Final Project
Computational Methods in Physics

By: Nikesh Maharjan

Language: Python

OBJECTIVES

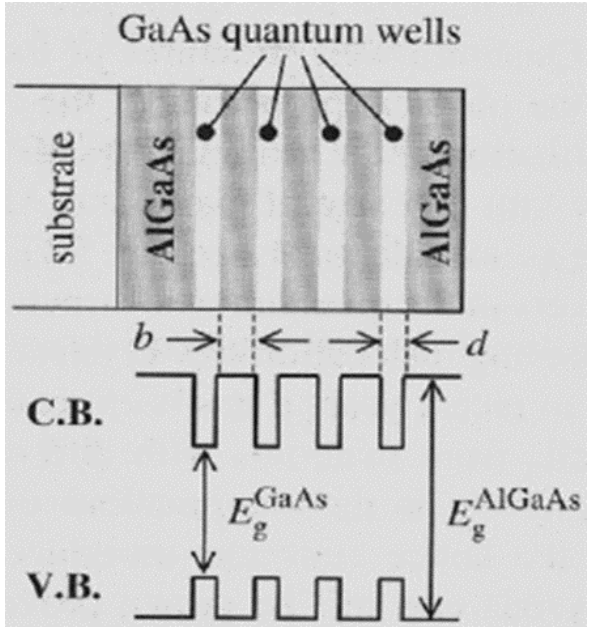
- To build an algorithm that solves a stationary one-dimensional Schrodinger equation to estimate the energy levels in Multiple Quantum Wells (MQWs) based Resonant Bragg Structure (RBS)
- To compare the results from the numerical calculation with the analytical solutions for the energy eigenvalues.

BACKGROUND

- Our RBS consists of 60 periods of AlGaAs/GaAs QWs and has intrinsic electronic excitations such as excitons.

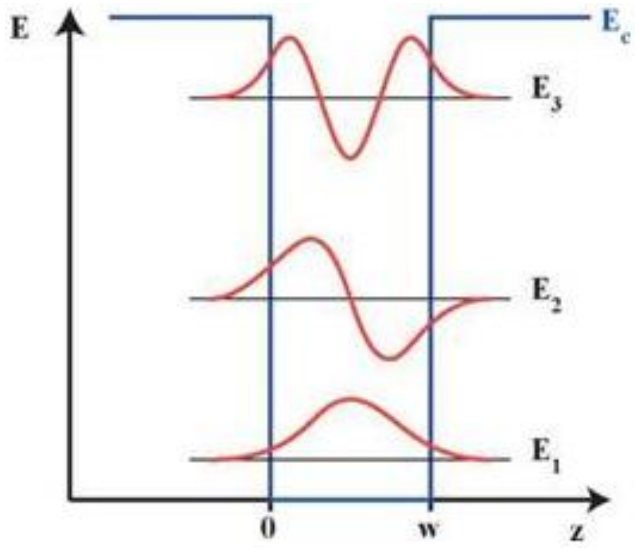
- Periodicity of the system provides the Bragg resonance condition at the photon energy equal to the energy of excitons in the QWs. It has thinner barriers, thus coupled by tunneling through it.

- Bragg diffraction of light by the QW excitons leads to the formation of a super-radiant optical mode at resonance frequency.



- Quantum well structure can be explained by the Particle in a box problem and the energy levels in the QWs can be calculated using one-dimensional Schrodinger equation.

$$-\frac{\hbar^2}{2m^*}\frac{d^2\phi_n}{dz^2}+V(z)\phi_n=E_n\phi_n$$



- Angle and temperature dependent Optical reflectance (OR) and contactless Electro-reflectance (ER) spectroscopy techniques are used to understand the Bragg resonance peak and exciton energy.

- Broad and enhanced OR and ER features are observed when resonance tuned to the second quantum state of QW excitons, showing a strong light matter interaction.

NUMERICAL METHOD

Solve Schrodinger equation, a second order ODE with only one dependent variable ϕ

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}z^2} = f\left(\phi, \frac{\mathrm{d}\phi}{\mathrm{d}z}, \mathrm{z}\right)$$

Define a new quantity ψ, such that

$$\frac{\mathrm{d}\phi}{\mathrm{d}z} = \psi, \qquad \frac{\mathrm{d}\Psi}{\mathrm{d}z} = f(\phi, \psi, z)$$

Hence, define f as:

$$\frac{\mathrm{d}\Psi}{\mathrm{d}z} = \frac{2m^*E\phi}{\hbar^2}$$

So we have two first order differential equation.
Solve it by Euler method:

$$\phi(\mathrm{z}+h) = \phi(z) + f(\phi, z) * h$$

Start with the BC: $\phi = 1$, and $\frac{\mathrm{d}\phi}{\mathrm{d}z} = \alpha$, $\alpha = \sqrt{\frac{2m^*(V_0 - E)}{\hbar^2}}$

