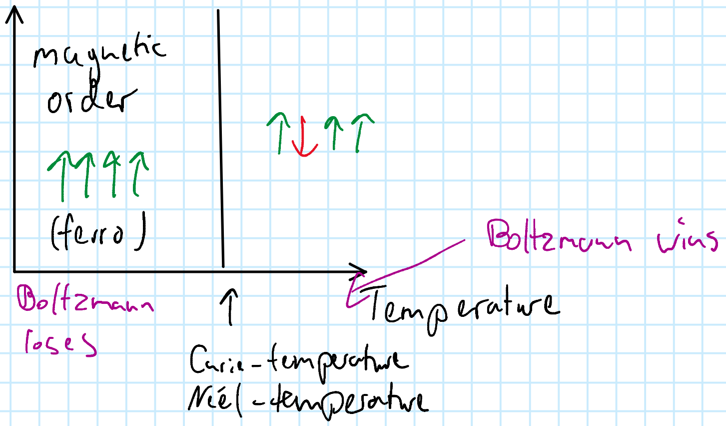
Lecture 20 - WiSe2022/2023

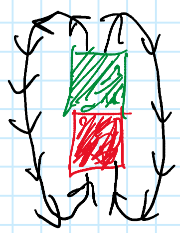
Monday, January 2, 2023 3:40 PM

3. Magnetic Interactions

- Like the coupling between S and L (spin-orbit: $\lambda \cdot \vec{S} \cdot \vec{L}$), spins of different spin centers can couple



3.1. Magnetic Dipole Interaction



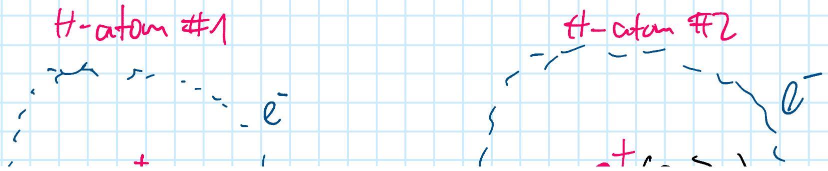
$$E_D = \frac{\mu_0}{4\pi} \cdot \frac{1}{r^3} \underbrace{\left[\vec{m}_1 \cdot \underbrace{\vec{m}_2}_{g_e \cdot \mu_B \cdot \vec{S}_2} - 3 \left(\vec{m}_1 \cdot \underbrace{\hat{r}}_{\text{connecting vector}} \right) \cdot \left(\vec{m}_2 \cdot \hat{r} \right) \right]}_{\text{MDI is anisotropic}}$$

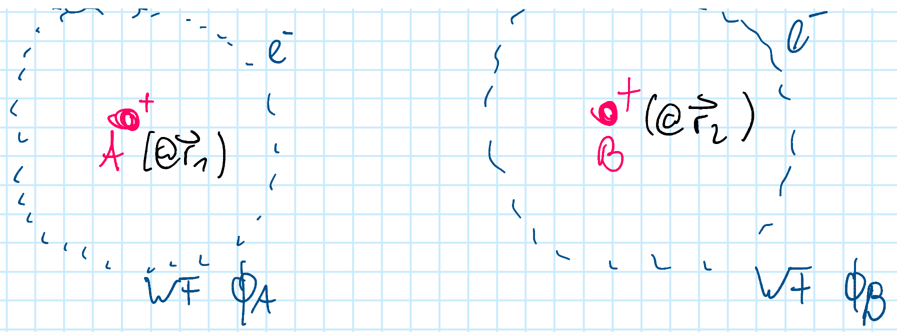
3.2. Magnetic Exchange Interaction

Exchange Interaction : overlap of wavefunctions

Interplay between : - Coulomb energy
- kinetic energy
- Pauli principle

- Introduction using the H_2 molecule





ϕ_A, ϕ_B : 1s wave functions of H

approach: linear combination of molecule orbitals

$$\psi^{sym}_{asym} = N \cdot \left(\phi_A \pm \phi_B \right) \qquad N = \frac{1}{\sqrt{2(1 \pm S_{AB})}}$$

(spatial wave function of $1e^-$)

overlap integral

$$S = \int \phi_A(\vec{r}) \, \phi_B(\vec{r}) d\vec{r}^3$$

→ for $2e^-$ we make an ansatz using the product

$$\psi(\vec{r}_1, \vec{r}_2) = \psi^{sym}(\vec{r}_1) \cdot \psi^{sym}(\vec{r}_2)$$

⇒ symmetric when swapping $\vec{r}_1$ and $\vec{r}_2$

↳ BUT: Pauli + Fermions → total WF must be antisymmetric

⇒ utilize the spin degree of freedom

$$\psi(\vec{r}_1, \vec{r}_2, \vec{s}_1, \vec{s}_2) = \psi^{sym}(\vec{r}_1) \cdot \psi^{sym}(\vec{r}_2) \cdot \chi^{asym}(\vec{s}_1, \vec{s}_2)$$

with $\chi_{asym} = \frac{1}{\sqrt{2}} \left[\sigma^+(\vec{r}_1) \cdot \sigma^-(\vec{r}_2) - \sigma^-(\vec{r}_1) \cdot \sigma^+(\vec{r}_2) \right]$

$= \frac{1}{\sqrt{2}} \left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right]$ (anti-symmetric Singlett state)

$+|\downarrow\uparrow\rangle \quad -|\uparrow\downarrow\rangle$

- analogously:

for $\psi_{asym}(\vec{r}_1) \longrightarrow \chi_{sym} = \begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{cases}$

$$\underbrace{|\downarrow\downarrow\rangle}_{\text{triplet}}$$

$$J = E_{sym} - E_{asym} = \overbrace{\frac{2}{1 - S_{AB}^2}}^{\approx 2} \cdot \left[A - C \cdot \underbrace{S_{AB}^2}_{\approx 0} \right] \approx 2 \cdot A$$

$S_{AB} < 1$

triplet

J

singlet

$J > 0 \rightarrow$ ferromagnetic coupling, triplet ground state

$J < 0 \rightarrow$ antiferromagnetic coupling $\rightarrow$ singlet ground state

3.9 Heisenberg model

solve XYZ-WF

↳ found J $\updownarrow J$

Pauli-Principle

define model Hamiltonian for spin-part only (push XYZ-WF into J)

$\underline{\text{two spin}}$ $\lambda \cdot \vec{S} \cdot \vec{L}$

$$H_{ex} = -J \cdot \frac{1}{\hbar^2} \cdot \vec{S}_1 \cdot \vec{S}_2$$

$\underline{\text{many spins}}$

$$H_{ex} = -\sum_{i \neq j, i > j} J^{ij} \cdot \frac{1}{\hbar^2} \vec{S}_i \cdot \vec{S}_j$$