Condensed Matter Physics - Electronic Properties - R.J. Nicholas HT 2010

Question Sheets

A. Free Electron Theory and Metals

A1. Explain what is meant by the *Fermi energy*, *Fermi temperature* and the *Fermi surface* of a metal.

Obtain an expression for the Fermi wavevector and the Fermi energy for a gas of electrons at absolute zero. Show that the density of states at the Fermi surface, dN/dE_F , can be written as $3N/2E_F$. Estimate the value of E_F for a monovalent metal such as copper.

- A2. Give simple derivations of the Fermi gas predictions for the heat capacity and susceptibility of the conduction electrons in metals. How do these two results differ from the predictions for theory based on assuming a classical gas of electrons? What other properties of metals might be different when described by the classical and Fermi gas theories?
- A3. The experimental heat capacity of potassium metal at low temperatures has the form:

$$C = (2.08T + 2.6 T^3) mJ mol^{-1} K^{-1}$$

where T is in Kelvin. Explain the origin of each of the two terms in this expression and make an estimate of the Fermi energy for potassium metal.

- A4. Assuming that the free electron theory is applicable:
 - (a) show that the speed v_F of an electron at the Fermi surface of a metal which has n electrons per unit volume is:

$$v_{\rm F} = \frac{\hbar}{m} \left(3\pi^2 n \right)^{\frac{1}{3}}$$

(b) show that the mean drift speed v_d of an electron in an applied electric field *E* is $v_d = \sigma E/(ne)$, where σ is the electrical conductivity, and show that σ is given in terms of the mean free path λ of the electrons by $\sigma = ne^2 \lambda/(mv_F)$.

Assuming that the free electron theory is applicable to copper:

(i) calculate the values of both v_d and v_F for copper at 300K in an electric field of 1 Vm^{-1} and comment on their relative magnitudes.

(ii) estimate λ for copper at 300K and comment upon its value compared to the mean spacing between the copper atoms.

[For copper: $n = 8.45 \times 10^{28} \text{m}^{-3}$, $\sigma = 5.9 \times 10^7 \Omega^{-1} \text{m}^{-1}$ at 300K]

A5. Define the Hall coefficient and obtain an expression for it using the free electron model. Estimate the magnitude of the Hall voltage for a specimen of sodium in the form of a rod of rectangular cross section 5mm by 5mm carrying a current of 1A in a magnetic field of 1T. (The bcc lattice of sodium has a cube edge of 0.42 nm). What practical difficulties would there be in measuring the Hall voltage and resistivity of such a specimen and how could this be done as a function of temperature?

B. Band Theory

B1. A specimen in the form of a cube of side L has a primitive cubic lattice whose mutually orthogonal fundamental translation vectors have length a. Show that the number of different allowed k states within the first Brillouin zone equals the number of unit cells forming the specimen.

Electrons in the conduction band of the solid experience a strong constant binding potential V_0 with a weak superimposed periodic component V_R representing the interaction with the lattice: $V = V_0 + V_R$, with $V_R \ll V_0$. Discuss qualitatively why the x-dependence of the wavefunction of the electrons can have the form $exp(ik_x x)$ when **k** is small, while functions of the form $cos(\pi x/a)$ or $sin(\pi x/a)$ are appropriate at the (100) boundaries of the first Brillouin zone.

- B2. Sketch the first two Brillouin zones for a two-dimensional square lattice. Taking the free electron picture with no electron-lattice interaction insert Fermi surfaces for a monovalent and for a divalent metal, each with one atom per unit cell. Sketch the modified Fermi surfaces that would result from weak electron-lattice interaction.
- B3. The energy of an electron in a two-dimensional layer of metallic atoms, in which the atoms lie on a square lattice of side a, is given by:

$$E(k_x, k_y) = C\{1 - \cos(k_x a) - \cos(k_y a)\}$$

where the wavevector of the electron is $\mathbf{k} = (k_x, k_y)$ and *C* is a positive constant. Draw labelled constant-energy contours when the wavevector of the electron is close to the bottom of the band, $k_x = k_y = 0$, and close to the Brillouin zone corner, $k_x = k_y = \pi/a$. What is the effective mass of an electron with each of these two wavevectors? Comment on the results.

B4. Discuss the general ideas which describe how the band theory of solids is related to the underlying atomic state of the atoms which make up the solid.

