Level 3 Condensed Matter Physics

Example Workshop 1

These are some questions to test your recall and understanding of Foundations of Physics 2B material. In the first couple of lectures I will be covering free electron theory and the nearly free electron model, using your newly-acquired quantum mechanical abilities. If you have any problems with the questions below, then maybe some reading of Simon (Solid State Basics) would be a good idea.

1. **Fermi energy**

   Give a definition of the *Fermi energy*. Describe, with the aid of a sketch, the Fermi surface in the free electron approximation for a three-dimensional solid. Explain why it has this shape.

2. **From FoP2B Exam 2015**

   (a) What does the *energy density of states* function $g(E)$ describe? How does the distribution of particles dN/dE vary with energy in three dimensions at low temperatures? Illustrate your answer with a diagram.

   (b) Explain the significance of the *Fermi energy* in a metal. Draw a diagram to illustrate the behavior of the Fermi-Dirac distribution function for a typical metal at both low temperatures close to absolute zero, and also at room temperature?

   (c) Silver has a free electron density of 6 x 10^{28} m^{-3} at 300 K. Determine the Fermi energy, Fermi velocity and Fermi temperature of free electrons in silver. Comment on your result in comparison to the thermal energy of electrons at room temperature.

3. **Square lattice, free electron energies.**
   Show that for a primitive square lattice (in two dimensions) that the kinetic energy of a free electron at a corner of the first Brillouin zone is higher than that of an electron at the midpoint of a side face of the zone by a factor of 2.
   What is the corresponding factor for a primitive cubic lattice in three dimensions?

4. **Kinetic energy of a free electron gas.**
   Show that the kinetic energy of a three-dimensional gas of N free electrons is
   $$U_0 = \frac{3}{5} N E_{\text{F}} \ .$$

Level 3 Condensed Matter Physics

Example Workshop 2

1. **Properties of electrons in Bloch energy bands.**

   This problem will look at the properties of electrons, and how they can be determined from knowledge of the *E-k* relationship (the energy band structure).

   (a) Write down the formula for the effective mass of an electron within an energy band *E(k)* of a simple one-dimensional crystal.

   (b) Obtain an expression for the effective mass of electrons in an energy band described by the energy wavevector relationship $E(k) = A\cos(ka)$ where $A > 0$ at the points *i)* $k = 0$, and *ii)* $k = \pi/a$.

   (c) What is the group velocity of electrons at $k = 0$ and $k = \pi/a$?

   (d) Consider the situation where the energy band is almost full except for a small number of states n_h per unit length near the top of the energy band ($k = 0$). Show that the total current carried by the band is equal to $+en_h v$ where v is the velocity of the missing electrons and $-e$ is the charge on an electron.

   (e) How do you interpret the result in part *(d)* in terms of positively charged pseudo-particles (called 'holes')?

   (f) Draw a simple sketch of the energy band structure for the first Brillouin zone indicating the position of electrons and holes as described in part *(d)*.

2. **The important ingredients of the quantum nearly free electron theory**

   (a) Consider a one-dimensional chain of atoms of lattice constant *a*. Starting from the energy - wavevector *E(k)* relationship for free electrons explain why the introduction of a periodic potential causes band gaps to open up at the wavevectors $k = \pm\pi/a$.

   (b) Show that the wavefunctions at $k = \pm\pi/a$ are not travelling waves of the form $\exp(\pm i\pi x/a)$ but are instead standing waves.

   (c) By considering the distribution of probability densities of these standing waves show that the energy gap, *U*, is equal to the Fourier component of the crystal potential.

   (d) Show that the group velocity of an electron at the bottom of an energy band in the nearly-free electron model is

   $$v_{\text{group}} = \frac{\hbar k}{m^*}$$

   where $\hbar k$ is the crystal momentum of the Bloch electrons and m^* is the effective mass of the electron. Use this to show that a completely filled band makes no contribution to the current carried by a crystal.

