

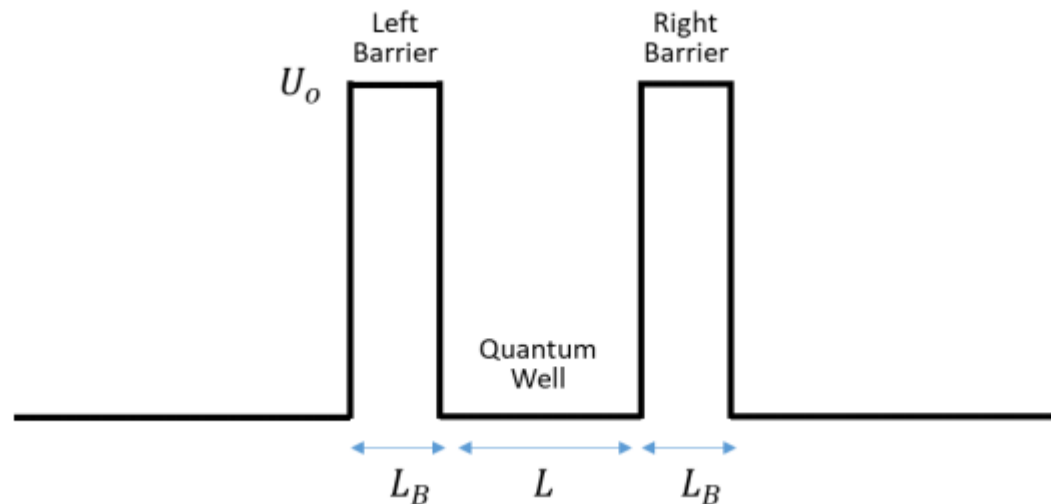
# Project-7

## Xichen Li, EE521 - Group 5

```
In [6]: import numpy as np
import matplotlib inline
import matplotlib.pyplot as plt
```

### Chapter-10 P7 :

(a) Calculate and plot the transmission probability versus energy through a double barrier structure shown below. On the same figure, plot  $t_1$  versus energy. Calculate  $t_1$ ,  $t_2$ ,  $r_1$ , and  $r_2$  using the expressions for a single barrier. What is the maximum value of transmission in your plots? What is the maximum theoretical value of transmission? Assume that  $L = 50\text{\AA}$ ,  $L_B = 10\text{\AA}$ , and  $U_o = 400\text{meV}$ .



(b) Plot and discuss the effect of making both barrier thinner,  $L_B = 6\text{\AA}$

### Answer

**(a)**

Define at the edge of the left barrier  $x = 0$ . According to the lecture, the boundary condition can be written as:

$$\begin{aligned} A_1 + B_1 &= C_1 + D_1 \\ ik(A_1 - B_1) &= \alpha(C_1 - D_1) \\ C_1 e^{\alpha L_B} + D_1 e^{-\alpha L_B} &= F_1 e^{i\beta L_B} \\ \alpha(C_1 e^{\alpha L_B} - D_1 e^{-\alpha L_B}) &= i\beta F_1 e^{i\beta L_B} \end{aligned}$$

where

$$\begin{aligned} k &= \sqrt{\frac{2mE}{\hbar^2}} \\ \alpha &= \sqrt{\frac{2m(|U_0| - E)}{\hbar^2}} \\ \beta &= \sqrt{\frac{2mE}{\hbar^2}} = k \end{aligned}$$

The  $\frac{B_1}{A_1}$  and  $\frac{F_1}{A_1}$  can be solved as:

$$\begin{aligned} \frac{B_1}{A_1} &= \frac{(\alpha + i\beta)(\alpha - ik)e^{-\alpha L_B} - (\alpha - i\beta)(\alpha + ik)e^{\alpha L_B}}{(\alpha + i\beta)(\alpha + ik)e^{-\alpha L_B} - (\alpha - i\beta)(\alpha - ik)e^{\alpha L_B}} e^{-i\beta L_B} \\ \frac{F_1}{A_1} &= \frac{-4i\alpha k}{(\alpha + i\beta)(\alpha + ik)e^{-\alpha L_B} - (\alpha - i\beta)(\alpha - ik)e^{\alpha L_B}} e^{-i\beta L_B} \end{aligned}$$

