

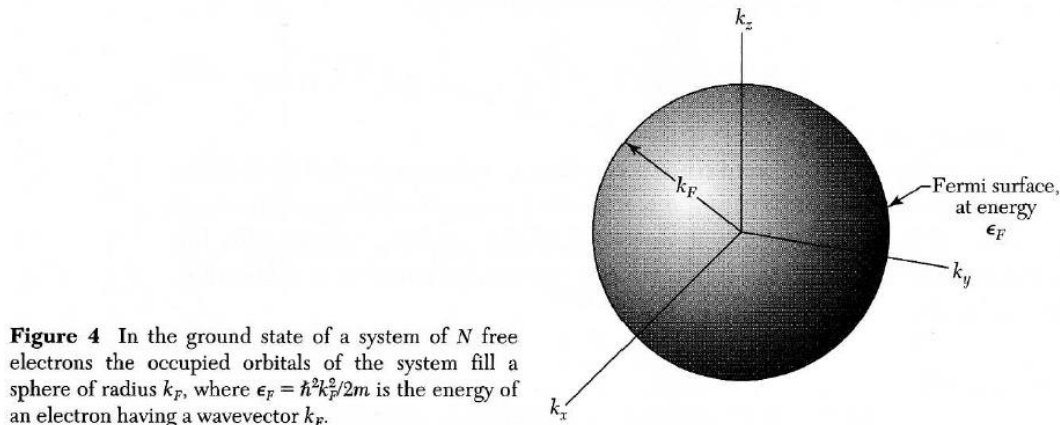
Level 3 Condensed Matter Physics Part 1

Example Workshop 1 – Solution

1. The Fermi energy is the highest occupied electron state in a system when it is in the ground state. From the solution of the free electron Schrodinger equation it can be shown that the energy of the electron state is related to its free electron wavevector by

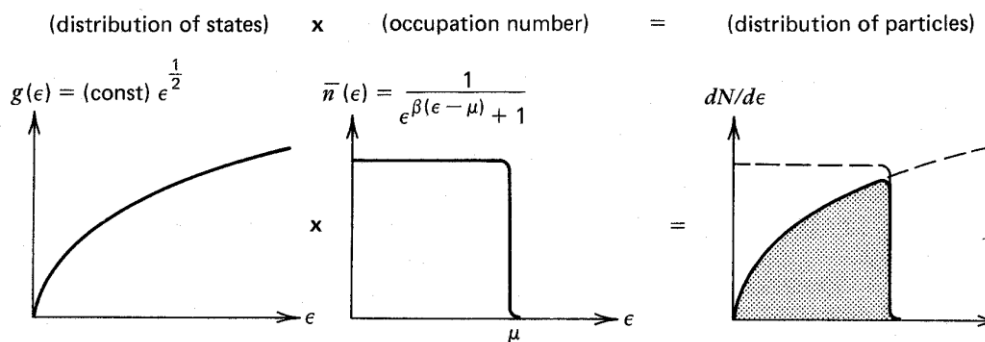
$$E = \frac{\hbar^2 k^2}{2m_e}$$

In three dimensions we have $k^2 = k_x^2 + k_y^2 + k_z^2$. The surface of constant energy in k -space, or reciprocal space, is therefore a surface of constant k^2 , or a sphere. This Fermi sphere is a sphere of radius equal to the Fermi wavevector, k_F , with all of the electron states on the Fermi surface having an energy equal to the Fermi energy, E_F , where $E_F = \frac{\hbar^2 k_F^2}{2m_e}$. This is shown below.

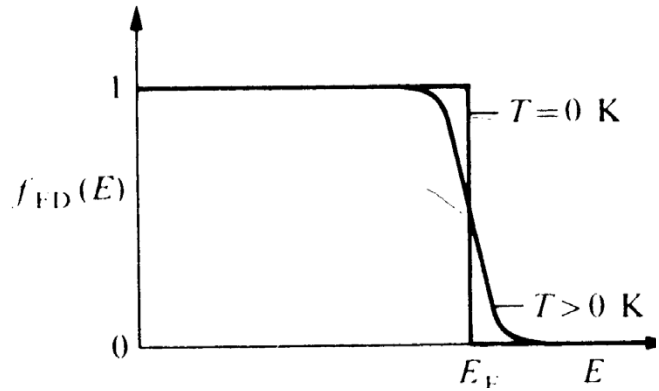


2. (a) The energy density of states function $g(E)$ describes the number of available energy states per unit volume of material, which can be occupied by electrons, per unit energy range. The probability of occupation of those states is given by the Fermi-Dirac equation (electrons are fermions). Multiplying these two together gives us the distribution of particles as a function of energy dN/dE where

$$N = \int_0^{\infty} g(E) f_{FD}(E) dE$$



(b) The Fermi energy is the energy of the highest occupied state in a metal (which is in its ground state). In a metal all energy states below the Fermi energy are occupied and all energy states above the Fermi energy are vacant. Note that at finite temperatures there is a thermal broadening of the transition from probability 1 to probability 0. The width of the transition is approximately $2k_B T$ around E_F . The diagram shows the behaviour of the Fermi-Dirac function at zero and finite temperatures.