Level 3 Condensed Matter Physics

Example Workshop 3

1. **Larmor precession**

   A uniform magnetic field **B** is applied along the *z*-axis. A magnetic moment **μ** due to an electron lies along the *xz*-plane at angle θ to the **B**-field.

   (a) Derive the *x,y* and *z*-components of the magnetic moment **μ** as a function of time in the presence of the **B**-field.
   (b) Show that the magnetic moment precesses about the **B**-field at frequency:

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

   where *e* and *m* are the charge and mass of the precessing electron.
   (c) Comment on the work done by the **B**-field on the precessing magnetic moment.

2. **Diamagnetism in Germanium.**

   Germanium is a diamagnetic semiconductor. The diamagnetic susceptibility is independent of temperature. When arsenic dopant atoms are added to the solid they behave as hydrogenic donors and it is assumed that the donors act paramagnetically at all temperatures. The paramagnetic susceptibility of the As donors follows Curie's Law, $\chi = {}^C/_T$, where Curie's constant, $C = N$ x 2.356 x 10^{-22} K, and *N* is the number of donor atoms per unit volume.

   (a) Calculate the diamagnetic susceptibility of undoped germanium given that the root mean square radius of the atom is 0.12 nm. The density of germanium is 5.323 x 10^3 kg m^{-3}.

   [*Hint:* the diamagnetic susceptibility is given by:

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

   where *n* is the number of atoms per unit volume, *Z* the atomic number, $\langle r^2\rangle$ the mean square radius of an electron orbit and *m* the electron mass].

   (b) A sample of germanium is doped with As atoms. A measurement of the magnetisation for *H* = 100 A m^{-1} indicates that at 2 K, *M* = 0 A m^{-1}. Use this information to calculate the number of donor atoms per unit volume stating any assumptions that you have made.

   (c) The relative permeability, μ_r = 1 + χ, of iron is about 10^5. At what temperature would the arsenic doped germanium sample achieve such a value of μ_r? If a sample with this relative permeability was placed at the centre of a very long solenoid having 1000 turns of wire per metre, what solenoid current would

be required to produce a flux density of 1 Tesla?

Magnetic constant: $\mu_0 = 4\pi \times 10^{-7}$ H m^{-1}
Bohr magneton: $\mu_B = 9.27 \times 10^{-24}$ A m^2
Boltzmann constant: $k = 1.38 \times 10^{-23}$ J K^{-1}
Relative atomic mass of germanium is 72.63×10^{-3} kg
Atomic number of germanium is $Z_{Ge} = 32$
Avogadro's number $N_A = 6.022 \times 10^{23}$ mol^{-1}
Mass of electron $m_e = 9.11 \times 10^{-31}$ kg

3. **Paramagnetism in a solid with angular momentum J (to be completed after Lecture 7).**

The paramagnetic susceptibility in the classical limit (Langévin theory) and a $J = \frac{1}{2}$ solid have been derived in the lectures. This question will examine paramagnetic susceptibility for intermediate values of J using quantum mechanics. The derivation is an extension of the methods used for a $J = \frac{1}{2}$ solid.

(a) For a given value of J write down the values the z-component, J_z, can take. Show that the partition function Z for the solid in a magnetic field B is:

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

where $x = g_J \mu_B B/kT$, with g_J being the Landé g-factor and m_J the quantum number for J_z.

(b) Show that the average magnetic moment $\langle \mu_z \rangle$ is given by:

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

(c) Hence if $y = xJ$ show that:

$$\frac{M}{M_s} = B_J(y)$$

where M_s is the saturation magnetisation and the Brillouin function is given by:

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

(d) Show that for $J = \infty$ the result in (c) leads to the Langévin equation:

$$\frac{M}{M_s} = \coth y - \frac{1}{y}$$

Level 3 Condensed Matter Physics

Example Workshop 4

1. **Hund's rules and magnetic levels in paramagnetic Cu^{2+} ions**

   (*a*) Calculate the principal quantum numbers S, L, and J of a Cu^{2+} ion
   ($1s^2 2s^2 2p^6 3s^2 3p^6 3d^9$) using Hund's rules. Make a sketch of the (ground state energy)
   levels associated with the magnetic moment of a Cu^{2+} ion in a magnetic field of flux
   density of 1 Tesla. Label each of the levels with the quantum number representing the
   projection of the total angular momentum on the field direction. Calculate the energy
   separation between the levels.

