



Keble College - Hilary 2010
B2: Condensed Matter Physics and Photonics
Tutorial 7 - Magnetism

Please leave your work in my Keble pigeon hole by Wednesday of 5th week.
Suggested reading: Hook & Hall 7,8; Kittel 11,12; Ashcroft/Mermin 31-33 (advanced treatment).

1 Diamagnetism

1. Give an heuristic, semi-classical argument to show that the diamagnetic susceptibility of a system of N atoms is:

$$\chi = -\frac{\mu_0 N Z e^2}{6m} \langle r^2 \rangle$$

The problem with this lies in the Bohr - van Leeuwen theorem which asserts that classically magnetism doesn't exist at all - thus we must use quantum mechanics. (As a corollary this means that simple fridge magnets are an everyday example of macroscopic quantum mechanics in action.) The Hamiltonian for a system of electrons in a uniform magnetic field is ¹:

$$H = \sum_i \left(\frac{(\mathbf{p}_i + e\mathbf{A}_i)^2}{2m} + g_s \mu_B \mathbf{S}_i \cdot \mathbf{B} \right)$$

where $\mathbf{A}_i = \frac{1}{2} \mathbf{B} \times \mathbf{r}_i$. Show that this can be rewritten as

$$H = \sum_i \left(\frac{p_i^2}{2m} + \mu_B (\mathbf{L} + g_s \mathbf{S})_i \cdot \mathbf{B} + \frac{e^2}{8m} (\mathbf{B} \times \mathbf{r}_i)^2 \right)$$

The second term gives rise to paramagnetism and the third to diamagnetism. Show that you can reproduce the semi-classical result for the susceptibility using a fully quantum argument.

2. Please attempt question D3 from Prof. Nicholas' problem set.

2 Paramagnetism

3. Consider the effect of a magnetic field on electrons in the conduction band and show that this leads to a paramagnetic susceptibility (Pauli paramagnetism) of

$$\chi = \frac{3N\mu_0\mu_B^2}{2k_B T_F}$$

Now consider the effect of the magnetic field on the ionic spins (assume they have spin J). Show that the magnetisation of the sample is given by

$$M = N g_J \mu_B J B_J(y)$$

¹If you are curious as to why the momentum has been replaced by $\mathbf{p} + e\mathbf{A}$, you are right to be. It isn't obvious how to generate a Hamiltonian for electromagnetic processes, and this turns out to work. Modern physics views charge and electromagnetism as arising from the need for the Hamiltonian to be invariant under the action of the group $U(1)$, which corresponds to multiplying wavefunctions by a complex number $\exp(i\alpha(x, t))$. In order to make the Hamiltonian invariant, terms of the form above are added which correspond to electromagnetic interactions.

where $y = g_J \mu_B B J / k_B T$ and $B_J(y)$ is the Brillouin function

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

Show that at high temperature this gives Curie's law for the magnetic susceptibility

$$\chi = \frac{N \mu_0 \mu_B^2 g_J^2 J(J+1)}{3k_B T}$$

while at low temperature the magnetisation saturates and is given by

$$M \simeq N g_J \mu_B J - N g_J \mu_B e^{-y/J}$$

4. State briefly what is meant by *ionic paramagnetism* and *orbital quenching*. It is observed that a crystal containing 4×10^{28} Fe^{3+} ions per cubic metre has a paramagnetic susceptibility that is approximately 1.45 times that for an equivalent crystal containing Mn^{3+} ions, and approximately 1.1 times that for a crystal containing N Gd^{3+} ions per cubic metre. Write down the ground state spectroscopic term for each ion. Explain the observations of paramagnetic susceptibility and find a value for N . [10]

[Ground state electronic configurations of outer shells: $\text{Fe}^{3+} 3s^2 3p^6 3d^5$, $\text{Mn}^{3+} 3s^2 3p^6 3d^4$, $\text{Gd}^{3+} 4f^7 5s^2 5p^6$.]