(c) The Fermi energy is determined from the free electron density:

$$E_F = \frac{\hbar^2 k_F^2}{2m_e}$$

where the Fermi wavenumber is given by $k_F = (3\pi^2 n)^{1/3}$. The Fermi wavenumber can therefore be determined from the radius of the Fermi sphere. Substituting in the electron density gives $k_F = (3\pi^2 \times 6 \times 10^{28})^{1/3} = 1.21 \times 10^{10} \text{ m}^{-1}$ giving an energy of $E_F = \frac{\hbar^2 (1.21 \times 10^{10})^2}{2m_e} = 8.96 \times 10^{-19} \text{ J} = 5.6 \text{ eV}$. The Fermi velocity is determined by $v_F = p/m_e = \hbar k/m_e = 1.4 \times 10^6 \text{ ms}^{-1}$, which is fast but not relativistic. The Fermi temperature is then $T_F = E_F/k_B = \frac{8.96 \times 10^{-19}}{1.38 \times 10^{-23}} = 6.4 \times 10^4 \text{ K}$. This demonstrates that silver at room temperature is a quantum degenerate material. The thermal energy at room temperature (300 K) is just

$E = k_B T = 1.38 \times 10^{-23} \times 300 = 4.14 \times 10^{-21} \text{ J} = 26 \times 10^{-3} \text{ eV}$, which is much, much smaller.

3. The wavevector at the corner is longer than the wavevector at the midpoint of a side by the factor $\sqrt{2}$. As $E \propto k^2$ for a free electron, the energy is higher by $(\sqrt{2})^2 = 2$. In three dimensions the energy at a corner is higher by $(\sqrt{3})^2 = 3$ than at the midpoint of a face.

4. The energy eigenvalues are

$$E_F = \frac{\hbar^2 k^2}{2m}$$

The mean value over the volume of a sphere in k space is

$$\langle E \rangle = \frac{\int_0^{k_F} \frac{\hbar^2 k^2}{2m} (4\pi k^2) dk}{\left(\frac{4\pi}{3} k_F^3\right)} = \frac{3}{5} \frac{\hbar^2}{2m} k_F^2 = \frac{3}{5} E_F$$

The total energy of N electrons is

$$U_0 = \frac{3}{5} N E_F$$

Condensed Matter Physics 3

Example Workshop 2 – Solution

1. Properties of electrons in Bloch energy bands.

(a) The effective mass is given by

$$m_{eff} = \hbar^2 \left(\frac{d^2 E}{dk^2} \right)^{-1}$$

[This is the inverse curvature of the energy band].

(b) To determine the effective mass we need to evaluate:

$$\frac{d^2 E}{dk^2} = -Aa^2 \cos(ka)$$

$$\text{At } k = 0, \quad m_{eff} = \frac{-\hbar^2}{Aa^2 \cos(0)} = \frac{-\hbar^2}{Aa^2}$$

$$\text{At } k = \pi/a \quad m_{eff} = \frac{+\hbar^2}{Aa^2 \cos(\pi)} = \frac{+\hbar^2}{Aa^2}.$$

[Note the change in sign from centre and edge of Brillouin zone. This is due to the opposite curvature of the energy bands.]

(c) The group velocity of the electrons is given by $v_g = \frac{1}{\hbar} \left(\frac{dE}{dk} \right)$. From the E - k relation given,

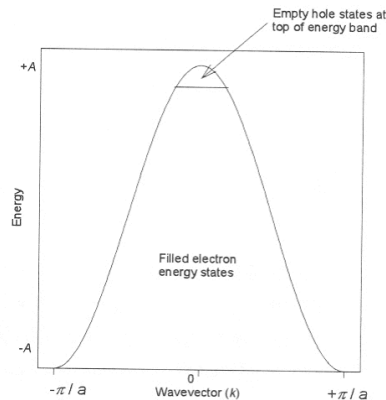
this is equal to 0 at both $k = 0$ and $k = \pi/a$.

(d) The total current carried by a completely full band is zero. (The average velocity distribution is zero, and this does not change under applied electric field – there are no empty electron states to move into so the average velocity distribution is still zero). The current carried by the nearly full band is then equal to the current carried by full band-current that would be carried by missing states = $0 - (-e)n_h v = +en_h v$.

(e) This is the same as a current that would be carried by n_h holes (of charge $+e$) per unit length moving with a velocity v .

(f) The diagram shows a sketch of the energy band from $k = -\pi/a$ to $+\pi/a$.

The vacant states at the top of the energy band can be thought of as full with positively charged holes.



2. Properties of electrons in Bloch energy bands.

(a) In one-dimensional free electron theory the allowed electron energy states are distributed over all energies

$$E(k) = \frac{\hbar^2 k^2}{2m}$$

The free electron wavefunctions are then of the form $\psi_k(x) = \exp(ikx)$ and they represent running (travelling) waves and carry momentum $p = \hbar k$. Consider a one-dimensional solid composed of a chain of atoms of lattice constant a . The Bragg condition $(k + G)^2 = k^2$ for diffraction of a wave of wavevector k then becomes (in one-dimension)

$$k = \pm \frac{1}{2} G = \pm n \pi / a$$

where $G = 2n\pi/a$ is a reciprocal lattice vector and n is an integer.

The first reflections and the first energy gap occur at $k = \pm \pi/a$. The region in k -space between $-\pi/a$ and $+\pi/a$ is the first Brillouin zone of the lattice. Other energy gaps occur for other values of the integer n .

(b) The wavefunctions at $k = \pm \pi/a$ are not the travelling waves of the form $\exp(i\pi x/a)$ or $\exp(-i\pi x/a)$ of free electrons we might expect. At these special values of k the wavefunctions are made up of equal parts of waves travelling to the right and waves travelling to the left. When the Bragg reflection condition $k = \pm \pi/a$ is satisfied by the wavevector, a wave travelling to the right is Bragg-reflected so as to travel to the left, and vice versa. Each subsequent Bragg reflection reverses the direction of travel of the wave. The time-independent result is a standing wave.

We can form two different standing waves from the two travelling waves $\exp(i\pi x/a)$, namely

$$\psi(+) = \exp(i\pi x/a) + \exp(-i\pi x/a) = 2\cos(\pi x/a)$$

$$\psi(-) = \exp(i\pi x/a) - \exp(-i\pi x/a) = 2i \sin(\pi x/a)$$

The standing waves are labelled (+) or (-) according to whether or not they change sign when $-x$ is substituted for x . Both standing waves are composed of equal parts of right- and left-directed traveling waves.

