Appendix D (Optional)†

- Magnetic Ordering comes from the "exchange interaction" (physical origin)
- Exchange interaction is a quantum effect
- Effective spin Hamltonian (Why is the form of Ising model a reasonable one?)
- Variations

† Optional because it is more related to quantum physics

Appendix D

Basic idea of exchange interaction (a Quantum Effect)

- To illustrate the idea, consider a 2-electron system with spin-independent Hamiltonian

Then,

$$\Psi_{total} = (\text{Spatial part}) \cdot (\text{spin part})$$

must be antisymmetric w.r.t. interchanging the coordinates of the two electrons (fermions)

$$\Psi_{total}(\underbrace{\vec{r}_1\, s_1}_{\text{coordinates of electron 1}}; \underbrace{\vec{r}_2\, s_2}_{\text{coordinates of electron 2}}) = -\Psi_{total}(\vec{r}_2\, s_2; \vec{r}_1\, s_1)$$

Spin Part

- Addition of two spin-½ angular momenta

$$\chi_S = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2\right)$$

antisymmetric w.r.t. $1 \leftrightarrow 2$

singlet state $S=0$ ($m_s = 0$ only 1 value)

$$\chi_T = \begin{cases} |\uparrow\rangle_1 |\uparrow\rangle_2 & (m_s = +1) \\ \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2\right) & (m_s = 0) \\ |\downarrow\rangle_1 |\downarrow\rangle_2 & (m_s = -1) \end{cases}$$

triplet state $S=1$

χ_T is symmetric w.r.t. $1 \leftrightarrow 2$

Total Spin $\hat{\vec{S}} = \hat{\vec{S}}_1 + \hat{\vec{S}}_2$ (Operator)

$$\begin{cases} \hat{\vec{S}}^2 \chi_S = 0 & (S=0,\ \text{so}\ S(S+1) = 0) \\ \hat{\vec{S}}^2 \chi_T = 2\hbar^2 \chi_T & (S=1,\ \text{so}\ S(S+1)\hbar^2 = 2\hbar^2) \end{cases}$$

$$\left.\begin{aligned} \hat{\vec{S}}_1^2 \chi_S &= \tfrac{3}{4}\hbar^2 \chi_S \\ \hat{\vec{S}}_1^2 \chi_T &= \tfrac{3}{4}\hbar^2 \chi_T \end{aligned}\right\} \text{(since "1" is a spin-½ electron)}$$

$$\left.\begin{aligned} \hat{\vec{S}}_2^2 \chi_S &= \tfrac{3}{4}\hbar^2 \chi_S \\ \hat{\vec{S}}_2^2 \chi_T &= \tfrac{3}{4}\hbar^2 \chi_T \end{aligned}\right\} \text{(since "2" is a spin-½ electron)}$$

$$\hat{\vec{S}}^2 = (\hat{\vec{S}}_1 + \hat{\vec{S}}_2)^2 = \hat{\vec{S}}_1^2 + \hat{\vec{S}}_2^2 + 2\underbrace{\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2}_{\text{relates to } \vec{\mu}_1 \cdot \vec{\mu}_2 \text{ for 2 electro}}$$

$$\Rightarrow \boxed{\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2 = \frac{1}{2}\left(\hat{\vec{S}}^2 - \hat{\vec{S}}_1^2 - \hat{\vec{S}}_2^2\right)}$$

$$\begin{cases} (\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2)\chi_S = -\frac{3}{4}\hbar^2 \chi_S \\ (\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2)\chi_T = +\frac{1}{4}\hbar^2 \chi_T \end{cases}$$

- χ_S and χ_T are eigenstates of $(\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2)$ with different eigenvalues
- this is why we work with χ_S and χ_T, instead of $|\uparrow\rangle_1, |\downarrow\rangle_1, |\uparrow\rangle_2, |\downarrow\rangle_2$.

Spatial Part

- Solving the Schrödinger equation
- single particle states $\psi_A(\vec{r})$, $\psi_B(\vec{r})$, ...

2-particle:

$$\psi_A(\vec{r}_1)\,\psi_B(\vec{r}_2) + \psi_A(\vec{r}_2)\,\psi_B(\vec{r}_1) \leftarrow \text{symmetric}$$

$$\psi_A(\vec{r}_1)\,\psi_B(\vec{r}_2) - \psi_A(\vec{r}_2)\,\psi_B(\vec{r}_1) \leftarrow \text{antisymmetric}$$

Total Wavefunctions

$$\Psi_{singlet} = \frac{1}{\sqrt{2}}\Big[\underbrace{\psi_A(\vec{r}_1)\,\psi_B(\vec{r}_2) + \psi_A(\vec{r}_2)\,\psi_B(\vec{r}_1)}_{\text{symmetric}}\Big]\cdot \underbrace{\chi_S}_{\text{antisymmetric}}$$

$$\Psi_{triplet} = \frac{1}{\sqrt{2}}\Big[\underbrace{\psi_A(\vec{r}_1)\,\psi_B(\vec{r}_2) - \psi_A(\vec{r}_2)\,\psi_B(\vec{r}_1)}_{\text{antisymmetric}}\Big]\cdot \underbrace{\chi_T}_{\substack{\text{3 choices}\\ \text{symmetric}}}$$

This is how the Pauli Exclusion Principle controls the total wavefunction.