Because  $\beta = k$ , then  $r_1 = \frac{B_1}{A_1}$  and  $t_1 = \frac{F_1}{A_1}$  can be re-written as :

$$\begin{aligned} r_1 &= \frac{B_1}{A_1} = \frac{(\alpha^2 + k^2)(e^{-\alpha L_B} - e^{\alpha L_B})}{(\alpha + ik)^2 e^{-\alpha L_B} - (\alpha - ik)^2 e^{\alpha L_B}} e^{-ik L_B} \\ t_1 &= \frac{F_1}{A_1} = \frac{-4i\alpha k}{(\alpha + ik)^2 e^{-\alpha L_B} - (\alpha - ik)^2 e^{\alpha L_B}} e^{-ik L_B} \end{aligned}$$

$r_2$  and  $t_2$  of the right barrier can be calculated similarly. The boundary condition needs to be re-written as:

$$\begin{aligned} A_2 e^{ikL_1} + B_2 e^{-ikL_1} &= C_2 e^{\alpha L_1} + D_2 e^{-\alpha L_1} \\ ik(A_2 e^{ikL_1} - B_2 e^{-ikL_1}) &= \alpha(C_2 e^{\alpha L_1} - D_2 e^{-\alpha L_1}) \\ C_2 e^{\alpha L_2} + D_2 e^{-\alpha L_2} &= F_2 e^{i\beta L_2} \\ \alpha(C_2 e^{\alpha L_2} - D_2 e^{-\alpha L_2}) &= i\beta F_2 e^{i\beta L_2} \end{aligned}$$

where  $L_1 = L_B + L$  and  $L_2 = L_B + L + L_B$ . And  $\alpha$ ,  $k$ , and  $\beta$  are the same as the left barrier.

$r_2 = \frac{B_2}{A_2}$  and  $t_2 = \frac{F_2}{A_2}$  are:

$$\frac{B_2}{A_2} = \frac{(\alpha + i\beta)(\alpha - ik)e^{-\alpha L_B} - (\alpha - i\beta)(\alpha + ik)e^{\alpha L_B}}{(\alpha + i\beta)(\alpha + ik)e^{-\alpha L_B} - (\alpha - i\beta)(\alpha - ik)e^{\alpha L_B}} e^{-i\beta L_2 + ikL_1}$$

$$\frac{F_2}{A_2} = \frac{-4i\alpha k}{(\alpha + i\beta)(\alpha + ik)e^{-\alpha L_B} - (\alpha - i\beta)(\alpha - ik)e^{\alpha L_B}} e^{-i\beta L_2 + ikL_1}$$

Again we have  $\beta = k$ , then

$$r_2 = \frac{B_2}{A_2} = \frac{(\alpha^2 + k^2)(e^{-\alpha L_B} - e^{\alpha L_B})}{(\alpha + ik)^2 e^{-\alpha L_B} - (\alpha - ik)^2 e^{\alpha L_B}} e^{-ikL_B}$$

$$t_2 = \frac{F_2}{A_2} = \frac{-4i\alpha k}{(\alpha + ik)^2 e^{-\alpha L_B} - (\alpha - ik)^2 e^{\alpha L_B}} e^{-ikL_B}$$

According to the lecture, the total transmission probability  $T$  is equal to:

$$T = \left| \frac{t_1 t_2}{1 - r_2 r_1 e^{i2kL}} \right|^2$$

The transmission probability  $T$  and  $t_1$  of the left barrier are plotted used the code below.

```

In [7]: eta = 6.63e-34/2/np.pi #Reduced Plank constant in eV.s
q = 1.6e-19
LB=10e-10
Lspace=50e-10
m = 9.11e-31 #Assuming the particle mass is equal to a free electron
Uo=0.4*q
E1=2*q
dE=0.0511e-2*q
E=np.arange(0, E1, dE)

k=np.sqrt(2*m*E/(eta**2))
alpha=np.sqrt(2*m*(Uo-E)/(eta**2)+0j)
beta=k
#print(alpha)

t1=-4j*alpha*k/((alpha+k*1j)**2*np.exp(-alpha*LB)-(alpha-k*1j)**2*np.exp(alpha*LB))*np.exp(-1j*k*LB)
T1=abs(t1)**2
r1=(alpha**2+k**2)*(np.exp(-alpha*LB)-np.exp(alpha*LB))/((alpha+k*1j)**2*np.exp(-alpha*LB)-(alpha-k*1j)**2*np
R1=abs(r1)**2
r2=r1
t2=t1

T=abs(t1*t2/(1-r1*r2*np.exp(1j*2*k*Lspace)))*2

plt.figure()
plt.plot(E/q, T1, color='b', ls='--')
#plt.plot(E/q, R1, color='g', ls='--')
#plt.plot(E/q, R1+T1, color='k', ls='--')

plt.plot(E/q, T, color='r', ls='--')

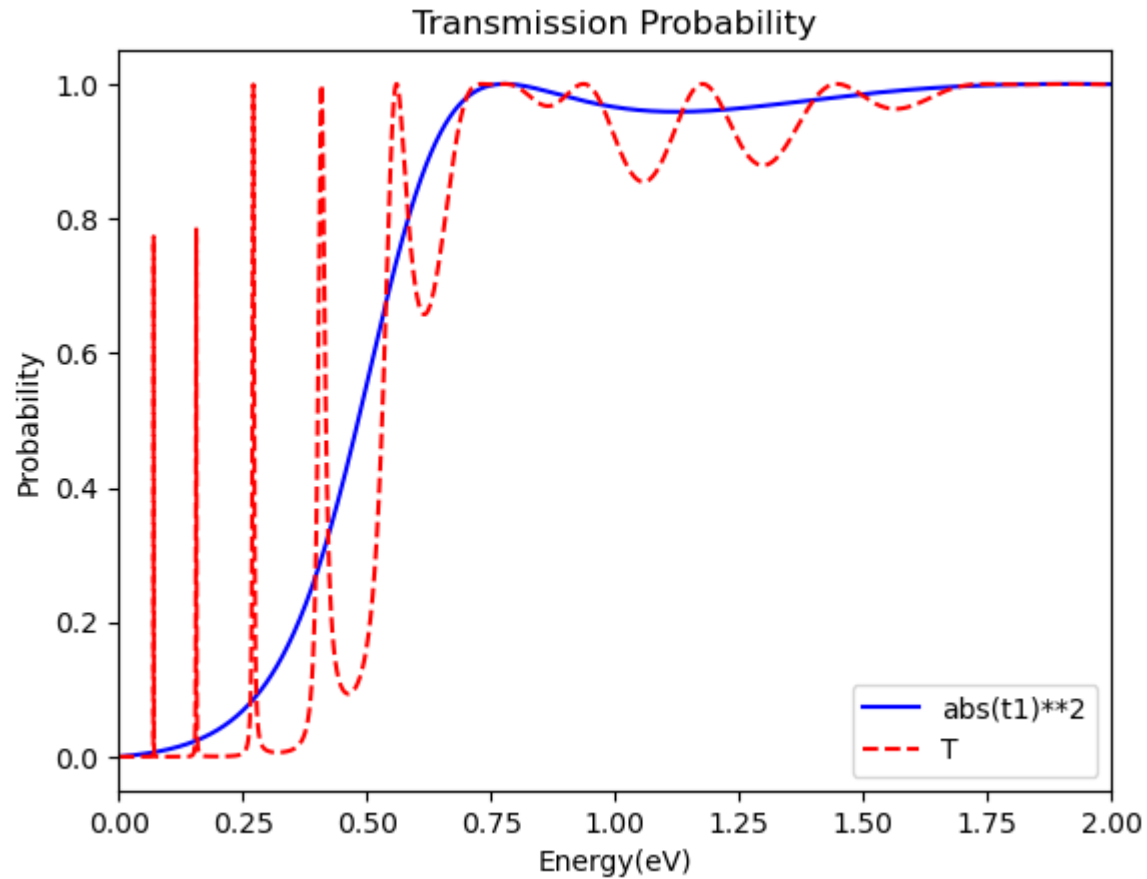
plt.legend(['abs(t1)**2', 'T'])
plt.title('Transmission Probability')
plt.xlabel('Energy(eV)')
plt.ylabel('Probability')
plt.xlim(0, E1/q)

```

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```
T=abs(t1*t2/(1-r1*r2*np.exp(1j*2*k*Lspace)))*2
```

Out[7]: (0.0, 2.0)



As we can tell from the plot above, the maximum value of the total transmission is close to 1. The maximum theoretical value of transmission will be equal to 1.

**(b) Plot and discuss the effect of making both barrier thinner,  $L_B = 6A$**

Repeat the code above by changing  $L_B = 6A$ . The transmission probability is plotted below:

In [8]: LB=6e-10

