PYL102 Practice problems:

Q-1: Metallic sodium crystalizes in body-centered cubic form, the length of the cube being 4.25 × 10-8 cm. Find the concentration of conduction electrons. Assume one conduction electron per atom. Adopting the free electron Fermi gas model for the conduction electrons, derive an expression for the Fermi energy (at 0 K) and show that it depends only on the concentration of conduction electrons, but not on the mass of the crystal.

Q-2: Consider an infinite row of identical atoms that are equidistant by a.

1) Find the general expression of the electron wavefunction that can move along the row.

2) This wavefunction satisfies periodic boundary conditions, PLC, with a periodicity L: w(x) = w(x + L). Find the wavevector quantization and the possible quantized energy levels for the electrons.

3) Find the expression and then the numerical value for the first three distinct energy levels in the case of a monovalent element (1e /at.) in which the atoms are equidistant by a = 3 A(take L = 3 mm). Find the expression and the numerical value characterizing the last occupied level at 0 K in terms of k and Er (the wave vector is in unit of $Å^{-1}$ and the Fermi energy in eV).

Q-3:

Consider an electron in 1D in the presence of the periodic potential (KP Model)

$$U(x) = \Sigma_{m=-\infty}^{\infty} U_o \Theta(x - ma)\Theta(ma + b - x)$$

a) Restrict your attention to a single unit cell and write down the boundary conditions for the wave function as required by Bloch's theorem.

b) Solve the Schrödinger equation by constructing ψ(x) from plane waves and imposing suitable boundary conditions at $x = 0, b, a$. The result is a relation between the Bloch index k and the energy.

c) Take the limit $b \to 0, U_o \to \infty \; with \; U_o b \to W_o a \frac{\hbar^2 a^{-2}}{m}$. Show that the condition for the Bloch index simplifies to

$$\cos(ka) = \frac{W_o}{qa}\sin(qa) + \cos(qa)$$

Where q is related to the eigenenergy ϵ via $q = \left(\frac{2m\epsilon}{\hbar^2}\right)^{1/2}$

Q-4:

He^3 atoms consist of an odd number of fermions (two electrons, two protons, and one neutron), and hence is itself a fermion. Consider a kilomole of He^3 atoms at standard temperature and pressure ($T = 293, K, p = 1 \; atm$).

What is the Fermi temperature of the gas?

Q-5: If free electron theory is applicable to Silver, then calculate the value of the mean drift velocity v_d at 300K under the electric field of 2V/m. Make a comment on the magnitude of the result obtained.

At 300 K assume the density of atoms in Silver to be $5.8X10^{28}$ m^{-3} and the conductivity to be $6.3X10^{7}$ $\Omega^{-1}m^{-1}$.

Q-6: A d-dimensional sample with volume L^d contains N electrons and can be described as a free electron model. Show that the Fermi energy is given by

$$E_F = \frac{\hbar^2}{2mL^2}(Na_d)^{2/d}$$

Find the numerical values of a_d for d= 1,2, and 3.

Q-7: For the delta-function potential and with $P \ll 1$, find at k = 0 the energy of the lowest energy band. (b) For the same problem find the bad gap at $k = \pi/a$

Q-8: Determine numerically the starting and ending energies of the first allowed band considering the Kronig-Penney model of a material with a_1=a_2= 7 Å and V_0= 0.8eV.

Q-9: If a Bloch state undergoes a translation by any lattice vector R, what is the effect on a) state wavefunction and b) the probability density?

Q-10: The electrons in a metal obey the Fermi-Dirac distribution.

$$n_F(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/kT+1}}$$

Find the Fermi-Dirac distribution function $n_F^{(0)}(\varepsilon)$at T = 0 by taking explicitly the $T \to 0$ limit of $n_F(\varepsilon)$. Note that $\mu(T = 0) = \varepsilon_F$ ·

Q-11: Consider one n-dimensional hypercube with length L for each side that contains free electrons. Answer the following questions:

a. What is the distance between nearest-neighbor points in k-space? Assume periodic boundary conditions. What is the density of k-points in n-dimensional k-space?

b. The number of k-points between k and (k+dk) is given by g(k)dk. Find g(k) for 1D, 2D and 3D, where g is the density of states.