(c) The two standing waves $\psi(+)$ and $\psi(-)$ pile up electron density in different regions and therefore have different potential energies. The probability density ρ of a particle is $\psi^* \psi = |\psi|^2$. For the standing wave $\psi(+)$ we have $\rho(+) = |\psi|^2 \propto \cos^2 \pi x/a$. For the other standing wave $\psi(-)$ the probability density is $\rho(-) = |\psi|^2 \propto \sin^2 \pi x/a$, which concentrates electron density between the positive ion cores.

The wavefunctions at the Brillouin zone boundary $k = \pi/a$ are $\sqrt{\frac{2}{a}} \cos \pi x/a$ and $\sqrt{\frac{2}{a}} \sin \pi x/a$, normalised over unit length of line. Let us suppose that the potential energy of an electron in the one-dimensional crystal at point x is $U(x) = U \cos 2\pi x/a$

The first-order energy difference between the two standing waves is

$$\begin{aligned} E_g &= \int_0^a dx U(x) [|\psi(+)|^2 - |\psi(-)|^2] \\ &= \frac{2}{a} \int_0^a U \cos(2\pi x/a) (\cos^2 \pi x/a - \sin^2 \pi x/a) dx = U \end{aligned}$$

Thus, the energy gap is equal to the Fourier component of the crystal potential.

(d) We know for ordinary travelling waves that the group velocity is given by

$$v_{\text{group}} = \frac{d\omega}{dk}$$

As $E = \hbar\omega$ then it follows that

$$v_{\text{group}} = \frac{1}{\hbar} \frac{dE(k)}{dk}$$

For an electron at the bottom of an energy band in the nearly-free electron model $E = \frac{\hbar^2 k^2}{2m^*}$ so

$$v_{\text{group}} = \frac{1}{\hbar} \frac{d}{dk} \left[\frac{\hbar^2 k^2}{2m^*} \right] = \frac{\hbar k}{m^*} = \frac{p}{m^*} = v$$

Where p is the crystal momentum of the Bloch electrons.

Once we know the velocity of an electron in a band we can determine the current carried by a collection of electrons in an energy band. The current density is given by $j = ne\langle v \rangle$ where $\langle v \rangle$ is the average velocity of electrons in the band. Suppose we have M energy states in an energy band occupied by $2M$ electrons. We then have

$$\langle v \rangle = \frac{a}{\hbar} \int_{k=-\pi/a}^{k=\pi/a} \frac{dE}{dk} \frac{dk}{2\pi}$$

or,

$$\langle v \rangle = \frac{a}{2\pi\hbar} [E(\pi/a) - E(-\pi/a)]$$

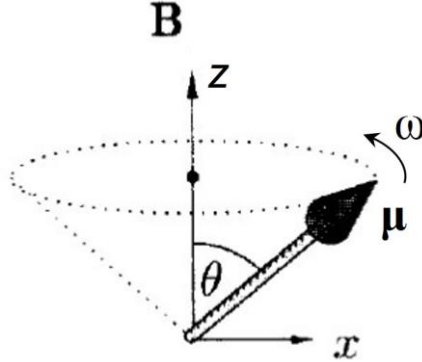
As we found earlier $k = \pm\pi/a$ are physically equivalent values of the Bloch wavevector. So $E(\pi/a) = E(-\pi/a)$ and $\langle v \rangle = 0$. If $\langle v \rangle = 0$ then $j = 0$ and the total current carried by the energy band is zero. This is an important result: a completely filled energy band makes no contribution to the current carried by a crystal.

Condensed Matter Physics 3

Example Workshop 3 – Solution

1. Larmor precession

(a) The schematic of the applied field \mathbf{B} and magnetic moment $\boldsymbol{\mu}$ is shown below:



From $\mathbf{B} = (0,0,B)$ and resolving the precession formula $\frac{d\boldsymbol{\mu}}{dt} = -\gamma(\boldsymbol{\mu} \times \mathbf{B})$ into individual components:

$$\frac{d\mu_x}{dt} = -\gamma B \mu_y \quad \dots (1a)$$

$$\frac{d\mu_y}{dt} = \gamma B \mu_x \quad \dots (1b)$$

$$\frac{d\mu_z}{dt} = 0 \quad \dots (1c)$$

Differentiating Eq. 1a w.r.t. t and substituting Eq. 1b gives:

$$\frac{d^2\mu_x}{dt^2} + (\gamma B)^2 \mu_x = 0 \quad \dots (2)$$

The solution to the above equation is of the form $\mu_x = C\sin(\gamma Bt) + D\cos(\gamma Bt)$, where C and D are constants that must satisfy the boundary conditions, namely $\mu_x = \mu\sin\theta$ at $t = 0$. This gives $C = 0$ and $D = \mu\sin\theta$, so that:

$$\mu_x = (\mu\sin\theta)\cos(\gamma Bt)$$

Using similar arguments, an Equation similar to Eq. 2 can be derived for μ_y , the solution for which is $\mu_y = C\sin(\gamma Bt) + D\cos(\gamma Bt)$. From the boundary conditions $\mu_y = 0$ at $t = 0$, it follows that $D = 0$. The value of C is obtained by noting that during precession $\sqrt{\mu_x^2 + \mu_y^2} = \mu\sin\theta$ (see figure), which implies $C = \mu\sin\theta$ and therefore:

$$\mu_y = (\mu\sin\theta)\sin(\gamma Bt)$$

From Eq. 1c the μ_z component is unchanged by precession, and therefore its value is (see figure):

$$\mu_z = \mu \cos \theta$$

(b) The magnetic moment components can be written as:

$$\begin{aligned}\mu_x &= (\mu \sin \theta) \cos(\omega t) \\ \mu_y &= (\mu \sin \theta) \sin(\omega t)\end{aligned}$$

where $\omega = \gamma B$. From the time-dependence of μ_x and μ_y it is clear that ω represents an angular frequency. Substituting $\gamma = e/2m$ for the gyromagnetic ratio gives the desired result:

$$\omega = \frac{eB}{2m}$$

(c) The energy of the magnetic moment is given by $E = -\boldsymbol{\mu} \cdot \mathbf{B}$. Since the angle θ between the vectors $\boldsymbol{\mu}$ and \mathbf{B} is constant during precession, there is no change in energy and therefore no work is done by the magnetic field.

