

## FoP3B Part I Lecture 12: Magnetism in Metals

In our discussion of long range magnetic ordering we implicitly assume that spins on neighbouring atoms interact *directly* with one another. In fact, the direct form of the exchange interaction is quite weak. In most cases the exchange interaction proceeds via an intermediary.

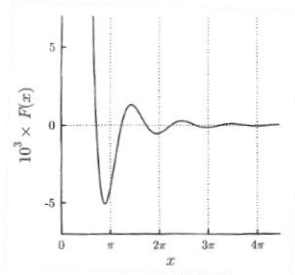


Figure 1

For example, in antiferromagnetic MnO magnetic moments on neighbouring  $\text{Mn}^{2+}$  ions interact via  $\text{O}^{2-}$  ions, a process known as *superexchange*. Similarly, in metals the conduction electrons serve as the intermediary in the so-called *RKKY interaction* (named after Ruderman, Kittel, Kasuya and Yosida). The exchange integral for the RKKY interaction has the form  $J_{\text{RKKY}}(r) \propto \frac{\cos(2k_F r)}{r^3}$ , where  $k_F$  is the Fermi wavenumber and  $r$  is the distance. Due to the cosine term the RKKY interaction has an oscillatory dependence (Figure 1).

In this final lecture we will look at magnetism in metals. Because the magnetic properties are determined by the conduction electrons we need to develop a *band theory of magnetism*. In particular, we will use these ideas to explore paramagnetism and ferromagnetism in metals. Diamagnetism in metals is slightly more complex and so will not be considered here<sup>1</sup>.

### Pauli Paramagnetism

The theory of paramagnetism in metals is due to Pauli. The density of states  $g(E)$  as a function of energy for the metal in the absence of an applied  $\mathbf{B}$ -field is shown in Figure 2a. The density of states curves for spin up and spin down electrons are shown separately. All the energy levels below the Fermi energy  $E_F$  are filled at absolute zero temperature. Assume a  $J = 1/2$  metal with  $\mathbf{L} = 0$  and  $S = 1/2$ . Using the fact that  $S_z = m_s \hbar = \pm 1/2 \hbar$  and  $g_s = 2$  the energy of a single spin in a magnetic field  $\mathbf{B}$  is:

$$-g_s \gamma \mathbf{S} \cdot \mathbf{B} = \mp \gamma \hbar B = \mp \mu_B B$$

Now consider applying a  $\mathbf{B}$ -field parallel to the spin up electrons. The spin down electron energies will increase by  $\mu_B B$ , while the energy of spin down electrons will be lowered by the same amount. Therefore, there is a relative energy shift  $2\mu_B B$  of spin up and spin down bands with respect to one another (Figure 2b). In order to have all energy levels below  $E_F$  occupied at absolute zero the spin down electrons within energy  $\mu_B B$  of  $E_F$  will be transferred to the spin up band (Figure 2b).

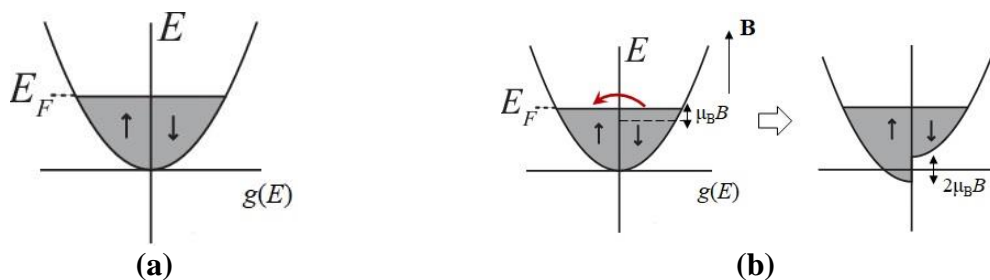


Figure 2: Spin up and spin down band structure in the (a) absence and (b) presence of a  $\mathbf{B}$ -field.

<sup>1</sup> The interested student is referred to section 7.6 on 'Landau diamagnetism' in Blundell's book *Magnetism in Condensed Matter*.

Assuming that the density of states at the Fermi energy  $g(E_F)$  does not change significantly within the energy range  $\mu_B B$  (a condition that is valid for small  $B$ ) the change in number of spin down electrons is  $\Delta n \downarrow = -\frac{1}{2} g(E_F) \mu_B B$ . The factor of  $\frac{1}{2}$  is included because  $g(E)$  is the density of states for *all* electrons, spin up and spin down.  $\Delta n \downarrow$  is equal in magnitude to the change in number of spin up electrons, i.e.  $\Delta n \uparrow = -\Delta n \downarrow = \frac{1}{2} g(E_F) \mu_B B$ . The magnetisation  $M = \mu_B (\Delta n \uparrow - \Delta n \downarrow) = g(E_F) \mu_B^2 B$ . For small magnetic fields the susceptibility  $\chi$ :

$$\chi = \frac{M}{H} \approx \frac{\mu_0 M}{B} = g(E_F) \mu_0 \mu_B^2$$

For a free electron metal the electron energy  $E = \frac{(\hbar k)^2}{2m}$  and  $\frac{dE}{dk} = \frac{\hbar^2 k}{m}$ . Therefore:

$$g(E) dE = 2 \frac{4\pi k^2}{(2\pi)^3} \frac{dk}{dE} dE = \frac{mk}{\pi^2 \hbar^2} dE$$

