Jahn Teller and Charge transfer Mott insulator

Exercise 1: Jahn-Teller Effect
Once the TM ions are placed in a crystal, the crystal field of the surrounding atoms splits the energy levels of the TM ion. The structure of these energy levels and their filling is determined by the crystal field, the Hund's, and Jahn Teller distortion. This exercise looks at some critical consequences of putting TM ion in an octahedral environment.

Consider an octahedral crystal field splitting given by Δ_{CF} and a Hund's coupling provided by J_H.

(a) For a d^4 electron configuration, what is the energy gained for an $S = 1$ as compared to an $S = 2$ configuration?

(b) What condition determines if the compound would have a high spin or a low spin state?

(c) What is the condition for a d^5 configuration?

(d) For a d^6 configuration, what is the energy difference between a high spin, low spin, and intermediate spin configuration?

Now consider an elongation of the octahedral along the z-axis (preserving the volume of the crystal to first order).

(e) What are the additional splitting in t2g and eg levels?

(f) Consider a d^4 electronic configuration in its high spin state. A Jahn-Teller distortion would split the energy levels with energy $\pm gu$, where g is the electron-phonon coupling constant. The energy cost corresponding to the distortion is Bu^2, where B is the bulk modulus. What is the distortion u_0 corresponding to the minimum energy of the eg electron?

(g) What is the energy difference between the zero distortion and u_0 distortion state?

Exercise 2: Charge transfer Mott insulator
The parent compound of the high T_c superconductor cuprates La_2CuO_2 is predicted to be metal from DFT calculations (see Figure 1). However, experiments demonstrated that it is an insulator with a gap width of 1 eV (see Figure 2). Which type of insulator is this system?

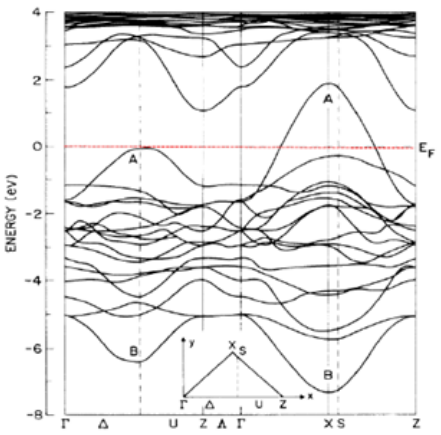

Figure 1: Electronic band structure of La_2CuO_2.

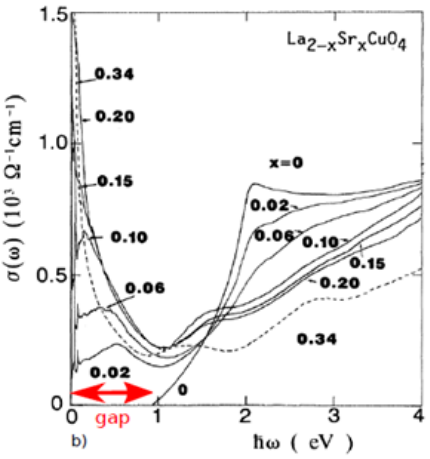

Figure 2: Optical conductivity of La_2CuO_2 for different doping, x.

How could you explain the gap of 1eV? Use the Hubbard model in your explanation.