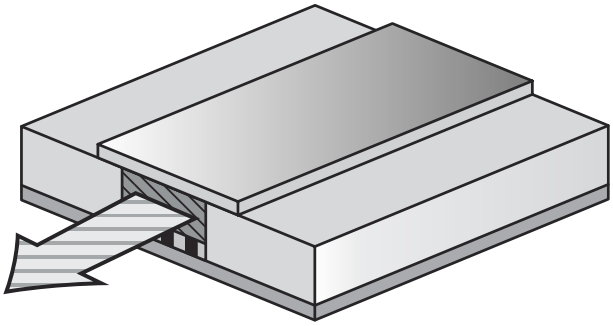
Semiconductor Optoelectronic Devices
Homework I



Filippos Tzimkas-Dakis
MSc. Photonics & Nanoelectronics
Faculty of Physics, University of Crete

November 13, 2020

Problem 1

Referring to a two-dimensional GaAs semiconductor system ($m_e = 0.07m_0$, $m_h = 0.4m_0$, $E_g = 1.4eV$):
(**a**) Calculate the density of states at the CB and VB band edges.
(**b**) Calculate the carrier densities in the CB and VB at T=300K, using the Boltzmann approximation and assuming intrinsic semiconductor.
(**c**) Find the quasi-Fermi levels, without using Boltzmann approximation, when the semiconductor is excited optically with $n = p = 10^{11}$ cm^{-2} carriers.
($^*k = 8.6173 * 10^{-5}\,\mathrm{eV}\cdot\mathrm{K}^{-1}$)

Solution
(**a**) For the density of states at the Conduction and Valence Band edges we have

- Conduction Band $\qquad N_{2\mathrm{D}}^{\mathrm{c}} = \dfrac{m_e}{\pi * \hbar^2} = 2.918 \cdot 10^{13}\ \mathrm{eV}^{-1}\mathrm{cm}^{-2}$
- Valence Band $\qquad N_{2\mathrm{D}}^{\mathrm{v}} = \dfrac{m_h}{\pi * \hbar^2} = 1.667 \cdot 10^{14}\ \mathrm{eV}^{-1}\mathrm{cm}^{-2}$

(**b**) At this point we calculate the carrier densities in the Conduction Band at $T = 300$ K,

$$n = \int_{E_c}^{\infty} f(E) \cdot N_{2\mathrm{D}}^{\mathrm{c}}(E)\,\mathrm{d}E = \frac{m_e}{\pi * \hbar^2} \int_{E_c}^{\infty} \frac{1}{\exp\left(\dfrac{E - E_F}{kT}\right) + 1}\mathrm{d}E \xrightarrow[\mathrm{E\text{-}E_F \gg kT}]{\text{Boltz.Appr.}}$$

$$\simeq \frac{m_e}{\pi * \hbar^2} \int_{E_c}^{\infty} \exp\left(\frac{E_F - E}{kT}\right)\mathrm{d}E = \frac{m_e}{\pi * \hbar^2} \cdot kT \left[-\mathrm{e}^{\left(\frac{E_F - E}{kT}\right)}\right]_{E_c}^{\infty}$$

$$= 7.45 \cdot 10^{11} \cdot \mathrm{e}^{\left(\frac{\mathrm{E_F - E_c}}{\mathrm{kT}}\right)}\ \ \mathrm{cm}^{-2}. \tag{1}$$

For the case of Valence Band we have

$$p = \int_{-\infty}^{E_v} (1 - f(E)) \cdot N_{2\mathrm{D}}^{\mathrm{v}}(E)\,\mathrm{d}E = \frac{m_h}{\pi * \hbar^2} \int_{-\infty}^{E_v} 1 - \frac{1}{\exp\left(\dfrac{E - E_F}{kT}\right) + 1}\mathrm{d}E$$

$$\xrightarrow[\mathrm{E\text{-}E_F \gg kT}]{\text{Boltz.Appr.}} \simeq \frac{m_h}{\pi * \hbar^2} \int_{-\infty}^{E_v} \exp\left(\frac{E - E_F}{kT}\right)\mathrm{d}E = \frac{m_h}{\pi * \hbar^2} \cdot kT \left[\mathrm{e}^{\left(\frac{E - E_F}{kT}\right)}\right]_{-\infty}^{E_v}$$

$$= 4.31 \cdot 10^{12} \cdot \mathrm{e}^{\left(\frac{\mathrm{E_v - E_F}}{\mathrm{kT}}\right)}\ \ \mathrm{cm}^{-2}. \tag{2}$$

