# Handout 26: Magnetic Moments and Fields

# **Handout 26: Magnetic Moments and Fields**

Introduction: In the first two parts of the course we have explored how light interacts with atoms and with solids. The aim of this part of the lecture course is to look at how solids respond to magnetic fields. Different types of material respond to magnetic fields in very different ways, and so the aim here is to provide an overview of magnetism in solids. Some materials contain magnetic moments that interact and produce a cooperative state of matter, and properties quite different to an array of isolated magnetic moments. There is a wide range of different types of interaction and this leads to a plethora of different cooperative states in materials. Magnetic materials have been known and exploited since ancient times, but it was only at the advent of quantum theory that a scientific description of magnetism began to emerge.

Lecture 26: We begin by revisiting ideas from electromagnetism and quantum mechanics to build up a picture of the individual magnetic moments

### 26.1 Magnetic Moments

The fundamental object in magnetism is the magnetic moment. Recall from Electromagnetism that an electric current I going round a closed loop of (vector) area S has magnetic moment vector, ( $\mu$  and m are both used as symbols for moment).

$$\mu = IS \tag{1}$$

 $\mu$  is normal to the plane enclosed by the loop with direction given by the right hand grip rule. The magnetic moment is also equivalent to, and sometimes describes as, a magnetic dipole. The dipole terminology is used by analogy to an electric dipole (two electric charges of opposite sign, separated by a small distance. It can sometimes be useful to imagine a magnetic moment as a two opposite magnetic charges separated by a small distance in the direction of the moment vector.

#### 26.2 Magnetization and Field

Let's begin with Maxwell's equations

Gauss's Law 
$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0} \tag{2}$$
 Gauss (magnetism) – no monopoles 
$$\nabla \cdot \mathbf{B} = 0 \tag{3}$$
 Ampere + Maxwell 
$$\nabla \times \mathbf{B} = \mu_0 \left( \mathbf{j} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right) \tag{4}$$
 Maxwell-Faraday (no magnetic charge current) 
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{5}$$

Ampere + Maxwell 
$$\nabla \times \mathbf{B} = \mu_0 \left( \mathbf{i} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial \mathbf{E}} \right) \tag{4}$$

Maxwell-Faraday (no magnetic charge current) 
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
 (5)

The Electric E and Magnetic B fields are related to each other. Critical parameters are the charge density  $\rho$  and the current density j. They are asymmetric because there magnetic charge density and magnetic current density are zero ( $\rho_m = j_m = 0$ ).  $\mu_0 = 4\pi \times 10^{-7} \text{Hm}^{-1}$  is the permeability of free space,  $\varepsilon_0 = 8.854 \times 10^{-12} \text{Fm}^{-1}$  is the permittivity of free space, E is the electric field with units of  $(Vm^{-1})$  and B is the induction or magnetic flux density with units of Tesla (T). Care is required with the use of magnetic fields because **B** is the measured quantity, but **H** is the applied magnetic field strength with units of Am<sup>-1</sup>.

In a vacuum there is no magnetization and the magnetic field is described by the vector fields **B** and **H** which are related as

$$\mathbf{B} = \mu_0 \mathbf{H} \tag{6}$$

A magnetic material consists of many atoms with magnetic moments. The magnetization  $\mathbf{M}$  is defined as the magnetic moment per unit volume. Generally the vector quantity M is treated in the 'continuum approximation', which means on a lengthscale large enough that the fluctuations of individual atomic moments are not seen. Thus M is a smooth vector field, continuous everywhere except at the edges of the magnetic material.

In a magnetic material the relationship between **B** and **H** is more complicated because the magnetization also contributes to the density of magnetic flux lines. In general

$$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M}) \tag{7}$$

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The magnetization is also generally related to the applied field H, by the magnetic susceptibility  $\chi$ . In many materials the susceptibility is linear and this preserves the linear relation between B and H.

$$M = \gamma H \tag{8}$$

$$\mathbf{B} = \mu_0 (1 + \chi) \mathbf{H} = \mu_0 \mu_r \mathbf{H} \tag{9}$$

Where  $\mu_r$  is the dimensionless relative permeability. The magnetization can also cause the internal magnetic field  $(\mathbf{H}_i)$  within the material to be very different to the externally applied magnetic field  $(\mathbf{H}_a)$ . This is characterized by the demagnetizing factor N, which is dependent on both the shape of the sample and the direction of the field.

$$H_i = H_a - NM \tag{10}$$

$$H_i = H_a - NM$$
 (10)  
 $B_i = \mu_0 (H_i + M) = B_a + \mu_0 (1 - N)M$  (11)

### 26.3 Angular momentum and magnetic moments

Current loops are associated with the motion of electrical charges that also have a mass. Thus there is always a connection between magnetic moments and angular momentum. In atoms the magnetic moment  $\mu$  associated with an orbiting electron is parallel to the angular momentum L of that electron. The two quantities are proportional to each other and their constant of proportionality is known as the gyromagnetic ratio,  $\gamma$ .

$$\mu = \gamma L \tag{12}$$

The relationship between magnetic moment and angular momentum is observed by the Einstein-de Haas effect, where the magnetization of an iron rod causes its rotation, and by the Barnett effect where rotation of the rod causes its magnetization. Both of these effects are caused by conservation of total angular momentum.

### 26.4 Precession

Consider a magnetic moment  $\mu$  in a magnetic field **B**. The energy of the magnetic moment is given by

$$E = -\mu \cdot B \tag{13}$$

Such that the energy is minimum when the moment is parallel to the field. There will be torque G on the magnetic moment

$$G = \mu \times B \tag{14}$$

If there were no angular momentum associated with the moment then this torque would turn the moment towards the field. As the magnetic moment is always associated with angular momentum the change in  $\mu$  can be expressed as

$$\frac{d\boldsymbol{\mu}}{dt} = \gamma \boldsymbol{\mu} \times \boldsymbol{B} \tag{15}$$

The cross product means that the change in  $\mu$  is perpendicular to both  $\mu$  and B.  $\mu$  is not turned towards B, but instead precesses around it. This is analogous to the spinning of a gyroscope.

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## 27. Magnetic Moments on atoms

Now let us consider the magnetic moment on individual atoms, starting with the Bohr model.

### 27.1. Bohr model of one electron atoms

This is revision of material you have already covered in the 2nd year Atomic, Nuclear & Particle course, so we will just emphasize the relevant points here. You will have encountered the Bohr model of the hydrogen atom before. Although the Bohr model is an ad hoc model, it gives many of the correct results for the hydrogen atom (as we'll see later), and it is a useful starting point for understanding the orders of magnitudes of various atomic properties. In the Bohr model, an electron of mass  $m_e$  and charge -e moves in a circular orbit around a much heavier nucleus of charge +e, and the angular momentum is quantized in integer units of  $\hbar$ . To keep the electron in orbit with radius r and speed v, the centrifugal and electrostatic forces must balance:

$$\frac{m_e v^2}{r} = \frac{e^2}{4\pi\epsilon_0 r^2} \tag{16}$$

The quantization of angular momentum (L) is expressed simply as

$$L = m_e v r = n\hbar \tag{17}$$

where n is an integer.

#### 27.1.1 The size of an atom and the Bohr radius

From these two equations we find the orbital radius as:

$$r = n^2 \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} = n^2 a_0 \tag{18}$$

Here we have defined the quantity

$$a_0 = \frac{4\pi\epsilon_0 \, \hbar^2}{m_e e^2} \tag{19}$$

which is known as the *Bohr radius*. It depends only on fundamental constants and has the value 5.292 x10<sup>-11</sup>m. This is (approximately) the size of hydrogen in its ground state. For many-electron atoms the greater Coulomb attraction to the nucleus is largely offset by the electron-electron repulsion, and so other atoms are roughly the same size as this.

