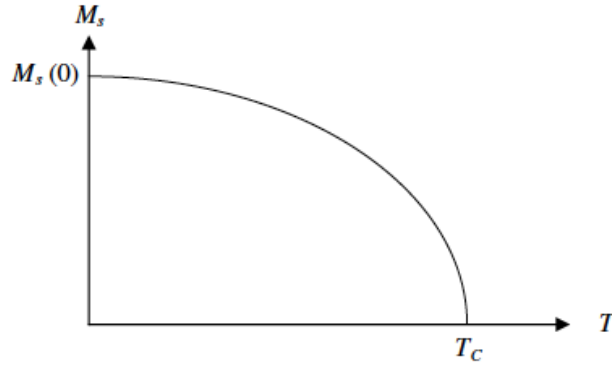


Condensed Matter Physics 3

Example Workshop 5 – Solution

1. Ferromagnetism

(a) See the figure below:



(b) Gd^{3+} ions have 7 electrons in the 4f shell hence,

m_s	1/2	1/2	1/2	1/2	1/2	1/2	1/2
m_l	-3	-2	-1	0	1	2	3

Hund's rules: $S = \sum m_s = 7 \times \frac{1}{2} = 3\frac{1}{2}$, $L = \sum m_l = 0$, $J = S = 3\frac{1}{2}$,

Hence the Landé g -factor $g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} = 2.0$.

Given that the solid has magnetic ions at the corners of a primitive cubic lattice of length $a = 0.75 \times 10^{-9}\text{m}$. The number of atoms per unit volume is therefore $N = 1/a^3 = 2.37 \times 10^{27}\text{m}^{-3}$.

i. At $T = 0\text{ K}$ the magnetisation is at its saturation value $M_{\text{sat}} = Ng_J\mu_B J$

$$M_{\text{sat}} = Ng_J\mu_B J = 2.37 \times 10^{27} \times 2.0 \times 9.27 \times 10^{-24} \times 3.5 = 1.53 \times 10^5 \text{Am}^{-1}$$

ii. Taking the alignment along the $[100]$ direction, $\theta_1 = 0^\circ$, $\theta_2 = \theta_3 = 90^\circ$, $\alpha_1 = \cos\theta_1 = 1$, $\alpha_2 = \cos\theta_2 = 0$, $\alpha_3 = \cos\theta_3 = 0$, and hence:

$$U_{\text{anis}} = 5.4 \times 10^5 (1^2 \times 0^2 + 1^2 \times 0^2 + 0^2 \times 0^2) + 5.1 \times 10^3 (1^2 \times 0^2 \times 0^2) = 0$$

Taking the alignment along the $[111]$ direction, $\theta_1 = \theta_2 = \theta_3 = 54.7^\circ$, $\alpha_1 = \alpha_2 = \alpha_3 = \cos\theta_1 = 0.577$, and hence:

$$U_{\text{anis}} = 5.4 \times 10^5 (3 \times (0.577)^4) + 5.1 \times 10^3 (0.577^6) = 1.8 \times 10^5 \text{Jm}^{-3}$$

i.e. the magnetisation alignment along the $\langle 100 \rangle$ axes leads to the lowest energy state and therefore, these axes are 'easy'. However, the $\langle 111 \rangle$ axes are 'hard' as magnetisation leads to high energy states.

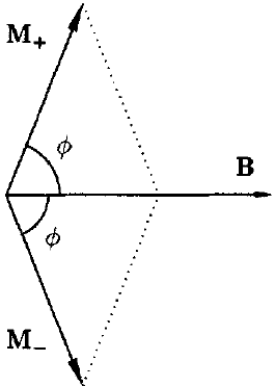
(c) Since $\kappa > 0$ the summation $\sum_i [(S_i^x)^4 + (S_i^y)^4 + (S_i^z)^4]$ must be as large as possible to lower the energy. We have:

$$(S_i^x)^4 + (S_i^y)^4 + (S_i^z)^4 = \left[(S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 \right]^2 - 2 \left[(S_i^x S_i^y)^2 + (S_i^x S_i^z)^2 + (S_i^y S_i^z)^2 \right] \\ = S^4 - 2 \left[(S_i^x S_i^y)^2 + (S_i^x S_i^z)^2 + (S_i^y S_i^z)^2 \right]$$

Since S is a constant we need to minimise $\left[(S_i^x S_i^y)^2 + (S_i^x S_i^z)^2 + (S_i^y S_i^z)^2 \right]$. This is satisfied for S along one of the cubic axes, e.g. $S_i^x = S, S_i^y = 0, S_i^z = 0$. Hence $\langle 100 \rangle$ directions are the easy axes of magnetisation.