For the analysis above we used Boltzmann approximation for both cases. More specifically, in Eq.(1) we assumed that

$$f(E) = \frac{1}{\exp\left(\frac{E-E_F}{kT}\right)+1} \simeq \exp\left(\frac{E_F-E}{kT}\right), \text{when } E-E_F \gg kT \quad (3)$$

and for the second case

$$1-f(E) = 1 - \frac{1}{\exp\left(\frac{E-E_F}{kT}\right)+1} \simeq \exp\left(\frac{E-E_F}{kT}\right), \text{when } E-E_F \gg kT. \quad (4)$$

For an intrisic semiconductor we know that $n \cdot p = {n_i}^2$, so we equate the Eqs.(1)-(2) and we get

$${n_i}^2 = n \cdot p = N_c \cdot N_v \cdot \mathrm{e}^{\frac{E_g}{kT}} = 10.876\,\mathrm{cm}^{-4}. \quad (5)$$

Now we can calculate the densities we where asked for as

$$\begin{aligned} n = n_i &= \sqrt{10.876} = 3.2978\,\mathrm{cm}^{-2}, \\ p = n_i &= \sqrt{10.876} = 3.2978\,\mathrm{cm}^{-2}. \end{aligned} \quad (6)$$

(**c**) Firstly, we calculate the integrals we need to calculate the quasi-Fermi levels,

$$\begin{aligned} &\int \frac{1}{\mathrm{e}^{a(x-x_o)}}\mathrm{d}x \to \left(u = \mathrm{e}^{a(x-x_o)}\right) \to \frac{1}{a}\int \frac{1}{u(u+1)}\mathrm{d}u \\ &= \frac{1}{a}\int \frac{1}{u} - \frac{1}{u+1}\mathrm{d}u = \frac{1}{a}\ln\left(\frac{u}{u+1}\right) \to \frac{1}{a}\ln\left(1 - \frac{1}{\mathrm{e}^{a(x-x_o)}+1}\right), \end{aligned} \quad (7)$$

and

$$\begin{aligned} &\int 1 - \frac{1}{\mathrm{e}^{a(x-x_o)}}\mathrm{d}x \to \left(u = \mathrm{e}^{a(x-x_o)}\right) \to \frac{1}{a}\int \frac{1}{u} - \frac{1}{u(u+1)}\mathrm{d}u \\ &= \frac{1}{a}\int \frac{1}{u+1}\mathrm{d}u = \frac{1}{a}\ln(u+1) \to \frac{1}{a}\ln\left(\mathrm{e}^{a(x-x_o)}+1\right), \end{aligned} \quad (8)$$

in our case $a = 1/kT$ and $x_o = E_F$.
Due to the optical excitation we have a change for the carries which is given as $\Delta_n = \Delta_p = 10^{11}\,\mathrm{cm}^{-2}$. Therefore, total amount of carriers in each case is given as

$$n = n_o + \Delta_n \simeq \Delta_n = 10^{11}\ \mathrm{cm}^{-2}, \quad (9)$$

$$p = p_o + \Delta_p \simeq \Delta_p = 10^{11}\ \mathrm{cm}^{-2}, \quad (10)$$

where for $n_o = p_o = 3.2978\,\mathrm{cm}^{-2}$ the values we found in (**a**). At this point, we do the same calculations as in (**a**) with the difference that here we do not make any approximation. So, the quasi-Fermi level of Coduction Band is given, via the Eq. (7),