## 27.1.2 The speed of the electron and the fine-structure constant

From the same equations, we get the speed of the electron as

$$v = \frac{1}{n} \frac{e^2}{4\pi\epsilon_0 \hbar c} c = \frac{1}{n} \alpha c \tag{20}$$

where we've defined the dimensionless quantity

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} c \tag{21}$$

which is known as the *fine structure constant*. It is a fundamental constant and has the approximate value 1/137. We see that the speed of the electron in the ground state is  $\sim 1/137c$ . Because the speed is a small fraction of the speed of light, we can use non-relativistic quantum mechanics to a fairly good approximation. However, to understand the finer details of atomic structure we will need to consider relativistic effects.

# 27.1.3 The energy levels and the Rydberg constant

Adding together the kinetic energy,  $0.5m_ev^2$  and the potential energy,  $e^2/_{4\pi\epsilon_0r}$ , and using the above formulae for v and r, we get the total energy to be

$$E_n = \frac{1}{2n^2} \alpha^2 m_e c^2 = \frac{1}{n^2} 13.6 eV$$
 (22)

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The factor of 13.6eV (electron volts) is known as the Rydberg energy.

# 27.1.4 The magnetic moment and the Bohr magneton

Recall from Electromagnetism that an electric current I going round a closed loop of (vector) area S has magnetic moment vector,  $\mathbf{\mu}=\mathrm{IS}$  with direction is given by the right hand grip rule. The orbiting electron is a current loop, and associated with this current loop is a magnetic dipole moment. The current  $I=\frac{dq}{dt}$ . In the lowest energy state of the hydrogen atom (n=1), the time taken to complete a single orbit is  $t=\frac{2\pi a_0}{v}$  so the current circulating is  $I=\frac{e\alpha c}{2\pi a_0}$ . The current loop encloses an area  $S=\pi a_0^2$  are therefore the magnetic moment can be defined as

$$\mu = \frac{1}{2} e a_0 \alpha c = \frac{e \hbar}{2m_e} = \mu_B = 9.274 \times 10^{-24} \text{J} T^{-1}$$
 (23)

 $\mu_B$  is known as the Bohr magneton. It is a fundamental constant and it defines the magnetic moment of a single electron and sets the scale for the magnetic moments of atoms.

(Note that we have used the angular momentum condition of the ground state  $L = m_e vr = \hbar$  to simplify this equation.)

## 27.2 (Semi)-classical model of Langevin paramagnetism

Consider a moment  $\mu$  of fixed magnitude. (If it were due to classical currents (orbital currents) it should decay. So this model already assumes some quantization and is semi-classical. The energy of  $\mu$  in a B field is a function of  $\theta$ , the angle between  $\mu$  and B.

$$E(\theta) = -\mathbf{\mu} \cdot \mathbf{B} = -\mu B \cos \theta \tag{24}$$

We can compose a partition function for this system:

$$Z = \int_0^{\pi} e^{(-E(\theta)/k_B T)} (2\pi \sin \theta d \theta) = \int_0^{\pi} e^{(+\mu B \cos \theta/k_B T)} (2\pi \sin \theta d \theta)$$
 (25)

The probability that the moment lies in the cone between angles  $\theta$  and  $(\theta + d\theta)$  is represented by the area of the annulus on the unit sphere  $(2\pi \sin \theta d \theta)$ . The Helmholtz free energy is  $F = -k_B T \ln(Z)$ .

The average magnetic moment in the z-direction (B-direction) is

$$\mathbf{M} = \langle \mu_z \rangle = -\left(\frac{\partial F}{\partial \mathbf{B}}\right) = \frac{k_B T}{Z} \left(\frac{\partial Z}{\partial \mathbf{B}}\right)$$
 (26)

$$\langle \mu_z \rangle = \frac{k_B T}{\int_0^{\pi} e^{(+mB\cos\theta/k_B T)} (2\pi \sin\theta d\theta)} \int_0^{\pi} \frac{\mu \cos\theta}{k_B T} e^{(+\mu B\cos\theta/k_B T)} (2\pi \sin\theta d\theta)$$
 (27)

$$\langle \mu_z \rangle = \frac{1}{\int_0^\pi e^{(+mB\cos\theta/k_BT)}(\sin\theta d\,\theta)} \int_0^\pi \frac{\mu\cos\theta}{1} e^{(+\mu B\cos\theta/k_BT)}(\sin\theta d\,\theta)$$
 (28)

Let  $x = \mu B \cos \theta / k_B T = a \cos \theta$ .;  $a = \mu B / k_B T$ . Then

$$\langle \mu_z \rangle = \frac{\int_a^{-a} k_B T \frac{x}{B} e^{(x)} \frac{1}{a} dx}{\int_a^{-a} e^{(x)} \frac{1}{a} dx}$$
 (29)

Then reversing limits on both integrals we get

$$\langle \mu_z \rangle = \frac{k_B T}{B} \frac{\int_{-a}^a x e^{(x)} dx}{\int_{-a}^a e^{(x)} dx}$$
 (30)

$$\langle \mu_z \rangle = \frac{k_B T}{B} \left[ \frac{\left[ x e^{(x)} \right]_{-a}^{a} - \int_{-a}^{a} e^{(x)} dx}{\int_{-a}^{a} e^{(x)} dx} \right]$$
(31)

$$\langle \mu_z \rangle = \frac{\mu}{a} \left[ \frac{a(e^a + e^{-a})}{e^a - e^{-a}} - 1 \right]$$
 (32)

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$$\frac{\langle \mu_z \rangle}{\mu} = \coth(a) - \frac{1}{a} \tag{33}$$

$$\frac{\langle \mu_z \rangle}{\mu} = \coth\left(\frac{\mu B}{k_B T}\right) - \frac{k_B T}{\mu B} \tag{34}$$

The Langevin function  $L(a) = \coth(a) - \frac{1}{a}$  approximates to  $\frac{a}{3}$  for small values of a.

At this point it is useful to define the **saturation magnetization**,  $M_S$ , which is the maximum magnetization when all the moments are aligned, so that  $M_S = n\mu$  where n is the number of moments per unit volume. When we measure magnetization, according to the Langevin model we would find that for small B, high T

$$\frac{M}{M_S} = \frac{\langle \mu_z \rangle}{\mu} \approx \frac{\mu B}{3k_B T} \tag{35}$$

Using  $\chi = M/H \approx \mu_0 M/B$  which is valid in low-fields

$$\chi = \frac{n\mu_0\mu^2}{3k_BT} = \frac{C}{T} \tag{36}$$

This is the Curie law  $^1/_T$  susceptibility of a paramagnet, where C is sometimes called the Curie constant. One way to consider it is that as the temperature of a paramagnet rises, there is in increase in disorder in the spins and the entropy increases  $(S = -\left(\frac{\partial F}{\partial T}\right)_B)$ . A decrease in temperature corresponds to an increase of order and a reduction in the entropy. The fact is exploited for a magnetic cooling application called adiabatic demagnetization.

### 27.3 From Paramagnetism to Magnetic Order: The Weiss Molecular Field

Weiss suggested that an internal molecular field provided the stabilising ordering force in ferromagnets. This is a mean field theory from the localized moments on the atoms. The magnitude of the internal field acting on a given atomic moment was assumed to be proportional to the magnetisation of the local vicinity of that moment. This field was around 1000 Tesla!

