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Exercise:1

For a d-d hopping(for example $d_{x^2-y^2}$ to adjacent $d_{x^2-y^2}$), if the hole occupies alternate e_g orbitals a hop can occur both when the spins on adjacent atoms are aligned and anti-aligned.

a) When the spins on the adjacent atoms are anti-aligned the effective energy gain due to a hop is obtained from second order perturbation as:

$$\Delta E_{\uparrow\downarrow} = -\frac{t^2}{U}$$

Note that unlike the case of a d-d hopping between same orbitals which has two exchange path ways, this process has only one exchange path way and hence there is no factor 2 in the above expression. When the spins on adjacent atoms are aligned we observe that the intermediate state has a net loss of J_H energy due to Hund's coupling. Hence the energy gain due to hop in this situation is:

$$\Delta E_{\uparrow\uparrow} = -\frac{t^2}{U - J_H}$$

Hence the difference in the energies is given by:

$$\Delta E_{\uparrow\uparrow} - \Delta E_{\uparrow\downarrow} = -t^2 \left(\frac{1}{U - J_H} - \frac{1}{U} \right) \simeq -\frac{t}{U} \frac{J_H}{U}$$

b) For a d^4 occupancy in High spin state the intermediate state in d-d hopping has an energy $U + 3J_H$. Hence the total energy gain of the hopping process is given by:

$$\Delta E_{\uparrow\downarrow} = -\frac{t^2}{U + 3J_H}$$

Similarly, the intermediate state in a aligned case would have energy $U - J_H$. Hence the energy gain is given by:

$$\Delta E_{\uparrow\uparrow} = -\frac{t^2}{U - J_H}$$

The difference between energies yields:

$$\Delta E_{\uparrow\uparrow} - \Delta E_{\uparrow\downarrow} = -t^2 \left(\frac{1}{U - J_H} - \frac{1}{U + 3J_H} \right) \simeq -\frac{t^2}{U} \frac{4J_H}{U}$$

Exercise:2

Similar to the above problem, we have a situation where the d^9 orbitals connected via the oxygen atom can have spins aligned or anti-aligned. In a anti aligned case we observe that

the intermediate state is at energy $2\Delta_{CT} + U_{pp}$ and in aligned case it is $2\Delta_{CT} + U_{pp} - J_H^p$, due to the hunds coupling on p-orbital. Hence the energy difference is given by:

$$\Delta E_{\uparrow\uparrow} - \Delta E_{\uparrow\downarrow} = -\frac{t_{pd}^4}{\Delta_{CT}^2} \left(\frac{1}{2\Delta_{CT} + U_{pp} - J_H^p} - \frac{1}{2\Delta_{CT} + U_{pp}} \right) = -\frac{t_{pd}^4}{\Delta_{CT}^2} \frac{J_H^p}{(2\Delta_{CT} + U_{pp})^2}$$

Exercise:3

The potential energy of the localized electrons in a 2D square lattice with canted ordering θ is given by

$$\frac{E_{pot}}{N} = 4JS^2 \cos \theta$$

The kinetic energy of the itinerant electrons at doping $x (<< 1)$ is given by:

$$\frac{E_{kin}}{N} = -4tx \cos \frac{\theta}{2}$$

Hence the total energy is given by:

$$\frac{E}{N} = 4JS^2 \cos \theta - 4tx \cos \frac{\theta}{2}$$

Minimizing the above energy we obtain:

$$\cos \frac{\theta}{2} = \frac{tx}{4JS^2}$$