QUEEN MARY, UNIVERSITY OF LONDON
SCHOOL OF PHYSICS AND ASTRONOMY

Structure and Properties of Functional Materials

Homework Set 5

Due Wednesday, 6 March, 2013 by 4 p.m.

Problem 1: Terms and definitions (8 marks)

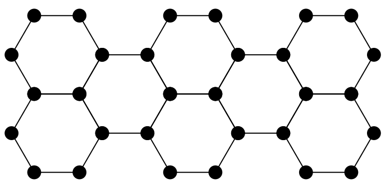
Explain the following terms or concepts, giving an example of their significance in condensed matter physics:

(a) Nearly free electron gas (4)

(b) Fermi level (4)

Problem 2: The free electron gas in two dimensions (18 marks)

Consider a single sheet of graphene:



Each atom contributes one electron to a cloud of delocalised electrons that can be modelled as a two-dimensional free electron gas.

(a) Repeat the calculations we did in class, but in only two dimensions, to calculate the Fermi wavevector k_F and the Fermi level E_F in terms of the electron density n. (Note that in two dimensions this is the number of electrons per unit *area*.) (9)

Hint: begin, as we did in class, by calculating the reciprocal space area of a single electronic state. The energy of each state, in terms of its wavevector, will be the same as in 3D.

(b) Calculate n for a graphene sheet in which the carbon-carbon bonds are $\ell = 1.4$ Å long. (7)

Hint: you will need to do a bit of geometry to show that the area of each hexagon is $(3\sqrt{3}/2)\ell^2$. Each hexagon contains six atoms, but each atom is shared between three hexagons, so the area per atom is half the area of a hexagon.

(c) Hence calculate numerical values for k_F and E_F for graphene. (2)

Problem 3: Bulk modulus of metals (14 marks)

(a) The total energy of a free-electron gas (at 0 K) can be calculated by integrating over each occupied state: (4)

$$E_{\text{total}} = \int_0^{k_F} E(k)g(k).$$

Evaluate this integral to find the total energy. Express your answer in terms of nE_F.

(b) The bulk modulus is a measure of the pressure needed to change the volume of a solid by a set amount; it is defined by (6)

$$B = -V\frac{\partial P}{\partial V}$$

so that the higher the bulk modulus, the harder it is to compress a solid. (Note that the negative sign is needed to keep B positive, since *increased* pressure will always cause a *decrease* in volume.)

The bulk modulus is related to the total energy of a solid by

$$B = -V\frac{\partial^2 E}{\partial V^2}$$

(where E is energy and V is volume). Evaluate this using your energy from part (a) to show that the bulk modulus of a free-electron gas is $B = \frac{2}{3}nE_F$.

Hint: the electron density n is just N/V, where N is the total number of electrons.

(c) Evaluate the value of B from (b) numerically for potassium. In the free-electron gas model, as you (should have) found in this week's tutorial, potassium has a Fermi level of $E_F = 2.04$ eV and an electron density of $n = 0.013$ Å^{-3}. Compare your answer to the experimental bulk modulus of 3.1 GPa. What can you conclude about the main force resisting compression in this metal? (4)

Data:

Electronic charge	$e = 1.6022 \times 10^{-19}$ C
Planck constant	$h = 6.626 \times 10^{-34}$ J s
	$\hbar = h/2\pi = 1.055 \times 10^{-34}$ J s
Boltzmann constant	$k_B = 1.3807 \times 10^{-23}$ J K^{-1}
Electron mass	$m = 9.109 \times 10^{-31}$ kg
Avogadro number	$N_A = 6.022 \times 10^{23}$ mol^{-1}