Explain the following:

- (a) sodium, which has 2 atoms in a (conventional cubic) bcc unit cell, is a metal;
- (b) calcium, which has 4 atoms in a cubic fcc unit cell, is a metal;
- (c) diamond, which has 8 atoms in a cubic fcc unit cell, is an electrical insulator, whereas silicon and germanium, which have similar structures, are semiconductors.

Condensed Matter Physics – Question Sheets C and D

Electronic Properties - R.J. Nicholas

C: Semiconductors

- C1. Outline the absorption properties of a semiconductor and how these are related to the band Explain the significance of the distinction between a direct and an indirect gap. semiconductor. What region of the optical spectrum would be being studied for a typical semiconducting crystal?
- C2. What is meant by the terms intrinsic and extrinsic when describing semiconductors? Describe and explain the temperature dependence of the carrier concentration and chemical potential in a typical semiconducting solid (a) when undoped and (b) when doped with acceptor impurities.
- Outline a model with which you could estimate the energy of electron states introduced by C3. donor atoms into an n-type semiconductor. Write down an expression for this energy, explaining why the energy levels are very close to the conduction band edge.
- C4. Show that in a pure semiconductor at a fixed temperature T the product of the number of conduction electrons (n) and holes (p) per unit volume depends only on the density of states in the conduction and valence bands (through the effective masses) and on the band gap energy E_g , assuming that $E_g >> kT$. Given that $np \approx 10^{32} \text{ m}^{-6}$ at room temperature for silicon, make a rough estimate of the

maximum concentration of ionised impurities which still allows intrinsic behaviour.

Estimate the conduction electron concentration for intrinsic Ge at room temperature, stating carefully any assumptions made (E_g for Si ≈ 1.1 eV and for Ge ≈ 0.75 eV).

- C5. What is meant by a hole in semiconductor physics and why is the concept useful? Explain how the following properties of a hole are related to the properties of the electron that is missing:
 - (i) wavevector,
 - (ii) energy,
 - (iii) velocity,
 - effective mass, (iv)
 - equation of motion in electric and magnetic fields. (v)
- C6. Describe experiments to determine the following properties of a semiconductor sample:
 - sign of the majority carrier, (i)
 - (ii) carrier concentration (assume that one carrier type is dominant),
 - (iii) band gap,
 - effective mass (iv)
 - mobility of the majority carrier, (v)

C7. A junction is formed between a p-type and an n-type semiconductor containing equal concentrations n of impurity atoms. Using a simple electrostatic model, show that a depletion layer is formed on either side of the junction of width δ given by:

$$\delta^2 = \frac{E_g \varepsilon}{e^2 n}$$

where E_g is the band gap energy, ε the permittivity and e the electronic charge.

Calculate the thickness of the depletion layer for Si with n- and p-type doping levels of 1 atom in 10^6 (relative atomic mass = 28, density = 2.3 x 10^3 kgm⁻³, relative permittivity = 12 and band gap energy = 1.1eV).

Obtain an approximate expression for the current through a p-n junction diode as a function of the voltage applied across it.

C8. A quantum well is formed from a layer of GaAs of thickness L nm, surrounded by layers of Ga_{1-x}Al_xAs. Sketch the shape of the potential for the electrons and holes. What approximate value of L is required if the band gap of the quantum well is to be 0.1eV larger than that of GaAs bulk material? You may assume that the band gap of the Ga_{1-x}Al_xAs is substantially larger than that of GaAs. How would it be possible to n-type dope the structure so that the electrons accumulate in a region of the structure away from the impurities? (The electron (hole) effective mass in GaAs is 0.068m_e (0.45m_e)).

Magnetic Properties

Diamagnetism

- D1. Explain the physical origin of diamagnetism. Derive an expression for the ratio (the gyromagnetic ratio) of the magnetic moment and the orbital angular momentum of an electron of charge e and mass m describing a circular orbit. Show that the diamagnetic susceptibility of a non-conducting material is negative and proportional to $\Sigma < r^2 >$ where $< r^2 >$ denotes the average value of the square of the radius of the electron orbit.
- D2. The wavefunction of an electron bound to an impurity in n-type silicon is hydrogenic in form. Estimate the impurity contribution to the diamagnetic susceptibility of a Si crystal containing 10^{20} m⁻³ donors given that the electron effective mass m^{*} = 0.4m_e and the relative permitivity is 12.
- D3. It is desired to magnetically levitate an animal, who's mass consists mainly of water, using a magnetic field of 15T. How large a magnetic field gradient is necessary in order to achieve this? [For water, the magnetic susceptibility is -9.03 x 10⁻⁶]. This really can be done! (for an example see: http://www.hfml.science.ru.nl/educational.shtml).

