Condensed Matter Physics: Workshop 4 (26 February - 2 March 2018)

Summary: The material in this workshop will explore the predictions of the free-electron (Sommerfeld) quantum model for electrons in metals in more detail. Problems **b** – **f** look at the density of states function in two dimensions (we derived the function for the 3D case in the lectures).

Problems **g** – **k** focus on predicting physical properties from the quantum free-electron model – specifically the Bulk Modulus, B, which measures how quickly the pressure increases when the volume of a solid is reduced.

a. In small groups discuss:
   i. What is the difference between the classical Drude model and the quantum free electron Sommerfeld model of electrons in metals?
   ii. What does the density of states function describe?
   iii. What is the significance of the Fermi Energy?

b. Consider a material in which the electrons are free to move only in a two-dimensional plane (this will occur in a very thin sheet of metal for example). We will assume that there are periodic boundary conditions over a length L in both dimensions in the plane.

Show that $\psi(x, y) = A\ \exp\left[i(k_x x + k_y y)\right]$ (where A is a normalisation constant) is a solution of the time-independent free-electron Schrödinger equation with energy eigenvalue $E = \hbar^2 k^2 / 2m_e$ (where m_e is the free-electron mass and $k^2 = k_x^2 + k_y^2$).

c. Show that this solution satisfies the periodic boundary conditions provided that:

$$k_x = \frac{2l\pi}{L}, k_y = \frac{2m\pi}{L}; l, m = 0, \pm 1, \pm 2, \ldots$$

d. Consider the two-dimensional space "*k*-space" formed by the values of k_x and k_y. Show that the number of electron states per unit area of "*k*-space" is $L^2 / 2\pi^2$ (remember to allow for the spin degeneracy of the electrons).

e. What is the area of the ring in *k*-space which encloses all vectors $\boldsymbol{k} = (k_x, k_y)$ with lengths between k and $k + \delta k$? Use your result to show that the number of allowed states whose k-value lies within this ring is $L^2 k \delta k / \pi$.

f. Use this result to calculate the density of states $n(E)$ per unit energy which is defined so that $n(E)\delta E$ is the total number of electron states with energy eigenvalues between E and $E + \delta E$.

g. Obtain an expression for the mean energy of an electron in the quantum free electron model in terms of the Fermi energy E_F.

h. Using this result for the average kinetic energy of an electron, show that the total kinetic energy of all the electrons N in a metal of volume V is $E_{\mathrm{TOT}} = AV^{-2/3}$ where:

$$A = \frac{3\hbar^2}{10m_e}(3\pi^2)^{2/3}N^{5/3}$$

i. The pressure P exerted by the electrons is equal to minus the partial derivative of the total energy with respect to the volume, $P = -\,\partial E_{\mathrm{TOT}}\ /\ \partial V$.

Show that the pressure satisfies the relationship $P = 2\,E_{\mathrm{TOT}}\ /\ 3V$.

j. The Bulk Modulus, B, of a material is defined by $B = -V\,\partial P\ /\ \partial V$. Show that for this system of electrons $B = 2n\,E_F\ /\ 3$ where $n = N\ /\ V$ is the electron density per unit volume.

k. Calculate the contribution of the conduction electrons to the bulk modulus of potassium which has a density of conduction electrons $n\ =\ 1.40\ \times\ 10^{28}\mathrm{m}^{-3}$. Compare your result with the experimental bulk modulus $2.81\ \times\ 10^{9}\mathrm{Pa}$.