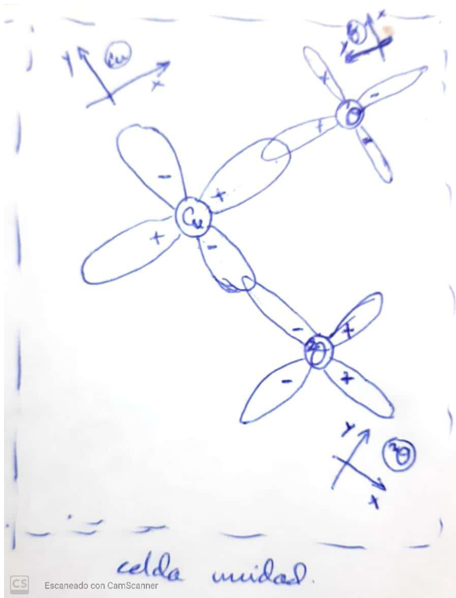

Figure 1: Unit cell CuO_2

1 Model

We consider two orbitals (p_x, p_y) for O atoms (two O per unit cell), one orbital (d_{xy}) for Cu atoms. The Hamiltonian is:

$$H = \sum_{iIJ\sigma} \Delta_{IJ} c^\dagger_{iI\sigma} c_{iJ\sigma} + \sum_{iIJ\sigma} t_{IJ} \left(c^\dagger_{iI\sigma} c_{i+1,J\sigma} + h.c. \right) + \sum_i \hat{V}_i \ ,$$

$$\Delta = \begin{pmatrix} 0 & 0 & t' & 0 & 0 \\ 0 & 0 & t_{CuO} & 0 & 0 \\ t' & t_{CuO} & -\mu_{Cu} & t_{CuO} & t' \\ 0 & 0 & t_{CuO} & 0 & 0 \\ 0 & 0 & t' & 0 & 0 \end{pmatrix}, \ t = \begin{pmatrix} t_{OO} & t_{OO} & t_{CuO} & 0 & 0 \\ t_{OO} & t_{OO} & t'_{CuO} & 0 & 0 \\ 0 & 0 & t_{CuCu} & 0 & 0 \\ 0 & 0 & t'_{CuO} & t_{OO} & t_{OO} \\ 0 & 0 & t_{CuO} & t_{OO} & t_{OO} \end{pmatrix}$$

where i is the lattice index and $I, J = p_x^{O_1}, p_y^{O_1}, d_{xy}^{Cu}, p_x^{O_2}, p_y^{O_2}$, are orbital indexes, Figure 1.

The local Coulomb interaction $\hat{V}_i$ is

$$\begin{aligned} \hat{V}_i = U \textstyle\sum_{I \neq d_{xy}^{Cu}} n_{iI\uparrow} n_{iI\downarrow} + \sum_{I=1,4,\sigma\sigma'} \left(U - 2J - J\delta_{\sigma\sigma'} \right) n_{iI\sigma} n_{i\bar{I}\sigma'} - \\ + J \textstyle\sum_{I \neq d_{xy}^{Cu}} \left(-c^\dagger_{iI\uparrow} c^\dagger_{i\bar{I}\downarrow} c_{i\bar{I}\uparrow} c_{iI\downarrow} + c^\dagger_{iI\uparrow} c^\dagger_{iI\downarrow} c_{i\bar{I}\downarrow} c_{i\bar{I}\uparrow} \right) + U_3 n_{i3\uparrow} n_{i3\downarrow}. \end{aligned} \tag{1}$$

We use the values: $t_{CuO} = 1.1$, $t'_{CuO} = 0.1$, $t_{CuCu} = 0.1$, $t_{OO} = -0.32$, $U_3 = 8$, $U = 2$, $J = 0.838$, $\mu_{Cu} = 0.5$. The global chemical potential μ should be tuned to obtain $n_{Cu} + n_O = 1$.

1.1 Spin rotation

Rotating the spins around y axis by

$$R_y(\theta) = \cos(\theta/2) I_2 - i \sin(\theta/2)\sigma_y = \cos(\theta/2)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sin(\theta/2)\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

gives the following transformation for $c^\dagger$ operators:

$$\begin{pmatrix} c_{iI\uparrow} \\ c_{iI\downarrow} \end{pmatrix} = \begin{pmatrix} c & -s \\ s & c \end{pmatrix}\begin{pmatrix} d_{iI\uparrow} \\ d_{iI\downarrow} \end{pmatrix},$$

where $c = \cos(\theta/2)$, $s = \sin(\theta/2)$. The idea is to rotate the site j the angle $j\theta$. The effect of this rotation can be written in terms of Δ and t matrices:

$$R(\theta) = I_5 \otimes \begin{pmatrix} c & -s \\ s & c \end{pmatrix},$$

$$\tilde{\Delta} = R(j\theta)^\dagger \left(\Delta \otimes I_2\right) R(j\theta) = \Delta \otimes I_2,$$

$$\tilde{t} = R(j\theta)^\dagger \left(t \otimes I_2\right) R\left((j+1)\theta\right) = \left(t \otimes I_2\right) R\left(\theta\right) = t \otimes \begin{pmatrix} c & -s \\ s & c \end{pmatrix}.$$

Finally, the Hamiltonian becomes:

$$H = \sum_{iIJ\sigma} \Delta_{IJ} d^\dagger_{iI\sigma} d_{iJ\sigma} + \sum_{iIJ\sigma\sigma'} \left(\tilde{t}_{I\sigma J\sigma'} d^\dagger_{iI\sigma} d_{i+1,J\sigma'} + h.c.\right) + \sum_i \hat{V}_i.$$

We can also incorporate twisted boundary conditions by setting $\tilde{t} \to \tilde{t}e^{i\phi}$.