   (*b*) How would your answer differ in Cu^{2+} was orbitally quenched (i.e. $L = 0$ and hence
   $J = S$)? Again calculate Make a sketch of the (ground state energy) levels associated with
   the magnetic moment of a Cu^{2+} ion in a magnetic field of flux density of 1 Tesla. Label the
   levels and calculate the energy separation between the levels.

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

   (a) Calculate S, L and J of the ground state of an Sm^{3+} ion ($4f^5$) stating any assumptions
   that you make.

   (b) Calculate the magnitudes of the atomic spin, orbital and total angular momenta of
   the Sm^{3+} ion in its ground state (in units of $\hbar$). What are the magnitudes of the three
   corresponding magnetic moments (in units of μ_B).

   (c) State the number of energy levels that correspond to the magnetic moment of an
   Sm^{3+} ion in the presence of a magnetic field. Calculate the smallest energy separation
   between two of these levels if the applied magnetic field strength is $H = 1.6 \times 10^6$ A m^{-1}.
   What frequency of electromagnetic radiation could be used to excite a transition
   between two of these levels?

   (d) Assuming the ions are magnetically isolated from one another in the solid, comment
   on the applicability of Curie's law to the paramagnetic susceptibility at 1 K and 300 K
   (**Hint**: Use the condition adopted to obtain Curie's law from the Brillouin function form
   of the magnetisation).

   (e) Calculate the maximum measureable magnetisation of a solid consisting of 1 mole of
   Sm^{3+} ions.

   (f) The spin-orbit interaction that couples $\underline{S}$ and $\underline{L}$ gives rise to the ground state (of part
   (a)) and to several excited states. The spin-orbit energy $E_{SO} = \lambda(\underline{L} \cdot \underline{S})$. If the spin-orbit
   coupling constant for Sm^{3+} is $\lambda = 28$ meV calculate the energy difference between the
   ground state and the first excited state. (**Hint**: Take the dot product of $\underline{J} = \underline{L} + \underline{S}$ with
   itself and re-arrange to obtain an expression for $\underline{L} \cdot \underline{S}$).

   (g) The effective number of Bohr magnetons of Sm^{3+} at room temperature is 1.5.
   Compare this value to your result from part (*b*) and explain any difference there may be.

(**Hint**: The effective number of Bohr magnetons, μ_{eff}, is defined via the equation $|\mu_J| = \{J(J+1)\}^{\frac{1}{2}} g_J \mu_B = \mu_{\text{eff}} \mu_B$).

$e = 1.60 \times 10^{-19} \text{ C}$
$\mu_B = 9.27 \times 10^{-24} \text{ J T}^{-1}$
$\mu_0 = 4\pi \times 10^{-7} \text{ H m}^{-1}$
$k_B = 1.38 \times 10^{-23} \text{ J K}^{-1}$
$h = 6.63 \times 10^{-34} \text{ J s}^{-1}$
$N_A = 6.022 \times 10^{23}$
$m_e = 9.11 \times 10^{-31} \text{ kg}$

Level 3 Condensed Matter Physics

Example Workshop 5

1.   Ferromagnetism

(*a*) Sketch the general form of the temperature dependence of the spontaneous magnetisation of a ferromagnet. Indicate both the Curie temperature, T_c, and the saturation magnetisation, M_{sat}, on you sketch.