According to the theory, a field of  $\mathbf{B} = \mathbf{B}_0 + \lambda \mathbf{M}$ , can be inserted into the previous model of paramagnetism where  $\lambda$  is a constant that parameterizes the strength of the molecular field, and is positive for a ferromagnet and negative for an antiferromagnets. It can be useful to consider  $\lambda$  as

$$\lambda = zI_{ii} \tag{37}$$

Such that z is the coordination number of an atom of position i (the number of equidistant atoms surrounding the ith atom at position j) and  $J_{ij}$  is the exchange interaction between the moments at i and j.

$$\frac{M}{M_S} = \frac{\langle \mu_z \rangle}{\mu} \approx \frac{\mu(\mathbf{B}_0 + \lambda \mathbf{M})}{3k_B T} \tag{38}$$

Essentially we are treating the system as a paramagnet which is experiencing an addition field. For ferromagnets a temperature emerges below which a spontaneous (B=0) magnetisation appears because the moments are aligned by the molecular field alone. Note that it is the alignment of moments that gives rise to the molecular field that causes the alignment, so this is something of a 'chicken-and-egg' model. Thus we need more formal quantum mechanics to fully explain ferromagnetism. Note also that M appears on both sides of the equation, so a numerical or graphical solution is required.

# 27.3.1 Ferromagnetism and the Weiss Model

Despite having limitations the Weiss model can predict some observed behaviour in magnetic materials. Above a critical temperature (The Curie temperature)  $T_C$ , thermal fluctuations are large enough to counteract the alignment of moments due to the molecular (or exchange) field, the zero field magnetization goes to zero and the behaviour is paramagnetic. This behaviour is shown for nickel in Figure 1 (left). In fact the mean field theory can predict a relation between  $T_C$  and  $J_{ij}$ .

$$T_C = 2zJ_{ii}J(J+1) (39)$$

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Additionally the Weiss model predicts that if M is plotted vs H/T then there will be a crossover in behaviour at T<sub>C</sub>. This is illustrated experimentally in Fig 1 (right). We will revisit the shape of these curves in the ferromagnetic state once we have introduced Quantum mechanics.

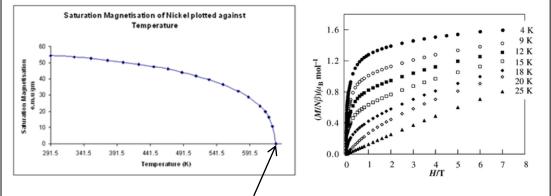


Figure 1: (left) Curie Temperature of Nickel. (Right) Magnetization vs H/T in a low temperature ( $T_c \sim 20K$ ) ferromagnet. At 4K (T <  $T_c$ ) in ferromagnetic state, at 25K (T >  $T_c$ ) it is in the paramagnetic state.

### 27.4 The Curie-Weiss Law

However the most important contribution of the Weiss model was in understanding magnetically ordered materials above their critical temperatures. We have seen for a paramagnet that

$$\chi = \frac{M}{H} = \frac{C}{T}$$
If we now add a Weiss molecular field to simulate the effect of the exchange interaction, then

$$\chi = \frac{M}{H} = \frac{C}{T - \theta_W} \tag{41}$$
 Where  $\theta_W$  is the Weiss constant. In a ferromagnet,  $\theta_W$  is positive and corresponds to  $T_C$ . In an antiferromagnet,

 $\theta_W$  is negative and the magnitude corresponds to the critical temperature, known as the Néel temperature,  $T_N$ . This is known as the Curie-Weiss law, which enables a moment sizes and interaction strengths to be extracted from a measurement of  $1/\chi$  vs T. C and  $\theta_W$  are the slope and the intercept and C can be related to the moment size using equation (36).

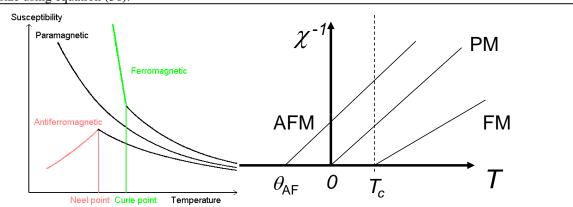


Figure 2: (left) Magnetic susceptibility vs Temperature in a paramagnet, and antiferromagnets and a ferromagnet. All obey the Curie-Weiss Law above their critical temperatures. (Taken from http://en.wikipedia.org/wiki/Magnetochemistry). The Curie Weiss Law is illustrated (right) by plotting inverse susceptibility vs Temperature, only using experimental data at temperatures above the critical temperature. In all cases the relationship is linear, the gradient is the Curie constant and by extrapolating to where the line crosses the Taxis (the intercept), the Weiss constant can be found. (In a pure paramagnet there is no critical temperature and the Weiss constant is zero).

### 28 Quantum Mechanics of Spin

Magnetization cannot be understood with purely classical mechanics. In the classical picture and applied B field would induce circular electron orbits that would have an associated moment. However a careful consideration of scattering at the edges of the material shows that the total moment associated with all the orbits cancels to zero. This is called the Bohr-van Leeuwen theorem. (This is beyond the scope of this course, but details can be found at for example Blundell p8.) Thus the properties of magnetic materials cannot be described without quantum mechanics.

### 28.1 Orbital and Spin Angular momentum

The electronic angular momentum that we calculated for the Bohr atom is known as the orbital angular momentum. In a real atom it depends on the electronic configuration, as described by the quantum numbers l and  $m_l$ , where  $m_l$  is the projection of the orbital angular momentum l on a fixed axis, which is usually taken to be the z-axis. The well-defined quantities are the projections on the z-axis and the square of the moments. The angular momentum operator  $\hat{L}^2$  has eigenvalue  $l(l+1)\hbar^2$  and operator  $\hat{L}_z$  has eigenvalue  $-m_l\hbar$ . Similarly the magnetic moment operator  $\hat{\mu}^2$  has eigenvalue  $l(l+1)\mu_B^2$  and operator  $\hat{\mu}_z$  has eigenvalue  $-m_l\mu_B$ . The component of the magnetic moment along the z-axis is  $-m_l\mu_B$  and the magnitude of the magnetic dipole is  $\sqrt{l(l+1)}\mu_B$ .

# 28.1.1 Zeeman Splitting of a spin

In addition each electron possesses an intrinsic angular momentum which is called spin. The spin quantum number of every electron is  $s=\frac{1}{2}$  and so this value is not usually listed in the electronic configuration. Any component of angular momentum can only have one of 2s+1 values,  $s\hbar$ ,  $(s-1)\hbar$ , ... ...,  $-s\hbar$ . The component of spin angular momentum is  $m_s\hbar$  ( $m_s$  is the projection of s on the z-axis). Thus for an electron with  $s=\frac{1}{2}$ , there are two possible values  $m_s=\pm\frac{1}{2}$ . The component of angular momentum along the z-axis is then  $+\hbar/2$ , which we call 'spin-up' and  $-\hbar/2$ , which we call 'spin-down'. The spin angular momentum gives rise to a magnetic moment, which can have a component along the z-axis of  $-g\mu_B m_s$  and a magnitude of  $\sqrt{s(s+1)}g\mu_B$  [the magnetic moment operator  $\mathbf{\hat{S}}^2$  has eigenvalue  $s(s+1)\hbar^2$ ]. The g-factor is a constant with a value of approximately 2, so the intrinsic magnetic moment of an electron is  $\approx \mp \mu_B$ . (There was no g-factor in the equivalent expression for orbital angular moment because in that case g=1.) The sign of the moment is inverted because the electron has negative charge, so the magnetic moment is antiparallel to the angular momentum. The energy of the electron in a magnetic field is

$$E = g\mu_B m_s B \tag{42}$$

The energy levels of an electron split in an applied field by  $g\mu_B B$ . This is called Zeeman splitting and the Zeeman energy.

