Level 3 Condensed Matter Physics- Part I Weekly problem 1

A Resume of the Properties of Free Electrons in Metals from FoP2B

- (1) Given a system of free electrons in a metal with chemical potential μ write an expression which gives the probability of an eigenstate of energy E being occupied. Draw this distribution as a graph of the probability of occupation against the free electron energy, labelling the position of the chemical potential and the Fermi energy. [2 marks]
- (2) By considering the free electron plane wavefunctions write an expression which relates the eigenstate energy to the wavevector. Use this expression to derive an expression for the Fermi energy and Fermi wavevector giving a definition of both. Draw a graph showing the E(k) dispersion curve. [3 marks]
- (3) Calculate the Fermi wavevector, Fermi energy and Fermi temperature of free electrons in copper metal given that copper crystallises in a fcc structure with a = 0.361 nm and is monovalent. What can you deduce about the properties of copper from these values? [3 marks]
- (4) Show that the kinetic energy of a three-dimensional gas of N free electrons is

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

[2 marks]

Level 3 Condensed Matter Physics- Part I Weekly problem 2

- (1) Define the term *group velocity* for nearly-free electrons in a metal. Explain how a nearly-free electron can have a velocity which changes with increasing wavevector k. Draw a sketch of a typical energy wavevector E(k) relationship for a nearly-free conduction electron in a metal across the first Brillouin zone. Use your diagram to show where the group velocity of electrons is zero and where it is a maximum. [4 marks]
- (2) A metal has an energy wavevector E(k) relationship given by: $E(k) = C(k^2 Dk^4)$ where C and D are constants. From this obtain an expression for the group velocity of an electron, v_g . From what you know about the behavior of v_g across the Brillouin zone, determine the value of D. [3 marks]
- (3) For the above metal the effective mass at the first Brillouin zone boundary $(k = \pi/a)$ is -0.5 times the effective mass at the centre of the Brillouin zone (k = 0), where a is the lattice spacing. Find the values for the effective masses at k = 0 and at $k = \pi/a$ in terms of the constant C. [3 marks]

Level 3 Condensed Matter Physics- Part I Weekly problem 3

This weekly problem concerns the derivation of the Hamiltonian for an atomic electron in a uniform magnetic field **B** (Lecture 5). It explores some facts implicitly assumed in the derivation, as well as some implications of the theory.

(1) For a uniform magnetic field $\bf B$ show that the magnetic vector potential is given by the so-called symmetric gauge:

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

where \mathbf{r} is the position vector.

[2 marks]

(2) Show that the symmetric gauge is rotationally invariant.

[2 marks]

(3) Show that the momentum operator $\mathbf{p} = -i\hbar \vec{\nabla}$ commutes with \mathbf{A} , i.e.

$$[\mathbf{p}, \mathbf{A}] = \mathbf{p} \cdot \mathbf{A} - \mathbf{A} \cdot \mathbf{p} = 0$$

[2 marks]

(4) In the presence of a magnetic field the velocity operator for an electron is given by:

$$\frac{(\mathbf{p} + e\mathbf{A})}{m}$$

where e and m are the charge magnitude and mass of an electron. Show that when an external magnetic field is applied to an atom a current density $\mathbf{J}(\mathbf{r})$ is generated, which is given by:

$$\mathbf{J}(\mathbf{r}) = \frac{e^2}{m} \rho(\mathbf{r}) [\mathbf{r} \times \mathbf{B}]$$

where $\rho(\mathbf{r})$ is the electron density within the atom. Is there a link between $\mathbf{J}(\mathbf{r})$ and diamagnetism?

[4 marks]

Level 3 Condensed Matter Physics- Part I Weekly problem 4

(1) How much work has been done?

Starting with an expression relating the work done by the torque, τ , when an object turns through a small angle $d\theta$, show that the potential energy of a magnetic dipole μ in a magnetic field is $E = -\mu \cdot \mathbf{B}$) [3 marks]

(2) Energy differences due to magnetism

An atom in a solid has a magnetic moment of $2\mu_B$ and it is in the presence of a magnetic field of flux density 1 T. Calculate the highest and lowest potential energy states of the atom. How does the difference between these two energy states compare to the thermal energy of the solid at room temperature? [3 marks]

(3) Diamagnetism in Bismuth

- (a) Bismuth (Z = 83, atomic mass = 208.98 u) is a diamagnetic material with a density of 9.75 x 10^3 kg m⁻³. Calculate the magnetic susceptibility of this element given that the root mean square atomic radius of bismuth is 0.16 nm. [2 marks]
- (b) A magnetic field of strength 3×10^3 A m⁻¹ is applied to a sample of bismuth of mass 1 gram. Calculate the magnetic moment induced in the sample by the applied field. [2 marks]

Magnetic constant: $\mu_0 = 4\pi \times 10^{-7} \text{ H m}^{-1}$

Bohr magneton: $\mu_{\rm B} = 9.27 \text{ x } 10^{-24} \text{ A m}^2$

Boltzmann constant: $k_{\rm B} = 1.38 \text{ x } 10^{-23} \text{ J K}^{-1}$

Unified atomic mass unit: $u = 1.66 \times 10^{-27} \text{ kg}$

Level 3 Condensed Matter Physics- Part I Weekly problem 5

- (1) What is meant by L-S (or Russell Saunders) coupling and under what conditions is it applicable? [1 mark]
- (2) The magnetisation of a paramagnet consisting of isolated atoms in their ground state with total angular momentum J is given by the Brillouin function,

$$M = M_S \left[\frac{(2J+1)}{2J} \coth\left(\frac{(2J+1)}{2J}y\right) - \frac{1}{2J} \coth\left(\frac{y}{2J}\right) \right]$$

where M_S is the saturated magnetisation value $ng\mu_B J$, $y = g_J \mu_B J B / (k_B T)$, B is the magnetic induction field and g_J is the Landé g-factor which is given by the expression,

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

Use the expression for *M* to derive Curie's law, stating any assumptions that you make.

[Hint:
$$\coth x \simeq \frac{1}{x} + \frac{x}{3}$$
 for $x \to 0$]

[2 marks]

- (3) Use Hund's rules to determine the ground state and excited total angular momentum states of an isolated Ti^{2+} ion which has a $3d^2$ electronic structure. Calculate the total magnetic moments of each of these states in units of μ_B . [3 marks]
- (4) The spin-orbit energy is given by $E_{SO}(J) = \frac{\lambda}{2} [J(J+1) L(L+1) S(S+1)]$. For a Ti²⁺ ion the spin-orbit coupling constant $\lambda = 4.5$ meV. Calculate the energies $E_{SO}(J)$ of the total angular momentum states determined in part (3). [2 marks]
- (5) Sketch the form of the temperature dependence of the inverse paramagnetic susceptibility of a solid of non-interacting Ti^{2+} ions, measured at low magnetic fields. Note that the probability of thermal occupation of the energy levels, determined in part (4), is proportional to $(2J + 1)\exp(-E_{SO}(J)/k_BT)$. [2 marks]