C3: Band Theory and Electronic Properties of Solids
MT 2013
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Problem Class 2

1. **Carbon nanotubes**
Graphene is formed by a hexagonal array of carbon atoms as shown in Figure 1, with nearest-neighbour carbon-carbon bond lengths a_{CC}. Single-walled carbon nanotubes are formed by rolling up the graphene sheet. A special kind of high-symmetry tube (an 'armchair' tube) can be made by rolling along the x-direction, so that the y-direction forms the tube axis. Show that the circumference of an armchair tube can only take the values $C_x = 3na_{\mathrm{CC}}$, where n is a positive integer.
a) By applying the appropriate boundary condition, find the permitted values of k_x, the Bloch wave vector in the circumferential direction.

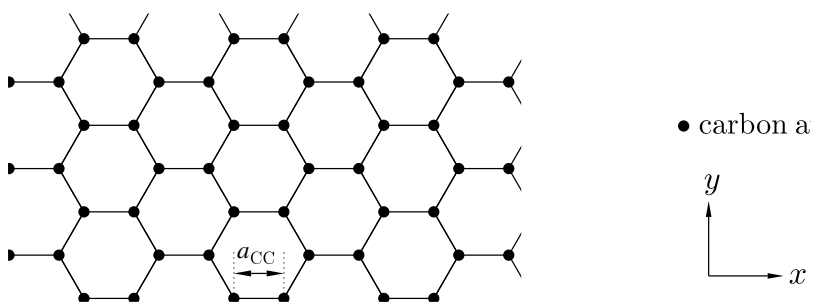

Figure 1: Graphene lattice

Figure 2(a) shows the Brillouin zone of graphene (which is divalent) and Figure 2(b) the electronic dispersion. The Brillouin zone crosses the axes at $k_x = 2\pi/(3a_{\mathrm{CC}})$ and $k_y = 4\pi/(3\sqrt{3}a_{\mathrm{CC}})$. The conduction and valence bands are degenerate at the K points.
b) Show that for an armchair nanotube there is always at least one circumferential sub-band with a continuous density of states at the Fermi energy (i.e. the tube is metallic).

c) A 'zig-zag' tube is made by rolling the graphene sheet in the y-direction. For which tube circumferences is a zig-zag tube metallic?

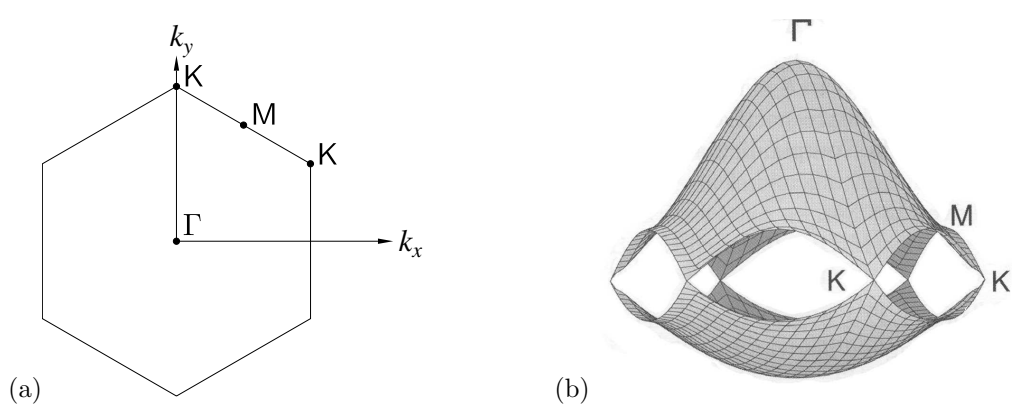

Figure 2: Representation of the first Brillouin zone (a) and dispersion relation (b) for graphene.

