Magnetism in materials

Solutions - Week 04

1. Consider the case of two interacting spin-$\frac{1}{2}$ electrons. The good quantum numbers are S = 0 and 1 so that there is a triplet state and a singlet state which will be separated by an energy gap Δ. We define the sign of Δ so that when $\Delta > 0$ the singlet state (S = 0) is the lower state and when $\Delta < 0$ the triplet state is the lower state. These situations are shown in Fig.1. For small B field and small χ, show that the susceptibility in this model is given by

$$\chi = \frac{2ng^2\mu_B^2\mu_0}{k_BT\left(3 + e^{\frac{\Delta}{k_BT}}\right)}$$

which is known as the Bleaney-Bowers equation. Use the script Bleaney_Bowers.ipynb to plot this function. Estimate the minimal temperature above which the susceptibility can be fitted with the Curie law.

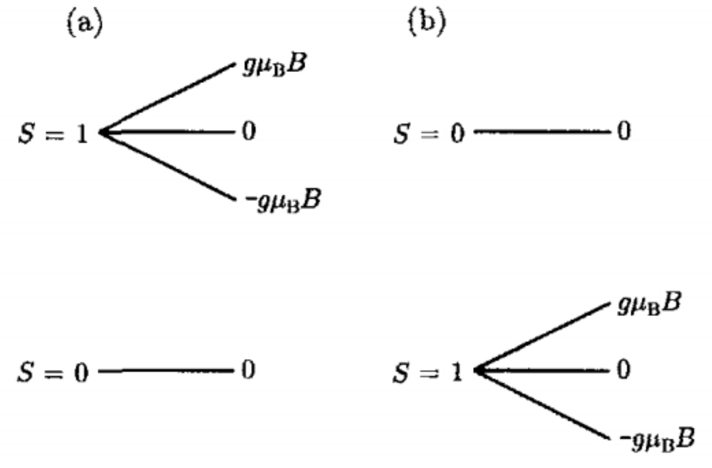

Figure 1: Energy levels if : (a)$\Delta > 0$, (b)$\Delta < 0$

Solution The energy of each state is the following :

$$\begin{aligned} E_s &= -\Delta \\ E_t(m_s = 1) &= g\mu_B B \\ E_t(m_s = 0) &= 0 \\ E_t(m_s = -1) &= -g\mu_B B \end{aligned}$$

Using the partition function :

$$Z = \sum_i e^{-E_i\beta}$$

with E_i the energy of the state i and $\beta = \frac{1}{k_B T}$, the mean magnetic moment can be found :

$$\begin{aligned} < M > &= \frac{\sum_i n g \mu_B m_i e^{-E_i \beta}}{Z} \\ &= n g \mu_B \frac{e^{g\mu_B B\beta} - e^{-g\mu_B B\beta}}{e^{\Delta\beta} + e^{-g\mu_B B\beta} + 1 + e^{g\mu_B B\beta}} \\ &\approx \frac{2ng^2\mu_B^2\beta B}{3 + e^{\Delta\beta}} \end{aligned}$$

Where the last step was done using that $B \ll 1$. In the small susceptibility limit : $B = \mu_0(1+\chi)H \approx \mu_0 H$. So we can found the magnetic susceptibility :

$$\begin{aligned} \chi &= \frac{M}{H} \approx \frac{\mu_0 M}{B} \\ &\approx \frac{2ng^2\mu_B^2\mu_0\beta}{3 + e^{\Delta\beta}} \end{aligned}$$

In the limit $T \gg \Delta/k_B$ the exponential part becomes 1 and we found the Curie law.

2. Calculate the magnitude of the magnetic field 1 Å and 10 Å from a proton in a direction (a) parallel and (b) perpendicular to the proton spin direction.

Solutions The proton magnetic moment is $\mu_p = 2.793\mu_n$ with $\mu_n = \frac{e\hbar}{2m_p}$. The dipole magnetic field is :

$$\vec{B} = \frac{\mu_0}{4\pi|\vec{r}|^3}(3(\vec{\mu}_p\hat{r})\hat{r} - \vec{\mu}_p)$$

(a)

$$\begin{aligned} |\vec{B}\left(\vec{r}\right)| &= \frac{\mu_0\mu_p}{2\pi|\vec{r}|^3} \\ |\vec{B}\left(1\text{Å}\right)| &= 2.82\text{mT} \\ |\vec{B}\left(10\text{Å}\right)| &= 2.82 \cdot 10^{-3}\text{mT} \end{aligned}$$

(b)

$$\begin{aligned} |\vec{B}\left(\vec{r}\right)| &= \frac{\mu_0\mu_p}{4\pi|\vec{r}|^3} \\ |\vec{B}\left(1\text{Å}\right)| &= 1.41\text{mT} \\ |\vec{B}\left(10\text{Å}\right)| &= 1.41 \cdot 10^{-3}\text{mT} \end{aligned}$$

3. Estimate the ratio of the exchange and dipolar coupling of two adjacent Fe atoms in metallic Fe.

Hint Iron has a BCC structure with a lattice constant of 286.65 pm. The magnetic dipole for each atom is $\mu = 2.2\mu_B$. The exchange constant in Fe can be crudely estimated by setting it equal to $k_B T_c$ where T_C is the Curie temperature. The curie temperature for iron is $T_C = 1043$ K.

