Exchange interactions

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Abstract

In the previous exercise we have seen how the super-exchange and semi-covalent exchange interaction occurs between d and p orbitals, and derived the exchange coupling in Mott-Hubbard and Charge-Transfer insulators. In this Exercise we will look at some exchange pathways through which super-exchange or semi-covalent exchange interaction can lead to a FM interaction. We also look at a new type of exchange interaction known as double exchange.

Exercise 1: Super-exchange to an empty orbital (GKA rule 2)

Consider CuO_2 planes in a cuprate,(d^9 occupancy) where the hole occupies the e_g orbital. Assume that the hole occupies alternate e_g orbitals on the adjacent Cu sites. Given that the hopping can occur only between same orbitals (due to 180° bond TM-O-TM) we observe that spin can hop for both aligned or non-aligned case.

a) Given a $d-d$ hopping t, coulomb interaction U and Hund's coupling $J_H(<< U)$ calculate the energy gain through a hop between Cu, both when spins on adjacent Cu atoms are aligned and non-aligned. Calculate the energy difference and show that the exchange path leads to an effective ferromagnetic coupling:

$$J \simeq \frac{-t^2}{U}\frac{J_H}{U}$$

b) Consider a d^4 occupancy in its high spin state with hopping between the e_g orbitals, and the high energy electron occupying the alternate orbitals. What is the exchange coupling in this case ?

Hint: Just have a look at the energy of the intermediate level in the exchange process, in both cases:

Exercise 2: Super-exchange between sites connected via perpendicular orbitals(GKA rule 3)

Consider a case where the TM ions are connected via a 90° bond instead of a 180° bond for e.g. edge sharing pervoskite MO_6. The nearest TM atoms are bonded via two perpendicular orbitals for e.g. p_x, p_y. If we imagine a d^9 configuration the only hopping process that can occur is between the $d_{x^2-y^2}$ orbitals and p orbitals. A super-exchange cannot occur but a semi-covalent exchange can occur.

a) Consider a p,d hopping energy given by t_{pd}, charge transfer energy Δ_{CT}, Coulomb energy on p orbitals U_{pp}(Note: All energies are given in hole picture as in Exercise-6

and the Δ_{CT} contains the Hund's energy of d-orbitals) and Hund's energy on p orbitals given by J_H^p. Show that this semicovalent exchange via perpendicular orbitals gives a FM coupling given by:

$$J_{90^\circ} \simeq -\frac{t_{pd}^4}{\Delta_{CT}^2(2\Delta_{CT}+U_{pp})}\frac{J_H^p}{(2\Delta_{CT}+U_{pp})}$$

Hint: Similar to previous case look at the energies of intermediate high energy state in the exchange process.

Exercise 3: Double exchange

Doping AFM Mott insulators with electrons(or holes) results in both itinerant and localized electrons and coupling between them could produce an exchange which can be Ferromagnetic. In FM ordering the loss in exchange energy of the localized electrons would be compensated by the gain of kinetic energy of the itinerant electrons. This phenomenon is called as 'double exchange'.

At low doping one can expect a canted ordering state with θ angle between the adjacent localized spins. The energy gain of hopping the itinerant electron can be approximately given by:

$$t_{eff} = t\cos\frac{\theta}{2}$$

where the effective Hamiltonian is given by:

$$H_{eff} = \underbrace{J\sum_{i,j} S_i \cdot S_j}_{localized} \underbrace{- t_{eff}\sum_{i,j} c_{i\sigma}^\dagger c_{j\sigma}}_{itinerent}$$

where J is the Heisenberg coupling. Consider a 2D square lattice with the above effective Hamiltonian:

a) For a canted ordering θ, what is the potential energy(magnetic) of the localized electrons, per site as function of θ?

b) For a doping concentration of x, where $x << 1$ what is the kinetic energy of itinerant electrons, per site, as function of θ ?

c) Minimize the total energy and find the angle θ, corresponding to a transition from canted state to a Ferromagnetic metallic state.

Hint: For calculating the kinetic energy follow the same process as **Exercise:1.2**