2. **Haas-van Alphen effect:**
A particular monovalent metal has the following properties:
(i) its Fermi surface is approximately spherical;
(ii) the Fermi wavevector is $9.1 \times 10^9 \mathrm{m}^{-1}$;
(iii) the electrons at the Fermi surface have an effective mass $m^* = 1.3 m_\mathrm{e}$, where m_e is the mass of a free electron.
a) Giving brief experimental details, explain how you would deduce properties (i), (ii) and (iii) using the *de Haas-van Alphen effect*.

b) Calculate the frequency of the de Haas-van Alphen oscillations that would be observed, the number density of electrons in the metal and its Fermi energy.

c) Figure 3 shows $F(P)/F(0)$, the ratio of the de Haas-van Alphen frequency measured with the metal subjected to pressure P to that measured with the metal *in vacuo*. Account for the form of the data, and use the Figure to estimate the actual bulk modulus B_act of the metal.

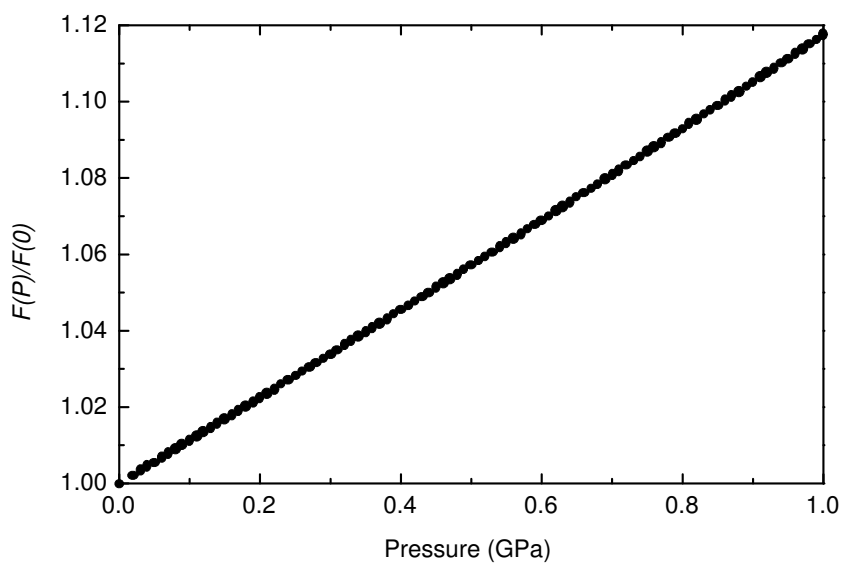

Figure 3: The Figure shows $F(P)/F(0)$, the ratio of the de Haas-van Alphen frequency measured with a metal subjected to pressure P to that measured with the metal *in vacuo*.

d) Calculate the bulk modulus that you would expect for the metal using the Sommerfeld model and comment on your answer.

e) Describe qualitatively how m^* might be expected to vary with pressure.

3. **Reciprocal mass tensor and effective mass tensor:**
The effective masses of electrons in anisotropic bands can be represented using tensors. This question exposes you to them.

a) Show that an electron in a crystal, with wave-vector $\mathbf{k}$ and energy $E(\mathbf{k})$ subjected to an applied electric field ϵ, will change its velocity $\mathbf{v}$ at a rate given by

$$\frac{\mathrm{d}\mathrm{v}_i}{\mathrm{d}t} = -e \sum_j (\mathbf{M}^{-1})_{ij} \epsilon_j \tag{1}$$

where the *reciprocal mass tensor* has components

$$(\mathbf{M}^{-1})_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}. \tag{2}$$

b) The highest occupied band of a particular substance is found to have the following reciprocal

mass tensor

$$\mathbf{M}^{-1} = \begin{pmatrix} \frac{1}{m_1} & 0 & 0 \\ 0 & \frac{1}{m_2} & 0 \\ 0 & 0 & \frac{1}{m_3} \end{pmatrix} \tag{3}$$

when a particular set of x, y and z axes are chosen. Sketch a constant energy surface (*i.e.* Fermi surface) of this substance, assuming that m_1, m_2 and m_3 are independent of E and $\mathbf{k}$ and that they differ in size.

c) As $\mathbf{M}^{-1}$ is diagonal, it is easy to invert it to get the *effective mass tensor* $\mathbf{M}$.

$$\mathbf{M} = \begin{pmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{pmatrix}. \tag{4}$$

A magnetic field $\mathbf{B}$ is applied to the sample in an arbitrary direction. By substituting $\mathbf{v} = \mathbf{v_0} e^{i\omega t}$ into the equation

$$\mathbf{M}\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -e\mathbf{v} \times \mathbf{B} \tag{5}$$

show that $\omega = \frac{eB}{m^*}$, with

$$m^* = \left(\frac{B^2 m_1 m_2 m_3}{m_1 B_x^2 + m_2 B_y^2 + m_3 B_z^2} \right)^{\frac{1}{2}}. \tag{6}$$

(Hint: write out all of the components of the equation and collect them into a matrix of coefficients of v_x, v_y and v_z; take a determinant of this and equate it to zero and everything should be OK.) This phenomenon is known as cyclotron resonance.