2. Diamagnetism in Germanium.

(a) The diamagnetic response of Ge will be

$$\chi_d = -\frac{\mu_0 n_{Ge} Z_{Ge} e^2 \langle r_{Ge}^2 \rangle}{6m_e}$$

The number of Ge atoms per unit volume is $n_{Ge} = \frac{N_A \rho}{M_{Ge}}$ where Avogadro's number $N_A = 6.023 \times 10^{23}$, the molar mass, in kg is $M_{Ge} = 72.63 \times 10^{-3}$ kg and the density is $\rho = 5.323 \times 10^3$ kg m⁻³.

$$n_{Ge} = \frac{N_A \rho}{M_{Ge}} = \frac{6.023 \times 10^{23} \times 5.323 \times 10^3}{72.63 \times 10^{-3}} = 4.41 \times 10^{28} \text{ m}^{-3}.$$

$$Z_{Ge} = 32; \quad \sqrt{\langle r_{Ge}^2 \rangle} = 0.12 \text{ nm}$$

$$\begin{aligned}\chi_d &= -\frac{\mu_0 n_{Ge} Z_{Ge} e^2 \langle r_{Ge}^2 \rangle}{6m_e} \\ &= -\frac{4\pi \times 10^{-7} \times 4.41 \times 10^{28} \times 32 \times (1.6 \times 10^{-19})^2 \times (0.12 \times 10^{-9})^2}{6 \times 9.11 \times 10^{-31}} \\ &= -1.197 \times 10^{-4}\end{aligned}$$

(b) Curie's Law, $\chi_p = \frac{C}{T} = \frac{N \times 2.356 \times 10^{-22}}{T}$. At 2 K the magnetisation, M , is zero and as $M = \chi H$, with $H = 100 \text{ A m}^{-1}$, this implies that $\chi = 0$.

Therefore at 2 K, the total measured magnetic susceptibility is $\chi = \chi_p + \chi_d = 0$.

We assume that we take the diamagnetic response of the arsenic atoms to be the same as germanium atoms (a reasonable assumption as they are neighbours in the 4th row of the periodic table), we have the situation where the diamagnetic contribution of the germanium cancels the paramagnetic susceptibility of the arsenic atoms.

Substituting for χ_p and χ_d and rearranging for N gives

$$N = \frac{-\chi_d T}{2.356 \times 10^{-22}} = \frac{1.197 \times 10^{-4} \times 2}{2.356 \times 10^{-22}} = 1.02 \times 10^{18} \text{ m}^{-3}.$$

(c) Relative permeability is related to susceptibility by $\mu_r = 1 + \chi$. To achieve a value of 10^5 we first substitute in for χ , $\mu_r = 1 + \chi = 1 + C/T + \chi_d$, and rearranging for T gives

$$T = C/(\mu_r - 1 - \chi_d) = \frac{1.02 \times 10^{18} \times 2.356 \times 10^{-22}}{10^5 - 1 + 1.197 \times 10^{-4}} = 2.40 \times 10^{-9} \text{ K}$$

To calculate the flux density at this value for the relative permeability we use $B = \mu_r \mu_0 H$ and for the infinite solenoid, $H = nI$ where n is the number of turns per unit length and I is the current through the solenoid. Substituting in for H and rearranging gives an expression for the current

$$I = B/(\mu_r \mu_0 n) = 1/(10^3 \times 10^5 \times 4 \times \pi \times 10^7) = 7.96 \times 10^{-3} \text{ A}$$

3. Paramagnetism in a solid with angular momentum J .

(a) We have $J_z = m_J \hbar$, where $m_J = -J, -J + 1, \dots, J - 1, J$.

The z -component of the magnetic dipole moment is $\mu_z = -\gamma g_J (m_J \hbar) = -\mu_B g_J m_J$ and the energy in a magnetic field is $-\mu_z B = \mu_B g_J m_J B$. The partition function Z is therefore:

$$Z = \sum_{m_J=-J}^J \exp\left(\frac{\mu_B g_J m_J B}{kT}\right) = \sum_{m_J=-J}^J \exp(m_J x)$$

Using the formula for a geometric series to solve for Z :

$$\sum_{m_J=-J}^J \exp(m_J x) = e^{-Jx} [1 + e^x + \dots + e^{2Jx}] = e^{-Jx} \left[\frac{e^{(2J+1)x} - 1}{e^x - 1} \right] = \frac{e^{(J+1)x} - e^{-Jx}}{e^x - 1}$$

Dividing numerator and denominator by $e^{x/2}$:

$$Z = \frac{e^{(2J+1)x/2} - e^{-(2J+1)x/2}}{e^{x/2} - e^{-x/2}} = \frac{\sinh[(2J+1)x/2]}{\sinh[x/2]}$$

(b) The average magnetic moment is given by:

$$\langle \mu_z \rangle = \frac{-\mu_B g_J \sum_{m_J=-J}^J m_J \exp(m_J x)}{\sum_{m_J=-J}^J \exp(m_J x)}$$

