

## Module III and V: Practical assignments

### Electrons I

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 the interatomic distance. If this assumption is questionable, it challenges interpretations of all transport properties in terms of the FEG model, specifically thermal ( $\kappa$ ) and electrical ( $\sigma$ ) conductivities. Nevertheless,
  - (a) Assuming the FEG model, derive and calculate the Wiedemann-Franz law coefficient  $L = \frac{\kappa}{\sigma T}$  and elaborate why it seems to be in remarkably good agreement with experiment, even if  $\kappa$  and  $\sigma$  reveal less trust individually.
  - (b) Refine the consideration by deriving  $L$  in terms of the free electron Fermi gas (FEFG) model, in particular taking into account that  $C_{\text{el}} = \frac{2\pi N k_B T}{2T_F}$  and using  $v_F$  for the electron velocity.
2. Introduce periodic (Born–von Karman) boundary conditions and derive the density of states (DOS) for a FEFG in a finite 3D sample. Calculate values of  $\epsilon_F$ ,  $k_F$ ,  $v_F$  and  $T_F$ , i.e., the Fermi energy, wavevector, velocity and temperature, respectively, for alkali metals. Explain the trend.
3. Implications of the Fermi-Dirac distribution ( $f_{\text{FD}}$ ) on the energies ( $\epsilon$ ) reachable by the FEFG in 3D, and the magnitude of the chemical potential ( $\mu$ ).
  - (a) Show that  $\mu = \epsilon_F$  at  $T = 0$  K in the in FEFG model. Tips: Recall that, at  $T = 0$  K, the Gibbs energy  $G = N\mu$ , where  $N$  is the number of particles; on the other hand, at  $T = 0$  K, this expression may be compared with  $G = E + pV$ , where  $E$ ,  $p$  and  $V$  are the total energy, pressure and volume of the system.  $E$  at  $T = 0$  K can then be readily calculated by integrating  $\text{DOS}(\epsilon) \cdot f_{\text{FD}} \cdot \epsilon$ . Further, calculate the pressure by choosing an appropriate thermodynamic relation, e.g.,  $p = -(\partial E / \partial V)$ ; the anticipated result is  $N\mu = E + pV = N\epsilon_F$ , i.e.  $\mu = \epsilon_F$ .
  - (b) Further, assume that this FEFG is heated up to  $T > 0$  K. Continue assuming that  $\mu = \epsilon_F$ , i.e., not changing with T. Plot  $f_{\text{FD}}$  as a function of  $\epsilon/\epsilon_F$  for  $T = 0.01 T_F$ ,  $0.1 T_F$ ,  $0.5 T_F$ ,  $1.0 T_F$  and  $1.2 T_F$ . Compare the result with literature data, e.g., Fig. 3 on p.136 in Kittel. Up to what temperatures, approximately, is the assumption of  $\mu = \epsilon_F$  reasonable?
  - (c) Now investigate the true temperature dependence of  $\mu$  and plot  $\mu/\epsilon_F$  as a function of  $T/T_F$ . Tips: Remember that the total number of FEFG particles ( $N$ ) is not changing with temperature. In other words, the integral of DOS at  $T = 0$  K (see Eqs. 19 and 20 on p.140 in Kittel) and the integral of  $\text{DOS} \cdot f_{\text{FD}}$  at  $T > 0$  K are both equal to  $N$ ; from here it only remains to evaluate the integral of  $\text{DOS} \cdot f_{\text{FD}}$  numerically, and to plot  $\mu/\epsilon_F$  as a function of  $T/T_F$ .
  - (d) Replot  $f_{\text{FD}}$  as a function of  $\epsilon/\epsilon_F$  for  $T = 0.01 T_F$ ,  $0.1 T_F$ ,  $0.5 T_F$ ,  $1.0 T_F$  and  $1.2 T_F$  using the  $\mu$  values found in part (c).
  - (e) Make an estimate for the electronic heat capacity, taking into account that only a fraction of the electrons – those in the vicinity of  $\epsilon_F$  – may contribute to an increase in the total energy due to heating. Explain why.

### Electrons II

1. Consider FEFG in 2D and 1D. Show that
  - (a) DOS is independent of energy ( $\epsilon$ ) for electrons in 2D;

- (b) DOS is proportional to  $\epsilon^{-1/2}$  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. Further, for a realistic quantum wire, a combination of the 1D DOS 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 the degeneracy taking place in quantum wires.

2. Solve the time-independent Schrödinger equation (TISE) using a potential energy in the form of a delta function having a magnitude of  $V_0$  between the atomic sites of a 1D periodic lattice, as shown in Fig. 1 below (often referred as Kronig-Penney model in the 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  $V_0 \rightarrow \infty$ .