From lecture 1 the electron density  $n = (k_F^3/3\pi^2)$  so that:

$$g(E_F) = \frac{mk_F}{\pi^2 \hbar^2} = \frac{mk_F^3}{\pi^2 (\hbar k_F)^2} = \frac{3n}{2E_F}$$

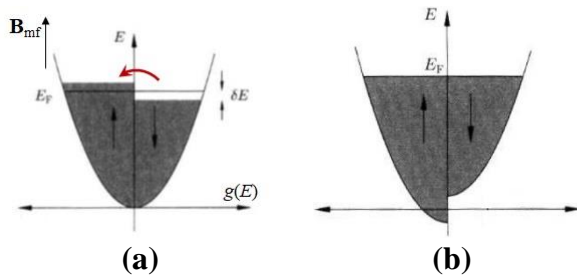
Substituting in the expression for susceptibility gives:

$$\chi = g(E_F) \mu_0 \mu_B^2 = \frac{3n \mu_0 \mu_B^2}{2E_F}$$

Note that  $\chi$  for Pauli paramagnetism is temperature independent, unlike the result for *localised* magnetic moments (Lecture 7) which predicted  $\chi \propto 1/T$  (Curie's law).

### ***Ferromagnetism and the Stoner criterion***

In ferromagnetism we have an internal molecular field  $\mathbf{B}_{mf}$  even in the absence of an external magnetic field. Let us assume that the direction of  $\mathbf{B}_{mf}$  is parallel to spin up electrons.



**Figure 3**

For a *spontaneous* magnetisation to take place spin down electrons within energy  $\delta E$  of  $E_F$  must be transferred to the spin up band. Two competing effects must however be taken into consideration: (i) increase in kinetic energy of transferred electrons (Figure 3a) and (ii) decrease in potential energy (Figure 3b).

Let us first consider the kinetic energy increase which is given by (the term within the curly brackets is the number of electrons transferred; Figure 3a):

$$\Delta E_{KE} = \left\{ \frac{1}{2} g(E_F) \delta E \right\} \delta E = \frac{1}{2} g(E_F) (\delta E)^2$$

Using the relation<sup>2</sup>  $dE = -\mathbf{B}(\mathbf{M}) \cdot d\mathbf{M}$  the potential energy decrease due to the molecular field  $B_{mf} = \lambda M$  is:

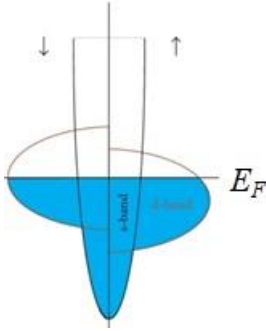
$$\Delta E_{PE} = - \int_0^M \lambda M' dM' = -\frac{\lambda M^2}{2}$$

From the previous analysis of paramagnetism the magnetisation:

$$M = \mu_B (\Delta n \uparrow - \Delta n \downarrow) = g(E_F) \mu_B \delta E$$

where the substitution  $\delta E = \mu_B B$  has been made.  $\therefore \Delta E_{PE} = -\frac{\lambda M^2}{2} = -\frac{1}{2} (\lambda \mu_B^2) [g(E_F) \delta E]^2$ . The term  $U = \lambda \mu_B^2$  is called the **Coulomb energy**, since it depends on  $\lambda$  and hence the molecular field which gives rise to the (Coulomb-based) exchange interaction. The net change in energy is therefore:

$$\Delta E = \Delta E_{KE} + \Delta E_{PE} = \frac{1}{2} g(E_F) (\delta E)^2 [1 - U g(E_F)]$$



**Figure 4:** density of states of  $s$  and  $d$ -bands

For ferromagnetism  $\Delta E < 0$ , which leads to the **Stoner criterion**  $U g(E_F) > 1$ . This condition predicts that ferromagnetism is favoured by a large Coulomb interaction ( $U$ ) and/or a high density of states at the Fermi level. The latter condition means ferromagnetism is more likely in transition metals (e.g. Fe, Co, Ni) where  $g(E_F)$  is large due to a narrow energy  $d$ -band (Figure 4). This means that electrons can be transferred from the low potential energy spin band without significantly increasing the kinetic energy of the transferred electrons.

<sup>2</sup> The equation  $dE = -\mathbf{B}(\mathbf{M}) \cdot d\mathbf{M}$  is slightly different to the more familiar expression  $-\mathbf{M} \cdot \mathbf{B}$  we have come across before for a fixed magnetisation  $\mathbf{M}$  in a magnetic field. The difference is due to the fact that the molecular  $\mathbf{B}$ -field is now a function of  $\mathbf{M}$  (i.e.  $\mathbf{B}_{mf} = \lambda \mathbf{M}$ )