From the definition of the partition function $Z = \sum_{m_J=-J}^J \exp(m_J x)$ it is clear that:

$$\frac{\partial Z}{\partial x} = \sum_{m_j=-J}^J m_j \exp(m_j x)$$

So that:

$$\langle \mu_z \rangle = \frac{-\mu_B g_J}{Z} \frac{\partial Z}{\partial x}$$

(c) The saturation magnetic moment $(\mu_z)_s = -\mu_B g_J J$ and consequently:

$$\frac{M}{M_s} = \frac{\langle \mu_z \rangle}{(\mu_z)_s} = \frac{1}{JZ} \frac{\partial Z}{\partial x}$$

Using the fact that $Z = \frac{e^{(2J+1)x/2} - e^{-(2J+1)x/2}}{e^{x/2} - e^{-x/2}}$ it follows that:

$$\frac{\partial Z}{\partial x} = \left(\frac{2J+1}{2} \right) \frac{\cosh[(2J+1)x/2]}{\sinh[x/2]} - \frac{1}{2} \frac{\cosh[x/2] \sinh[(2J+1)x/2]}{\sinh^2[x/2]}$$

Hence:

$$\frac{M}{M_s} = \frac{1}{JZ} \frac{\partial Z}{\partial x} = \left(\frac{2J+1}{2J} \right) \coth[(2J+1)x/2] - \frac{1}{2J} \coth[x/2]$$

Making the substitution $y = xJ$ we obtain the desired result.

(d) The Brillouin function:

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

For $J = \infty$ the first term is simply $\coth(y)$. For the second term:

$$\begin{aligned} \lim_{J \rightarrow \infty} \coth\left(\frac{y}{2J}\right) &= \lim_{J \rightarrow \infty} \frac{e^{\frac{y}{2J}} + e^{-\frac{y}{2J}}}{e^{\frac{y}{2J}} - e^{-\frac{y}{2J}}} \\ &= \frac{\left(1 + \frac{y}{2J}\right) + \left(1 - \frac{y}{2J}\right)}{\left(1 + \frac{y}{2J}\right) - \left(1 - \frac{y}{2J}\right)} = \frac{2J}{y} \end{aligned}$$

Substituting we obtain:

$$B_{\infty}(y) = \coth y - \frac{1}{y}$$

Condensed Matter Physics 3

Example Workshop 4 – Solution

1. Hund's rules and magnetic levels in paramagnetic Cu²⁺ ions

(a) Cu²⁺ (all other shells filled) d⁹

m_l	-2	-1	0	1	2
m_s	$\frac{1}{2}$	$\frac{1}{2}, -\frac{1}{2}$	$\frac{1}{2}, -\frac{1}{2}$	$\frac{1}{2}, -\frac{1}{2}$	$\frac{1}{2}, -\frac{1}{2}$

Hund's 1st rule: Total spin should be maximised, $S = \sum m_s = 1 \times \frac{1}{2} = \frac{1}{2}$

Hund's 2nd rule: Orbital angular momentum should be maximised consistent with the value of S,
 $L = \sum m_l = 2 + 2 + 1 + 1 + 0 + 0 - 1 - 1 - 2 = 2$

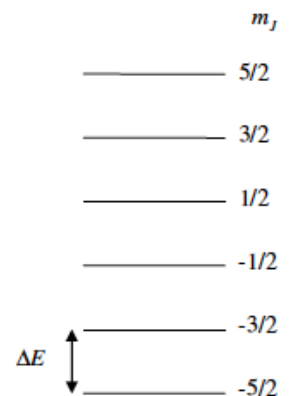
Hund's 3rd rule: The value of the total angular momentum, J , for a more than half filled shell is
 $J = L + S = 2 + \frac{1}{2} = \frac{5}{2}$

$\Delta E = g\mu_B B \Delta m_J$ where $\Delta m_J = 1$ and $B = 1$

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

$$g = 1 + \frac{\frac{5}{2}\left(\frac{7}{2}\right) + \frac{1}{2}\left(\frac{3}{2}\right) - 2(3)}{5\left(\frac{7}{2}\right)} = 1 + \frac{35/4 + 3/4 - 6}{35/4} = 1.20$$

$$\Delta E = 1.20 \times 9.27 \times 10^{-24} \times 1 \times 1 = 1.11 \times 10^{-23} \text{ J} = 6.95 \times 10^{-5} \text{ eV}.$$



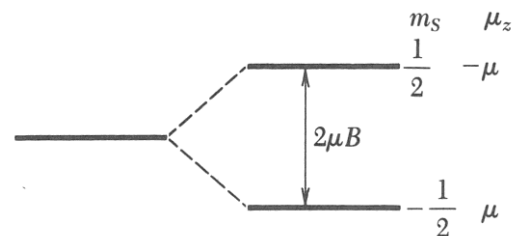
(b) If Cu²⁺ is orbitally quenched then $L = 0$

m_l	0	0	0	0	0
m_s	$\frac{1}{2}$	$\frac{1}{2}, -\frac{1}{2}$	$\frac{1}{2}, -\frac{1}{2}$	$\frac{1}{2}, -\frac{1}{2}$	$\frac{1}{2}, -\frac{1}{2}$

Then $J = S = \frac{1}{2}$. There are just two levels $-1/2$ and $+1/2$ with $g = 1 + \frac{\frac{1}{2}(\frac{3}{2}) + \frac{1}{2}(\frac{3}{2}) - 0}{1(\frac{3}{2})} = 1 + \frac{3/2}{3/2} = 2$

but with an increased (but still very small) splitting

$$\Delta E = 2 \times 9.27 \times 10^{-24} \times 1 \times 1 = 1.85 \times 10^{-23} \text{ J} = 1.16 \times 10^{-4} \text{ eV}.$$



2. Paramagnetism, Hund's rules and spin-orbit coupling in Sm^{3+} ions.

(a) Assuming L-S, or Russell-Saunders coupling we need only consider the outermost unfilled shell.
5 electrons in the f -shell: $l = 3$, $s = \frac{1}{2}$

m_l	-3	-2	-1	0	1	2	3
m_s			$+\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{2}$

Hund's 1st rule: Total spin should be maximised, $S = \sum m_s = 5 \times \frac{1}{2} = 5/2$.