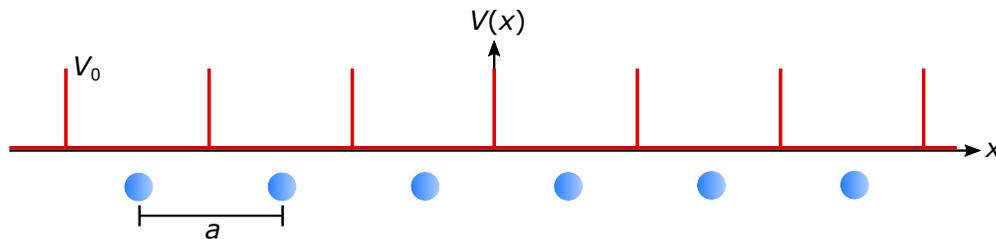


Figure 1: Potential consisting of delta functions with magnitude  $V_0$ .

3. Assume monovalent atoms crystallizing in a simple cubic (SC) lattice with a lattice parameter  $a$ .
- Calculate the magnitude of  $k_F$  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 ( $k_{BZ}$ ) in a SC lattice.
  - 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 a SC lattice to make  $k_F < k_{BZ}$  in the alloy. Would such alloying result in an improvement or degradation of electrical conductivity?
  - Repeat the calculations in part (a) for Na, which crystallizes in a BCC structure with 2 atoms in each conventional unit cell;
  - Calculate how much Mg should be added to Na to make  $k_F$  equal to  $k_{BZ}$  in the shortest possible direction from the  $\Gamma$  point, assuming the alloy to maintain the original BCC form.
  - Discuss the electrical conductivity evolution in such an alloy as a function of composition.
4. Introduce the idea of using effective mass by comparing the dispersion relations for FEEG and an arbitrary  $E(k)$  as expanded in a Taylor series in the vicinity of minimum/maximum points. Plot such  $E(k)$ , its first and second derivatives, as well as the effective mass as a function of  $k$  within the the 1<sup>st</sup> Brillouin zone (BZ) for a 1D crystal.
- Why is the effective mass different from that of the electron rest mass?
  - Can the effective mass be negative? What does this mean? Introduce the concept of holes.
  - Assume the energy of electrons near the conduction band edge to be  $E(k) = Ak^2$ , with  $A = 5 \times 10^{-37} \text{ Jm}^2$ . Compute the effective mass of electrons at the conduction band edge.

5. A 2D  $1 \times 1$  cm metallic sample consists of monovalent atoms crystallized in a simple rectangular primitive cell having parameters  $a = 2 \text{ \AA}$  and  $b = 4 \text{ \AA}$ . Calculate and make a scaled drawing of the 1<sup>st</sup> Brillouin zone and the free electron Fermi sphere. Discuss why and how the situation changes for the case of nearly free electrons and make a corresponding drawing.

6. Consider a 2D graphene sheet. The primitive vectors of the honeycomb lattice are given by

$$\mathbf{a}_1 = \frac{3a}{2}\mathbf{e}_x + \frac{\sqrt{3}a}{2}\mathbf{e}_y \quad \mathbf{a}_2 = \frac{3a}{2}\mathbf{e}_x - \frac{\sqrt{3}a}{2}\mathbf{e}_y,$$

where  $a = 0.142 \text{ nm}$ . The energy bands of the graphene sheet are found to be given by

$$E_{c,v}(\mathbf{k}) = \pm t \left[ 1 + 4 \cos \frac{\sqrt{3}\mathbf{k}_y a}{2} \cos \frac{3\mathbf{k}_x}{2} + 4 \cos^2 \frac{\sqrt{3}\mathbf{k}_y a}{2} \right]^{1/2},$$

with  $t = 3 \text{ eV}$

- (a) Plot  $E_{c,v}(\mathbf{k})$  along  $[10]$ ,  $[01]$  and  $[11]$  directions. Indicate the band gap.
  - (b) Derive a general expression for the effective mass of electrons in the conduction band of the graphene sheet. Find its values at the  $\Gamma$  point and  $[01]$  edge of the 1<sup>st</sup> Brillouin zone.
7. GaAs is a semiconductor with a direct band gap of  $\sim 1.42 \text{ eV}$  at room temperature. The experimental values for the effective mass (in units of the free electron rest mass,  $m_e$ ) are 0.067, 0.082 and 0.45 for electrons in the conduction band as well as light and heavy holes at the top of the valence bands, respectively. Compute the corresponding energy dispersion relations and sketch the band structure of GaAs in the vicinity of  $\Gamma$  point. What is the origin of “light” and “heavy” holes?
8. Consider P donors in Si in terms of a hydrogen-like model in the effective mass approximation.
- (a) Calculate the value of the ionization level for electrons to be excited to the conduction band.
  - (b) Calculate the Bohr orbit for these electrons and estimate the doping concentration required to transform localized states into an impurity band.
9. Consider the carrier concentration evolution as a function of temperature in  $10^{17} \text{ P/cm}^3$  homogeneously P-doped Si. Choose several characteristic temperature limits, specifically low, intermediate, and high – corresponding to donor freeze-out, full donor activation, and overtaking by intrinsic carriers, respectively. For these limits, compute
- (a) The equilibrium concentration of electrons and holes.
  - (b) The position of  $E_F$  relative to  $E_F$ .