And, get $\phi(\mathrm{z}+\mathrm{h})$ and $\Psi(\mathrm{z}+\mathrm{h})$ until cover the whole range we want

$$\phi \mathrel{+}= \Psi * h$$

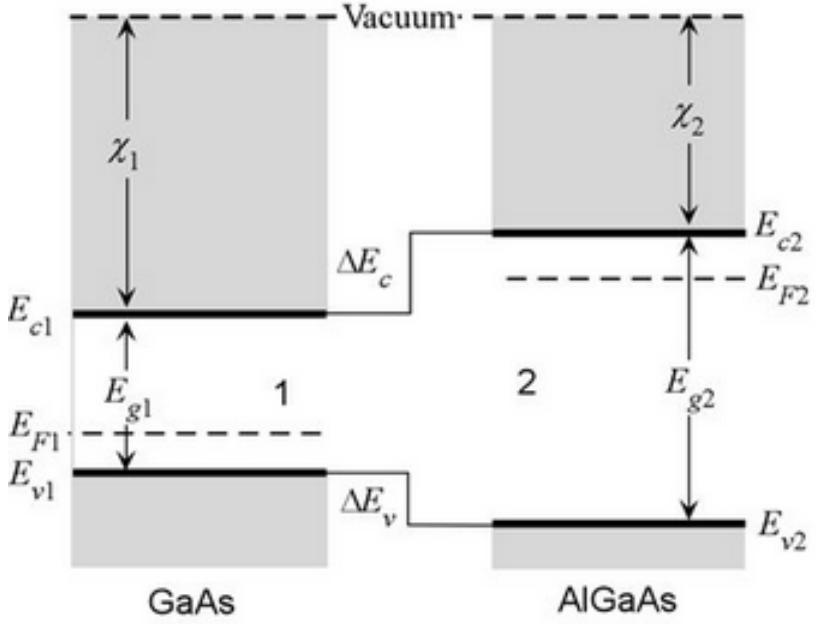
$$\Psi \mathrel{+}= f(\Psi, z) * h$$

SOME PARAMETERS

 # Constants
m0 = 9.10938291E-31 # Free electron rest mass
h = 6.62606957E-34 # Plank constant
hbar = h/(2*pi) # Reduced Plank constant
ee = 1.60217657E-19 # Electron charge

#Parameters GaAs/AlGaAs
L = 14.5E-9 # GaAs QW width
N = 1000 # Number of steps
h = L/N # Step size
Eg_well = 1.518 # Bandgap eV
Eg_barrier = 2.5753
dEc = 0.4729 # conduction band discontinuity
exciton_binding = 8.5E-3 # Exciton binding energy (eV)

 # Electron
V0_ee = (Eg_barrier - Eg_well)*dEc*ee # Barrier height
m_ee = 0.067 # Effective electron mass
 # Light hole
V0_lh = (Eg_barrier - Eg_well)*(1 - dEc)*ee # Barrier height
m_lh = 0.087 # Effective hole mass
 # Heavy hole
V0_hh = (Eg_barrier - Eg_well)*(1 - dEc)*ee # Barrier height
m_hh = 0.62 # Effective hole mass