# 28.1.2 Spin-orbit coupling

In general

$$\mu = -g \times \left(\frac{angular\ momentum}{\hbar}\right)\mu_B \tag{43}$$

Or more precisely we can write the magnetic moment operator

$$\hat{\mu} = \mu_B (g_L \hat{L} + g_S \hat{S}) \tag{44}$$

Where  $g_L=1$  for orbital angular momentum, and  $g_S=2$  for spin angular momentum. Now spin(S) and orbital (L) angular momentum may not be 'good quantum numbers', and instead J,  $m_J$  are the relevant quantities, where

$$J = L + S \tag{45}$$

and all momenta have units of  $\hbar$ . Now

$$\hat{\boldsymbol{\mu}} = -g_I \mu_B \hat{\boldsymbol{J}} \tag{46}$$

Where  $g_J$  is a constant, between 1 and 2, that depends on the relative strength of **S** and **L**. The angular momentum operator  $\hat{J}^2$  has eigenvalue  $j(j+1)\hbar^2$  and operator  $\hat{J}_z$  has eigenvalue  $m_J h$ . Similarly the magnetic moment operator  $\hat{\mu}^2$  has eigenvalue  $j(j+1)g_J^2\mu_B^2$  and operator  $\hat{\mu}_z$  has eigenvalue  $-g_J m_j \mu_B$ . The component of the magnetic moment along the z-axis is  $-g_J m_j \mu_B$  and the magnitude of the magnetic dipole is  $g_J \sqrt{j(j+1)}\mu_B$ .

It can be shown that the Landé g-factor

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$$g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} \tag{47}$$

It is enough for you to be aware of this. A full derivation can be found in Blundell, Appendix C9. Then the potential energy of a quantum dipole in a magnetic field  $B_Z$  is

$$E = -\boldsymbol{\mu} \cdot \boldsymbol{B} = +g_I m_I \mu_B B \tag{48}$$

This leads to a 'quantum' version of Langevin paramagnetism, where instead of considering a smoothly rotating angle of magnetization, we instead have a sum over the allowed values of  $m_J$ .

$$M = \langle \mu_z \rangle = \frac{\sum_{m_J = -J}^{m_J = +J} \left( -g_J m_J \mu_B \right) exp\left( \frac{-g_J m_J \mu_B B}{k_B T} \right)}{\sum_{m_J = -J}^{m_J = +J} exp\left( \frac{-g_J m_J \mu_B B}{k_B T} \right)}$$

$$(49)$$

By using the partition function

$$Z = \sum_{m_I = -J}^{m_J = +J} exp\left(\frac{-g_J m_J \mu_B B}{k_B T}\right)$$
(50)

Which produces a Brillouin function.

$$M = M_S B_I(\alpha) \tag{51}$$

where

$$M_S = ng_I \mu_B J \tag{52}$$

And n is the density of magnetic atoms (number per unit volume).

We define  $\alpha = g_I \mu_B J B / k_B T$  and the Brillouin function

$$B_{J}(\alpha) = \frac{2J+1}{2J} \coth\left(\frac{2J+1}{2J}\alpha\right) - \frac{1}{2J} \coth\left(\frac{\alpha}{2J}\right)$$
 (53)

For  $J = \infty$  the Brillouin function reduces to the Langevin function we derived previously.

$$B_{\infty}(\alpha) = L(\alpha) \tag{54}$$

For  $J = \frac{1}{2}$  the Brillouin function reduces to a tanh function

$$B_{\frac{1}{2}}(\alpha) = \tanh(\alpha) \tag{55}$$

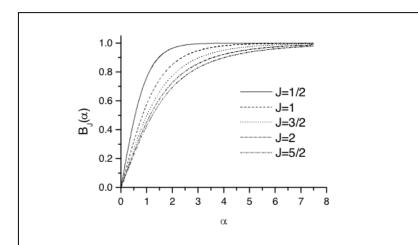


Figure 3: Brillouin function for different J. Taken from http://moxbee.blogspot.co.uk/

## 28.2 Magnetic Susceptibility of materials

The elements show a strength variation in magnetic properties, and the magnetic susceptibility of the elements fluctuates strongly in both sign and magnitude. This is illustrated in Figure 4, and here we explore the causes of this. Susceptibility is dimensionless, but it is an extensive quantity (it depends on how much material is present.

Previously we defined it as  $\mathbf{M} = \chi \mathbf{H}$  and here the susceptibility was per unit volume. It is often more usefully stated per unit mass  $(\chi_q)$ , or per mole  $(\chi_m)$ 

$$\chi_m = \chi V_m 
\chi_g = \frac{\chi}{\rho}$$
(56)

Where  $V_m$  is the molar volume and  $\rho$  is the density.

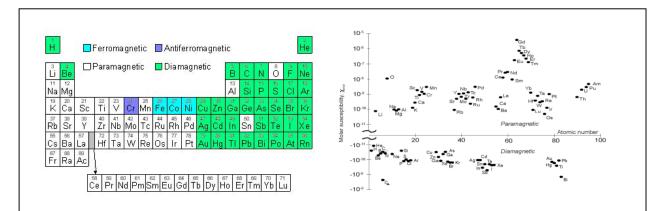


Figure 4: (left) Magnetic periodic table and (right) Molar Susceptibility of the elements vs Atomic Number. The ferromagnetic elements Fe, Co, Ni are not shown and have much larger positive susceptibility. Taken from Coey (http://magnetism.eu/esm/2009/slides/coey-slides-1.pdf)

## 28.3 A quantum atom in a magnetic field

To understand this variation in the susceptibility, first let us consider an atom in a magnetic field. A spin in a magnetic field has energy  $E = g\mu_B m_s B \approx \pm \mu_B B$ . In addition electrons will have an orbital angular momentum. Define the *i*th electron to have position  $r_i$  and momentum  $p_i$ . The total angular momentum is

$$\hbar L = \sum_{i} r_i \times p_i \tag{58}$$

Consider a Hamiltonian which is a sum of the electron kinetic and potential energies.

$$\widehat{H}_0 = \frac{\widehat{\boldsymbol{p}}^2}{2m_e} + V_i \tag{59}$$

We now add a magnetic field as a perturbation. This makes solving the Schrodinger equation much more difficult. You do not need to be able to evaluate the perturbation in field for the course, only be aware of the result. It is shown briefly here – a fuller explanation can be found in Coey (p88) or Blundell (p7).

$$B = \nabla \times A \tag{60}$$

Where  ${\bf A}$  is the magnetic vector potential. We choose a gauge such that  ${\bf A}$  and  $\widehat{{\boldsymbol p}}$  commute and

$$A(r) = \frac{B \times r}{2} \tag{61}$$

A charged particle moving in both electrical and magnetic fields is subject to the Lorentz force  $F = qE + v \times B$ . The momentum and kinetic energy are both the sum of the kinetic and potential terms. The (canonical) momentum becomes  $\hat{p} = \widehat{p_{kin}} + qA$  and the Hamiltonian becomes

$$\widehat{H} = \frac{1}{2m} (\widehat{p} + eA)^2 + V_i$$
(62)

becomes 
$$p = p_{kin} + qA$$
 and the Hamiltonian becomes
$$\widehat{H} = \frac{1}{2m_e} (\widehat{p} + eA)^2 + V_i$$
In our gauge we can expand  $(\widehat{p} + eA)^2 = \widehat{p}^2 + e^2A^2 + 2eA \cdot \widehat{p}$  so there are 3 terms in the Hamiltonian
$$\widehat{H} = \left[ \frac{\widehat{p}^2}{2m_e} + V_i \right] + \frac{e}{m_e} (A \cdot \widehat{p}) + \left( \frac{e^2}{2m_e} \right) A^2$$

or

$$\widehat{H} = \widehat{H}_0 + \widehat{H}_1 + \widehat{H}_2 \tag{64}$$

Where  $\widehat{H}_0$  is the original (unperturbed) Hamiltonian,  $\widehat{H}_1$  gives the paramagnetic response and  $\widehat{H}_2$  describes the small diamagnetic response.