2. Antiferromagnetism and Ferrimagnetism

(a)



i. The exchange energy is given by $\sum_{i,j} -J_{\text{ex}} \mathbf{S}_i \cdot \mathbf{S}_j$. Treating the magnetisation as free vectors and making use of the fact that $J = S$ the exchange interaction has the form $-2J_{\text{ex}} M^+ M^- \cos(2\phi) = -2J_{\text{ex}} M^2 \cos(2\phi)$, where for an antiferromagnet $M = M^+ = M^-$. The magnetocrystalline anisotropy energy, $K \sin^2 \theta$, is minimum for $\theta = 0, \pi$ rad (i.e. spin 'up' and spin 'down'). Therefore, the anisotropy energy is $K \sin^2 \left(\frac{\pi}{2} - \phi \right) = K \cos^2 \phi$. The Zeeman energy is $-(M^+ + M^-) B \cos \phi = -2MB \cos \phi$. The total energy is therefore:

$$E = -2J_{\text{ex}} M^2 \cos(2\phi) + K \cos^2 \phi - 2MB \cos \phi$$

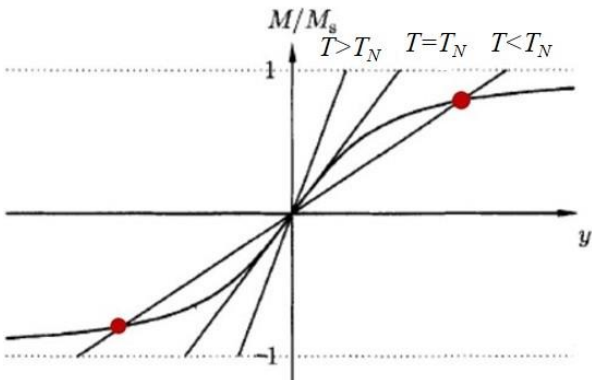
ii. The equilibrium angle ϕ is determined by $\frac{dE}{d\phi} = 0$.

$$\frac{dE}{d\phi} = 4J_{\text{ex}} M^2 \sin(2\phi) - K \sin(2\phi) + 2MB \sin \phi = 0$$

Using the fact that $\sin(2\phi) = 2 \sin \phi \cos \phi$, we have:

$$\cos \phi = \frac{MB}{K - 4J_{\text{ex}} M^2}$$

(b) i. The Weiss model treats the exchange energy due to neighbouring spins as an effective 'molecular field' B_{mf} . For example, the molecular field experienced by a spin 'up' electron is due to the spin 'down' sub-lattice, and is proportional to the magnetisation of the spin 'down' sub-lattice, i.e. $B_{\text{mf}}^+ = -\lambda M^-$ and $B_{\text{mf}}^- = -\lambda M^+$, where the '+' and '-' superscripts refer to spin 'up' and spin 'down' sub-lattices.



The magnetisation must simultaneously satisfy the equations:

$$\frac{M^\pm}{M_s^\pm} = B_J(y^\pm) \text{ and } y^\pm = \frac{g_J \mu_B J^\pm (B + B_{\text{mf}}^\pm)}{k_B T} = \frac{g_J \mu_B J^\pm (B - \lambda M^\mp)}{k_B T}$$

where B_J is the Brillouin function and B is the applied magnetic field. The graphical solution for zero applied field is shown opposite.

It is clear that in a ferrimagnet the magnetisation of a given sub-lattice is a function of its saturation magnetisation M_s and J angular momentum. Therefore, the temperature dependence of the magnetisation for the two sub-lattices will be different, such that at the compensation temperature the magnetisation of the spin ‘up’ sub-lattice will cancel that of the spin ‘down’ sub-lattice.

ii. In the paramagnetic phase under small applied \mathbf{B} -fields the term y^\pm is small. Using the approximation $B_J(y) \approx \frac{(J+1)}{3J} y$, we have:

$$\frac{M^\pm}{M_s^\pm} = B_J(y^\pm) \approx \frac{(J^\pm + 1)}{3J^\pm} y^\pm = \frac{g_J \mu_B (J^\pm + 1) (B - \lambda M^\mp)}{3k_B T}$$

Rearranging:

$$M^\pm = \frac{C_\pm}{T} (B - \lambda M^\mp) \text{ where } C_\pm = \frac{g_J \mu_B (J^\pm + 1) M_s^\pm}{3k_B}$$

Hence:

$$M^+ = \frac{C_+}{T} (B - \lambda M^-) = \frac{C_+ B}{T} - \frac{\lambda C_+}{T} \left[\frac{C_-}{T} (B - \lambda M^+) \right] \text{ or}$$

$$M^+ \left[1 - \frac{\lambda^2 C_+ C_-}{T^2} \right] = \left[\frac{C_+}{T} - \frac{\lambda C_+ C_-}{T^2} \right] B$$

Similarly, it easy to show that:

$$M^- \left[1 - \frac{\lambda^2 C_+ C_-}{T^2} \right] = \left[\frac{C_-}{T} - \frac{\lambda C_+ C_-}{T^2} \right] B$$

For weak magnetisations the susceptibility $\chi = \frac{M}{H} = \frac{\mu_0 M}{B}$. The susceptibility is due to both the spin ‘up’ and spin ‘down’ sub-lattices, i.e. $\chi = \frac{\mu_0 (M^+ + M^-)}{B}$. Hence:

$$\chi = \frac{\mu_0 \left[\frac{(C_+ + C_-)}{T} - \frac{2\lambda C_+ C_-}{T^2} \right]}{\left[1 - \frac{\lambda^2 C_+ C_-}{T^2} \right]} = \frac{\mu_0}{T^2 - \theta^2} [(C_+ + C_-)T - 2\lambda C_+ C_-]$$

where $\theta^2 = \lambda^2 C_+ C_-$.