Problem sheet 4: Magnetic order and Magnetic couplings **18.12.2024**

4.1. Dipolar couplings (5 P)

Estimate the dipolar coupling energy in metallic Fe (bcc structure with $a = 2.86\,\text{Å}$) and compare it to the experimental Curie temperature, $T_C = 1043\,\text{K}$. Consider three possible scenarios:

(a) spins parallel to the Fe-Fe bonds

(b) spins perpendicular to the Fe-Fe bonds

(c) spins are at 45° with respect to the Fe-Fe bonds

The magnetic moment of an Fe atom in metallic iron is $2.3\,\mu_B$.

4.2. Mean-field theory for a ferrimagnet (8 P)

Consider a ferrimagnet with sublattices 1 and 2 built by two different magnetic ions with the different Curie constants C_1 and C_2. The coupling λ between the sublattices contributes to the effective (molecular) field experienced by the ions in each of the sublattices:

$$\mathbf{B}_1 = \mathbf{B}_{\text{ext}} + \lambda \mathbf{M}_2, \qquad \mathbf{B}_2 = \mathbf{B}_{\text{ext}} + \lambda \mathbf{M}_1$$

(a) Show that the high-temperature magnetic susceptibility is given by

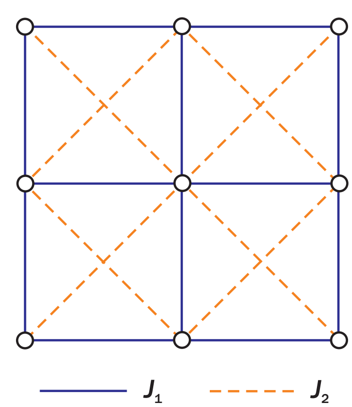
$$\chi = \frac{(M_1 + M_2)}{B_{\text{ext}}} = \frac{(C_1 + C_2)T + 2\lambda C_1 C_2}{T^2 - \lambda^2 C_1 C_2}$$

(b) Show that this expression reduces to the Curie-Weiss law for an antiferromagnet when $C_1 = C_2$.

(c) Determine the magnetic ordering temperature from the condition $\chi^{-1} = 0$.

4.3. Square-lattice antiferromagnet (7 P)

Consider a square-lattice antiferromagnet with the nearest-neighbor coupling J_1 and next-nearest-neighbor coupling J_2, as shown in the figure.



(a) Compare the $\mathbf{k} = (\frac{1}{2}, \frac{1}{2})$ and $\mathbf{k} = (\frac{1}{2}, 0)$ ordered states and determine their stability regions with respect to the J_2/J_1 ratio. To this end, write down the energies of these states using the Heisenberg model.

(b) Download the experimental magnetic susceptibility data for $Pb_2VO(PO_4)_2$ and fit them with the Curie-Weiss law. You will notice that $1/\chi$ is not quite linear at high temperatures. This is due to the temperature-independent terms, such as core diamagnetism. You can fix this problem by using $\chi(T) = \chi_0 + C/(T - \theta)$.

(c) What is the effective moment and how does it compare to the expected value for vanadium? Note that you should get a reasonable match for μ_{eff}. Otherwise, your fit is probably not good enough to determine θ.

(d) Write the Curie-Weiss temperature θ as a linear combination of J_1 and J_2. Determine the values of these exchange couplings using the Curie-Weiss temperature obtained from the fit and considering the experimental saturation field of 21 T. Note that you will obtain two solutions from the two possible ordered states.