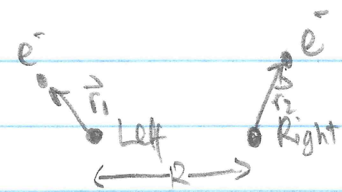
Lecture 9

10/8

Magnetic Interaction :

1. Direct Exchange



$$H_{11} = \frac{-\hbar^2}{2m} \nabla^2 + V_0(\vec{r})$$

H_{11}: # of atom, 1 electron

$$H_{21} = H_{11}(\vec{r}) + V_0(|\vec{r} - \vec{R}|)$$

$$H_{22} = H_{21}(\vec{r}_1) + H_{21}(\vec{r}_2) + V_c(\vec{r}_1, \vec{r}_2)$$

$$|n\rangle = C_1|LL\rangle + C_2|LR\rangle + C_3|RL\rangle + C_4|RR\rangle$$

$|C_n|^2$ = prob of state n

$$U = \langle LL|V_c|LL\rangle = \langle RR|V_c|RR\rangle$$

Coulomb integral $U > 0$

$$J_D = \langle LR|V_c|RL\rangle = \langle RL|V_c|LR\rangle$$

J_D is exchange integral

$$\mathcal{H} = 2\varepsilon_0 + \begin{pmatrix} U & t & t & J_D \\ t & 0 & J_D & t \\ t & J_D & 0 & t \\ J_D & t & t & U \end{pmatrix} |n\rangle$$

$$t = \langle L|T|R\rangle \Rightarrow T = \frac{-\hbar^2}{2m} \nabla_e^2$$

$$|n\rangle = C_1|LL\rangle + C_2|LR\rangle + C_3|RL\rangle + C_4|RR\rangle$$

Eigenvalues : $E_1 = 2E_0 - J_D$

$E_2 = 2E_0 + U - J_D$

$E_3 = 2\varepsilon_0 + \frac{U}{2} + J_D - \sqrt{4t^2 + \frac{U^2}{4}}$

$E_4 = 2\varepsilon_0 + \frac{U}{2} + J_D + \sqrt{4t^2 + \frac{U^2}{4}}$

AS $|1\rangle = \frac{1}{\sqrt{2}}\left(|LR\rangle - |RL\rangle\right)$ parallel spin - singlet

S $|2\rangle = \frac{1}{\sqrt{2}}\left(|LL\rangle - |RR\rangle\right)$ anti parallel spin - triplet

S $|3\rangle = \frac{\sin\varphi}{\sqrt{2}}\left(|LL\rangle + |RR\rangle\right) + \frac{\cos\varphi}{2}\left(|LR\rangle + |RL\rangle\right)$

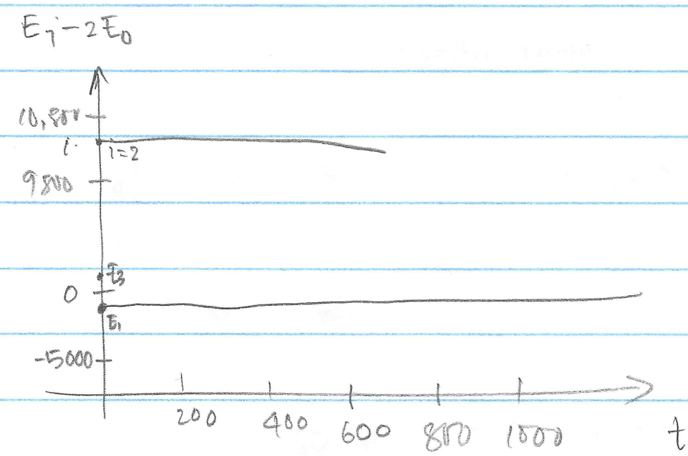
S $|4\rangle = \frac{\cos\varphi}{\sqrt{2}}\left(|LL\rangle + |RR\rangle\right) - \frac{\sin\varphi}{\sqrt{2}}\left(|LR\rangle + |RL\rangle\right)$

$\tan 2\varphi = \frac{-4t}{U}$, $t \ll U$

Example :

$J_D = 100K$

$U = 10^4 K$



Define exchange parameter :

$$J = E_3 - E_1$$
$$= 2J_D + \frac{u}{2} - \sqrt{4t^2 + \frac{u^2}{4}}$$

Why do you call this exchange?
E_4 & E_2 are high in energy!

Heisenberg Hamiltonian
$$\mathcal{H}_{Heis} = -J\,\vec{S_1}\cdot\vec{S_2}$$

$$(\vec{S_1}+\vec{S_2})^2 = \vec{S}^2 = S_1^2 + S_2^2 + 2\vec{S_1}\cdot\vec{S_2}$$

eigenvalues : $E_S = -\frac{J}{2}\left[S(S+1) - S_1(S_1+1) - S_2(S_2+1)\right]$

two spin $\frac{1}{2}$s $\quad 0 < S < 1$

$$E_{S=0} = \frac{3}{4}J$$
$$E_{S=1} = -\frac{1}{4}J$$
$$\Delta E = J$$

generalized $\mathcal{H} = -J(S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z})$

B is always in z-direction $\mathcal{H} = -J\left(\alpha(S_{1x}S_{2x} + S_{1y}S_{2y}) + \beta S_{1z}S_{2z}\right)$

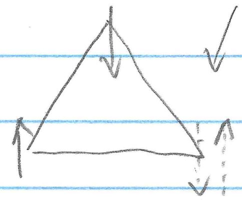
$\alpha = \beta = 1$ isotropic 3D Heisenberg spin

$\alpha \neq \beta \neq 0$ anisotropic Heisenberg

$\alpha = 1,\ \beta = 0$ xy spins

$\alpha = 0,\ \beta = 1$ Ising spins

Frustration



2 states
degenerate

AF- Ising spins

$J < 0$ AF

$$\frac{1}{m^*} = \frac{1}{\hbar} \frac{\partial^2 E}{\partial k^2}$$