FYS3410 Spring 2017

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,
   (a) 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.
   (b) 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 periodic (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. Implications of the Fermi-Dirac distribution (FDD) on the energies (ε) reachable by the FEFG in 3D and the magnitude of the chemical potential (μ).
   (a) Show that in FEFG $\mu=\varepsilon_F$ at T=0K. Tips: recall that at T=0K the Gibbs energy $G = N\cdot\mu$, where N is the number of particles; on the other hand at T=0K the expression above may be compared with $G = E + pV$, where E, p and V are the total energy, pressure and volume of the system; E can be readily calculated by integrating DOS·FDD·ε at T=0K; further, calculate the pressure choosing an appropriate thermodynamic relation, e.g. $p = - (\partial E/\partial V)$; the anticipated result is $N\cdot\mu = E + pV = N\cdot\varepsilon_F$, i.e. $\mu=\varepsilon_F$.
   (b) Further, assume this FEFG is heated up to T >0K. Continue assuming $\mu= \varepsilon_F$, i.e. not changing with T. Plot FDD as a function of $\varepsilon/\varepsilon_F$ for T = 0.01T_F, 0. 1T_F, 0.5T_F, T_F, 1.2T_F; compare with literature data, e.g Fig.3 in p.136 in Kittel. Up to what temperatures, approximately, the assumption of $\mu= \varepsilon_F$ was reasonable?
   (c) Now investigate the true temperature dependence of μ and plot μ/ε_F as a function of T/T_F. Tips: remember that the total number of FEFG particles (N) is not changing with temperature, or in other words the integral of "DOS" at T=0K (see Eqs.19 and 20 in p.140 in Kittel) and the integral of "DOS·FDD" at T > 0K are both equal to N; from here it only remains to evaluate the integral of "DOS·FDD" numerically, and plot μ/ ε_F as a function of T/T_F.
   (d) Replot FDD as a function of $\varepsilon/\varepsilon_F$ for T = 0.01T_F, 0. 1T_F, 0.5T_F, T_F, 1.2T_F plugging μ values as found in part (c).

(e) 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 (ε) for electrons in 2D;
   (b) DOS is proportional to $\varepsilon^{-1/2}$ 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 having a magnitude of V_0 at the atomic sites of a 1D periodic lattice (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 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, in terms of available electron states in the band it means, 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 calculations from part (a) for Na;
   (d) Calculate how much of Mg should be added to Na to make it k_F equal to 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.

7. Introduce the idea of using "effective mass" by comparing the dispersion relations for FEFG and an arbitrary $E(k)$ as expanded in Taylor series in the vicinity of minima/maxima points. Plot such $E(k)$, its first and second derivatives, as well as the effective mass as a function of k within the the 1st Brillouin zone (BZ) for a 1D crystal.
   (a) Why the effective mass is different from that of the electron rest mass?
   (b) Can the effective mass be negative? What does it mean? Introduce the concept of holes.

(c) Assume the energy of electrons in the vicinity of the conduction band edge to be $E(k)=Ak^2$, with A=5e-37 J·m². Compute the effective mass of electrons at the conduction band edge.