Magnetic Ordering and Spin Waves

10.1 Ferromagnetism

10.1.1 Heisenberg Exchange Interaction

The origin of the Weiss effective field is found in the exchange field between the interacting electrons on different atoms. For simplicity, assume that atoms A and B are neighbors and that each atom has one electron. Let $\Psi_A$ and $\Psi_B$ be the wave functions of the electron on atoms A and B, respectively. The Pauli principle requires that the wave function for the pair of electrons be antisymmetric. If we label the two indistinguishable electrons 1 and 2, this means

$$\Psi(1,2) = -\Psi(2,1). \quad (10.1)$$

The wave function for an electron has a spatial part and a spin part. Let $\eta_{i\uparrow}$ and $\eta_{i\downarrow}$ be the spin eigenfunctions for electron $i$ in spin up and spin down states, respectively. There are two possible ways of obtaining an antisymmetric wave function for the pair (1,2).

$$\Psi_I = \Phi_S(r_1,r_2)\chi_A(1,2) \quad (10.2)$$
$$\Psi_{II} = \Phi_A(r_1,r_2)\chi_S(1,2). \quad (10.3)$$

The wave function $\Psi_I$ has a symmetric space part and an antisymmetric spin part, and the wave function $\Psi_{II}$ has an antisymmetric space part and a symmetric spin part. In (10.2) and (10.3), the space parts are

$$\Phi_S(r_1,r_2) = \frac{1}{\sqrt{2}} [\Psi_a(1)\Psi_b(2) \pm \Psi_a(2)\Psi_b(1)], \quad (10.4)$$

and $\chi_A$ and $\chi_S$ are the spin wave functions for the singlet ($s = 0$) spin state (which is antisymmetric) and for the triplet ($s = 1$) spin state (which is symmetric).
\[ \chi_A(1, 2) = \frac{1}{\sqrt{2}} [\eta_{1\uparrow}\eta_{2\downarrow} - \eta_{1\downarrow}\eta_{2\uparrow}] ; \quad S_z = 0 \]  
\[ \chi_S(1, 2) = \begin{cases} 
\frac{1}{\sqrt{2}} [\eta_{1\uparrow}\eta_{2\downarrow} + \eta_{1\downarrow}\eta_{2\uparrow}] & S_z = 0 \\
\eta_{1\downarrow}\eta_{2\uparrow} & S_z = -1 
\end{cases} \]  

If we consider the electron–electron interaction

\[ V = \frac{e^2}{r_{12}}, \]  

we can evaluate the expectation value of \( V \) in state \( \Psi_I \) or in state \( \Psi_{II} \). Since \( V \) is independent of spin it is simple enough to see that

\[ \langle \Psi_I | V | \Psi_I \rangle = \langle \Phi_S | V | \Phi_S \rangle = \langle \Psi_a(1)\Psi_b(2) | V | \Psi_a(1)\Psi_b(2) \rangle + \langle \Psi_a(1)\Psi_b(2) | V | \Psi_a(2)\Psi_b(1) \rangle. \]  

When we do the same for \( \Psi_{II} \), we obtain

\[ \langle \Psi_{II} | V | \Psi_{II} \rangle = \langle \Phi_A | V | \Phi_A \rangle = \langle \Psi_a(1)\Psi_b(2) | V | \Psi_a(1)\Psi_b(2) \rangle - \langle \Psi_a(1)\Psi_b(2) | V | \Psi_a(2)\Psi_b(1) \rangle. \]  

The two terms are called the direct and exchange terms and labeled \( V_d \) and \( \mathcal{J} \), respectively. Thus, the expectation value of the Coulomb interaction between electrons is given by

\[ \langle V \rangle = \begin{cases} 
V_d + \mathcal{J} & \text{for the singlet state } (S = 0) \\
V_d - \mathcal{J} & \text{for the triplet state } (S = 1). 
\end{cases} \]  

Now, \( \mathbf{S} = \hat{s}_1 + \hat{s}_2 \) and \( \mathbf{S}^2 = (\hat{s}_1 + \hat{s}_2)^2 = \hat{s}_1^2 + \hat{s}_2^2 + 2\hat{s}_1 \cdot \hat{s}_2 \). Therefore, \( \hat{s}_1 \cdot \hat{s}_2 = \frac{1}{2} (\hat{s}_1 + \hat{s}_2)^2 - \frac{1}{2}\hat{s}_1^2 - \frac{1}{2}\hat{s}_2^2 = \frac{1}{2} S(S + 1) - \frac{3}{4}. \) Here, we have used the fact that the operator \( \mathbf{S}^2 \) has eigenvalues \( S(S + 1) \) and \( \hat{s}_1^2 \) and \( \hat{s}_2^2 \) have eigenvalues \( \frac{1}{2}(\frac{3}{2} + 1) = \frac{3}{4} \). Thus, one can write

\[ \hat{s}_1 \cdot \hat{s}_2 = \begin{cases} 
-\frac{3}{4} & \text{if } S = 0 \\
\frac{1}{4} & \text{if } S = 1. 
\end{cases} \]  

Then, we write

\[ \langle V \rangle = V_d + \mathcal{J} \left(1 - \mathbf{S}^2 \right) = V_d - \frac{1}{2} \mathcal{J} - 2\mathcal{J}\hat{s}_1 \cdot \hat{s}_2. \]  

Here, \( -2\mathcal{J}\hat{s}_1 \cdot \hat{s}_2 \) denotes the contribution to the energy from a pair of atoms (or ions) located at sites 1 and 2. For a large number of atoms we need only sum over all pairs to get

\[ E = \text{constant} - \frac{1}{2} \sum_{i \neq j} 2\mathcal{J}_{ij}\hat{s}_i \cdot \hat{s}_j. \]