Lecture 3 (Jan. 16th)

Note Title 20/09/2009

Heisenberg model

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

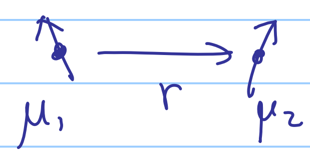
$\boxed{Q}$ What is the physical origin of J, $\vec{S}_i$ ...?

① J: magnetic energy scale

Can it be from magnetic dipole interaction?

$$E = \frac{1}{r^3}\left[\vec{\mu}_1 \cdot \vec{\mu}_2 - \frac{3}{r^2}(\vec{\mu}_1 \cdot \vec{r})(\vec{\mu}_2 \cdot \vec{r})\right]$$

Order of magnitude estimate



$\mu_1 = \mu_2 \cong g\mu_B$

$r \sim a_H$

Then $E = \dfrac{(g\mu_B)^2}{a_H^3} \sim \alpha^2 R_y \sim 0.1\,\mathrm{meV} \sim 1\,\mathrm{K}$

This is too small for magnetic order in Fe.

(Fe : $T_c \sim 1000\,\mathrm{K}$)

c.f. dipole interaction sometimes <u>does</u> play a major role. A good example is $LiHoF_4$ (Transverse-field Ising model)

$\boxed{\text{Side note:}}$ for electrons

$$hf \longleftrightarrow k_B T \longleftrightarrow \left(\frac{1}{2}mv^2\right)$$

$$0.24\,\text{THz} \longleftrightarrow 11.6\,\text{K} \longleftrightarrow 1\,\text{meV}$$

Characteristic energy scale in

E-M: $\dfrac{e^2}{(1\,\text{Å})} \sim 2.3\times 10^{-11}\,\text{erg} \sim 14\,\text{eV}$

QM: 1D box $E = \dfrac{\hbar^2}{2m}\left(\dfrac{\pi}{a}\right)^2 \sim 37\,\text{eV}$

Energetics in solids;

Kinetic energy lowering by $a \to \infty$

+

Coulomb interaction (potential energy)

Therefore, large J (of order of eV) must arise from Coulomb interaction.

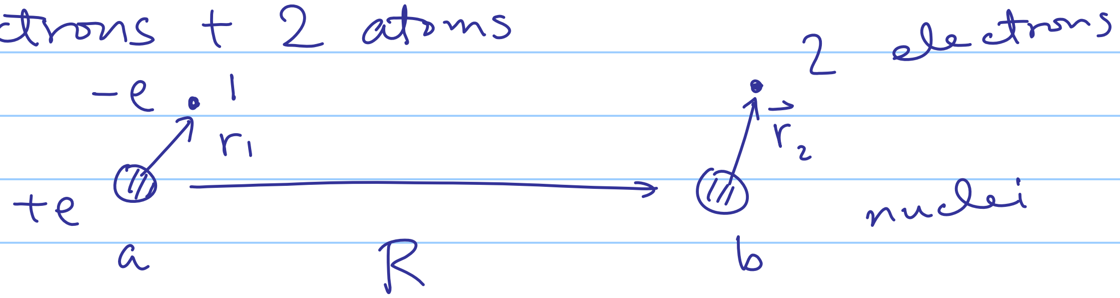
Consider 2 electron spins $\vec{S}_1$ & $\vec{S}_2$ $(s = 1/2)$

Since $\vec{S}_1 \cdot \vec{S}_2 = \dfrac{1}{2}\left[S_{tot}^2 - S_1^2 - S_2^2\right]$, where

$S_1^2 = s_1(s_1+1) = 3/4$, $S_{tot}^2 = 0$ or 2

$$\vec{S}_1 \cdot \vec{S}_2 = \begin{cases} 1/4 & \text{for } S=1 \quad \text{triplet} \\ -3/4 & \phantom{\text{for }} S=0 \quad \text{singlet} \end{cases}$$

2-electrons + 2 atoms



$$\mathcal{H}_0 = \frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) - \frac{e^2}{r_1} - \frac{e^2}{r_2}$$

Electron wavefns. are

$$\left[\frac{\hbar^2}{2m}\left(\nabla_1^2\right) - \frac{e^2}{r_1}\right]\phi_a(\vec{r}_1) = E_a\,\phi_a(\vec{r}_1)$$

$$\left[\frac{\hbar^2\nabla_2^2}{2m} - \frac{e^2}{r_2}\right]\phi_b(\vec{r}_2) = E_b\,\phi_b(\vec{r}_2)$$

When $R \gg a_0$, classical problem (spin-part ignored
$\Rightarrow$ Van der Waals interaction.