4. **Cyclotron resonance in metals and semiconductors:**
a) A very pure sample of a metal at a temperature of 1 K is illuminated by microwaves of frequency 72 GHz. At this temperature and frequency the skin depth is less than the electron mean free path. A magnetic flux density $\mathbf{B}$ is applied parallel to the surface of the sample and at right angles to the electric vector of the radiation. As B is varied the power absorbed by the sample passes through maxima and minima. Maxima are observed when $nB = 0.95$ tesla, where n is an integer. Account for this behaviour and deduce the electronic dynamical (cyclotron) mass.

b) A nominally undoped piece of semiconductor is illuminated with above-band-gap radiation and a cyclotron absorption measurement is performed at a frequency of 300 GHz and a temperature of 1.5 K. Cyclotron resonances are observed at 1.1 T and 5.8 T; the width (full width at half maximum) of the lower field resonance is 0.2 T and that of the higher field resonance is 1 T. Estimate the masses and mobilities of the carriers induced by the illumination. How might the measurement be modified to determine which resonance was due to holes and which was due to electrons?

5. **Two carrier Hall effect:**
a) (i) In the limit of small magnetic field, show that the Hall coefficient for a sample containing both electrons and holes is given by:

$$R_H = \frac{1}{|e|} \frac{(p - nb^2)}{(p + nb)^2}$$

, where $|e|$ is the magnetude of the electronic charge, n is the concentration of electrons and p is the concentration of holes. (ii) Find an expression for the dimensionless parameter b in terms of the electron mobility μ_e and the hole mobility μ_h. List the approximations used in your derivation.

b) Explain why μ_e is generally much greater than μ_h in many direct gap semiconductors such as InSb and GaAs.

c) Figure 4 shows The Hall coefficient R_H plotted as a function of the inverse temperature for a sample of InSb. R_H is observed to change sign between 0.005 and 0.006 K^{-1}. Describe the mechanisms responsible for the form of the curve and estimate (i) the concentration and type of impurities in the sample and (ii) the band gap of InSb. What temperature dependence would be expected for the mobilities of the carriers over the temperature range shown?

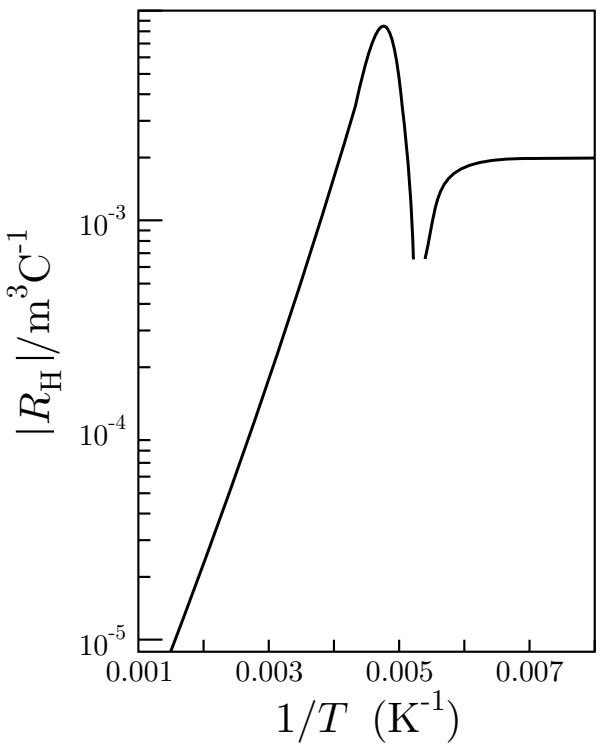

Figure 4: Hall coefficient of an InSb sample versus $1/T$.