Hund's 2nd rule: Orbital angular momentum should be maximised consistent with the value of S , $L = \sum m_l = 3 + 2 + 1 + 0 - 1 = 5$.

Ground state given by Hund's 3rd rule: The value of the total angular momentum, J , for a less than half filled shell is $J = |L - S| = 5 - \frac{5}{2} = 2\frac{1}{2}$.

(b) The magnitudes of the angular momenta are:

$$|S| = \{S(S+1)\}^{\frac{1}{2}}\hbar = \left\{2\frac{1}{2}\left(2\frac{1}{2}+1\right)\right\}^{\frac{1}{2}} = 2.96\hbar$$

$$|L| = \{L(L+1)\}^{\frac{1}{2}}\hbar = \{5(5+1)\}^{\frac{1}{2}} = 5.47\hbar$$

$$|J| = \{J(J+1)\}^{\frac{1}{2}}\hbar = \left\{2\frac{1}{2}\left(2\frac{1}{2}+1\right)\right\}^{\frac{1}{2}} = 2.96\hbar$$

The magnitudes of the magnetic moments are:

$$|\mu_S| = \{S(S+1)\}^{\frac{1}{2}}g_S\mu_B = 2.96 \times 2\mu_B = 5.92\mu_B$$

$$|\mu_L| = \{L(L+1)\}^{\frac{1}{2}}\mu_B = 5.47\mu_B$$

Calculating the Landé g -factor

$$g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} = 1.5 + \frac{8.75 - 30}{17.5} = 0.29$$

Therefore

$$|\mu_J| = \{J(J+1)\}^{\frac{1}{2}}g_J\mu_B = 2.96 \times 0.29\mu_B = 0.86\mu_B$$

(c) There are $2J+1 = 6$ levels. The energy of each level has the form

$$E = -\mu_J \cdot \underline{B} = m_J g_J \mu_B B$$

The magnetic flux density is,

$$B = \mu_0 H = 4\pi \times 10^{-7} \times 1.6 \times 10^6 = 2 \text{ T},$$

and the smallest separation between the two levels is

$$\Delta E = \Delta m_J g_J \mu_B B = 1 \times 0.29 \times 9.27 \times 10^{-24} \times 2 = 5.38 \times 10^{-24} \text{ J}.$$

The energy of the photons required to excite a transition between the two levels is $h\nu = \Delta E$. Therefore, the frequency of the electromagnetic radiation is $\nu = 5.38 \times 10^{-24} / 6.63 \times 10^{-34} = 0.81 \times 10^{10} \text{ Hz}$ i.e. 8.1 GHz. This corresponds to microwaves, which are typically used in electron spin resonance.

(d) We expect Curie's law to be applicable when $\frac{g_J \mu_B B}{k_B T} \ll 1$, (or usually, $B/T \ll 1$). For the solid containing Sm^{3+} ions,

$$\frac{g_J \mu_B B}{k_B T} = \frac{0.29 \times 9.27 \times 10^{-24} \times 2.5 \times 2}{1.38 \times 10^{-23} \times T} = 0.97/T.$$

hence at 300 K, $y = B/T = 0.97/300 = 3.3 \times 10^{-3}$ and we would expect Curie's law to be applicable. Whilst at $T = 1$ K, $y = B/T = 0.97/1 = 0.97$ and it is unlikely that Curie's law would be applicable.

(e) The maximum magnetisation value of the solid will occur when the saturation magnetisation, $|M_{\text{sat}}| = ng_J\mu_B J$. Therefore, the maximum magnetic moment of the solid will be $|m_{\text{sat}}| = Ng_J\mu_B J$ where N is the total number of atoms in the solid. Hence for 1 mole of solid containing Avogadro's number of atoms we expect the maximum magnetisation

$$|m_{\text{sat}}| = N_A g_J \mu_B J = 6.022 \times 10^{23} \times 0.29 \times 9.27 \times 10^{-24} \times 2.5 = 4.05 \text{ A m}^2$$

(f) The first excited state occurs at $J = |L - S + 1| = 3.5$. The spin-orbit energy of each state is $E_{SO} = \lambda(\underline{L} \cdot \underline{S})$ where $\underline{L} \cdot \underline{S}$ may be determined by starting with $\underline{J} = \underline{L} + \underline{S}$ and taking the dot product of itself:

$$\begin{aligned} \underline{J} \cdot \underline{J} &= (\underline{L} + \underline{S}) \cdot (\underline{L} + \underline{S}) \\ J(J+1) &= L(L+1) + S(S+1) + 2\underline{L} \cdot \underline{S} \end{aligned}$$

Re-arranging gives

$$\underline{L} \cdot \underline{S} = \frac{J(J+1) - L(L+1) - S(S+1)}{2}$$

Hence,

$$E_{SO} = \lambda \frac{J(J+1) - L(L+1) - S(S+1)}{2}.$$

For the ground state $S = 2\frac{1}{2}$, $J = 2\frac{1}{2}$, and $L = 5$

For the 1st excited state $S = 2\frac{1}{2}$, $J = 3\frac{1}{2}$, and $L = 5$

Therefore, as S and L are common to both states,

$$\Delta E_{SO} = E_{SO}(J = 3.5) - E_{SO}(J = 2.5) = \lambda \frac{[3.5(3.5 + 1) - 2.5(2.5 + 1)]}{2} = 28 \times \frac{7}{2} = 99.5 \text{ meV}$$

