Entanglement in CuO

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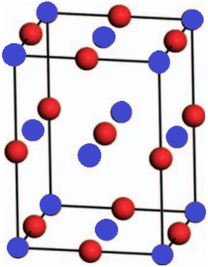
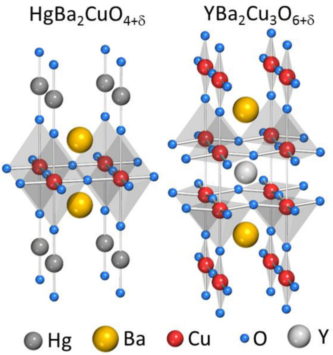
Scheme of the presentation

- Tetragonal CuO structure
- Entanglement as the Von-Neumann entropy
- Affection of states by E_{gap}
- High charge for low entangled states

Introduction

- Quantum correlation in cuprates (CuO) $\rightarrow$ Understanding superconductivity
- Two-holes states in the *CuO* layer as quantum bipartite states.


CuO



Measure of Entanglement

- Given $|\chi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$, if $\exists\, |\phi\rangle \in \mathcal{H}_1$ and $\exists\, |\psi\rangle \in \mathcal{H}_2$ such that

$$|\chi\rangle = |\phi \otimes \psi\rangle \rightarrow \textit{separable} \tag{1}$$

$$|\chi\rangle \neq |\phi \otimes \psi\rangle \rightarrow \textit{entangled} \tag{2}$$

- Given $\rho = |\chi\rangle \langle\chi|$ and $\rho_1 = Tr_2(\rho)$,

$$S(\rho) = -Tr(\rho_1 log(\rho_1))$$

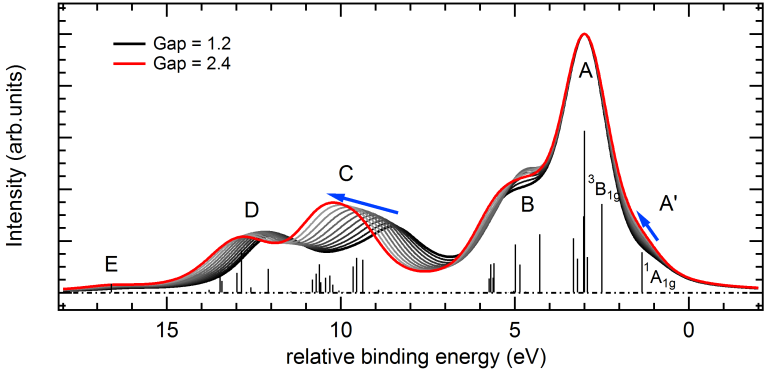
- If $|\chi\rangle = \sum_i \sqrt{\lambda_i}\, |\xi_i\rangle_1 \otimes |\xi_i\rangle_2$ in its singular basis (Schmidt decomposition)

$$S(\rho) = -\sum_n \lambda_n log(\lambda_n)$$

- $$S(sep.) = 0 \quad and \quad 0 < S(ent.) \leq log(\frac{1}{d})$$

Photoemission spectrum of CuO

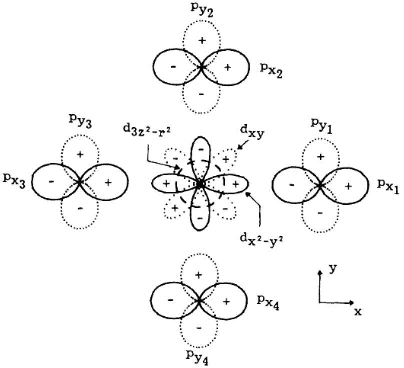
- Each vertical line describes a two-hole state (59 total)
- Variable E_{gap}



The *CuO* cluster model

3 different orbitals:

- $3d^8$- 2 holes on Cu
- $3d^9L$ - 1 hole on Cu, 1 hole on O
- $3d^{10}L^2$ - 2 holes on O



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Symmetry classes

- States gathered in symmetry classes
- Elements of C depending on parameters that can be changed in experiments

$$C = \left[\begin{array}{c|c|c|c|c|c|c} {}^3A_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & {}^3E & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & {}^1E & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & {}^1A_1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & {}^1A_2 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & {}^3B_1 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & {}^1B_1 \end{array}\right] \tag{3}$$

