Heisenberg coupling in Mott and Charge transfer insulator

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Abstract

Apart from the on-site coulomb energy U another important scale that determines the nature of the insulating phase is the charge transfer energy Δ_{CT}. In this exercise we look at how Δ_{CT} effects the exchange paths and the final Heisenberg coupling in a charge transfer(CT) insulator.

Exercise 1: Exchange interaction in CT insulator

Consider a CuO_2 plane of a HTS,(d^9 configuration) with hopping energy between p and d orbitals given by t_{pd}. Consider a hole representation, in which transferring one hole from d orbitals to p orbital,($d^9p^6 \rightarrow d^{10}p^5$), costs an energy of Δ_{CT}(charge transfer energy).

a)Using the second order perturbation,(same as problem 2a in Exercise-2) show that the effective hopping energy between two adjacent d orbitals following the process $d^9p^6d^9 \rightarrow d^{10}p^5d^9 \rightarrow d^{10}p^6d^8$ is given by:

$$t_{dd}^{eff} = \frac{t_{pd}^2}{\Delta_{CT}}$$

b) If the energy cost of putting two holes on a Cu site is U_{dd}, show that the effective Heisenberg exchange for process,

$$d_i^n p^6 d_j^n \rightarrow d_i^n p^5 d_j^{n+1} \rightarrow d_i^{n-1} p^6 d_j^{n+1} \rightarrow d_i^n p^5 d_j^{n+1} \rightarrow d_i^n p^6 d_j^n$$

is given by:

$$J_{dd}^{(1)} = \frac{2t_{pd}^4}{\Delta_{CT}^2 U_{dd}}$$

Hint: Use part 'a' to re-write the process as effective hopping between d-d orbitals and use the Heisenberg coupling formula derived in Exercise-2.

c) If the energy cost of putting two holes on a oxygen atom is U_{pp}, show that the effective coupling due to the below process

$$d_i^n p^6 d_j^n \rightarrow d_i^n p^5 d_j^{n+1} \rightarrow d_i^{n+1} p^4 d_j^{n+1} \rightarrow d_i^n p^5 d_j^{n+1} \rightarrow d_i^n p^6 d_j^n \quad (0.1)$$

is given by:

$$J_{dd}^{(2)} = \frac{2t_{pd}^4}{\Delta_{CT}^2(\Delta_{CT} + \frac{U_{pp}}{2})}$$

Hint: Use the same method as part 'b'. Note that there are twice the number of exchange paths when compared to the previous case.

d) Which is the dominant exchange for $\Delta_{CT} >> U_{dd}$(Mott-Hubbard) and $U_{dd} >> \Delta_{CT}$(Charge transfer).