```

t1=-4j*alpha*k/((alpha+k*1j)**2*np.exp(-alpha*LB)-(alpha-k*1j)**2*np.exp(alpha*LB))*np.exp(-1j*k*LB)
T1=abs(t1)**2
r1=(alpha**2+k**2)*(np.exp(-alpha*LB)-np.exp(alpha*LB))/((alpha+k*1j)**2*np.exp(-alpha*LB)-(alpha-k*1j)**2*np
R1=abs(r1)**2
r2=r1
t2=t1

T=abs(t1*t2/(1-r1*r2*np.exp(1j*2*k*Lspace)))**2

plt.figure()
plt.plot(E/q, T1, color='b', ls='-')
#plt.plot(E/q, R1, color='g', ls='-')
#plt.plot(E/q, R1+T1, color='k', ls='-')

plt.plot(E/q, T, color='r', ls='--')

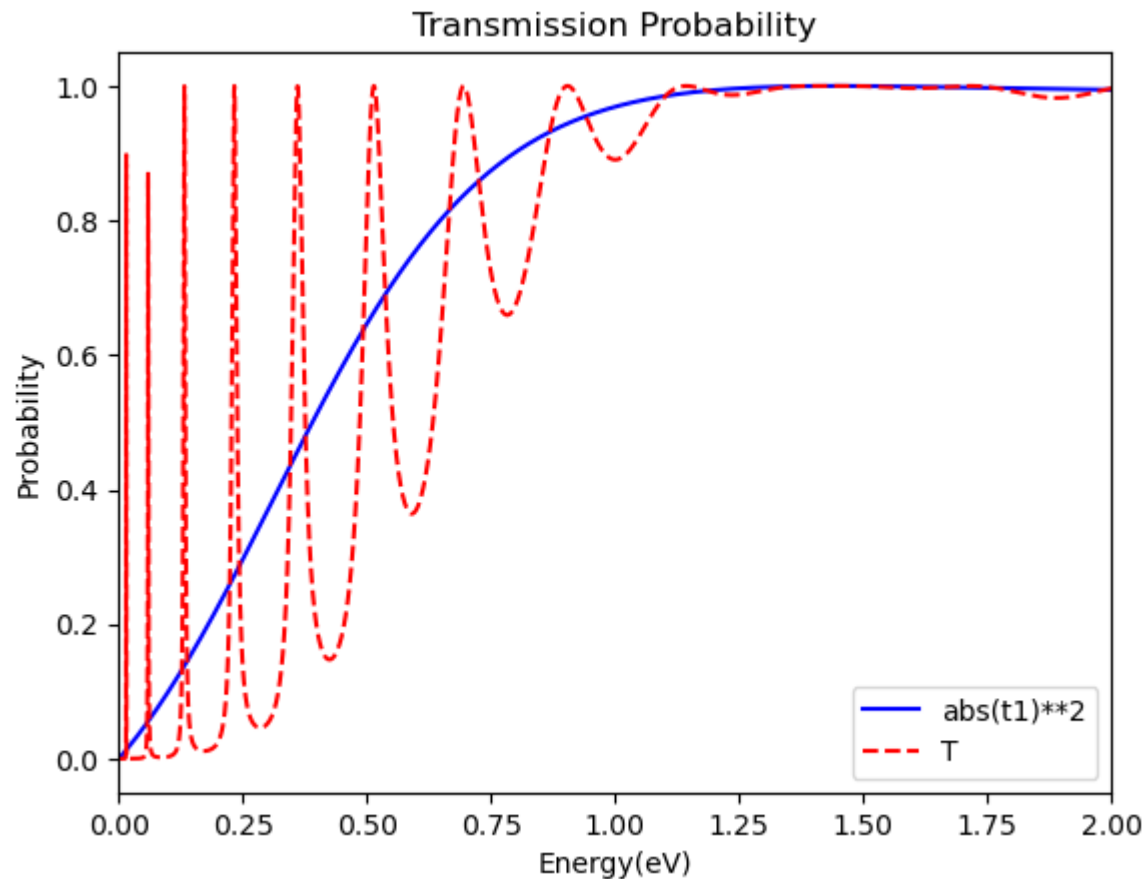
plt.legend(['abs(t1)**2', 'T'])
plt.title('Transmission Probability')
plt.xlabel('Energy(eV)')
plt.ylabel('Probability')
plt.xlim(0, E1/q)

```

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```
T=abs(t1*t2/(1-r1*r2*np.exp(1j*2*k*Lspace)))**2
```

Out[8]: (0.0, 2.0)



As we can observe from the figure above, decreasing the thickness of the barrier can decrease the energy of the resonances.