(g) From part (b) the effective number of Bohr magnetons, μ_{eff} , is

$$|\mu_J| = \{J(J+1)\}^{\frac{1}{2}} g_J \mu_B = \mu_{\text{eff}} \mu_B = 0.86 \mu_B$$

while the experimental value at room temperature is $1.5\mu_B$. The result of part (f) suggests that, given the room temperature thermal energy is about 26 meV, partial occupation of the first excited state is likely. This state has $S = 2\frac{1}{2}$, $J = 3\frac{1}{2}$, and $L = 5$

$$g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} = 1.5 + \frac{8.75 - 30}{7 \times 4.5} = 0.83$$

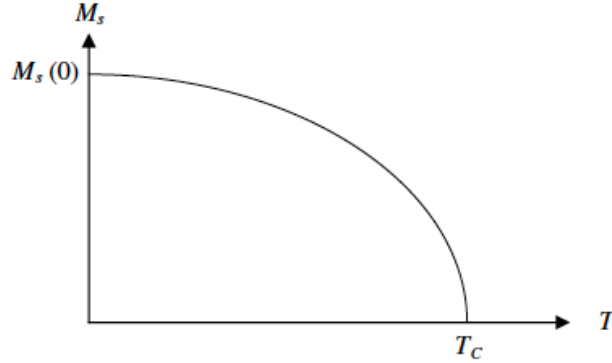
and $|\mu_J| = \{J(J+1)\}^{\frac{1}{2}} g_J \mu_B = \mu_{\text{eff}} \mu_B = 3.4 \mu_B$.

Condensed Matter Physics 3

Example Workshop 5 – Solution

1. Ferromagnetism

(a) See the figure below:



(b) Gd^{3+} ions have 7 electrons in the 4f shell hence,

m_s	1/2	1/2	1/2	1/2	1/2	1/2	1/2
m_l	-3	-2	-1	0	1	2	3

Hund's rules: $S = \sum m_s = 7 \times \frac{1}{2} = 3\frac{1}{2}$, $L = \sum m_l = 0$, $J = S = 3\frac{1}{2}$,

Hence the Landé g -factor $g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} = 2.0$.

Given that the solid has magnetic ions at the corners of a primitive cubic lattice of length $a = 0.75 \times 10^{-9}\text{m}$. The number of atoms per unit volume is therefore $N = 1/a^3 = 2.37 \times 10^{27}\text{m}^{-3}$.

i. At $T = 0\text{ K}$ the magnetisation is at its saturation value $M_{\text{sat}} = Ng_J\mu_B J$

$$M_{\text{sat}} = Ng_J\mu_B J = 2.37 \times 10^{27} \times 2.0 \times 9.27 \times 10^{-24} \times 3.5 = 1.53 \times 10^5 \text{Am}^{-1}$$

ii. Taking the alignment along the $[100]$ direction, $\theta_1 = 0^\circ$, $\theta_2 = \theta_3 = 90^\circ$, $\alpha_1 = \cos\theta_1 = 1$, $\alpha_2 = \cos\theta_2 = 0$, $\alpha_3 = \cos\theta_3 = 0$, and hence:

$$U_{\text{anis}} = 5.4 \times 10^5 (1^2 \times 0^2 + 1^2 \times 0^2 + 0^2 \times 0^2) + 5.1 \times 10^3 (1^2 \times 0^2 \times 0^2) = 0$$

Taking the alignment along the $[111]$ direction, $\theta_1 = \theta_2 = \theta_3 = 54.7^\circ$, $\alpha_1 = \alpha_2 = \alpha_3 = \cos\theta_1 = 0.577$, and hence:

$$U_{\text{anis}} = 5.4 \times 10^5 (3 \times (0.577)^4) + 5.1 \times 10^3 (0.577^6) = 1.8 \times 10^5 \text{Jm}^{-3}$$

i.e. the magnetisation alignment along the $\langle 100 \rangle$ axes leads to the lowest energy state and therefore, these axes are 'easy'. However, the $\langle 111 \rangle$ axes are 'hard' as magnetisation leads to high energy states.

(c) Since $\kappa > 0$ the summation $\sum_i [(S_i^x)^4 + (S_i^y)^4 + (S_i^z)^4]$ must be as large as possible to lower the energy. We have:

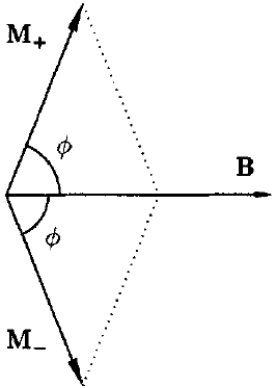
$$(S_i^x)^4 + (S_i^y)^4 + (S_i^z)^4 = \left[(S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 \right]^2 - 2 \left[(S_i^x S_i^y)^2 + (S_i^x S_i^z)^2 + (S_i^y S_i^z)^2 \right]$$

$$= S^4 - 2 \left[(S_i^x S_i^y)^2 + (S_i^x S_i^z)^2 + (S_i^y S_i^z)^2 \right]$$

Since S is a constant we need to minimise $\left[(S_i^x S_i^y)^2 + (S_i^x S_i^z)^2 + (S_i^y S_i^z)^2 \right]$. This is satisfied for S along one of the cubic axes, e.g. $S_i^x = S, S_i^y = 0, S_i^z = 0$. Hence $\langle 100 \rangle$ directions are the easy axes of magnetisation.

