

## FYS3410 Spring 2014

### Module III

#### Practical assignments:

1. One of the basic assumptions of the free electron gas (FEG) - or Drude model for electrons in solids - is that the mean free path for electrons is of the order of an interatomic distance. If this assumption is questionable, it challenges interpretations of all transport properties in terms of FEG, specifically thermal ( $\kappa$ ) and electrical ( $\sigma$ ) conductivities. Nevertheless, assuming FEG model, derive and calculate Wiedemann-Franz law coefficient  $L = \kappa / (\sigma T)$  and elaborate why  $L$  seems to be in remarkably good agreement with the experiment even if  $\kappa$  and  $\sigma$  reveal less trust individually. Refine the consideration by deriving  $L$  in terms of free electron Fermi gas (FEFG), in particular accounting that  $C_{el} = \pi^2 N k_B T / (2T_F)$  and using  $v_F$  for the electron velocity.
2. Introduce Born – von Karman boundary conditions and derive the density of states (DOS) for FEFG in a finite 3D sample. Calculate values of  $\epsilon_F$ ,  $k_F$ ,  $v_F$ , and  $T_F$ , i.e. Fermi energy, wavevector, velocity and temperature, respectively, for alkali metals. Explain the trend .
3. Consider the heating of the 3D FEFG up to  $T > 0$ . Make an estimate for the electronic heat capacity, accounting that only a fraction of the electrons - in the vicinity of  $\epsilon_F$  - may contribute to the increase in the total energy due to heating. Explain why.
4. Consider FEFG in 2D and 1D. Show that
  - (a) DOS is independent of energy ( $E$ ) for electrons in 2D;
  - (b) DOS is proportional to  $E^{-1/2}$  in 1D;

Taking into account the quantization of states in the 3<sup>rd</sup> dimension, the result obtained for 2D is directly applicable to represent DOS in a quantum well, specifically its step-like form. In its turn, for a realistic quantum wire, a combination of the 1D result with the idea of the state quantization in the 2<sup>nd</sup> and 3<sup>rd</sup> dimensions, leads to a reasonable interpretation of DOS in quantum wires.

- (c) Explain DOS trends for quantum wells and quantum wires in comparison with 3D;
- (d) Explain degeneracy taking place in quantum wires.

5. Solve time independent Schrödinger equation (TISE) employing potential energy in form of a delta function at the atomic sites of a 1D periodic lattice having a magnitude of  $V_0$  (often referred as Kronig-Penney model in literature). Illustrate – e.g. using a graph – that the discontinuities in the solution correlate with the idea of forbidden energy states. Further, using this solution, investigate limits of  $V_0 = 0$  and  $V_0 \rightarrow \infty$ .

1. Assume monovalent atoms crystallizing in a simple cubic (SC) lattice with a lattice parameter  $a$ .

- (a) Calculate the magnitude of the Fermi wavevector ( $k_F$ ) and compare it with the shortest possible distance from the origin of the k-space ( $\Gamma$  point) to the edge of the 1<sup>st</sup> Brillouin zone – BZ – ( $k_{BZ}$ ) in SC lattice.
- (b) If  $k_F < k_{BZ}$  holds it means, in terms of available electron states in the band, there are empty states available up to  $k = k_{BZ}$ . Compute how much of divalent atoms should be added to such SC lattice to make  $k_F = k_{BZ}$  in the alloy. Would such alloying result in an improvement or degradation of electrical conductivity?

Na is known as one of the best behaving metals. Notably, Na crystallizes in a BCC structure with 2 atoms in each conventional unit cell.

- (c) repeat calculation (a) for the BCC structure representing Na;
- (d) Calculate how much of Mg should be added to Na so that  $k_F$  equals  $k_{BZ}$  in the shortest possible direction from  $\Gamma$  point, assuming the alloy to maintain the original BCC form;
- (e) propose a scenario for the electrical conductivity evolution in such alloy as a function of composition.