Magnetism in materials

Solutions - Week 10

1. Let's consider a system of n spin $J = 1/2$ per unit volume, with no interaction. Using the partition function for a spin in a field B, calculate the entropy and the heat capacity per unit volume.
   Useful thermodynamic functions :

$$
\begin{aligned}
E &= -n\frac{\partial \ln(Z)}{\partial B} \\
F &= -\frac{n}{\beta}\ln(Z) \\
M &= -\left(\frac{\partial F}{\partial B}\right)_{T,V,n} \\
S &= -\left(\frac{\partial F}{\partial T}\right)_{B,V,n} \\
C_P &= T\left(\frac{\partial S}{\partial T}\right)_{B,P,n}
\end{aligned}
$$

   Where Z is the partition function for one spin, E is the energy per unit volume, F the free energy per unit volume, M the magnetization, S the entropy, C_P the heat capacity and $\beta = \frac{1}{k_B T}$

   Solution

$$
\begin{aligned}
Z &= e^{g\mu_B B\beta/2} + e^{-g\mu_B B\beta/2} = 2\cosh\left(\frac{g\mu_B B\beta}{2}\right) \\
E &= -n\frac{\partial \ln(Z)}{\partial B} = -n\frac{g\mu_B B}{2}\tanh\left(\frac{g\mu_B B\beta}{2}\right) \\
F &= -\frac{n}{\beta}\ln(Z) = -\frac{n}{\beta}\ln\left[2\cosh\left(\frac{g\mu_B B\beta}{2}\right)\right] \\
S &= -\left(\frac{\partial F}{\partial T}\right)_{B,V,n} = nk_B\ln\left[2\cosh\left(\frac{g\mu_B B\beta}{2}\right)\right] - \frac{ng\mu_B Bk_B\beta}{2}\tanh\left(\frac{g\mu_B B\beta}{2}\right) \\
C_P &= T\left(\frac{\partial S}{\partial T}\right)_{B,P,n} = n\left(\frac{g\mu_B B\beta}{2}\right)^2 k_B\left[1-\tanh^2\left(\frac{g\mu_B B\beta}{2}\right)\right]
\end{aligned}
$$

2. Use the script ESR.ipynb to simulate an ESR measurement.

   - Assuming a g-factor $g = 2$, and that the ESR machine works around 1T, estimate what frequency you should use for the microwave signal. Change in the simulation the value of the g factor and of the GHz frequency used to see how the value of the resonant field changes.

- What would happen to the signal if the system is spin $S = 3/2$, and a zero field energy splitting is present between the states $m_z = \pm 1/2$ and $m_z = \pm 3/2$? how could you estimate the zero-field splitting?
- In the simulation you can change the linewidth of the magnetic resonance by adjusting its quality factor Q. The linewidth of the ESR signal also depends on experimental parameters such as the the amplitude of the field modulation. Change the settings of experimental parameters in the simulation to see how they affect the signal.
- ESR employs the lock-in technique to recover a weak signal from a noisy environment. To observe that set the integration time to a very low value (for instance 1 μs), this will give you the result of a measurement performed without field modulation, repeat after turning the option to add noise.

Solution

- $E = g\mu_B B = h\nu$ $\nu \approx 28$GHz
- with zero-field splitting, the gaps get on resonance with the microwave frequency at different field values. Measuring the three resonance fields and knowing the g factor you can infer the zero-field splitting Figure 1.

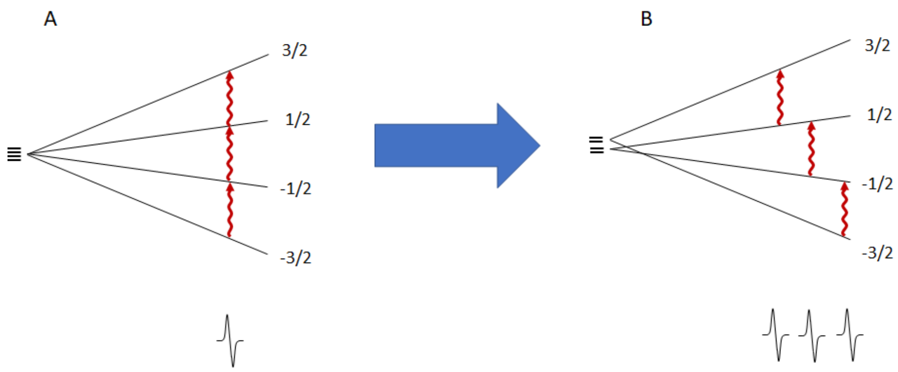

Figure 1: (A) Zeeman splitting of system with $S = 3/2$ without zero-field splitting, the gaps get on resonance at the same field and give a single ESR signal. (B) with zero-field splitting, the gaps get on resonance with the microwave frequency at different field values.