3.225 Quiz 2003: Electronic and Optical Properties

\[ e = 1.602 \times 10^{-19} \text{ C} \quad m_0 = 9.11 \times 10^{-31} \text{ kg} \quad c = 2.998 \times 10^8 \text{ m/sec} \quad \varepsilon_0 = 8.854 \times 10^{-12} \text{ F/m} \]

\[ k_b = 1.38 \times 10^{-23} \text{ J/K} \quad h = 6.626 \times 10^{-34} \text{ J-sec} \quad \hbar = 1.054 \times 10^{-34} \text{ J-sec} \]

For this exam, consider a 3-D crystal of NaCl. It is a thin slab such that in the z-direction, the crystal is only 1 unit cell thick! How exciting.

**Crystal Structure of NaCl:**

\[ \varepsilon_r (w << 10^{14} \text{Hz}) = 5.9 \]

n = index of refraction = 1.5

\[ a = 0.5 \text{nm} \]

**Shape of Crystal:**

Thickness = 0.5 nm

1 cm
1. Assume the Drude Model to predict the electronic and optical properties
   (a) What would be the expected conductivity of NaCl in this model at room temperature?

   (b) What is the average electron velocity and maximum electron velocity at T=0 and T=300K?
(c) What are the optical properties of NaCl at room temperature (for example, sketch R vs. frequency of the light, and label).
2. Now consider upgrading to the Sommerfeld (i.e. free electron wave) model
   (a) The conductivity at room temperature is the same as it is for the Drude
   model. Make arguments to show that:

   \[ \sigma = \frac{k_B e^2}{m^*} \cdot g(E_F) \cdot \tau_F T \]

   and determine \( \tau_F \) to make \( \sigma \) agree with Drude if we assume \( m^* = m_o \).
(b) What is the maximum and average velocity at $T=0$ and $T=300K$?
(c) Describe any changes in optical properties as compared to the Drude model
(Hint: don’t forget to consider the geometry of the sample on electron waves)
3. Now consider the Nearly Free electron model. Assume that there is the same average potential $U$ at every lattice site (i.e. that Na and Cl sites have the same $U$; of course, in reality they are different, but for the exam let’s assume the $U$ on Na and Cl are the same).

(a) Draw the first 2 bands in the 100 direction and the 001 direction. Make the energy axis in units of $\frac{\pi^2 \hbar^2}{2ma^2}$. Assume $U=1 \frac{\pi^2 \hbar^2}{2ma^2}$. 
(b) Describe how a very large U in an ionic material can make an insulator, making the conductivity zero instead of the conductivity predicted by Drude/Sommerfeld.

(c) Roughly, what value of U (in eV) would make a ‘well-controlled’ semiconductor at room T (for any material, i.e. this question is not asking about the NaCl in this particular problem)? Explain.
4. Since real NaCl has a large U and is an insulator, it has no free carriers and its optical properties are dominated by bound charge. What are the relative contributions of electronic and ionic polarization in NaCl based on the supplied data?