$$n = \Delta_n = \frac{N_c}{kT}\int_{E_c}^{\infty} f\,(E)\mathrm{d}E = N_c \cdot \ln\left(1 - \frac{1}{\exp\left(\frac{E_c - E_{Fn}}{kT}\right) + 1}\right) \Rightarrow$$

$$\exp\left(\frac{\Delta_n}{N_c}\right) = 1 - \frac{1}{\exp\left(\frac{E_c - E_{Fn}}{kT}\right) + 1} \Rightarrow$$

$$E_c - E_{Fn} = kT \cdot \ln\left(\frac{\mathrm{e}^{\frac{\Delta_n}{N_c}}}{1 - \mathrm{e}^{\frac{\Delta_n}{N_c}}}\right) = 0.054\,\mathrm{eV}. \tag{11}$$

Regarding quasi-Fermi level of Valence band, we use Eq. (8) and we get

$$p = \Delta_p = \frac{N_v}{kT}\int_{-\infty}^{E_v} (1 - f\,(\,E\mathrm{d}E = N_v \cdot \ln\left(\exp\left(\frac{E_v - E_{Fv}}{kT}\right) + 1\right) \Rightarrow$$

$$\exp\left(\frac{\Delta_p}{N_v}\right) = \exp\left(\frac{E_v - E_{Fv}}{kT}\right) + 1 \Rightarrow$$

$$E_v - E_{Fv} = kT \cdot \ln\left(\mathrm{e}^{\frac{\Delta_p}{N_v}} - 1\right) = -0.0972\,\mathrm{eV} \quad . \tag{12}$$

As we expected, the quasi-Fermi energy of the conduction band is lower than the band's energy level, but in the case of valence band the scheme is inverted, i.e. the quasi-Fermi energy is higher.

Problem 2

The following photoluminescence spectrum, obtained at $T = 2$ K, is the outcome of electron-heavy hole recombination in GaAs/$\mathrm{Al}_{0.26}\,Ga_{0.74}As$ quantum wells of different thicknesses. It is given that $m_e = 0.07m_o$, $m_h = 0.4m_o$, $E_g(\mathrm{GaAs}) = 1.51$ eV and $E_g(\mathrm{Al}_{0.26}\mathrm{Ga}_{0.74}\mathrm{As}) = 1.91$ eV at $T = 2$ K.Also, that the partition of band gap difference between GaAs and AlGaAs in CB and VB is 2:1. Calculate the thicknesses of the two quantum wells that correspond to

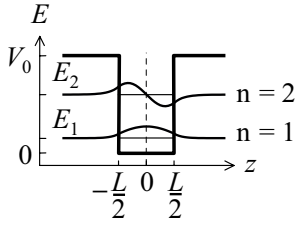


Figure 1: Finite square well potential, with thickness L and potential $\mathrm{V_o}$.

the lowest and highest emission energy.

Solution

Firstly, we have to solve the finite square well potential depicted in Fig.(1) in order to find the relation that connects the energy E and the thickness of each well. This potential is one a part of the total super-lattice which is shown in Fig.(2). So, if you solve this one-dimensional square well we get two relations from the continuity condition of the wavefunction and its derivative, and combining those two relations we get

$$\tan(\xi) = \frac{\sqrt{\lambda^2 - \xi^2}}{\xi}, \tag{13}$$

with

$$\xi = \sqrt{\frac{2m^* \cdot E}{\hbar^2}}\frac{L}{2}, \qquad \lambda = \sqrt{\frac{2m^* \cdot V_o}{\hbar^2}}\frac{L}{2}, \tag{14}$$

where m^* is the effective mass of the electron inside the well, E is the energy the even solutions and L is the thickness/width of the quantum well.