The (orbital) paramagnetic term  $(\widehat{H}_1)$   $\widehat{H}_1 = \frac{e}{m_e} (\mathbf{A} \cdot \widehat{\mathbf{p}}) = \frac{e}{2m_e} (\mathbf{B} \times \mathbf{r}) \cdot \widehat{\mathbf{p}} = \frac{e}{2m_e} \mathbf{B} \cdot (\mathbf{r} \times \widehat{\mathbf{p}}) = \frac{e}{2m_e} \mathbf{B} \cdot \widehat{\mathbf{l}}$ (65)

Thus  $\hat{H}_1$  is the Zeeman interaction for the orbital moment. For a field along the z-axis it becomes

$$\hat{H}_1 = \left(\frac{\mu_B}{\hbar}\right) \hat{\boldsymbol{l}}_z B \tag{66}$$

The eigenvalues of  $\hat{\boldsymbol{l}}_z$  are  $m_l h$ .  $\widehat{H}_1$  thus gives an average orbital magnetic moment of

$$\langle m_z \rangle = \frac{\sum_{-l}^{l} - m_l \mu_B exp(m_l \mu_B B / k_B T)}{\sum_{-l}^{l} exp(m_l \mu_B B / k_B T)}$$

$$(67)$$

The orbital paramagnetic term, for any fully occupied shell or subshell of orbitals this tends to zero because  $\sum_{-l}^{l} - m_l$  tends to zero.

The diamagnetic term  $(\hat{H}_2)$ 

$$\widehat{H}_2 = \left(\frac{e^2}{2m_e}\right) A^2 = \left(\frac{e^2}{2m_e}\right) \left(\frac{\mathbf{B} \times \mathbf{r}}{2}\right)^2 = \left(\frac{e^2}{8m_e}\right) B^2 (x^2 + y^2)$$
(68)

For spherically symmetric orbitals  $\langle x^2 \rangle = \langle y^2 \rangle = \frac{1}{3} \langle r^2 \rangle$  and so the shift in the ground state energy corresponding to  $\widehat{H}_2$  is

$$\Delta E_0 = \left(\frac{e^2 B^2}{12m_e}\right) \langle r^2 \rangle \tag{69}$$

As the Magnetization

$$M = -\left(\frac{\partial F}{\partial B}\right) = \frac{N}{V} \left(\frac{-\partial \Delta E_0}{\partial B}\right) = \frac{N}{V} \frac{e^2 B}{6m_e} \sum_{i=1}^{Z} \langle r_i^2 \rangle$$
 (70)

Where F is the Helmholtz function. The diamagnetic susceptibility  $\chi = \left(\frac{M}{H}\right) \approx \frac{\mu_0 M}{B}$  the diamagnetic susceptibility is

$$\chi = \frac{N}{V} \frac{\mu_0 e^2}{6m_e} \sum_{i=1}^{Z} \langle r_i^2 \rangle \tag{71}$$

This relationship can be tested by making the assumption that the outer shell electrons dominate, all the electrons in the outer shell have the same radius which corresponds to the measured atomic radius, r, and the number of electrons in the outer shell is  $Z_{\text{eff}}$  such that

$$\sum_{i=1}^{Z_{eff}} \langle r_i^2 \rangle \approx Z_{eff} r^2 \tag{72}$$

This relationship that  $\chi_{dia} \propto Z_{eff} r^2$  gives an excellent fit to the diamagnetic susceptibility of many ions in solids – see Blundell p22.

### 28.4 Orbitals

As you have seen in your Quantum Mechanics courses, solving the Schrödinger equation for a many electron atom is challenging. However we can use a central potential theorem to separate the radial and angular parts of the wavefunction, and the strength of the central potential only affects the radial parts. The angular distribution of each electronic configuration (described by the quantum numbers, n, l,  $m_l$ ,  $m_s$ ) around the nucleus is the same for all atoms. These characteristic shapes (angular eigenfunctions for a central potential) are described by the 'spherical harmonics' or 'orbitals' and are shown in the polar plots in Figure 5.

Any magnetic response other than diamagnetism requires unpaired spins, or put another way partially-filled orbitals. The s-orbitals (l=0) and p-orbitals (l=1) are 'bonding orbitals' and are almost always fully occupied in stable compounds. (This is sometimes called the 'Octet rule'.) By the time the d and f orbitals of the same shell (n) start to fill up the nucleus has a much greater positive charge (Z), which is only partially screened by the other

# Handout 28: Quantum Mechanics of Spin

electrons in that shell. For example sodium has Z=11 and the electronic configuration  $1s^22s^22p^63s^1$  (or [Ne]3s<sup>1</sup>). Because the 10 [Ne] core electrons are much closer to the nucleus on average, they screen the nuclear charge almost perfectly, and so the effective charge (Zeff) felt by the 3s1 electron is  $Z_{eff}\sim 1$ . This means that the energy of the 3s1 orbital in sodium is similar to that in hydrogen, and so it is very unstable (reactive). In constrast iron has Z=26 and the electronic configuration  $1s^22s^22p^63s^22p^64s^23d^6$ . The 10 [Ne] core electrons still screen the nuclear charge almost perfectly, but there are now 16 electrons from unfilled (n=3,4) shells and so the effective charge (Z<sub>eff</sub>) felt by the electrons in the partially filled 3d subshell is  $Z_{\text{eff}} >> 1$ . This means that an electron in a 3d orbital in iron is much more closely bound to the nucleus, lower in energy and

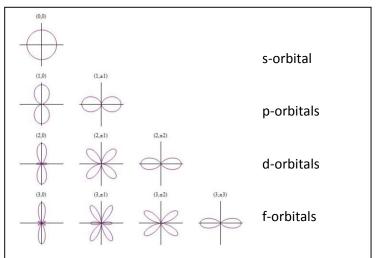


Figure 5: The angular distribution of the s, p, d and forbitals. Labels give  $(l, m_l)$  quantum numbers.

so far more stable than a 3d electron in hydrogen. For this reason the 3d, 4d, 5d, 4f and 5f orbitals are often described as 'core-like' orbitals that do participate much in bonding. This is why magnetism is usually associated with these particular orbitals.

#### 28.5 Hund's rules

Hund's three rules are processed in order. Once S, L and J have been found the state can be given a term symbol of the form  $^{2S+1}L_J$ . Here L is written not with a number, but with the characteristic letter that matches the orbital names, except it is the capital letter e.g. S for L=0, P for L=1, D for L=2, F for L=3 etc... 2S+1 is the spin multiplicity.

$$Maximise S (73)$$

(2) Consistent with (1); 
$$Maximise L$$
 (74)

(3) If shell 
$$<$$
 half full;  $J = |L - S|$  If shell  $>$  half full:  $J = |L + S|$ 

## 28.6 Orbital Quenching

The model we defined previously to define the magnetic moment in terms of the total angular momentum, J, works exceptionally well for f-orbital magnets, but does not work at all well for the most common (3d) magnets. The d-metal ions are often much better described if we set L~0, because there is an effect known as orbital quenching (the orbital angular momentum is reduced to zero, or close to zero).