- 2 electrons will interact with each other and with ions

$U(\vec{r}_1,\vec{r}_2)$ = potential energy due to interactions

$$= \underbrace{V_{ee}(|\vec{r}_1-\vec{r}_2|)}_{\substack{\text{Coulomb repulsion}\\ >0}} + \underbrace{V_{e,ions}(\vec{r}_1)}_{\substack{\text{attractive}\\ <0}} + \underbrace{V_{e,ions}(\vec{r}_2)}_{\substack{\text{attractive}\\ <0}}$$

- Want to evaluate $\langle U\rangle_{singlet}$ and $\langle U\rangle_{triplet}$

<u>if</u> $\langle U\rangle_{triplet} < \langle U\rangle_{singlet}$

$\Rightarrow \chi_T$ $(S=1)$ is preferred $\Rightarrow$ two spins tend to align! (ferromagnetic interaction)

- $\langle U\rangle_{singlet} = \langle \Psi_{singlet} | U | \Psi_{singlet}\rangle$

$$= \int d^3r_1\, d^3r_2\; |\psi_A(\vec{r}_1)|^2\, U(\vec{r}_1,\vec{r}_2)\, |\psi_B(\vec{r}_2)|^2 \leftarrow \text{"direct" term}$$

$$+ \int d^3r_1\, d^3r_2\; \psi_A^*(\vec{r}_1)\,\psi_B^*(\vec{r}_2)\, U(\vec{r}_1,\vec{r}_2)\, \psi_B(\vec{r}_1)\,\psi_A(\vec{r}_2)$$

$$\equiv U_0 + \underbrace{J_{ex}}_{\text{exchange integral (can be positive or negative)}}$$

- Similarly, $\langle U\rangle_{triplet} = \langle \Psi_{triplet}|U|\Psi_{triplet}\rangle$

$$= U_0 - J_{ex}$$

If $J_{ex}>0$, $\langle U\rangle_{singlet} > \langle U\rangle_{triplet}$

$\Rightarrow \chi_T$ spin state preferred

$\Rightarrow$ parallel alignment of spins preferred

$\Rightarrow$ ferromagnetic interaction

If $J_{ex}<0$, $\langle U\rangle_{singlet} < \langle U\rangle_{triplet}$

$\Rightarrow \chi_S$ spin state preferred

$\Rightarrow$ anti-parallel alignment of spins preferred

$\Rightarrow$ anti-ferromagnetic interaction

Note: $\langle U\rangle_{singlet} - \langle U\rangle_{triplet} = 2J_{ex}$

This is how QM and Coulomb interaction govern the internal interaction of neighboring magnetic moments.

It is a <u>quantum effect</u>!

<u>Effective spin-dependent interaction</u>

Aim: Write down an <u>effective Hamiltonian</u> that gives

$$\langle H\rangle_{singlet} - \langle H\rangle_{triplet} = 2J_{ex}$$

Try

$$\boxed{\hat{H}_{spin} = U_0 - \underbrace{\frac{2J_{ex}}{\hbar^2}\hat{\vec{S}}_1\cdot\hat{\vec{S}}_2}_{\text{an effective spin-spin interaction that mimics the effect of QM + Coulombic interaction}} \qquad (*)}$$

$\hat{H}_{spin}$: effective Hamiltonian

U_0: a constant

<u>Check</u>: $\langle\chi_S|\hat{H}_{spin}|\chi_S\rangle = U_0 - \frac{2J_{ex}}{\hbar^2}\langle\chi_S|\hat{\vec{S}}_1\cdot\hat{\vec{S}}_2|\chi_S\rangle$

χ_S: spin singlet state ($S=0$)

$$= U_0 - \frac{2J_{ex}}{\hbar^2}\left(-\frac{3}{4}\hbar^2\right) \quad \text{(see XI)}$$

$$= U_0 + \frac{3}{2}J_{ex}$$

$$\langle\chi_T|\hat{H}_{spin}|\chi_T\rangle = U_0 - \frac{2J_{ex}}{\hbar^2}\langle\chi_T|\hat{\vec{S}}_1\cdot\hat{\vec{S}}_2|\chi_T\rangle$$

$$= U_0 - \frac{1}{2}J_{ex}$$

Thus

$\langle\hat{H}_{spin}\rangle_{singlet} - \langle\hat{H}_{spin}\rangle_{triplet} = 2J_{ex}$ as required.

(*) is a reasonable form of $\hat{H}_{spin}$

This also justifies the use of

$$H_{ferro} = -\sum_{\langle ij \rangle} J_{ij}\, \vec{\mu}_i \cdot \vec{\mu}_j + \sum_i \left(-\vec{\mu}_i \cdot \vec{B}_{applied}\right)$$

OR

$$H_{spin} = -\sum_{\langle ij \rangle} J_{ij}\, \vec{S}_i \cdot \vec{S}_j + \sum_i \left(-\vec{B} \cdot \vec{S}_i\right)$$

as the starting point in investigating magnetic ordering. The physical origin of the first term is the (Heisenberg) exchange interaction. Heisenberg proposed the model in 1928 (Heisenberg model) for which the spins were not restricted to up or down only.

- $J_{ex} > 0$ ferromagnetic interaction

  $J_{ex} < 0$ anti-ferromagnetic interaction
- <u>Short-range interaction</u> can lead to <u>long-range order</u>!

- <u>Variations</u>
  - Spins in 1D chain, 2D & 3D lattices
  - Classical (not to worry about commutation relations of spin components) and Quantum Models
  - Components of a spin
    - Up/down only (Ising)
    - X-Y model
    - Heisenberg
  - Random field Ising Model
    - $\vec{B}_{applied}(\vec{x})$ is positional dependent
  - Spin Glass

    J_{ij} between neighboring sites are chosen from a distribution, e.g.