Solution The dipole interaction energy is given by

$$E = \frac{\mu_0}{4\pi}\left[\frac{\vec{\mu}_1\vec{\mu}_2}{r^3} - \frac{3(\vec{\mu}_1\vec{r})(\vec{\mu}_2\vec{r})}{r^5}\right] \approx \frac{\mu_0\mu_{Fe}^2}{4\pi r^3}$$

Using the hints and the fact that the closest neighbour in a bcc structure is given by $r = \frac{3a}{\sqrt{2}}$ with a the lattice constant, we found that $E \approx 1.15\mu$eV. The exchange constant being $J \approx 0.09$eV, the exchange dominate in pure iron.

4. Provide a rough estimate of the size of the exchange constant in a magnetic oxide which is coupled by superexchange using the measured value of the electronic bandwidth (determined by inelastic neutron scattering) of 0.05 eV. Take the Coulomb energy to be 1 eV. Hence estimate the antiferromagnetic ordering temperature.

Solution $J \approx \frac{-t^2}{U}$ with $t = 0.05$eV and $U = 1$eV. Hence the Néel temperature can be estimated using $J \approx k_B T_N$:

$$T_N \approx \frac{t^2}{Uk_B} \approx 29\text{K}$$

5. Dzyaloshinskii–Moriya interaction is a magnetic exchange interaction between two neighboring magnetic spins, $\vec{S}_i$ and $\vec{S}_j$, described by the Hamiltonian $\vec{D}\cdot(\vec{S}_i \times \vec{S}_j)$. In the two spin system depicted here, $\vec{D}$ is along $\hat{x}$, and $\vec{S}_1 = \frac{1}{\sqrt{2}}(-\hat{x}+\hat{z})$ and $\vec{S}_2 = -\hat{y}$. Find and sketch the direction of $\vec{S}_1 \times \vec{S}_2$. Now, assume that $\vec{S}_1 = \frac{1}{\sqrt{2}}(\hat{x}-\hat{z})$ and repeat the same exercise. Which of these two configurations have lower energy?
Use the script DMI.ipynb to visualize how the vector $\vec{D}$ changes when the central ligand is moved around. What symmetries are broken when you move it?

Solution

$$\vec{S}_1 \times \vec{S}_2 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{1}{\sqrt{2}}(-1) & 0 & \frac{1}{\sqrt{2}}(1) \\ 0 & -1 & 0 \end{vmatrix} = \frac{1}{\sqrt{2}}(\hat{x}+\hat{z})$$

Now, if we assume that $\vec{S}_1 = \frac{1}{\sqrt{2}}(\hat{x}-\hat{z})$, we can repeat the same steps to find $\vec{S}_1 \times \vec{S}_2$:

$$\vec{S}_1 \times \vec{S}_2 = \frac{1}{\sqrt{2}}(-\hat{x}-\hat{z})$$

Comparing the two configurations, we see that the direction of $\vec{S}_1 \times \vec{S}_2$ differs in sign for the $\hat{x}$ component. The second configuration has lower energy as the $\hat{x}$ component in negative.

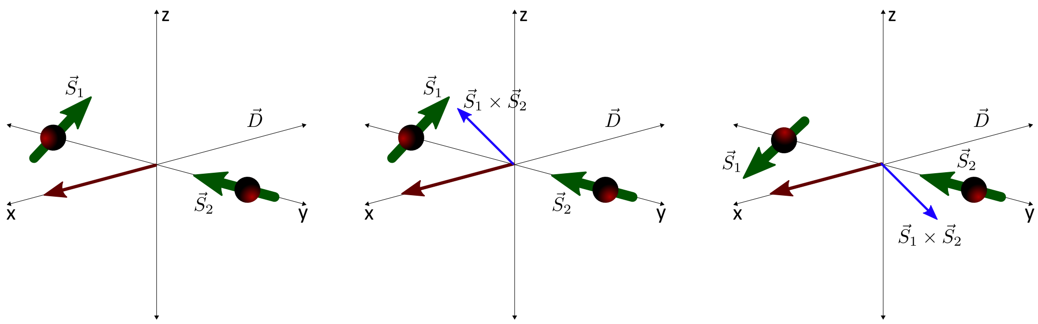
z
$\vec{S}_1$
$\vec{D}$
$\vec{S}_2$
x
y
z
$\vec{S}_1$
$\vec{S}_1 \times \vec{S}_2$
$\vec{D}$
$\vec{S}_2$
x
y
z
$\vec{D}$
$\vec{S}_1$
$\vec{S}_2$
x
y
$\vec{S}_1 \times \vec{S}_2$

Figure 2: