Faculté de physique et ingénierie Université de Strasbourg

University of Strasbourg

Problem Set 8

R. Jalabert, O. Ersen, D. Weinmann

Transcribed by

Pierre Guichard

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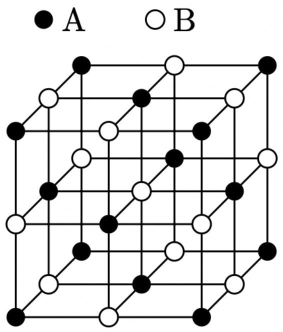
Exercise 1 : Mean field theory for Ferro- and Antiferromagnetism



We consider a cubic lattice system containing $N/2$ atoms of type A and $N/2$ atoms of type B, which are located on sub-lattices A and B. Each atom of type A (B) has four nearest neighbors of type B (Aà. The atoms have a total angular momentum $\vec{J}$ with projections J_z on the quantization axis $\hat{z}$ that can take the values $J_z = m\hbar$ with $m = \{-j, -1+1, \cdots, j-1, j\}$, where j is the quantum number associated with the angular momentum $\vec{J}$. Such an angular momentum is related to a magnetic moment $\vec{\mu} = -g\mu_B \vec{J}/\hbar$, where g is the Landé factor and μ_B the Bohr magneton. The system is in thermal equilibrium at temperature T.

a) Explain how a generalization of the usual mean (molecular) field theory leads to the expressions

$$\vec{H}_A^m = \gamma_{AA}\vec{M}_A + \gamma_{AB}\vec{M}_B \quad (1)$$
$$\vec{H}_B^m = \gamma_{BA}\vec{M}_A + \gamma_{BB}\vec{M}_B \quad (2)$$

for the internal mean fields seen by the atoms A and B with constants γ_{AA}, γ_{AB}, γ_{BA}, γ_{BB} and the magnetization $\vec{M}_A$, $\vec{M}_B$ of the subsystems A and B.

Trivial

b) We now assume that the system is under the effect of an eternal magnetic field $\vec{H}_{\text{ext}} = H_{\text{ext}}\vec{e}_z$, oriented in z-direction. Use the mean fiedl approximation to derive the coupled equations

$$M_A^z = M_0[(H_{\text{ext}} + \gamma_{AA}M_A^z + \gamma_{AB}M_B^z)/T] \quad (3)$$
$$M_B^z = M_0[(H_{\text{ext}} + \gamma_{BA}M_A^z + \gamma_{BB}M_B^z)/T] \quad (4)$$

for the magnetizations along the $\hat{z}$-axis. Give the function $M_0[x]$.

$$B_j(x) = \frac{2j+1}{2j}\coth\left(\frac{2j+1}{2j}x\right) - \frac{1}{2j}\coth\left(\frac{x}{2j}\right)$$

And in the general case,

$$M^z = ng\mu_B j B_j\left(\right)$$

$$\begin{cases} M_A^z = n_A g\mu_B j B_j(g\mu_B j\mu_0[H_{\text{ext}}^z + \gamma_{AA}M_A^z + \gamma_{AB}M_B^z]/k_BT) \\ M_B^z = n_B g\mu_B j B_j(g\mu_B j\mu_0[H_{\text{ext}}^z + \gamma_{BB}M_B^z + \gamma_{BA}M_A^z]/k_BT) \end{cases}$$

In this case $n_A = n_B = n/2$. We take

$$M_0(x) = \frac{ng\mu_B j}{2} B_j\left(\frac{g\mu_B j\mu_0}{k_B}x\right)$$

c) Calculate the magnetic susceptibility χ_m of the system at high temperatures, above the critical temperature, where the functions $M_0[x]$ can be linearized.

$T \to +\infty$ meaning that $x \to 0$.

$$\coth(x) \sim \frac{1}{x} + \frac{x}{3} + \mathcal{O}(x^3)$$

$$\begin{aligned} B_j(x) &\sim \frac{2j+1}{2j}\left(\frac{2j}{2j+1}\frac{1}{x} + \frac{1}{3}\frac{2j+1}{2j}x\right) - \frac{1}{2j}\left(\frac{2j}{x} + \frac{1}{6j}x\right) \\ &= \frac{(2j+1)^2}{3(2j)^2}x - \frac{1}{12j^2}x \\ &= \frac{x}{12j^2}\left((2j+1)^2 - 1\right) \\ &= \frac{x}{3j}(j+1) \end{aligned}$$

Thus,

$$M_0(x) \sim \frac{ng\mu_B j}{2}\frac{g\mu_B j\mu_0 x}{3k_B j}(j+1) = \frac{ng^2\mu_B^2 j(j+1)\mu_0}{6k_B}x = \alpha x$$

$$\begin{aligned} M_A^z &= \alpha[(H_{\text{ext}} + \gamma_{AA}M_A^z + \gamma_{AB}M_B^z)/T] \\ M_B^z &= \alpha[(H_{\text{ext}} + \gamma_{BA}M_A^z + \gamma_{BB}M_B^z)/T] \end{aligned}$$

$$\begin{aligned} M_A^z &= \alpha H_{\text{ext}}\frac{T - \alpha(\gamma_{BB} - \gamma_{AB})}{(T - \alpha\gamma_{BB})(T - \alpha\gamma_{AA}) - \alpha^2\gamma_{AB}\gamma_{BA}} \\ M_B^z &= \alpha H_{\text{ext}}\frac{T - \alpha(\gamma_{AA} - \gamma_{BA})}{(T - \alpha\gamma_{AA})(T - \alpha\gamma_{BB}) - \alpha^2\gamma_{BA}\gamma_{AB}} \end{aligned}$$

$$
\begin{aligned}
M_A + M_B &= \alpha H_{\text{ext}} \frac{2T - \alpha(\gamma_{AA} + \gamma_{BB} - \gamma_{AB} - \gamma_{BA})}{(T - \alpha\gamma_{AA})(T - \alpha\gamma_{BB}) - \alpha^2\gamma_{BA}\gamma_{AB}} \\
&= \chi_m H
\end{aligned}
$$

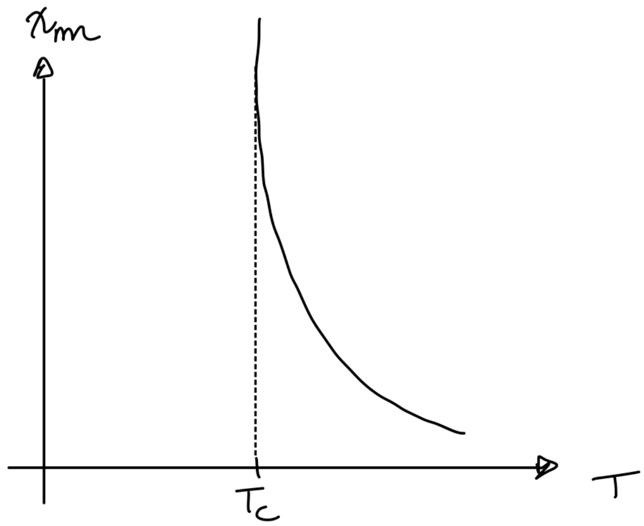
So,

$$
\chi_m = \alpha \frac{2T - \alpha(\gamma_{AA} + \gamma_{BB} - \gamma_{AB} - \gamma_{BA})}{(T - \alpha\gamma_{AA})(T - \alpha\gamma_{BB}) - \alpha^2\gamma_{BA}\gamma_{AB}}
$$

d) Show that the usual Curie-Weiss law for the temperature-dependence of the magnetic susceptibility, $\chi_m(T) = C/(T - T_c)$, is obtained in the simple ferromagnetic case $\gamma_{AA} = \gamma_{BB} = \gamma_1 > 0$; $\gamma_{AB} = \gamma_{BA} = \gamma_3 \geq 0$. Express C and T_c as a function of the parameters of the problem and sketch $\chi_m(T)$.

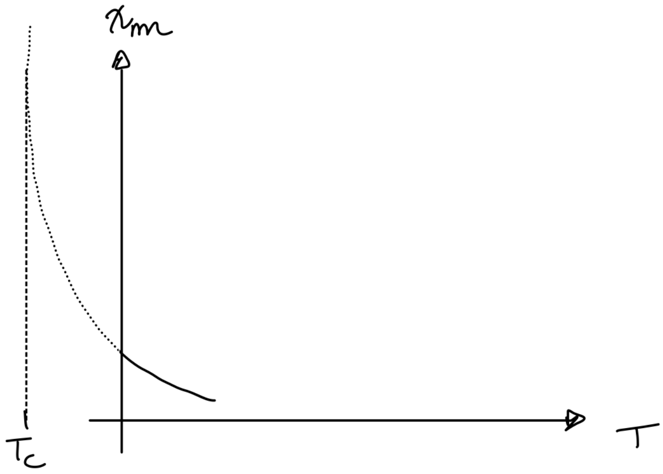
$$
\begin{aligned}
\chi_m &= 2\alpha \frac{T - \alpha(\gamma_1 - \gamma_3)}{(T - \alpha\gamma_1)^2 - \alpha^2\gamma_3^2} \\
&= 2\alpha \frac{T - \alpha(\gamma_1 - \gamma_3)}{(T - \alpha\gamma_1 + \alpha\gamma_3)(T - \alpha\gamma_1 - \alpha\gamma_3)} \\
&= \frac{2\alpha}{T - \alpha(\gamma_1 + \gamma_3)} \\
&= \frac{C}{T - T_c}
\end{aligned}
$$