(*b*) A ferromagnetic solid contains Gd^{3+} ions arranged in a primitive cubic arrangement with a unit cell of 0.75 nm. Each gadolinium ion has 7 electrons in its *4f* shell. At very low temperatures close to absolute zero the magnetocrystalline anisotropy is described by the constants K_1 = 5.4 x 10^5 J m^{-3} and K_2 = 5.1 x 10^3 J m^{-3}. Use this information to:

i. Calculate the saturation magnetisation of the ferromagnetic solid at absolute zero.

ii. Demonstrate that <100> directions in the crystal are '*easy*' axes for magnetisation, whereas <111> are '*hard*' directions for magnetisation.

 (**Hint**: For a cubic crystal the anisotropic energy density is:
$$U_{anis} = K_1(\alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_3^2 + \alpha_2^2\alpha_3^2) + K_2(\alpha_1^2\alpha_2^2\alpha_3^2)$$

where $\alpha_1 = \cos\theta_1$, $\alpha_2 = \cos\theta_2$ and $\alpha_3 = \cos\theta_3$, are the direction cosines of the magnetisation with respect to the [100], [010] and [001] directions).

(c) The Hamiltonian for a cubic ferromagnetic material is given by:

$$\widehat{H}_{mag} = \sum_{i,j} -J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - \kappa \sum_i \left[(S_i^x)^4 + (S_i^y)^4 + (S_i^z)^4 \right]$$

where the first term represents the exchange interaction and the second term is the magnetocrystalline anisotropy, with κ being a positive constant. S_i^x, S_i^y, S_i^z are the *x,y,z* components of the spin angular momentum for atomic site '*i*'. If the spin angular momentum magnitude S is constant for all atomic sites, show that the easy axis for magnetisation is along the cubic <100> directions.

2.   Antiferromagnetism and Ferrimagnetism

(a)
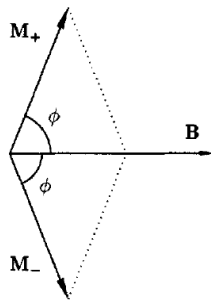
The figure opposite shows the stable configuration for an antiferromagnet with external **B**-field applied at right angles to the easy magnetisation axis. The magnetisations M⁺ and M⁻ of the spin 'up' and spin 'down' sub-lattices are at an angle ϕ to the **B**-field.

i. Write down an expression for the total energy, taking into account contributions due to the exchange interaction, magnetocrystalline

anisotropy and (Zeeman) potential energy. You may assume that $J = S$ and that the anisotropy energy density has the form $K\sin^2\theta$, where K is a positive constant and θ is the angle between the magnetisation vector and easy axis of the crystal.

ii. Using your expression for the total energy determine the equilibrium value for the angle ϕ.

(b) A ferrimagnet displays antiferromagnetic ordering, but with the magnetisation of the spin 'up' and spin 'down' sub-lattice being unequal. Ferrimagnets therefore have a net magnetisation (unlike antiferromagnets). For some ferrimagnets it is found that at the so-called 'compensation temperature' the net magnetisation drops to zero.

    i.   Using the Weiss model explain qualitatively the origin of the compensation temperature.

    ii. At high temperature the ferrimagnet undergoes a transformation to the paramagnetic state. Show that the paramagnetic susceptibility is given by:

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

where θ is a constant, T is temperature and the Curie constant $C = \frac{g_J\mu_B(J+1)M_S}{3k_B}$, with the subscripts '+' and '-' denoting spin 'up' and spin 'down' sub-lattices with corresponding saturation magnetisation M_S. The molecular field due to a sub-lattice of magnetisation M is represented by $-\lambda M$, where λ is a constant.

(**Hint**: For small y the Brillouin function $B_J(y) \approx \frac{(J+1)}{3J}y$).

$e = 1.60 \times 10^{-19}$ C
$\mu_B = 9.27 \times 10^{-24}$ J T^{-1}
$\mu_0 = 4\pi \times 10^{-7}$ H m^{-1}
$k_B = 1.38 \times 10^{-23}$ J K^{-1}
$h = 6.63 \times 10^{-34}$ J s^{-1}
$N_A = 6.022 \times 10^{23}$
$m_e = 9.11 \times 10^{-31}$ kg