Paramagnetism

- D4. Outline the quantum theory of paramagnetic susceptibility for an assembly of n spin 1/2 atoms per unit volume in which the mutual interactions are negligibly small. Show that it leads to Curie's law for the susceptibility, χ , in small magnetic fields at temperature T, of the form $\chi = \mu_0 n \mathbf{m}^2/3k$ T, where *k* is Boltzmann's constant, and derive an expression for \mathbf{m}^2 .
- D5. A crystalline insulator contains N magnetic ions per mole having spins $S = \frac{1}{2}$. The magnetic susceptibility obeys Curie's law to below 0.1 K. Show that the magnetic contribution to the molar specific heat at temperatures above 1 K is given by

$$C_{mag} = Nk (\epsilon/kT)^2 [e^{\epsilon/kT}/(1+e^{\epsilon/kT})^2]$$

where ε is the magnetic level splitting.

Give approximate expressions for C_{mag} at temperatures high and low compared with ϵ/k . Sketch the variation of C_{mag} as a function of temperature.

The lattice specific heat of the insulator obeys the low temperature limit of Debye theory very closely below 20 K, with a Debye temperature $\vartheta_D = 158$ K. In zero applied magnetic field the molar specific heat is measured to be 0.0592R at 10 K. Values of the total molar specific heat measured in an applied field of 0.75 T are given in the table. Obtain a value for the g-factor of the magnetic ions.

Temperature	Specific heat
10.0 K	0.0617 R
7.0 K	0.0254 R
5.0 K	0.0173 R
3.0 K	0.0286 R

D6. Estimate the relative magnitude of the contributions to the susceptibility of copper from the conduction electrons and the filled d-shell $(3d^{10})$. Do you expect copper metal to be diamagnetic or paramagnetic?

Ferromagnetism

- D7. Magnetic ions with S=1/2 and L=0 are spaced 0.5nm apart. Calculate the magnetic dipolar energy of one ion due to the field of its neighbour. At approximately what temperature would the moments be aligned due to this type of interaction?
- D8. Explain what is meant by the molecular or mean field model of the interaction between ions in a solid. Outline how the model can be used to account for the onset of a ferromagnetic state, with a large spontaneous magnetisation in the absence of an externally applied magnetic field, when the temperature is below a critical temperature T_c . What is the nature of the interaction which is represented by the mean molecular field? The ferromagnet gadolinium has a Curie temperature of 298 K and each atom has J=7/2 and g=2. Find the value of the molecular field at low temperatures.
- D9. Why do domains form in ferromagnetic materials? What determines the shape and size of the domains? Describe what happens when a magnetic field is applied to a ferromagnetic sample with an initial bulk magnetisation very much lower than the saturation value. Why must impurities be introduced into iron to make permanent magnets? Calculate the width of a domain wall, given that the exchange constant $J = 10^{-21}$ J, the anisotropy energy per unit volume is $K = 4x10^4$ Jm⁻³, the atomic spacing is 0.3 nm, and S=1 for all atoms in the wall.

Antiferromagnetism

D10. Use mean field theory to show that the paramagnetic susceptibility of a two sublattice antiferromagnet may be written in the form

$$\chi(T) = C / (T + T_N)$$

where C is a constant and T_N is the ordering temperature for the antiferromagnet. Compare this result with the magnetic susceptibility of a ferromagnet. [You may assume that for an antiferromagnet the only interaction of importance is an antiparallel interaction between the two sublattices]

Superconductivity

- D11. Explain why a superconductor cannot be regarded simply as a perfect conductor. Explain why a strong enough magnetic field applied to a superconductor will cause a phase transition to the normal state.
- D12. (a) What indications are there that the phenomenon of superconductivity is connected with an *energy gap*? How large is the energy gap in a typical superconductor?
 (b) How do Type I and Type II superconductors differ?
- D13. Discuss briefly flux quantisation, including a derivation of the size of the flux quantum and one example in which it can be observed.