment)

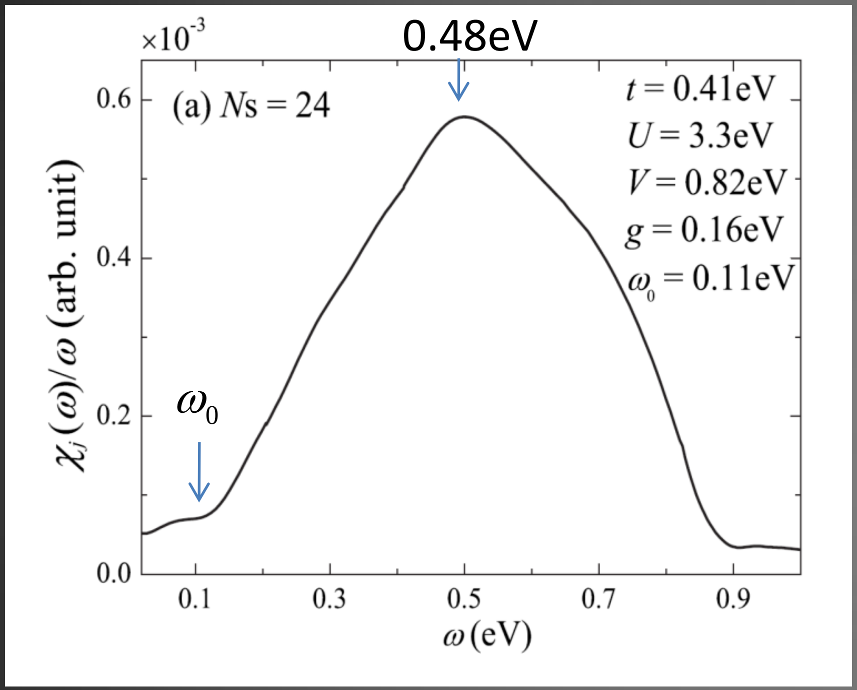
$\omega_0 = 0.11\text{eV}$

$g = 0.16\text{eV}$

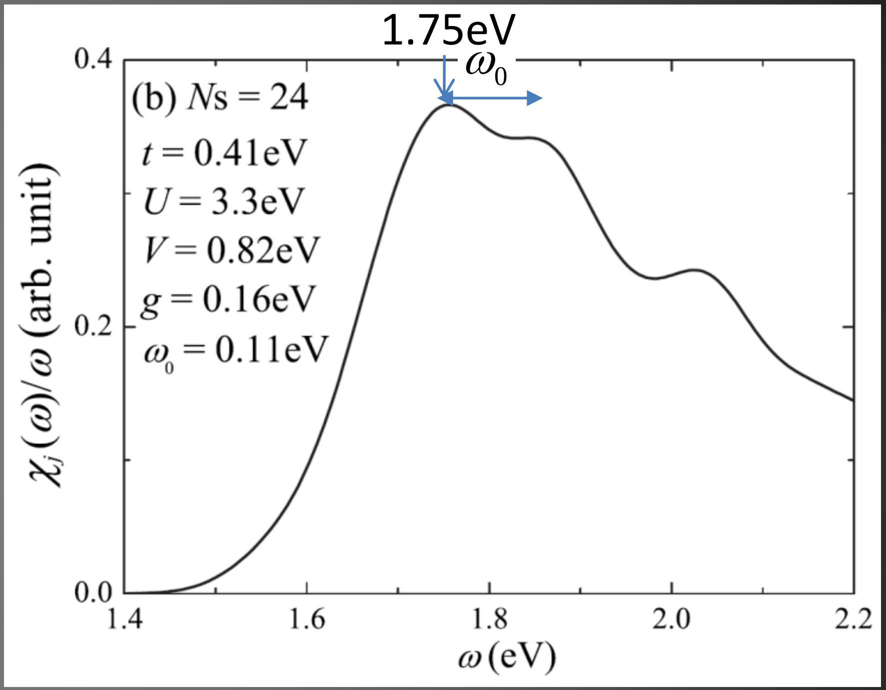
- phonon structure
- Mott gap

results

- Phonon-assisted spin excitation



- Charge-transfer excitation



Hubbard-Holstein model

$$t = 0.41\text{eV},\ U = 3.3\text{eV},\ V = 0.82\text{eV},\ g = 0.16\text{eV},\ \omega_0 = 0.11\text{eV}$$

→ One-dimensional electron system of Sr_2CuO_3