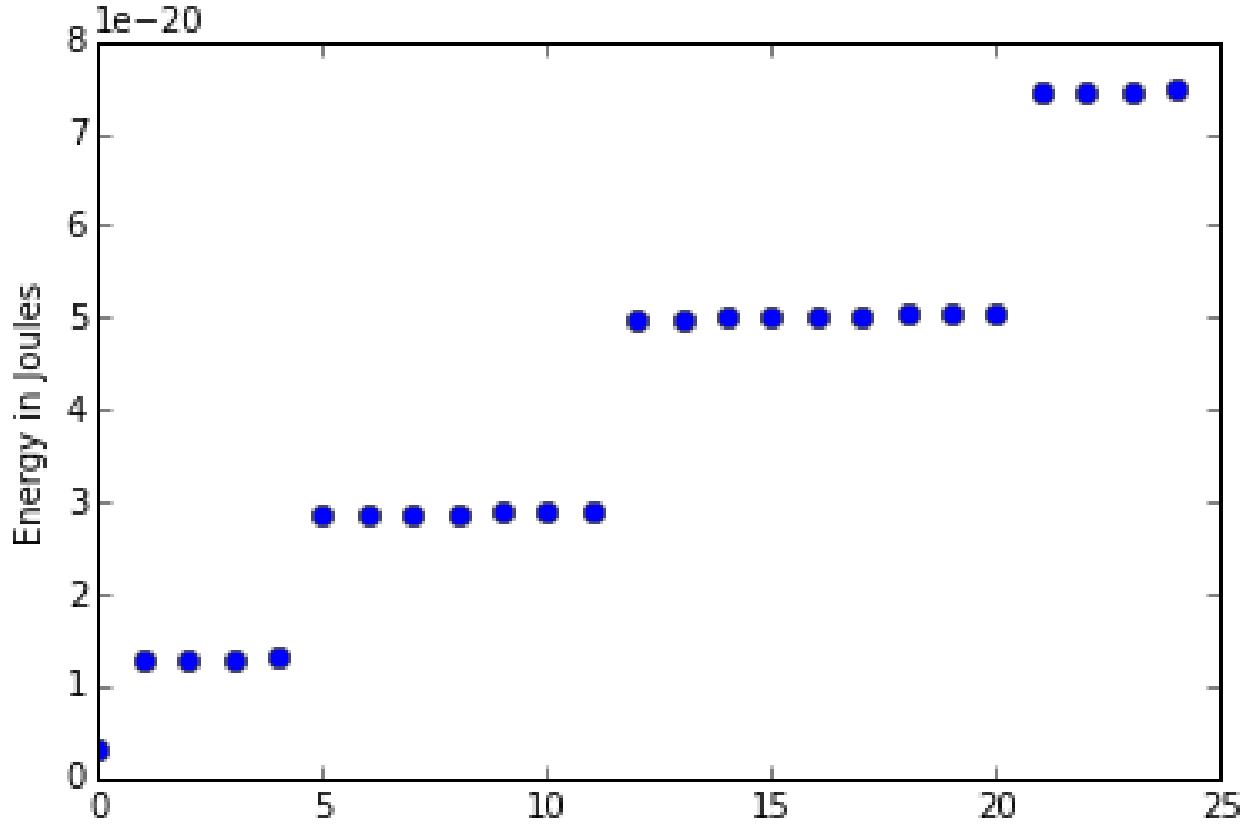


PROGRAM THAT CALCULATES THE ELECTRON ENERGY EIGENVALUES

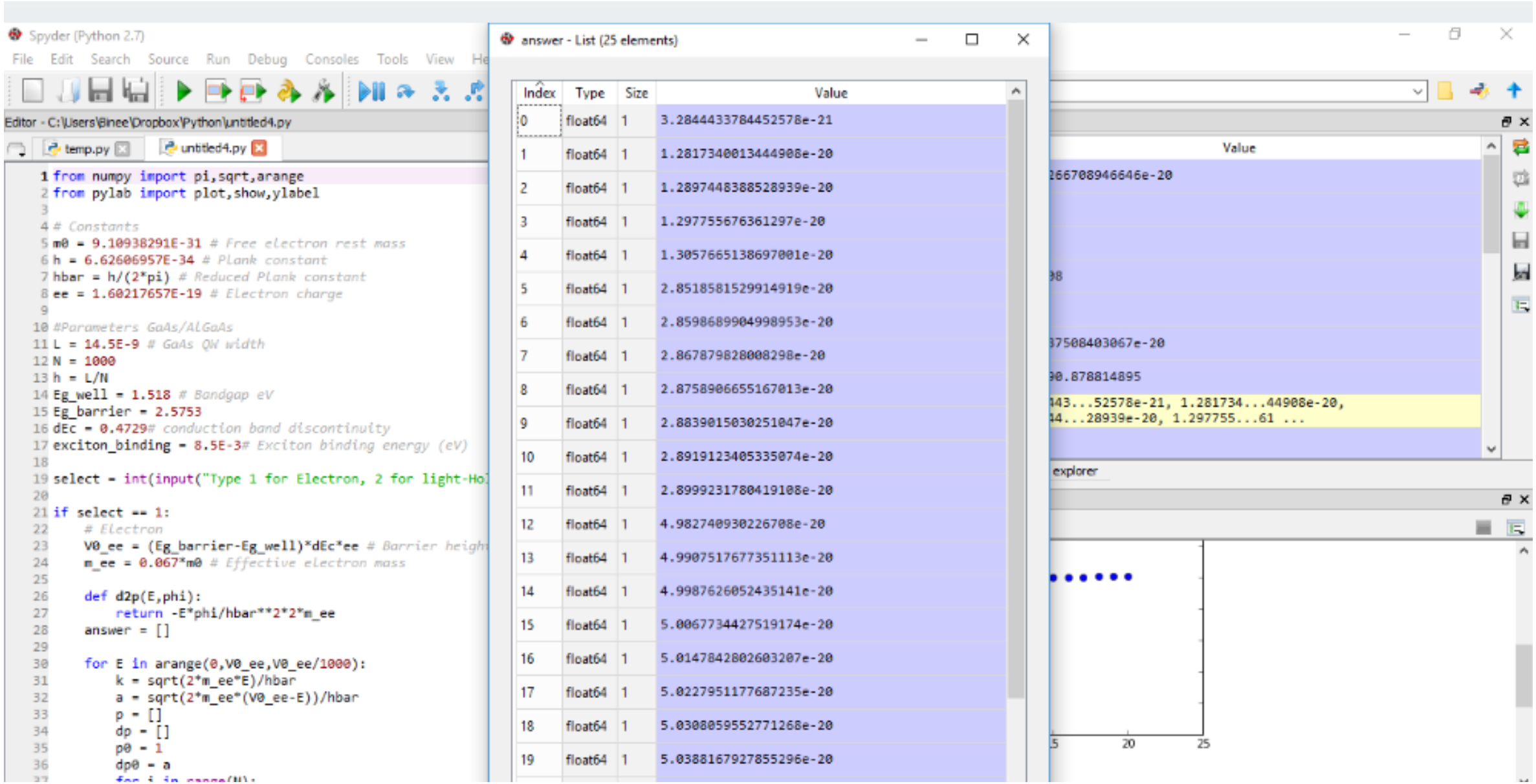
```
# Electron
V0_ee = (Eg_barrier-Eg_well)*dEc*ee      # Barrier height
m_ee = 0.067*m0          # Effective electron mass

def d2p (E, phi):
    return -E*phi/hbar**2*2*m_ee
answer = []

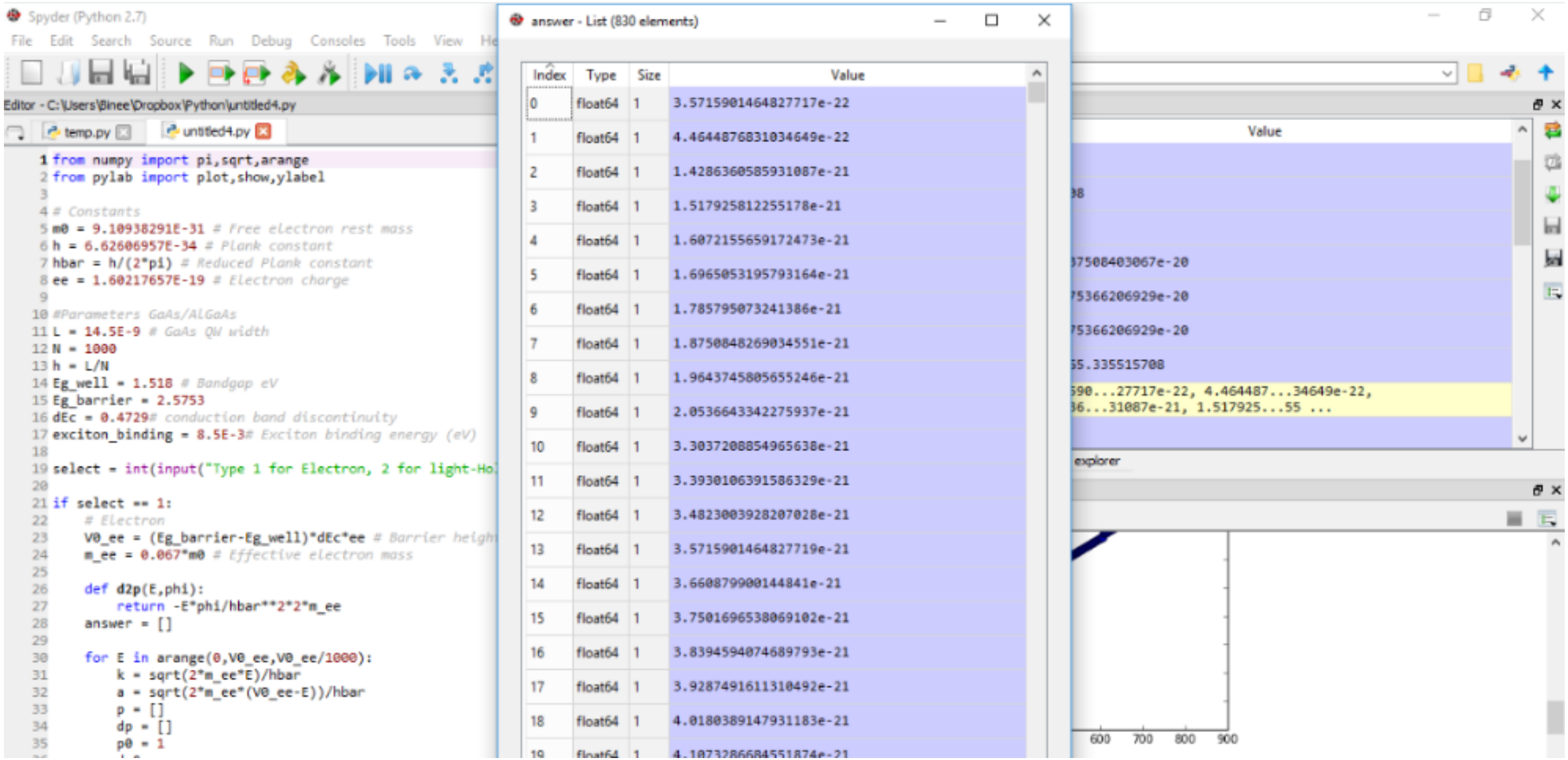
for E in arange (0, V0_ee, V0_ee/1000):
    k = sqrt (2*m_ee*E)/hbar
    alpha = sqrt (2*m_ee*(V0_ee - E))/hbar
    p = []
    dp = []
    p0 = 1
    dp0 = alpha
    for i in range (N):
        p.append (p0)
        dp.append (dp0)
        dp0 += d2p (E,p0)*h     # Euler Method  of solving ODEs
        p0 += dp0*h
    if abs (1 + alpha*p[-1]/dp[-1]) < 1e-1:
        answer.append (E)
```