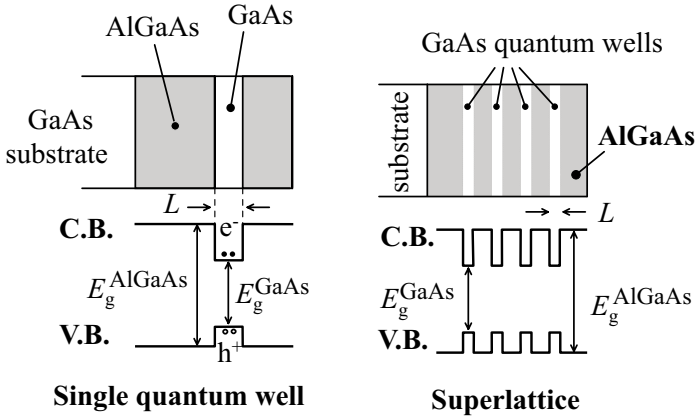


Figure 2: The left schematic depicts the layout of one single quantum well, while the right one shows the superlattice which is composed of many single quantum wells.

Anyone familiar with the equations we are about to solve can understand that we have a transcendental equation which can only be solved graphically, as shown in Fig.(3), or by using a recursive method. We chose the second option for two reasons, (a) it is much more efficient and precise, and (b) we need to make a parametric analysis to solve our problem, so the recursive method is much more

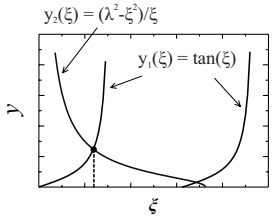


Figure 3: Finite square well potential, with thickness L and potential V_o.

rapid.
Before we reveal our results it is convenient to make some comments about the process. We solve the transcendental Eq.(13) two times, one for the quantum well of electrons and one for the quantum well of holes. In each case we used the given effective masses and we calculated the potential V_o as it is shown below

$$\Delta E_g = E_g^{AlGaAs} - E_g^{GaAs} = 1.91 - 1.51 = 0.4\,\text{eV} \Rightarrow$$

$$V_e = \frac{2}{3}\Delta E_g = 0.2667\,\text{eV}\,, \tag{15}$$

$$V_h = \frac{1}{3}\Delta E_g = 0.133\,\text{eV} \tag{16}$$

We calculated all the ground state energies E_e and E_h for values of width $L \in [1, 50]$nm and the results are depicted in Fig.4. Figure 4(a) shows how we used the total energy (i.e. $E_g + E_{ee} + E_{hh}$) to find the respective widths L_1 and L_2, while Figure 4(b) shows only the energies E_{ee} and E_{hh} separately. The two peaks were located at $\lambda_1 = 979\,\text{nm}$ and $\lambda_2 = 745$ nm, wavelengths

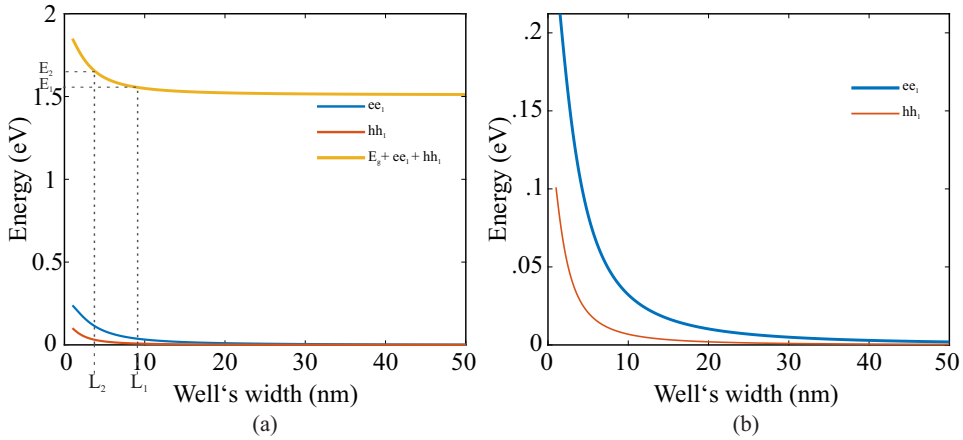


Figure 4: (a) Shows the total energy versus the width L and also reveals the difference between the ground state energies of the two potential wells. (b) Depicts the ground state energy of each potential well, with blue(bold line) for the carriers n and with red(thin line) for the holes p, versus the width L.