Metal	3d (spins)					4s (spins)
Sc	1					↑ ↓
Ti	1	1				↑↓
V	1	1	1			1 ↑ ↓
Cr	1	1	1	1	1	1
Mn	1	1	1	1	1	1 ↑ ↓
Fe	↑↓	1	1	1	1	1 ↑ ↓
Co	↑↓	1 ↑ ↓	1	1	1	↑↓
Ni	1 ↑ ↓	1 ↑ ↓	1 ↑ ↓	1	1	1 ↑ ↓
Cu	↑↓	1 ↑ ↓	1 ↑ ↓	↑↓	1 ↑ ↓	1

Figure 6: Electron spin configurations for isolated atoms of the transition metals.

We expect that Hund's first rule should be satisfied, as shown in Figure 6, and that we should maximise the total spin on each atom. However, that relies on the near-degeneracy of the 5 d-orbital energy levels. Magnetic ions sit in an **environment** which we will assume to be crystalline and well-ordered. The electronic bonding and crystal symmetry will change the energy of the electron levels on the mangetic ion site. The effective field that causes

this is known as the '**crystal field**'. Only s-orbitals are spherically symmetric, all others have a pronounced angular dependence as shown in Figure 5. This crystal field removes the degeneracy of the energy levels, as shown in figure 7. Hund's 3<sup>rd</sup> rule assumes that the spin-orbit interaction is the most significant term in the Hamiltonian after Coulombic effects, but this is incorrect here. Thus in this case the effective dipole moment is better described by  $\mu_{eff} = 2\sqrt{S(S+1)}\mu_B$  than it is by  $\mu_{eff} = g_I\sqrt{J(J+1)}\mu_B$  as in equation (48).

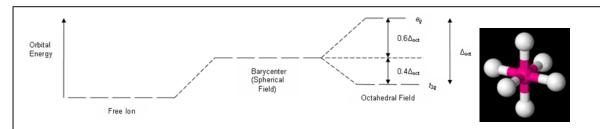


Figure 7: (left) Octahedral crystal field stabilization energy of the 3d orbitals and (right) schematic of a metal ion in an octahedral environment. The spherical field raises the average electron energy because there is a surrounding field of negatively charged ions. The octahedral field accounts for the spatial distribution of the surrounding negative charge. Some d-orbitals (labelled  $e_g$ ) have more probability density close to the negative charge and are raised in energy, whilst others (labelled  $t_{2g}$ ) have less probability density close to the charges and so are lowered in energy compared to a spherical charge distribution. Taken from http://upload.wikimedia.org/wikipedia/commons/8/83/Crystal\_Field\_Splitting\_4.png

## 29 Magnetic order and the Exchange interaction

### 29.1 Revisiting the Weiss Molecular Field

Now that we have the partition function and Brillouin function established, the Weiss Molecular field can explain the function form of a ferromagnets magnetization quite well.

Inserting the mean field of  $\mathbf{B} = \mathbf{B}_0 + \lambda \mathbf{M}$ , into the partition function in equation (50).

$$Z = \sum_{m_J = -J}^{m_J = +J} exp\left(\frac{-g_J m_J \mu_B(B_0 + \lambda M)}{k_B T}\right)$$
(76)

Thus the magnetization takes the form of the Brillouin function,

$$\frac{\mathbf{M}}{M_S} = B_J(\alpha_w) \tag{77}$$

$$\alpha_w = \frac{g_J J \mu_B (\pmb{B}_0 + \lambda \pmb{M})}{k_B T}$$
 which is a good description of the ferromagnetic behaviour in Figure 1. In this model the Saturation magnetization

is given by  $M_S = n\mu_B g_I J$  or (spin-only)  $M_S = n\mu_B 2S$ .

At low temperatures the magnetic order is self-sustaining. As the temperature is raised, thermal fluctuations begin to destroy the order (and so the molecular field) and at a critical temperature the order will be destroyed. To find the transition temperature equations (77) and (78) must be simultaneously solved by graphical methods. This is beyond the scope of this course, but the Curie temperature result obtained is

$$T_C = \frac{g_J \mu_B (J+1) \lambda M_S}{3k_R} = \frac{n \lambda \mu_{eff}^2}{3k_R}$$
 (79)

### 29.1.1 Implications of the Weiss Model

At low temperatures, where  $\lambda M$  is significant compared to  $k_B T$ , there will be a spontaneous magnetization in zero field. If a field is applied along the direction (z) and then removed, the spontaneous magnetization, and so the molecular field, will point along the z-axis. If a field is now applied along the direction (-z) and then removed the spontaneous magnetization, and so the molecular field, will point in the (-z) direction. Both of these magnetization states are stable (and in this model any other direction of magnetization will also be stable once set up.) In fact the magnetization along a certain axis (z) can take any value  $-M_S \le M_z \le M_S$ . This property is what enables ferromagnets to be used to store data and is usually described by the hysteresis loop (see Fig 8). M<sub>z</sub> can have any value because a large ferromagnet can break up into domains, as shown in Fig 8. The atomics moments within one domain are all parallel, but different domains point in different directions. The size of domains in ferromagnets typically range from 10nm to 10000nm in each dimension. (In a given material there is a typical domain sixe and little variation, but there is a strong variation in domain sizes between different materials.)

### 29.1.2 Why Weiss was right: The exchange interaction (and the birth of solid state magnetism)

In fact, the molecular field model strictly only applies to materials in which the magnetism come from electrons that are strongly localised at ion cores. Rare earth magnets are examples of such localised magnetism; materials such as iron, cobalt or nickel, in which the conduction and magnetic electrons are one and the same are known as itinerant magnets.

Let us examine the localised case in more detail and, in particular the origin of Weiss' molecular field. This field is a purely quantum phenomenon, resulting from spin state-dependence of the electrostatic energy due to the Pauli exclusion principle.

The exchange interaction is caused by a Coulombic perturbation to the single-electron Hamiltonian. This has been covered earlier in the Physics course, for example in the formation of singlet and triplet states in the Helium atom (2<sup>nd</sup> year Advanced Quantum Mechanics).

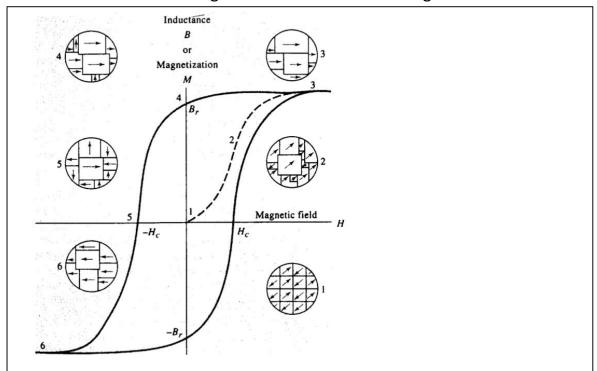


Figure 8: The ferromagnetic hysteresis loop. The sample starts in a 'virgin state' with zero net magnetization from a ferromagnetic domain pattern as shown in (1). A field is then applied until magnetic saturation is reached in the positive direction ( $M=M_s$ ) in state (3). The field is then removed to leave the remanent state (4) with remanent magnetization  $M=-M_r$  (or induction  $B_r$ ). Field is then applied in the negative direction until the magnetization reaches zero in state (5). The magnitude of the field needed to reach this state is called the coercive field ( $H_c$ ). Further field is then applied in the negative direction until saturation is reached in this direction ( $M=-M_s$ ) in state (6). If the field is now removed the remanent state has magnetization ( $M=-M_r$ ) Taken from from D. R. Askeland, "The Science and Engineering of Materials". PWS. 1994.

