Magnetism in ionic solids

Pauli principle: The total e^- wavefunction has to be antisymmetric with respect to the exchange of two e^-.

$$\Psi(\vec{r}_1 s_1, \vec{r}_2 s_2) = -\Psi(\vec{r}_2 s_2, \vec{r}_1 s_1)$$

$$\Psi(\vec{r}_1 s_1, \vec{r}_2 s_2) = \phi(\vec{r}_1, \vec{r}_2)\,\chi(s_1, s_2)$$

- ϕ symmetric $\Rightarrow$ χ antisymmetric $\Rightarrow$ $\underbrace{s_1 = -s_2}_{\text{spins align antiparallel}}$
  $\Rightarrow$ total spin $S = 0$
  Spin singlet $S = 0,\ m_s = 0$
- ϕ antisymmetric $\Rightarrow$ χ symmetric $\Rightarrow$ $\underbrace{s_1 = s_2}_{\text{spins align parallel}}$
  $\Rightarrow$ total spin $S = 1$
  Spin triplet $S = 1,\ m_s = 0, \pm 1$

$$\Psi_{\text{singlet}} = \frac{1}{\sqrt{2}}\left[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) + \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)\right]\chi_S$$

$$\Psi_{\text{triplet}} = \frac{1}{\sqrt{2}}\left[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) - \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)\right]\chi_T$$

Energies are given by:

$$E_{S/T} = \int d\vec{r}_1 \int d\vec{r}_2 \; \Psi^*_{S/T} \, H \, \Psi_{S/T} = 4 \text{ terms each}$$

$$E_S - E_T = 2 \int d\vec{r}_1 \int d\vec{r}_2 \; \phi_1^*(\vec{r}_1) \, \phi_2^*(\vec{r}_2) \, H \, \phi_1(\vec{r}_2) \, \phi_2(\vec{r}_1)$$

Energy difference between singlet and triplet states

Parametrize effective Hamiltonian by intermediate states between $|\uparrow\uparrow\rangle \longleftrightarrow |\uparrow\downarrow\rangle$

$\vec{S}_1 \cdot \vec{S}_2$

$$J \equiv \frac{E_S - E_T}{2} \Rightarrow H = J \, \vec{S}_1 \cdot \vec{S}_2$$

Exchange interaction

$\Downarrow$ generalize for many spins

"Heisenberg model" $H = \sum_{i \neq j} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$

$J_{ij} > 0$ reduces energy for antiparallel spin ordering, $\vec{S}_1 = -\vec{S}_2$

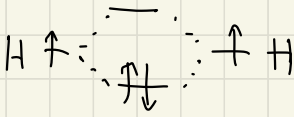
$J_{ij} < 0$ reduces energy for parallel spin ordering, $\vec{S}_1 = \vec{S}_2$

Hubbard model

$a_i^\dagger, a \rightarrow s_i^\dagger s$

$\frac{t^2}{U} \rightarrow J$

- If spins sit on the same atom : antisymmetric ϕ
  minimizes Coulomb repulsion between e^- by keeping them apart
  $\Rightarrow$ χ symmetric $\Rightarrow$ triplet $S = 1$ favored
  First Hund's rule (maximize spin angular momentum)
- If spins sit on neighboring atoms:



  Molecular orbital can be

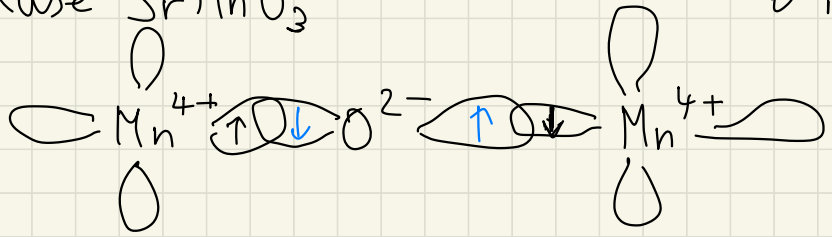
  - bonding (ϕ symmetric) $\Rightarrow$ χ antisymmetric $\Rightarrow$ singlet $S = 0$
  - antibonding (ϕ antisymmetric) $\Rightarrow$ χ symmetric $\Rightarrow$ triplet $S = 1$

  For many 3d magnetic compounds in insulating state, antiparallel alignment is favored

For "transition-metal oxides" & other ionic solids :

Superexchange is the primary mechanism

Case $SrMnO_3$



$\Rightarrow$ Mn antiferromagnetic alignment

Generally: 180° exchange favors AFM ordering

90° exchange favors FM ordering

There are only few FM insulators