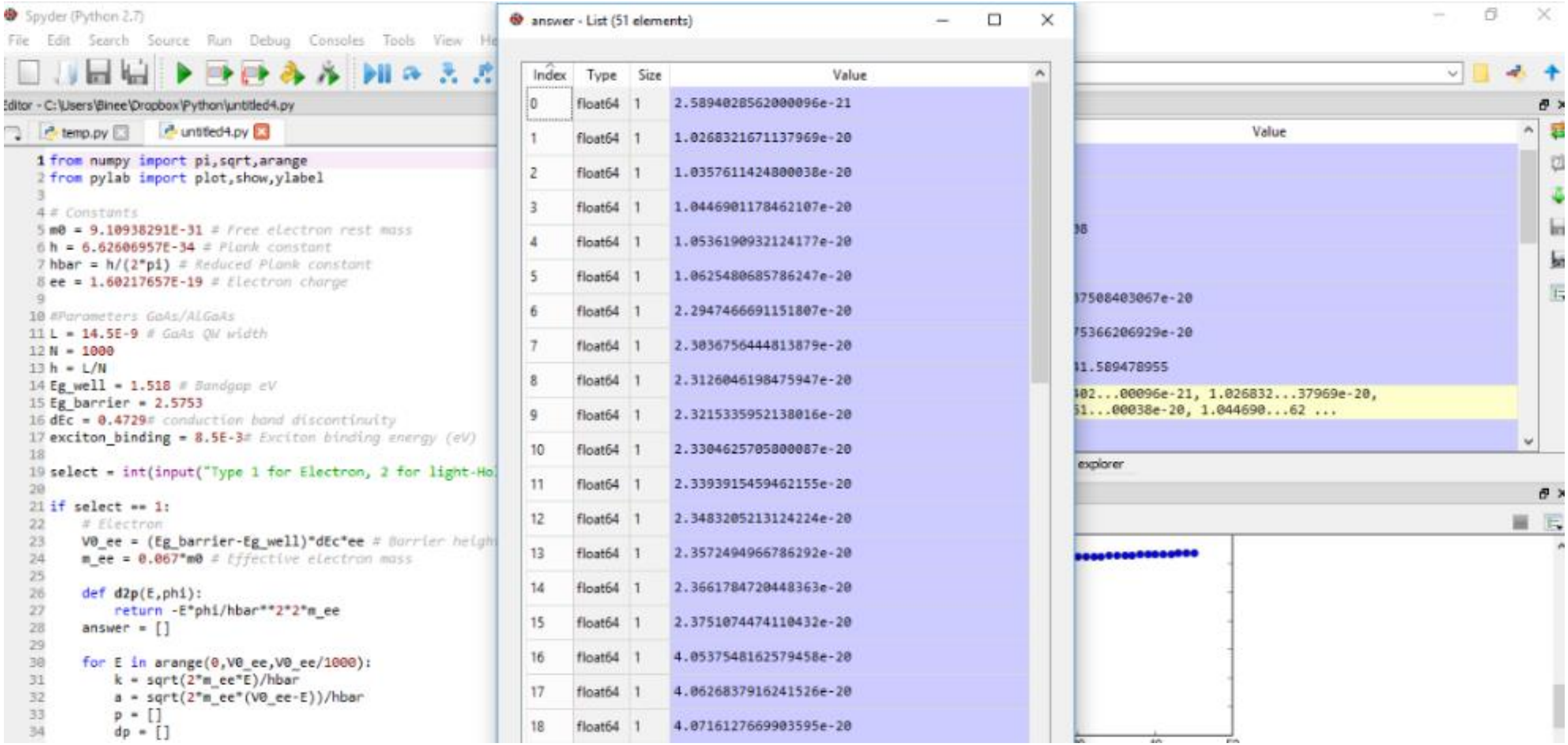
ELECTRON ENERGY EIGENVALUES



HEAVY-HOLE ENERGY EIGENVALUES



LIGHT-HOLE ENERGY EIGENVALUES



ANALYTICAL METHOD OF SOLVING SCHRODINGER EQUATION

$$-\frac{\hbar^2}{2m^*}\frac{d^2\phi_n}{dz^2}+V(z)\phi_n=E_n\phi_n$$

We got solution of two forms:

$$u=\begin{cases}\text{v tan v (symmetric)}\\ \text{-v cot v (antisymmetric)}\end{cases} \qquad k=\frac{\sqrt{2mE}}{\hbar} \qquad \alpha=\frac{\sqrt{2m^*(v_0-E)}}{\hbar}$$

$$\text{Using } u^2+v^2=u_0^2 \text{ and, } u_0^2=\frac{m^*L^2V_0}{2\hbar^2} \qquad u=\alpha\left(\frac{L}{2}\right), \text{ and } \frac{kL}{2}=v,$$

$$\sqrt{u_0^2-v^2}=\begin{cases}\text{v tan v (symmetric)}\\ \text{-v cot v (antisymmetric)}\end{cases}$$

The energy eigen values is given by: $E=\frac{2\hbar^2}{m^*L^2}v_n^2$

The inter-section between the curves $\sqrt{u_0^2-v^2}$ and $v\tan v$ or $-v\cot v$

gives the v-values and eventually gives the energy values.

SHORT PROGRAM THAT GIVES THE INTERSECTION OF THREE FUNCTIONS

 # Electron

```
u0_2_ee = m_ee*m0*power (L,2)*V0_ee/(2.0*power (hbar,2) )    # u0 square
f = lambda v: sqrt (u0_2_ee - power (v,2) )
g = lambda v: v*tan (v)
h = lambda v: - v*cot (v)
v = arrange (0, 8, 0.001)
plot ( [f, g, h], ylim = [0,8], xlim = [0,8] )
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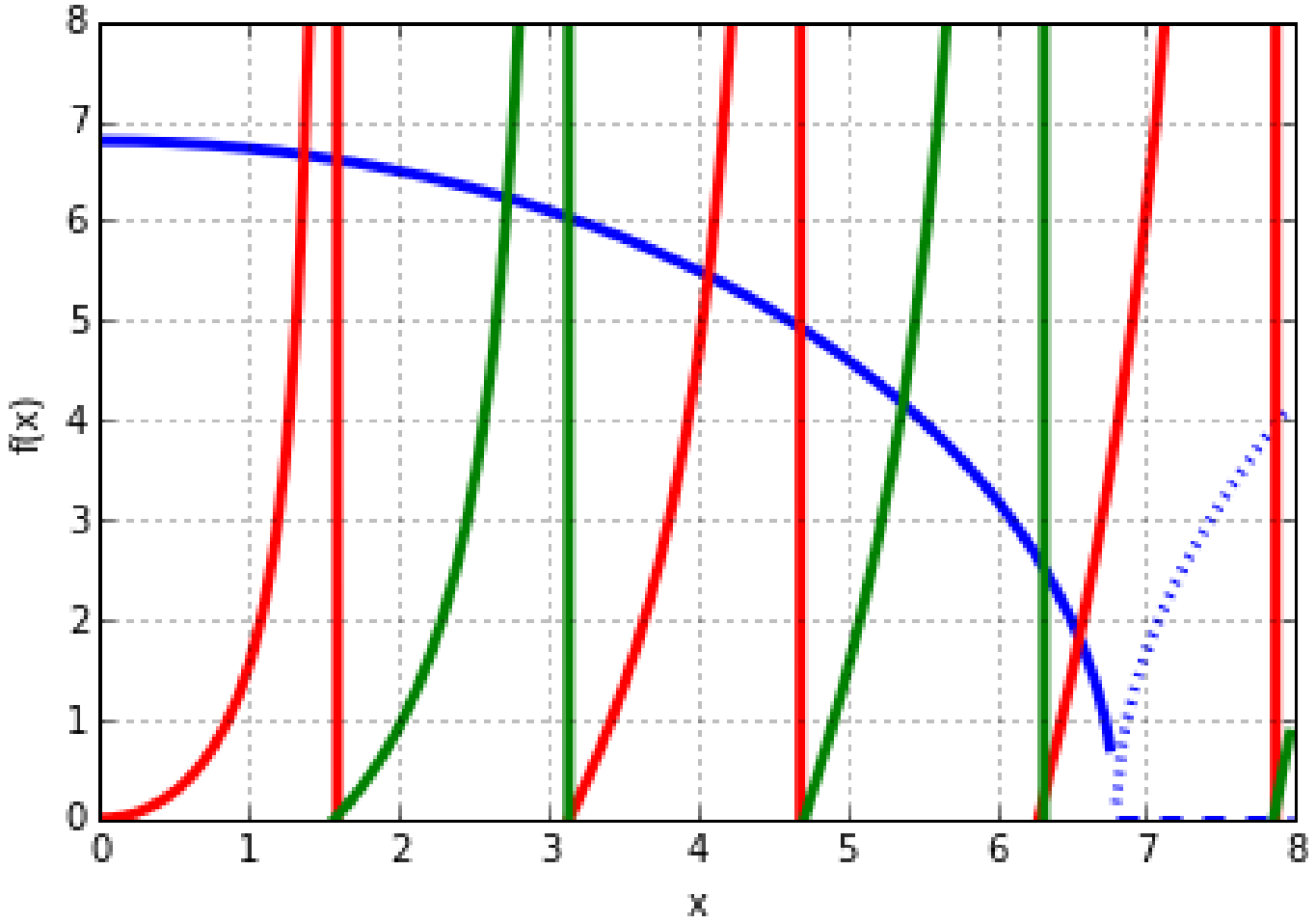
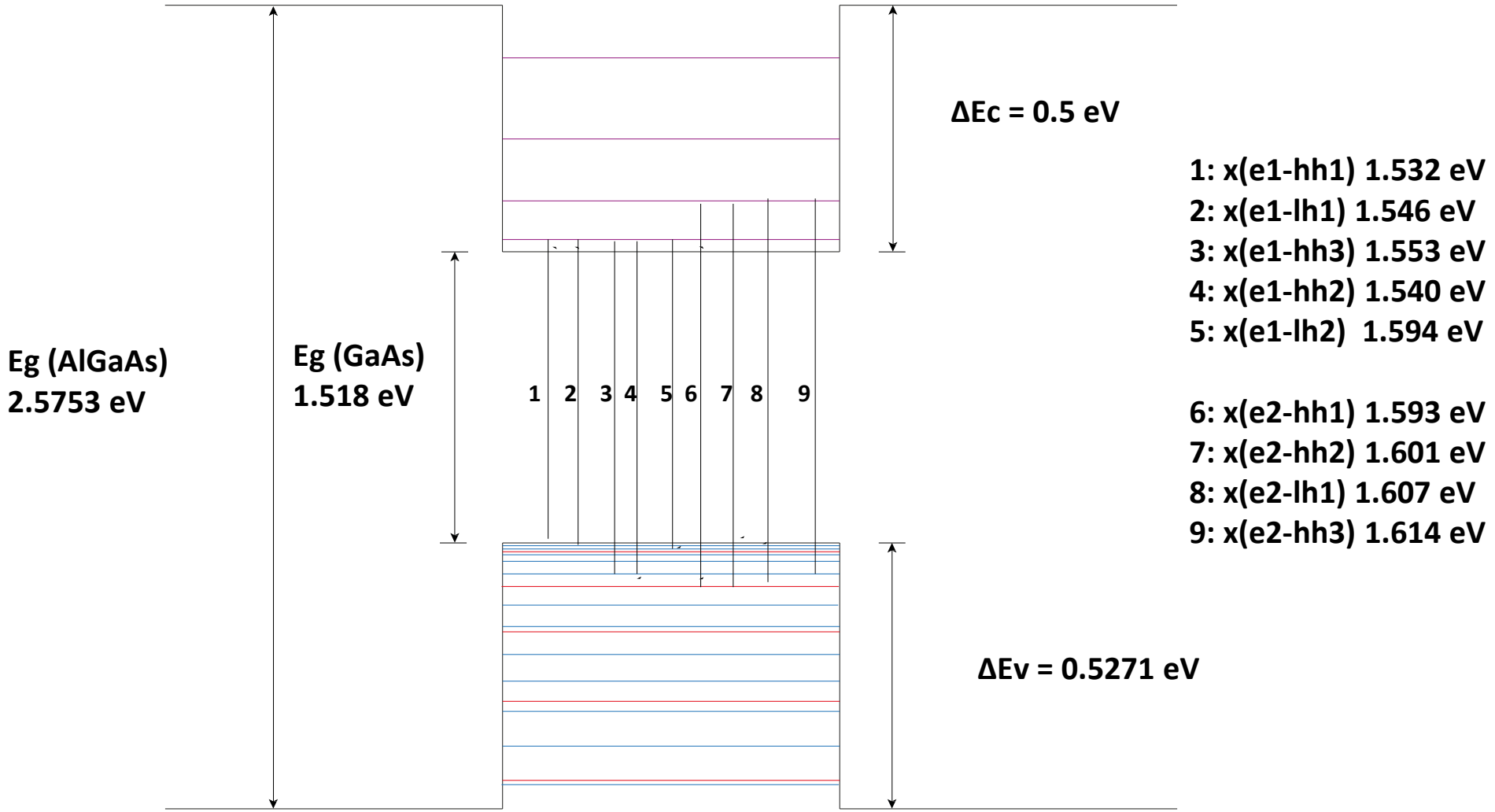


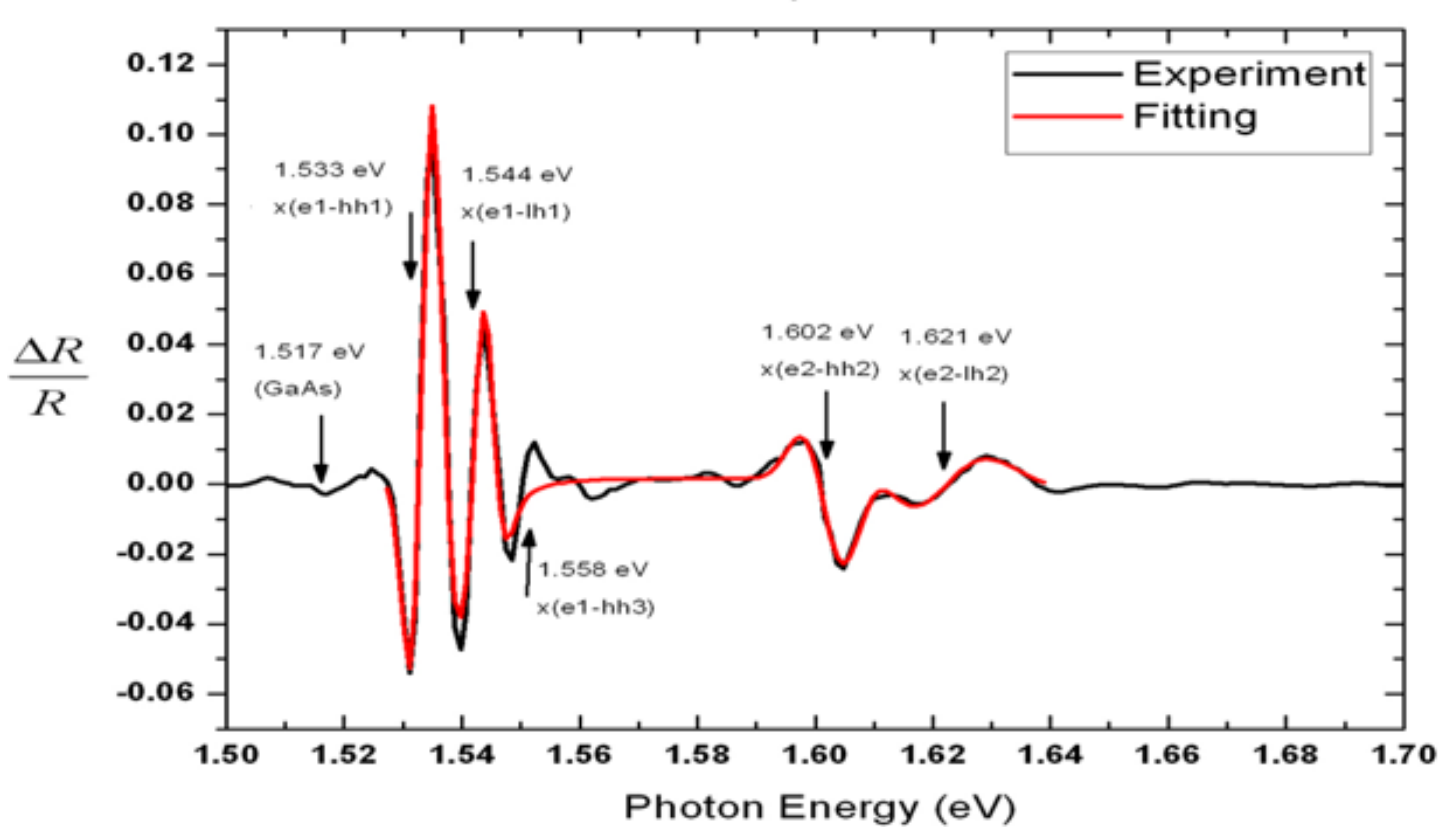
CALCULATED EXCITON ENERGY VALUES IN QUANTUM WELLS

QW width, **L = 14.5nm**



ER SPECTRUM OF THE RBS STRUCTURE

- ER measurement at 20 Kelvin with an angle of 23 degree incident photon
- Excitonic features are fitted using the first derivative of the Lorentzian line shape.
- Transition energies from fitting are marked by arrows



CONCLUSION

- Energy eigenvalues for electron, heavy-hole and light-hole calculated using the numerical methods are comparable to the analytic solutions.

- Fitted excitonic features from the ER spectrum are best matched up-to two decimal places from the numerical calculations.

Thank you for your time