that can be converted to the respective energies as $E_1 = 1.55174$ eV and $E_2 = 1.66422$ eV, respectively. Thus, using the above mentioned method we find

$$L_1 = 9.58\,\text{nm}$$
$$L_2 = 3.54\,\text{nm}\ .$$

Code

In this section we attach the MATLAB code that has been used to produce the above mentioned results. For comments, mistakes, clarifications etc. please send a message to dakisfilippos@gmail.com.

```
% Filippos Tzimkas-Dakis  UoC October 2020
% Homework 1 ------- Optoelectronics and Lasers


% Solving the square welll potential
%------ Even solutions -------------
eV2J      = 1.60218e-19;            % converts eVolts to Joules
J2eV      = 6.241509e+18;           % converts Joules to eVolts
% c        = 3*1e8;                 % speed of light (m/s)
Eg_GA     = 1.51;                   % E-Bandgap @ GaAs(eV)
Eg_AGA    = 1.91;                   % E-Bandgap @ AlGaAs(eV)
Delta_Eg  = Eg_AGA -Eg_GA;
Eg        = Eg_GA;
me        = 9.1093837015*1e-31;          % electron mass in (Kg)
h_eV      = 6.582119569*1e-16;           % h-bar in (eV*s)
h_J       = 1.054571817*1e-34;           % h-bar in (J*s)
L         = (1:0.02:50)*1e-9;            % creates the a vector with widths
% h_ev^2 /me
%% Pure Mathematical way for ee1
m    = 0.07*me;               % effective mass of the electron
Vo   = (2/3)*Delta_Eg;        % well's potential in (eV)
Vo   = Vo*eV2J;
Uo   = 2*m*Vo/h_J^2;          % defines a new normalized potential value
y    = sqrt(Uo)*L/2;

Eee     = 0.*L;
options = optimset('Display','off'); %meaningless input for fsolve
out     = 0.1;

for i = 1:length(L)
    % using "fsolve()" to solve the trascedental equation
    out  = fsolve(@(t)tan(t) - sqrt(y(i)^2 - t^2)/t,out,options);
    % Eee(i) stores the g.s. energy for every L
    Eee(i) = (2*out/L(i))^2*(h_J^2 /2/ m)*J2eV;
end
%% Pure Mathematical way for hh1
m    = 0.4*me;                % effective mass of the electron
Vo   = (1/3)*Delta_Eg;        % well's potential in (eV)
Vo   = Vo*eV2J;
Uo   = 2*m*Vo/h_J^2;          % defines a new normalized potential value
```

```
y     = sqrt(Uo)*L/2;

Ehh      = 0.*L;
options = optimset('Display','off'); % meaningless input for
    fsolve
out      = 0.1;

for i = 1:length(L)
    % fsolve, solves the trascedental equation
    out   = fsolve(@(t)tan(t) - sqrt(y(i)^2 - t^2)/t,out,options
    ); %solver
    % Ehh(i) stores the g.s. energy for every L
    Ehh(i) = (2*out/L(i))^2*(h_J^2 /2/ m)*J2eV;
end

%%
close all
E_tot = Eg + Ehh + Eee;

figure(1)                              % Ploting results
plot(L*10^9,Eee,'LineWidth',1.5)
hold on
plot(L*10^9,Ehh,'LineWidth',1.5)
plot(L*10^9,E_tot,'LineWidth',1.5)
axis on
xlabel('Well's width (nm)')
ylabel('Energy (eV)')
legend('ee_1','hh_1','E_g + ee_1 + hh_1')

E1 = 1.55174; % eV @ 799 nm
E2 = 1.66422; % ev @ 745 nm
[~,j1] = min(abs(Eg + Ehh+Eee - E1));
L(j1)                                  % returns the width L_1
[~,j2] = min(abs(Eg + Ehh+Eee -E2));
L(j2)                                  % returns the width L_2
% 1.55174 ev  @ 799
% 1.55564 ev  @ 797
% 1.66422 ev  @ 745
```