When $R \approx a_0$, Pauli exclusion principle should be considered.

Since electron wavefn. should be antisym.

$$\Psi_S = \frac{1}{\sqrt{2}}\left[\phi_a(\vec{r}_1)\,\phi_b(\vec{r}_2) + \phi_a(\vec{r}_2)\,\phi_b(\vec{r}_1)\right]\chi_S$$

$$\Psi_T = \frac{1}{\sqrt{2}}\left[\phi_a(\vec{r}_1)\,\phi_b(\vec{r}_2) - \phi_a(\vec{r}_2)\,\phi_b(\vec{r}_2)\right]\chi_T$$

Spin w.f.

With a perturbation $\boxed{V = \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}, \quad \mathcal{H} \equiv \mathcal{H}_0 + V}$

$$E_{S,T} = \int d\vec{r}_1 d\vec{r}_2 \, \Psi^*_{S,T} \mathcal{H} \Psi_{S,T}$$

$$= \frac{1}{2} \int d\vec{r}_1 d\vec{r}_2 \left(\phi_a^* \phi_b^* \pm \phi_b^* \phi_a^* \right) \mathcal{H} \left(\phi_a \phi_b \pm \phi_b \phi_a \right)$$

$$E_S = \varepsilon_a + \varepsilon_b + K + J$$

$$E_T = \varepsilon_a + \varepsilon_b + K - J$$

$$K = \int d\vec{r}_1 d\vec{r}_2 \, |\phi_a(\vec{r}_1)|^2 V |\phi_b(\vec{r}_2)|^2$$: Coulomb integral

$$J = \int d\vec{r}_1 d\vec{r}_2 \, \phi_a^*(\vec{r}_1) \phi_b^*(\vec{r}_2) V(\vec{r}_1, \vec{r}_2) \phi_a(\vec{r}_2) \phi_b(\vec{r}_1)$$

; exchange integral

The difference between E_S and E_T is $2J$.

Utilizing $\vec{S}_1 \cdot \vec{S}_2 = 1/4$ for triplet and $-3/4$ for a singlet, the following effective Hamitonian has the same eigenvalues and eigenstates as the original Hamiltonian $\mathcal{H}$.

$$\mathcal{H}_{eff} = \frac{1}{4} \left(E_S + 3 E_T \right) - \left(E_S - E_T \right) \vec{S}_1 \cdot \vec{S}_2$$

$$= \begin{cases} E_S & \text{for } \vec{S}_1 \cdot \vec{S}_2 = -3/4 \\ E_T & \vec{S}_1 \cdot \vec{S}_2 = 1/4 \end{cases}$$

$$\mathcal{H}_{eff} = \text{const} - 2J\,\vec{S}_1 \cdot \vec{S}_2$$

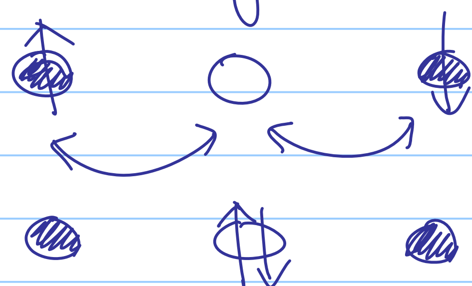
exchange interaction

Typically, one drops -2 in front, and just write the spin Hamiltonian as

$$\mathcal{H}_{spin} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \qquad \begin{array}{ll} J>0 & \text{for AFM} \\ J<0 & \text{FM} \end{array}$$

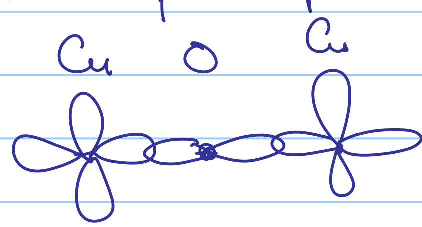
<u>However,</u> this direct exchange interaction is not usually the strongest magnetic interaction.

$\Rightarrow$ Need superexchange (Kinetic exchange)



If spins on are aligned AFM, they can hop to the middle orbital to lower kinetic energy, but still satisfy Pauli principle

e.g. Cuprates



<u>superexchange</u> mediated by oxygen.

In Hubbard model t is hopping parameter, and U is Coulomb energy, the superexchange $J = \frac{t^2}{4U}$