Problem Set 9
Magnetic ordering

1 Ferromagnetism

We consider a cubic lattice system (with coordination number $z = 6$) of volume V and containing N atoms. Each atom has a total angular momentum (in units of $\hbar$) $\mathbf{J} = \mathbf{S} + \mathbf{L}$, with $\mathbf{S}$ and $\mathbf{L}$ the spin and orbital angular momentum, respectively. The absolute square value $\mathbf{J}^2 = J(J+1)$, where J is the quantum number of the total angular momentum. The magnetic moment of an atom is given by $\boldsymbol{\mu} = -g\mu_\mathrm{B}\mathbf{J}$, where g is the Landé factor and μ_B the Bohr magneton. An external magnetic field in the z direction (which defines the quantization axis) $\mathbf{B} = B\,\hat{z}$ is applied, and we consider a ferromagnetic exchange interaction $\gamma > 0$ between nearest neighbor atoms. The Hamiltonian of the system reads

$$H = -\gamma \sum_{\langle i,j\rangle} J_i^z J_j^z + g\mu_\mathrm{B} B \sum_{i=1}^{N} J_i^z, \tag{1.1}$$

where J_i^z is the z component of the total angular momentum, while $\langle i,j\rangle$ represents a summation over nearest neighbors.

For $\gamma = 0$, the average magnetization of the sample is given by (*cf.* Problem Set 6, Exercice 2)

$$\langle M^z\rangle = M_\mathrm{s} B_J(\beta g\mu_\mathrm{B} J B),$$

with $M_\mathrm{s} = ng\mu_\mathrm{B}J$ the saturation magnetization ($n = N/V$ is the density), $\beta = 1/k_\mathrm{B}T$ the inverse temperature, and where

$$B_J(x) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}\,x\right) - \frac{1}{2J}\coth\left(\frac{1}{2J}\,x\right)$$

denotes the Brillouin function. Note that for $x \ll 1$, the latter reads

$$B_J(x) = \frac{J+1}{3J}\,x - \zeta_J\,x^3 + \mathcal{O}\left(x^5\right), \qquad \text{with} \quad \zeta_J = \frac{(J+1)[2J(J+1)+1]}{90J^3}.$$

(a) At zero temperature ($T = 0$) and vanishing magnetic field ($B = 0$), what are the two degenerate ground states of the system?

(b) By writing down the energy of one lattice site and within the mean (molecular) field approximation due to Pierre Weiss (1907), argue that the effective magnetic field seen by the spin J_i^z is given by $B_\mathrm{eff} = B + B_\mathrm{m}$, where $B_\mathrm{m} = \lambda\langle M^z\rangle$. Determine the expression of the constant λ.

(c) Deduce from the preceding question that the magnetization obeys the self-consistent equation

$$\langle M^z\rangle = M_\mathrm{s} B_J(\beta g\mu_\mathrm{B} J[B + \lambda\langle M^z\rangle])$$

(d) Let us first consider the case $B = 0$. Show that the system presents a spontaneous magnetization below the critical temperature[1]

$$k_\mathrm{B}T_\mathrm{c} = \frac{J(J+1)}{3}\,z\gamma. \tag{1.2}$$

Sketch $\langle M^z\rangle$ as a function of temperature.

[1]To simplify the notation, you may want to introduce the dimensionless quantity $m = \langle M^z\rangle/M_\mathrm{s}$.

(e) Show that the critical temperature (1.2) can be re-expressed as

$$k_{\mathrm{B}}T_{\mathrm{c}} = \frac{J+1}{3}\, g\mu_{\mathrm{B}}\lambda M_{\mathrm{s}}$$

and estimate the molecular field B_{m} for a ferromagnet with $J = 1/2$ and $T_{\mathrm{c}} = 10^3\,\mathrm{K}$. How does this value compare to typical applied magnetic fields that can be found in the lab?

(f) Still for $B = 0$, determine an approximate expression of $\langle M^z \rangle$ for temperatures in the vicinity of T_{c}.

(g) Determine the zero-field magnetic susceptibility χ in the vicinity of the phase transition, for $T \gtrsim T_{\mathrm{c}}$.

2 Antiferromagnetism

We now consider a similar system as in Exercice 1, but with an *anti*ferromagnetic exchange interaction $\gamma < 0$, so that we rewrite the Hamiltonian (1.1) as

$$H = |\gamma| \sum_{\langle i,j \rangle} J_i^z J_j^z + g\mu_{\mathrm{B}} B \sum_{i=1}^{N} J_i^z, \tag{2.1}$$

(a) Let us consider for this question that $T = 0$ and $B = 0$. Justify that the system splits into two sublattices A and B, such that the angular momenta take the value $+J$ or $-J$ depending on the sublattice to which they belong. These states are called *Néel states*. How many Néel states are there?

(b) Let us call $\langle M_A^z \rangle$ ($\langle M_B^z \rangle$) the average magnetization of the A (B) sublattice. Using the Weiss molecular field approximation, show that these two quantities are determined by the two self-consistent coupled equations

$$\langle M_A^z \rangle = \frac{M_{\mathrm{s}}}{2} B_J(\beta g\mu_{\mathrm{B}} J[B - 2|\lambda| \langle M_B^z \rangle])\,, \tag{2.2a}$$

$$\langle M_B^z \rangle = \frac{M_{\mathrm{s}}}{2} B_J(\beta g\mu_{\mathrm{B}} J[B - 2|\lambda| \langle M_A^z \rangle])\,, \tag{2.2b}$$

where the notation is the same as in the first exercice.

(c) For $B = 0$, assuming that $\langle M_A^z \rangle = -\langle M_B^z \rangle$, show that there exists a phase transition for a temperature T_{N} (called the Néel temperature) between a phase where $\langle M_A^z \rangle = -\langle M_B^z \rangle = 0$ and a phase where $\langle M_A^z \rangle = -\langle M_B^z \rangle = M_0(T)$. Give an expression for T_{N}. Sketch $M_0(T)$ as a function of temperature.

(d) Still for $B = 0$, sketch the total magnetization $M_{\mathrm{tot}} = \langle M_A^z \rangle + \langle M_B^z \rangle$ and the staggered magnetization $M_{\mathrm{sta}} = \langle M_A^z \rangle - \langle M_B^z \rangle$ as a function of T. Which quantity is the order parameter of the antiferromagnetic-paramagnetic phase transition?

(e) Using Eqs. (2.2), determine the zero-field magnetic susceptibility χ for $T \gtrsim T_{\mathrm{N}}$.

3 Experimental considerations

As we have seen in the previous exercices, in both the ferromagnetic and antiferromagnetic cases, the susceptibility is given, above the critical temperature of the phase transition, by

$$\chi \sim \frac{1}{T - \theta},$$

where $\theta = T_{\mathrm{c}}$ in the ferromagnetic case, while $\theta = -T_{\mathrm{N}}$ in the antiferromagnetic one. What is the value of θ for a paramagnet, *i.e.*, $\gamma = 0$ in Eq. (1.1) or (2.1)? Sketch χ^{-1} as a function of temperature in all three cases, and discuss how experimentalists determine that a sample is para-, ferro-, or antiferromagnetic.