Parameters can be found in PhysRevB.41.288

$^3A_2$ contains : $|b_1, b_2\rangle$,$|\underline{b_1}, b_2\rangle$,$|\underline{b_1}, \underline{b_2}\rangle$,$|b_1, \underline{b_2}\rangle$,$|e_1^2\rangle$,$|\underline{e_1}, e_1\rangle$,$|\underline{e_1^2}\rangle$. Thus it appears in C as:

$$\left[\begin{array}{c|c|c|c|c|c|c|c}
 & |b_1, b_2\rangle & |\underline{b_1}, b_2\rangle & |\underline{b_1}, \underline{b_2}\rangle & |b_1, \underline{b_2}\rangle & |\underline{e_1^2}\rangle & |\underline{e_1}, e_1\rangle & |e_1^2\rangle \\ \hline
|b_1, b_2\rangle & & & & & & & \\ \hline
|\underline{b_1}, b_2\rangle & & & & & & & \\ \hline
|\underline{b_1}, \underline{b_2}\rangle & & & & & & & \\ \hline
|b_1, \underline{b_2}\rangle & & & & & & & \\ \hline
|\underline{e_1^2}\rangle & & & & & & & \\ \hline
|\underline{e_1}, e_1\rangle & & & & & & & \\ \hline
|e_1^2\rangle & & & & & & &
\end{array}\right] \tag{4}$$

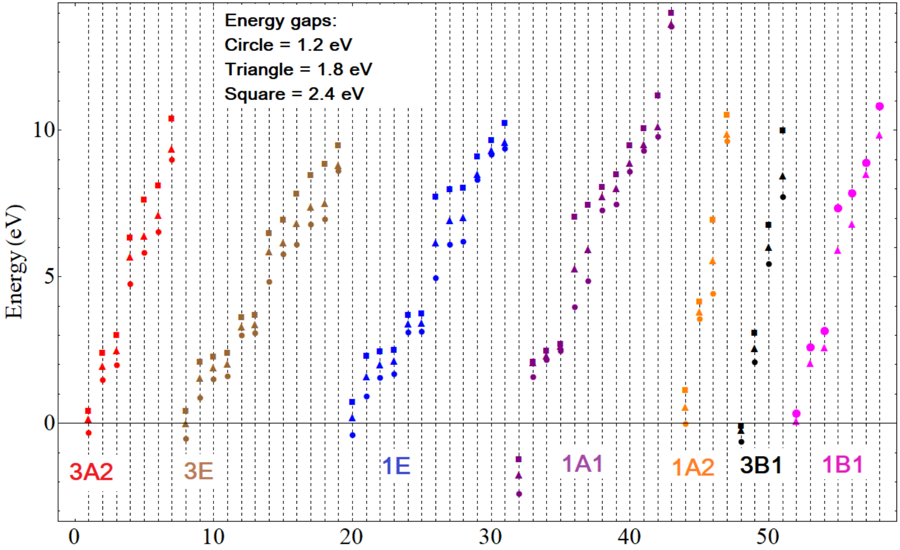
Once it is diagonalized, eigenvectors are of the form

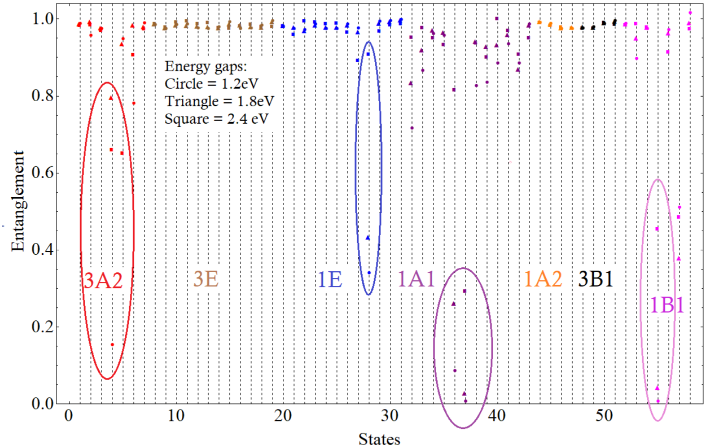
$$|\alpha_1\rangle = \beta_1 \, |b_1, b_2\rangle + \beta_2 \, |\underline{b_1}, b_2\rangle \, ...\beta_7 \, |e_1^2\rangle$$

To build the matrix of ONE two particle state:

$$state = \left[\begin{array}{c|c|c|c|c|c|c}
 & b_1 & \underline{b_1} & b_2 & \underline{b_2} & e_1 & \underline{e_1} \\ \hline
b_1 & 0 & 0 & \beta_1 & & & \\ \hline
\underline{b_1} & 0 & 0 & & & & \\ \hline
b_2 & -\beta_1 & & & & & \\ \hline
\underline{b_2} & & & & & & \\ \hline
e_1 & & & & & & \\ \hline
\underline{e_1} & & & & & &
\end{array}\right] \tag{5}$$

