Homework 4

Due Friday, May 2, 2025, 11:59 PM, by electronic upload

Problem 1. Consider a 1D lattice with lattice constant *a* and two atoms (A and B, with masses M_A and M_B, respectively) in each unit cell. Nearest-neighbor A and B atoms are connected via springs of lattice constant γ.

a) How many lattice wave branches do you expect? How many acoustic, how many optical?

b) Calculate and plot the dispersion relations for all branches for $M_A/M_B=1$ and $M_A/M_B=10$. Clearly denote the acoustic and optical branches.

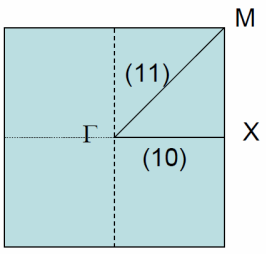
c) Calculate the ratio of displacements of atom A and atom B in the same unit cell for each normal mode of oscillation of the chain (a normal mode is a wave with a given **Q** and $\omega_{\mathbf{Q}}$).

Problem 2. Consider a 1D lattice with lattice constant *a* and three atoms in each unit cell. The atoms are A and B, with masses M_A and M_B, respectively, sand the lattice basis is A-B-A, i.e. the chain looks like this: —A-B-A—A-B-A—A-B-A—A-B-A—A-B-A Nearest-neighbor A and B atoms are connected via springs of lattice constant $,_1\gamma$ while nearest-neighbor A and A atoms are connected via springs of lattice constant $._2\gamma$

a) How many lattice wave branches do you expect? How many acoustic, how many optical?

b) Calculate and plot the dispersion relations for all the branches for $M_A/M_B=1$ and $M_A/M_B=10$ and $\gamma_1/\gamma_2=1$ and $\gamma_1/\gamma_2=10$ (there are 4 combinations, two of mass and two of spring constants, so you should have four sets of dispersion curves). Clearly denote the acoustic and optical branches.

Problem 3. Consider a 2D square lattice, with lattice constant *a*. The basis contains two atoms, A and B, with masses M_A and M_B, respectively. With respect to the unit cell located at the coordinate origin, atom A is at (0,0) and atom B is at (*a*/2,*a*/2). Springs of spring constant γ connect each atoms just to their nearest neighbors. Compute the phonon modes for this lattice, and plot them along the following high-symmetry directions in the Brillouin zone : M–⟶Γ–⟶X–⟶ M. Make sure you denote the acoustic and optical branches on the plot [High symmetry points in the Brillouin zone of the square lattice are Γ , M, and X, located at (0,0), (π/*a* ,π/*a*), and (*π*/*a* ,0) respectively (see Figure)].



Go through the details of the derivations of the transition rates, relaxation rates, and momentum relaxation rates for all the scattering mechanisms covered in the ECE 745 class.

Problem 4. a) Calculate and plot the relevant scattering rates and momentum relaxation rates for electrons in GaAs at room temperature (300 K):

- acoustic phonon scattering (absorption and emission together, within the elastic and equipartition approximations);
- polar optical phonon scattering (absorption and emission separately) for electrons in the Γ valley;
- intervalley scattering (Γ→L and L→Γ, together in one graph; Γ→X and X→Γ together, X→L and X→L together, L→L, X→X)
- ionized impurity scattering at doping densities of 10^{17} and 10^{19} cm-3.

The electron energy range should be 0 to 2 eV. Use the data from the table provided. Intervalley spacing is $\Delta E_{L\Gamma} = 0.29$ eV, $\Delta E_{X\Gamma} = 0.48$ eV. Assume m*=0.067m_0 for electrons in the Γ valley (not 0.063 as the table suggests). A good repository of data on various semiconductors is the Ioffe institute page http://www.ioffe.ru/SVA/NSM/Semicond/index.html

b) Calculate and plot the relaxation rates and momentum relaxation rates for POP and ionized impurity scattering in the same energy range. (Note how different they are.)

Hint: You have done this problem already when you took ECE 745. The point is to find your old scattering rate data in preparation for the Monte Carlo simulation project.

Problem 5. (*Lundstrom, problem 3.8*) Derive the Boltzmann transport equation for a semiconductor with a slowly varying (in space) effective mass. (Hint: First derive an expression for $d\vec{p}/dt$).

Problem 6. a) Prove that the relaxation time approximation (RTA) can be employed only for elastic and isotropic scattering processes. Which relaxation time should be used as the characteristic relaxation time τ in the RTA for isotropic, and which for elastic processes?

b) Dominant scattering mechanisms in bulk Si are acoustic phonon scattering, ionized impurity scattering, and equivalent intervalley scattering. For which ones among them can we employ the RTA?

c) Dominant scattering mechanisms in bulk GaAs at low fields are acoustic phonon scattering, ionized impurity scattering, and the most efficient one is the polar-optical-phonon scattering (at higher electric fields, nonequivalent intervalley scattering starts to be appreciable). For which ones among these scattering mechanisms can we employ the RTA?

Problem 7.

a) For a uniform sample of GaAs doped *n*-type to 10^{17}cm^{-3} and kept at room temperature (300 K), calculate the position of the Fermi level with respect to the conduction band.
b) For the same sample, using the relaxation-time approximation, calculate the mobility limited only by acoustic phonon scattering, then only by ionized impurity scattering, and finally only by polar-optical-phonon scattering. (For some of these mechanisms the RTA is technically not justified, but is still widely used to produce order-of-magnitude estimates).
c) Use Matthiessen's rule to calculate the mobility and from it the conductivity of this sample. How does it compare to the experimentally measured value ?
d) Do not use Matthiessen's rule, but rather sum up the momentum relaxation rates for every given energy, then invert the sum to get the total momentum relaxation rate, and then find the average of that time, $\langle\langle\tau_m\rangle\rangle$. With it, calculate the mobility and conductivity. How does it compare to that obtained using Matthiessen's rule? How does it compare to experiment/your calculation using Rode's method?

Problem 8. (*Lundstrom, problem 3.14*)

In metals, we often assume that $\partial f_S/\partial t \approx -\delta(\varepsilon-\varepsilon_F)$.

a) Explain and justify the approximation (e.g., why can it be used in metals, and not in semiconductors)
b) Derive an expression for the mobility of electrons in a metal and compare the result to Eq. (3.61).

Problem 9. (*Lundstrom, problem 3.10*)

Use the principle of detailed balance in equilibrium [i.e., that $\partial f_0/\partial t = 0$] , and answer the following questions:

a) Establish the following relation between the equilibrium transition rate and its inverse:

$$\frac{S_0(\vec{p}',\vec{p})}{S_0(\vec{p},\vec{p}')} = \exp\left(\frac{\varepsilon(\vec{p}')-\varepsilon(\vec{p})}{k_B T_L}\right)$$

(This relation is often true away from equilibrium, because S are determined by the scattering potentials and are relatively insensitive to the applied fields.)

b) Use physical arguments to explain why transitions to higher energy states are less probable than transitions to lower energy states.