6. **Quantum Hall effect:**
A semiconductor quantum well is made from a 30 nm thick layer of GaAs (with an effective mass $m^*/m_e = 0.07$) surrounded by $Ga_xAl_{1-x}As$.

a) Sketch the spatial dependence of the potential for the conduction band. Estimate the values for the first two energy levels of the electrons in the quantum well relative to the GaAs band edge, assuming that the potential well is infinitely deep. The quantum well is doped with electrons using the technique of 'modulation doping'. Explain what this term means and calculate the value of the Fermi Energy when the carrier density is $3\times10^{15}\,m^{-2}$.

b) Measurements of the resistivity components ρ_{xx} and ρ_{xy} for such a quantum well at low temperature are shown in figure 5**a** as a function of magnetic field applied perpendicular to the layer. Sketch the electronic Landau level density of states for a quantum well under such conditions, indicating *localised states*, *extended states* and *spin splitting*. Describe briefly how the changing position of the chemical potential in the Landau levels as a function of magnetic field produces data such as those in Figure 5**a**. **c)** Show that the magnetic field values of the minima in ρ_{xx} are consistent with the carrier density and deduce the mean free path length of the electrons (you may assume that the electrons have effective mass $m^* = 0.07m_e$). Calculate the theoretically expected value for ρ_{xy} in the region of 12 T.

d) A second quantum well of the same width but a higher carrier density shows oscillations in ρ_{xx} as shown in figure 5**b**. Explain the reasons for the different form of the oscillations and use them to deduce the total carrier density. How would the oscillations change if the width of this quantum well were to be reduced to 10nm while the carrier density is kept constant?

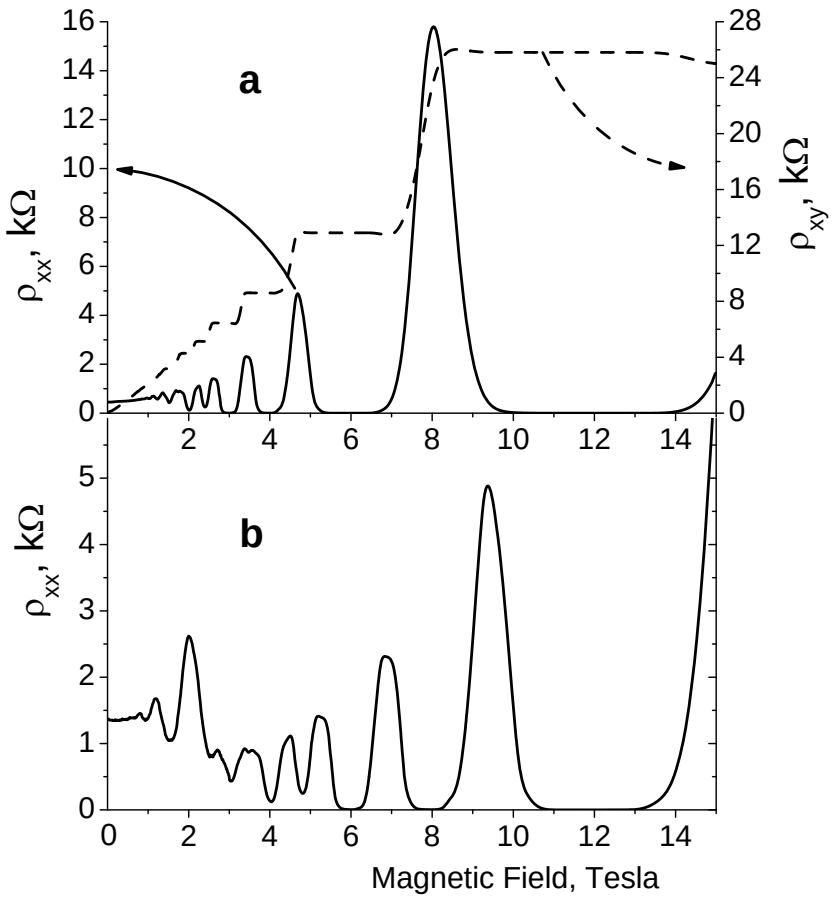

Figure 5: Resistivity components for two different quantum wells (**a** and **b**) measured at low temperatures.