# 29.2 Heisenberg Exchange

Heisenberg worked out the effective Hamiltonian of spin-spin interactions. The energy of this exchange is given by

$$E_{ex} = -2J_{ij}(\mathbf{S}_i \cdot \mathbf{S}_j) \tag{80}$$

The exchange constant  $J_{ij}$  is related to the energy **difference** between singlet and triplet states (between antiparallel and parallel spins). IMPORTANT! Don't confuse this  $J_{ij}$  (often just written as J) with the total angular momentum (also "J"). Look out for the context when reading a textbook or other source. On the same atom,  $J_{ij}$  is usually positive (Hund's first rule). Between different atoms  $J_{ij}$  can be either positive (Ferromagnetic interaction) or negative (Antiferromagnetic interaction).

In fact there are many different types of exchange, some of which are illustrated in Figure 9. The sign of the interaction is governed by the orbitals involved in the overlap, the Pauli exclusion principle and Hund's rules. The strength of the interaction (magnitude of  $J_{ij}$ ) depends on the extent of the overlap and the separation of the spins.

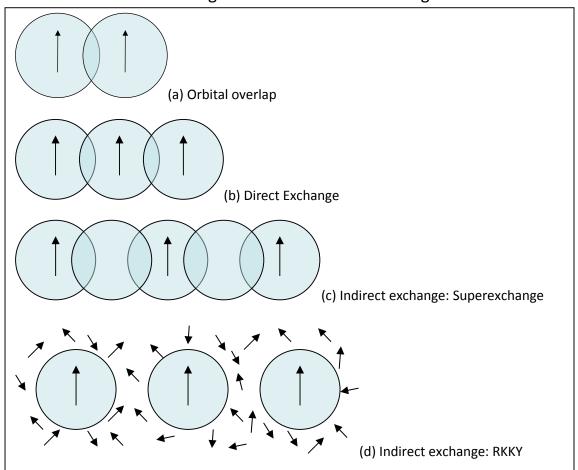


Figure 9: Exchange schematics. (a) Schematic of orbital overlap. The electrostatic energy of e<sup>-</sup> overlap region determined by relative orientation of neighbouring spins. (b) Direct exchange between directly overlapping orbitals. (c) Indirect exchange (Superexchange) between two magnetic atoms, mediated by orbitals in a single non-magnetic atom (e.g. Mn-O-Mn interaction in Manganese oxide, MnO.) (d) RKKY (Ruderman-Kittel-Kasuya-Yosida) exchange coupling of localized magnetic moments mediated by the conduction electrons.

## 29.3 Types of magnetic order

So far we have mostly looked at localised ferromagnetism, which we can describe as a very simple type of order, where the spin is on average the same on each atomic site, and so the unit cell of the material does not change. However many other types of magnetic order are possible. The exchange interaction gives rise to possibilities for ordered phases, including negative  $J_{ij}$  (antiferromagnetic coupling) and hence antiferromagnets and ferromagnets. Let us examine an antiferromagnetically ordered, or "broken symmetry" phase.

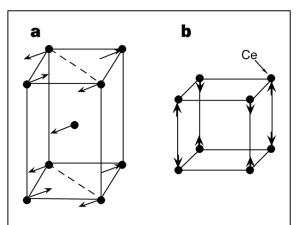


Figure 10: Spin structures in (a) CePd<sub>2</sub>Si<sub>2</sub> and (b) CeIn<sub>3</sub>, showing Ce atoms only (Mathur *et al.*, *Nature 1998*).

Handout 29: Magnetic order and the Exchange Interaction

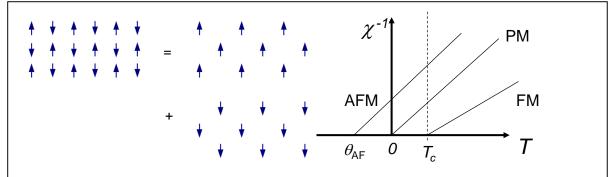


Figure 11: (left) Localized moments in the two sublattice model of antiferromagnetism. Right Inverse susceptibility vs T for a n AFM, PM and FM material.

### 29.4 Localised Antiferromagnetism

Antiferromagnets (AFM) show ordered, zero net moment up to the Néel temperature,  $T_N$ . Examples are shown in Figure 10. It can be due to multiple magnetic *sublattices* with different ordering directions, as illustrated in Figure 11.

Each sublattice (labelled (+) and (-)) has a molecular field dependent on opposite spin nearest neighbours.

$$B_{(+)} = -\lambda M_{(-)} \tag{81}$$

$$B_{(-)} = -\lambda M_{(+)} \tag{82}$$

The effect of the molecular field is to reduce the total flux density

$$\mathbf{B} = \mathbf{B_0} - \lambda \mathbf{M} \tag{83}$$

The total magnetization of one of the two sublattices and can also be estimated using a Weiss model treatment as in equation (77).

$$\boldsymbol{M}_{(\pm)} = \frac{M_S B_J \left( g_J J \mu_B | \lambda | \boldsymbol{M}_{(\mp)} \right)}{k_B T}$$
(84)

In a simple antiferromagnet the two sublattices are equivalent in everything except direction so that

$$|M_{(+)}| = |M_{(-)}| \tag{85}$$

As the two magnetizations are is opposite directions the net magnetization will be zero. It can also be useful to define a quantity known as the staggered magnetization, which is the difference between the two sublattices,  $M_{(+)} - M_{(-)}$  which is the order parameter for antiferromagnets. In the same fashion as equation (79) we can obtain a critical (Néel) temperature.

$$T_{N} = \frac{g_{J}\mu_{B}(J+1)|\lambda|M_{S}}{3k_{B}} = \frac{n|\lambda|\mu_{eff}^{2}}{3k_{B}}$$
 (86)

If the Brillioun function is expanded out one finds

$$B_J(\alpha) = \frac{(J+1)\alpha}{3J} + O(\alpha^3)$$
(87)

And so the magnetic susceptibility is

$$\chi = \lim_{B \to 0} \frac{\mu_0 M}{B} \propto \frac{1}{T + T_N} = \frac{1}{T - \theta_W}$$
(88)

This is the proof that the Curie-Weiss law really does describe the high temperature susceptibility of an antiferromagnet.

# 29.4.1 How do you prove that a zero-moment system isn't just a paramagnet?

The experimental proof of antiferromagnetic order was provided by *neutron diffraction* studies, pioneered by Brockhouse and Shull (1940s and 1950s, Nobel Prize 1994). They observed an extra peak from magnetic order below Néel temperature (neutrons "see" magnetic structure, due to their own magnetic moment). Because

antiferromagnetism is symmetry breaking, the magnetic unit cell is bigger than the structure (or chemical) unit cell, and so there are Bragg peaks that cannot be indexed in the structural unit cell. Figure 12 shows neutron diffraction patterns for MnO at room temperature and 80K (above and below  $T_{\rm N}$ .)

# 29.4.2 Ferrimagnets

If the two sublattices of an antiferromagnets have different magnitudes of magnetic moment, then these is a non-zero net magnetization below the Néel temperature. This means that it can be experimentally difficult to distinguish from a ferromagnetic, even though the exchange constant is negative. A material of this type is called a ferromagnet.

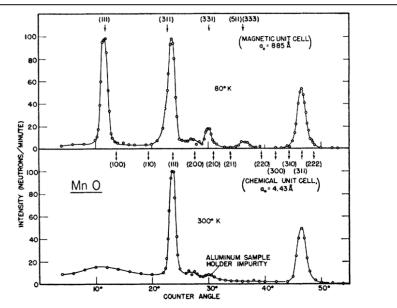


Fig. 1. Neutron diffraction patterns for MnO at room temperature and at  $80^{\circ}K_{\bullet}$ 

Figure 12: Original Neutron diffraction pattern for an antiferromagnets. C.G. Shull and J.S. Smart, Phys. Rev. 76 1256 (1949).