$$
T_c = \alpha(\gamma_1 + \gamma_2)
$$



e) Take the simple case of antiferromagnetic coupling $\gamma_{AA} = \gamma_{BB} = \gamma_1 > 0$; $\gamma_{AB} = \gamma_{BA} = \gamma_3 < 0$. Express C and T_c as a function of the problem parameters and give the condition for which the critical temperature becomes negative. Sketch $\chi_m(T)$ for this case.

The critical temperature becomes negative when $|\gamma_3| > |\gamma_1|$



We linearized because of the high-temperature regime, so this situation is non-sense.

f) Determine the magnetization in the zero-temperature limit and in the limit of vanishing external magnetic field for $\gamma_1 > 0$, for the cases $\gamma_3 > \gamma_1$ and $\gamma_3 < -\gamma_1$. Sketch $\chi_m(T)$ and give a physical interpretation of the result. What happens when $|\gamma_3| < \gamma_1$?

In zero-temperature limit,

$$B_j(x) \sim \pm 1$$

$$M_0(x) = \frac{ng\mu_B j}{2}\text{sgn}(x) = M_S\text{sgn}(x)$$

Where M_S is the saturation magnetization. We can plug this into M_A and M_B,

$$\begin{cases} M_A = M_S\text{sgn}(\gamma_1 M_A + \gamma_3 M_B) \\ M_B = M_S\text{sgn}(\gamma_1 M_B + \gamma_3 M_A) \end{cases}$$

- if $\gamma_1 > 0$ and $\gamma_3 > \gamma_1$,

$$\text{sgn}(\gamma_1 M_B + \gamma_3 M_A) = \text{sgn}(\gamma_3 M_A) = +1$$

  And thus, both are aligned : $M_B = M_A$.

- if $\gamma_3 < \gamma_1$,

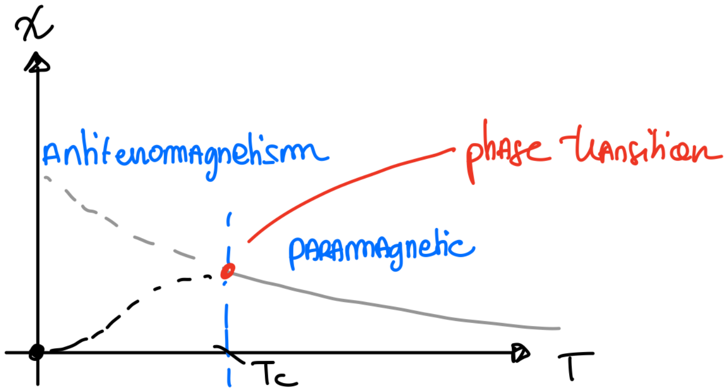
$$\text{sgn}(\gamma_1 M_B + \gamma_3 M_A) = \text{sgn}(\gamma_1 M_B)$$

  And thus, $M_B = \text{sgn}(\gamma_1 M_B)M_S$, meaning we have decoupled the two equations : anything is a solution.

- If $\gamma_1 > 0$ and $\gamma_3 < -\gamma_1$,

$$M_A = M_S \text{sgn}(\gamma_3 M_B) = -\text{sgn}(M_B) M_S \quad M_B = M_S \text{sgn}(\gamma_3 M_A) = -\text{sgn}(M_A) M_S$$

$M_A = -M_B$, they are anti-aligned, meaning a total magnetization of 0.



Exercise 2 : Ferrimagnetism

Consider the system of Exercise 2, but with atoms A and B that have different total angular momentum $\vec{J}_X$ ($X = \{A, B\}$), different quantum number j_X, and different magnetic moment $\vec{\mu}_X$. Discuss the new situation and revisit the aspects of Exercise 2 b-f, paying particular attention to the similarities and differences with respect to the situation of Exercise 2.