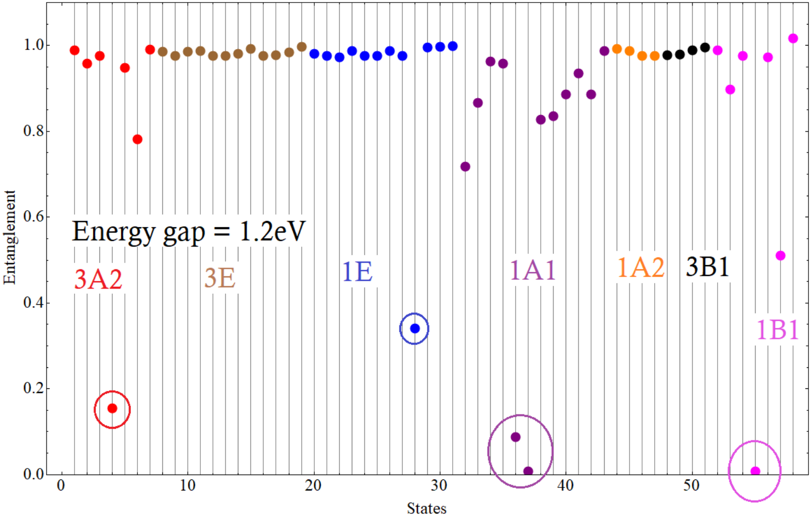
States ordered by energy ($\hat{H}\,|n\rangle = E_n\,|n\rangle$)





- For most states Ent.=1
- Different behavior of symmetry classes
- Low E_{gap} → Low entanglement

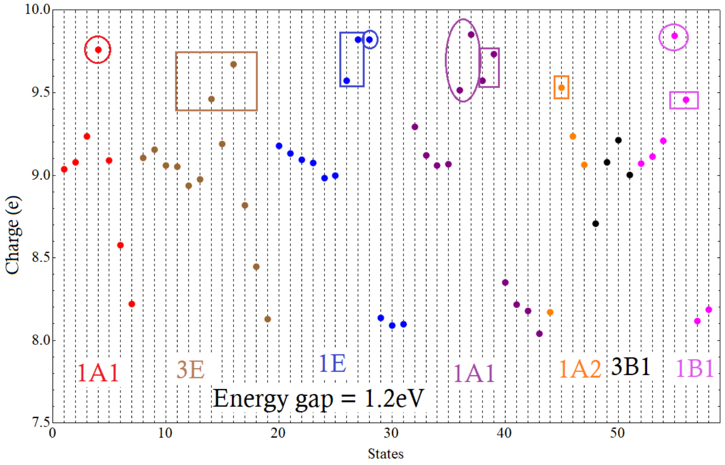
Entanglement (1.2eV)



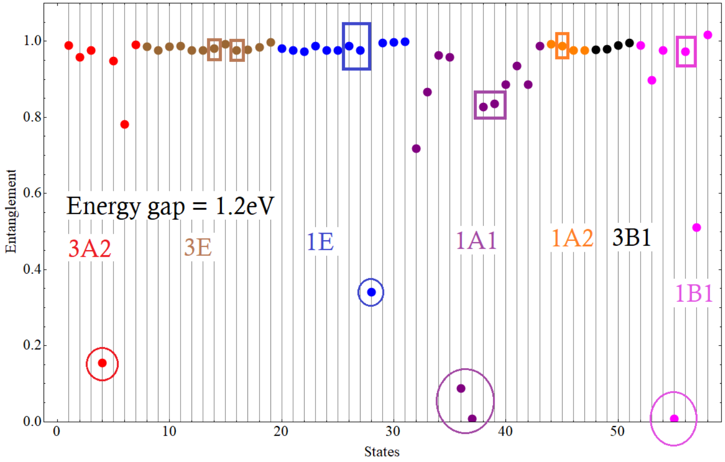
5 states with ent.<0.4

Charge

- $Q(|\phi\rangle) = 8|\langle 3d^8|\phi\rangle|^2 + 9|\langle 3d^9 L|\phi\rangle|^2 + 10|\langle 3d^{10}L^2|\phi\rangle|^2$
- Charge(e) on Cu atom for $E_{gap} = 1.2eV$
- High charge for multiple states



Entanglement fo $E_{gap} = 1.2eV$



$$\text{Low entanglement} \implies \text{High charge}$$
$$\text{High charge} \not\Longrightarrow \text{Low entanglement}$$

Conclusions

Most important results:

- Entanglement of 3E,1A2 and 3B1 hardly affected by E_{gap}
- Low entangled states for $E_{gap} = 1.2eV$
- Low entanglement $\rightarrow$ High charge

Future researches

- Why do low entangled states have high charge?
- Focus on Zhang-Rice singlet (lowest energy state)

Frame Title

$$3B1 = \begin{matrix} \mathrm{AA}-8B & \mathrm{Ta1} & \mathrm{Tb1} & 0 \\ \mathrm{Ta1} & -A+\mathrm{Da1} & 0 & \mathrm{Tb1} \\ \mathrm{Tb1} & 0 & -A+\mathrm{Db1} & \mathrm{Ta1} \\ 0 & \mathrm{Tb1} & \mathrm{Ta1} & -2A+\mathrm{Da1}+\mathrm{Db1}+\mathrm{Upp} \end{matrix}$$