# Handout 30: Other types of order and Applications

30 Other types of Order and Magnetic Data Storage

## 30.1 Beyond the Localized Moment Model: The Itinerant electron model.

The most common ferromagnets (Fe, Ni, Co) don't obey the local moment model. In transition metals, the itinerant conduction electrons are often also those responsible for magnetism. Again we can regard, in a mean field way, an effective exchange energy that can stabilise a system towards ferromagnetism. This time we express it by adding a term to the energy of an electron, depending on its spin state (-ve sign for spin in direction of polarisation,  $\mathbf{M}$ , +ve for spins against  $\mathbf{M}$ ): This is known as the Stoner model of itinerant electron ferromagnetism.

$$E = \frac{\hbar^2 k^2}{2m} \pm \lambda \mu_B M \tag{89}$$

From this starting point, we can find that the magnetisation is a function of the electron Density of States (DoS) and so therefore, the effective moment per ion is not an integer number of Bohr magnetons (see Figure 13). Paramagnetism, diamagnetism and antiferromagnetic states are also possible within the itinerant electron model. AFM states correspond to finite wavevector ("q value") spin ordering.

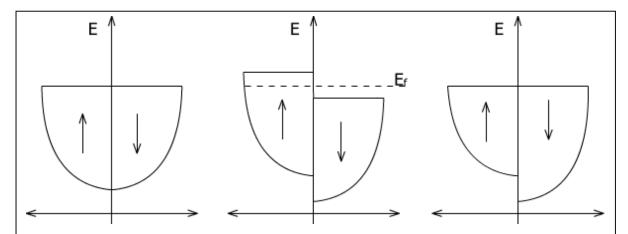


Figure 13: Spin Dependent Density of states (DoS). (left) Energy vs DoS in a paramagnetic metal. (middle) Zeeman energy splitting of the paramagnetic metal density of states. In this figure the total energy is unchanged and the net magnetization is zero. This middle case will not occur naturally because the spins can redistribute to a lower energy state. (right) Lowest energy state after Zeeman splitting of the spin-up and spin-down bands. The spins redistribute until the both bands are filled to the Fermi energy. Here there is a non-zero net magnetization and the total energy is lower than in the original paramagnetic case.

# 30.2 Single domain nanoparticles and Superparamagnetism

As stated in section 29.1, ferromagnetic domains have a natural size. This varies strongly between materials but is typically of the order of 100nm. As the size of particles decreases to this size, the ferromagnetic structure can no longer break up into domains and so all the moments in the material point in the same direction. These are single domain nanoparticles. The defining property of a ferromagnet is that the energy barrier to switching the magnetization is greater than  $k_BT$ . This energy barrier can either come from anisotropy or from the molecular field associated with the magnetization, and in both cases it is proportional to the volume of ferromagnetic material. If the size of single domain ferromagnetic nanoparticles is further decreases there comes a point where the volume of magnetic material is not sufficient to support a stable direction of magnetization in zero field at all temperatures. In that case, above the blocking temperature ( $T_B$ ) thermal activation can cause the magnetization direction to switch. If the energy barrier is  $K_1V$  where  $K_1$  is an anisotropy constant with units of  $kJ/m^3$  and V is the volume, then the blocking temperature  $T_B$  is given by

$$T_B \sim \frac{K_1 V}{k_B} \tag{90}$$

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And the rate of magnetic switching  $(1/\tau)$  can be described by an Arrhenius rate equation

$$\frac{1}{\tau} = \Omega \exp\left(\frac{-K_1 V}{k_B T}\right) \tag{91}$$

Where  $\Omega$  is the attempt frequency, which is up to  $10^9/s$ .

### 30.3 Superconductivity

Superconductivity was discovered by Kammerlingh Onnes in 1911. It is characterized by the expulsion of magnetic fields and exactly zero electrical resistance. The quantum mechanical nature of the superconducting phase transition is demonstrated by the Meissner effect, in which a superconductor expels magnetic field lines from its interior. There is an energy cost to this, so there is a maximum amount of field that can be excluded. Thus the phase transition has both a critical temperature  $T_C$ , and a critical field,  $H_C$ .

### 30.3.1 Classification

In fact there are two types of superconductors with distinct critical field behaviour: A type I superconductor has a single critical field above which there is no superconductivity. A type II superconductor has two critical fields, above the lower critical field ( $H_{C1}$ ) there is a mixed state where some magnetic flux enters the interior of the superconductor, yet superconductivity still persists, and above the upper critical field ( $H_{C2}$ ) there is no superconductivity. Superconductors are also sometimes classified by their  $T_C$  or my the mechanism of superconductivity. High Temperature superconductivity generally refers to materials that are superconducting above liquid nitrogen temperature (77K). A conventional superconductor is well described by the BCS theory (below) and an unconventional superconductor is not. As a general rule, high temperature superconductors are unconventional and low temperature superconductors are conventional.

## 30.3.2 Theories of Superconductivity

In 1950 Maxwell and Reynolds showed the  $T_C$  depends on the isotopic mass of the elements, which implies that lattice vibrations, specifically the electron-phonon interaction, play an important role. Aso in 1950, Ginzburg and Landau combined the theory of second-order phase transition and the Schrodinger equation and were able to explain a number of the properties of superconductors. In this theory the electrons which contribute to superconductivity form a superfluid and the superconductor is described by a coherence length and a penetration depth, which describes how the magnetic field decays inside the superconductor. A complete microscopic theory of superconductivity was developed by Bardeen, Cooper and Schreiffer in 1957 (BCS theory). In this theory the superconducting current is described as a superfluid of 'Cooper pairs' of electrons, which interact via the exchange of phonons.

### 30.3.3 Cooper pairs

Cooper pairing is a quantum effect, but the underlying physics can be understood with a classical argument. Usually, an electron in a metal acts as a free particle. Coulombic interactions cause it to be repelled by other electrons, and attracted to the positively charged nuclei in the solid. This attraction can slightly distort the lattice of charged ions, moving them towards the electron, and creating a build-up of positive charge in the vicinity. This positive charge can them attract other electrons, at long distances it can overcome the mutual repulsion of two electrons, leaving a favourable pairing energy, so the electrons pair up. The paired electrons do not need to be physically close together, in fact they can be thousands of atom apart, and many Cooper pairs can occupy the same space. The pairing energy is very weak (~10<sup>-3</sup>eV) and so the pairing is broken by thermal energy at most temperatures, and conventional (BCS) superconductivity is a very low temperature phenomenon. Because a Cooper pair is composed of two electrons, its total spin is an integer (0 or 1) and so it is a (composite) Boson rather than a Fermion, and a superconductor is a Bose-Einstein condensate. Cooper pairs are also responsible for the superfluids, such as helium-3.

# 30.4 Magnetic Data Storage

# Light and Matter 2015: *Matter and Magnetic Fields* (Will Branford) Handout 30: Other types of order and Applications

Magnetic storage was originally developed as 'sequential access memory' such as tape drives, audio and video cassettes. This means that when writing to or reading from the tape you must start and the start and then access the bits of information one after the other. Now this has been superseded by 'random access memory' in which the read/write head can be moved to address any magnetic bit as desired. In a hard disk this is achieved by storing the data on tracks of ferromagnetic recording layer on a spinning platter, and putting the read/write head on an arm which moves freely over the platter to any desired position. The write head is a solenoid with a soft ferromagnetic core, and the read head is a magneto-resistive sensor. There are two main designs, called longitudinal and perpendicular recording, as shown in Figure 14. The names refer to the orientation of the magnetic moments storing the information.

A very nice video describing the operation of a hard disk (shown in lecture) can be found at the following link: <a href="https://www.youtube.com/watch?v=4iaxOUYalJU">https://www.youtube.com/watch?v=4iaxOUYalJU</a>

