FYS3410 Spring 2015

Module III

Practical assignments:

1. One of the basic assumptions of the free electron gas (FEG) - or Drude model for elections in solids - is that the mean free pass for electrons is of the order of the interatomic distance. If this assumption is questionable, it challenges interpretations of all transport properties in terms of FEG, specifically thermal (κ) and electrical (σ) conductivities. Nevertheless, assuming FEG model, derive and calculate Widemann-Franz law coefficient $L=\kappa/(\sigma T)$ and elaborate why L seems to be in remarkably good agreement with the experiment even if κ and σ reveal less trust individually. Refine the consideration by deriving L in terms of the 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 ε_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 ε_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 3rd dimension, the result obtained for 2D is directly applicable to represent DOS in a quantum well, specifically its step-like form. Further, for a realistic quantum wire, a combination of the 1D DOS with the idea of the state quantization in the 2nd and 3rd 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 $V_0 \rightarrow \infty$.

6. 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 (Γ point) to the edge of the 1st 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 add to Na so that k_F equals k_{BZ} in the shortest possible direction from Γ 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.