[from 2003 A4 question 6 (old course)]

3 Ferromagnetism and Antiferromagnetism

5. Explain the physical basis for the Weiss molecular field theory of ferromagnetism, and show that the Curie temperature T_c of a material with $S = 1/2$ and $g_J = 2$ is given according to Weiss theory by

$$T_c = \frac{n \mu_0 \mu_B^2 \lambda}{k_B}$$

where n is the number of ions per unit volume, and λ is the molecular field constant. [10]

Iron has a body centred cubic structure with lattice constant $a = 0.287 \text{ nm}$, and is a ferromagnet with a Curie temperature of $T_c = 1043 \text{ K}$ and a saturated magnetic moment of $2.2 \mu_B$ per atom. Calculate the molecular field inside Fe at temperature $T \ll T_c$. Compare the calculated molecular field with an estimate of the field at a distance a from a magnetic dipole of magnitude $2.2 \mu_B$. [7]

Account for the following observations:

- (a) a bar of soft iron is usually unmagnetised at room temperature;
 (b) the observed saturated moment on the Cr ions in ferromagnetic CrO_2 is $2.0 \mu_B$, while Hund's rules predict that the ground state angular momentum quantum numbers of Cr^{4+} are $S = 1$, $L = 3$ and $J = 2$. [8]

[1999 A4 question 5 (old course)]

6. Please attempt question D9 from Prof. Nicholas' problem set.
 7. Please attempt question D10 from Prof. Nicholas' problem set.

The next question is optional and is included only to provide you with a more complete picture. It is hoped that you will find time to read through it and think about the ideas it contains. These are the core ideas behind ferromagnetism which you should at least be aware of for the exam. If you wish to attempt a solution, Ashcroft and Mermin (chapter 32) provides a good guide.

4 Exchange Interactions and Ferromagnetism

8. When we discussed the tight binding model we considered wavefunctions of a *single* electron in a two proton system. Now we consider a *two* electron system - we assume that the coulomb repulsion is so large that two electrons are *never* bound to the same atom. Specifically, letting $|i; j\rangle = \Psi_1(r_i)\Psi_2(r_j)$ denote a state in which electron i is bound to site 1 and electron j is bound to site 2, we consider the two states:

$$\begin{aligned} |\psi_S\rangle &= \frac{1}{\sqrt{2}} (|1; 2\rangle + |2; 1\rangle) , \\ |\psi_A\rangle &= \frac{1}{\sqrt{2}} (|1; 2\rangle - |2; 1\rangle) . \end{aligned}$$

For appropriately chosen Ψ , these will be approximate eigenstates under the assumption that two electrons never occupy the same site. Note that this correlation between the electrons arises entirely from considerations of coulomb interactions. So far we have ignored the spin part of the wavefunction: from exchange symmetry, what is the spin of each of these states? What is the value of $\mathbf{S}_1 \cdot \mathbf{S}_2$ for each state? Hence show that the Hamiltonian may be written as

$$H = \frac{1}{4} (3E_A + E_S) + (E_A - E_S) \mathbf{S}_1 \cdot \mathbf{S}_2 .$$

Explain why $E_A - E_S$ is referred to as an *exchange* energy. Remember this comes solely from Coulomb interactions but it gives us a Hamiltonian with spin-spin interactions, i.e., it gives us (ferro)magnetism.

The generalisation to more particles is obvious;

$$H = - \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{h}_i \cdot \mathbf{S}_i ,$$

where $\langle ij \rangle$ means a sum over *pairs* i and j and \mathbf{h}_i is an applied external field (in suitable units) at site i . (This is known as the Heisenberg model.)

In what follows you may take $J_{ij} = J/N$ and $\mathbf{h}_i = \mathbf{h}$, for simplicity.

By writing

$$\mathbf{S}_i = \langle \mathbf{S} \rangle + (\mathbf{S}_i - \langle \mathbf{S} \rangle) ,$$

and keeping terms in fluctuations to first order only, show that

$$H \simeq -\mathbf{h}^{eff} \cdot \sum_i \mathbf{S}_i ,$$

where \mathbf{h}^{eff} is an effective field which you should give an expression for. (This general process is referred to as *mean field theory*, although in the context of ferromagnetism it is also called the Weiss molecular field.)

Hence obtain the mean field partition function and a self-consistency equation for the magnetisation $m = \langle S \rangle$. Show that, below a critical temperature, T_c , which you should give an expression for, the susceptibility diverges as $(T_c - T)^{-1}$.