2. Antiferromagnetism and Ferrimagnetism

(a)



i. The exchange energy is given by $\sum_{i,j} -J_{\text{ex}} \mathbf{S}_i \cdot \mathbf{S}_j$. Treating the magnetisation as free vectors and making use of the fact that $J = S$ the exchange interaction has the form $-2J_{\text{ex}} M^+ M^- \cos(2\phi) = -2J_{\text{ex}} M^2 \cos(2\phi)$, where for an antiferromagnet $M = M^+ = M^-$. The magnetocrystalline anisotropy energy, $K \sin^2 \theta$, is minimum for $\theta = 0, \pi$ rad (i.e. spin 'up' and spin 'down'). Therefore, the anisotropy energy is $K \sin^2 \left(\frac{\pi}{2} - \phi \right) = K \cos^2 \phi$. The Zeeman energy is $-(M^+ + M^-) B \cos \phi = -2MB \cos \phi$. The total energy is therefore:

$$E = -2J_{\text{ex}} M^2 \cos(2\phi) + K \cos^2 \phi - 2MB \cos \phi$$

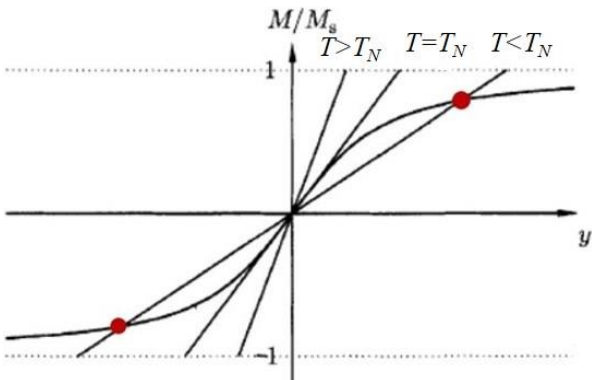
ii. The equilibrium angle ϕ is determined by $\frac{dE}{d\phi} = 0$.

$$\frac{dE}{d\phi} = 4J_{\text{ex}} M^2 \sin(2\phi) - K \sin(2\phi) + 2MB \sin \phi = 0$$

Using the fact that $\sin(2\phi) = 2 \sin \phi \cos \phi$, we have:

$$\cos \phi = \frac{MB}{K - 4J_{\text{ex}} M^2}$$

(b) i. The Weiss model treats the exchange energy due to neighbouring spins as an effective 'molecular field' B_{mf} . For example, the molecular field experience by a spin 'up' electron is due to the spin 'down' sub-lattice, and is proportional to the magnetisation of the spin 'down' sub-lattice, i.e. $B_{\text{mf}}^+ = -\lambda M^-$ and $B_{\text{mf}}^- = -\lambda M^+$, where the '+' and '-' superscripts refer to spin 'up' and spin 'down' sub-lattices.



The magnetisation must simultaneously satisfy the equations:

$$\frac{M^\pm}{M_s^\pm} = B_J(y^\pm) \text{ and}$$

$$y^\pm = \frac{g_J \mu_B J^\pm (B + B_{\text{mf}}^\pm)}{k_B T} = \frac{g_J \mu_B J^\pm (B - \lambda M^\mp)}{k_B T}$$

where B_J is the Brillouin function and B is the applied magnetic field. The graphical solution for zero applied field is shown opposite.

It is clear that in a ferrimagnet the magnetisation of a given sub-lattice is a function of its saturation magnetisation M_s and J angular momentum. Therefore, the temperature dependence of the magnetisation for the two sub-lattices will be different, such that at the compensation temperature the magnetisation of the spin ‘up’ sub-lattice will cancel that of the spin ‘down’ sub-lattice.

ii. In the paramagnetic phase under small applied \mathbf{B} -fields the term y^\pm is small. Using the approximation $B_J(y) \approx \frac{(J+1)}{3J} y$, we have:

$$\frac{M^\pm}{M_s^\pm} = B_J(y^\pm) \approx \frac{(J^\pm + 1)}{3J^\pm} y^\pm = \frac{g_J \mu_B (J^\pm + 1) (B - \lambda M^\mp)}{3k_B T}$$

Rearranging:

$$M^\pm = \frac{C_\pm}{T} (B - \lambda M^\mp) \text{ where } C_\pm = \frac{g_J \mu_B (J^\pm + 1) M_s^\pm}{3k_B}$$

Hence:

$$M^+ = \frac{C_+}{T} (B - \lambda M^-) = \frac{C_+ B}{T} - \frac{\lambda C_+}{T} \left[\frac{C_-}{T} (B - \lambda M^+) \right] \text{ or}$$

$$M^+ \left[1 - \frac{\lambda^2 C_+ C_-}{T^2} \right] = \left[\frac{C_+}{T} - \frac{\lambda C_+ C_-}{T^2} \right] B$$

Similarly, it easy to show that:

$$M^- \left[1 - \frac{\lambda^2 C_+ C_-}{T^2} \right] = \left[\frac{C_-}{T} - \frac{\lambda C_+ C_-}{T^2} \right] B$$

For weak magnetisations the susceptibility $\chi = \frac{M}{H} = \frac{\mu_0 M}{B}$. The susceptibility is due to both the spin ‘up’ and spin ‘down’ sub-lattices, i.e. $\chi = \frac{\mu_0 (M^+ + M^-)}{B}$. Hence:

$$\chi = \frac{\mu_0 \left[\frac{(C_+ + C_-)}{T} - \frac{2\lambda C_+ C_-}{T^2} \right]}{\left[1 - \frac{\lambda^2 C_+ C_-}{T^2} \right]} = \frac{\mu_0}{T^2 - \theta^2} [(C_+ + C_-)T - 2\lambda C_+ C_-]$$

where $\theta^2 = \lambda^2 C_+ C_-$.