### Chapter-10 P8 :

For a double barrier resonant tunneling barrier, show that the transmission probability as a function of energy near a resonant energy level  $E_1$  in the well is,

$$T = \frac{\Gamma_1 \Gamma_2}{(E - E_1)^2 + (\frac{\Gamma_1 + \Gamma_2}{2})^2}$$

Assume the transmission through the individual barriers are both smaller than one.

(a) Express  $\Gamma_1$  and  $\Gamma_2$  in terms of the length of the quantum well (box)  $L$ , mass  $m$ , and the transmission amplitude through the two barriers. What are the units of  $\Gamma_1$  and  $\Gamma_2$  ?

(b) What physical quantity does  $\frac{\hbar}{\Gamma_1 + \Gamma_2}$  represent?

(c) Using the expression for the transmission probability given in equation 10-36, find the maximum possible transmission probability through the double barrier structure. Give an example of the device's barrier heights and widths that will have the highest possible transmission probability (You should not have to calculate anything significant for this part).

### Answer

Because the reflected electromagnetic wave has to be 180 degrees out of phase,  $r_1$  and  $r_2$  can be written as :

$$r_1 \sim -\sqrt{1 - |t_1|^2}$$

$$r_2 \sim -\sqrt{1 - |t_2|^2}$$

Then the transmission probability can be expressed as:

$$T = \left| \frac{t_1 t_2}{1 - r_2 r_1 e^{i2kL}} \right|^2 \approx \frac{|t_1|^2 |t_2|^2}{|1 - \sqrt{1 - |t_1|^2} \sqrt{1 - |t_2|^2} e^{i2kL}|^2}$$

Noting that  $\sqrt{1 - |t_i|^2} = 1 - \frac{|t_i|^2}{2} + \frac{|t_i|^4}{4} - \dots$ , we can neglect  $|t_i|^4$  and higher order terms when  $|t_i|^2 \ll 1$ . Thus  $T$  simplifies to:

$$T \approx \frac{|t_1|^2 |t_2|^2}{|1 - [1 - \frac{|t_1|^2}{2}][1 - \frac{|t_2|^2}{2}] e^{i2kL}|^2}$$

The denominator of the equation above can be expanded and rewritten as by neglecting terms of the order of  $|t_1|^2 |t_2|^2$ :

$$|1 - [1 - \frac{|t_1|^2}{2}][1 - \frac{|t_2|^2}{2}] e^{i2kL}|^2 \sim |1 - e^{i2kL} + \frac{|t_1|^2 + |t_2|^2}{2} e^{i2kL}|^2$$

Then  $T$  can be further simplified to:

$$T \approx \frac{|t_1|^2 |t_2|^2}{|1 - e^{i2kL} + \frac{|t_1|^2 + |t_2|^2}{2} e^{i2kL}|^2}$$

At energies  $E_n + \Delta E$  close to the resonances, the wavefactor is

$$k = \sqrt{\frac{2m(E_n + \Delta E)}{\hbar^2}} \sim \sqrt{\frac{2mE_n}{\hbar^2}} \left(1 + \frac{\Delta E}{2E_n}\right) = k_n \left(1 + \frac{\Delta E}{2E_n}\right)$$

Using the above equation,  $e^{i2kL}$  can be expressed as:

$$e^{i2kL} \sim e^{i2k_n L} e^{ik_n L \frac{\Delta E}{E_n}}$$

Because close to these resonance energies, we also have  $k_n L = n\pi$ . As  $e^{i2k_n L} = 1$ , we can simplify the above equation:



$$e^{i2kL} \sim e^{ik_n L \frac{\Delta E}{E_n}}$$

The classical velocity at energy level in the well  $E_n$  is given by:

$$v = \frac{\hbar k_n}{m}$$

and we also have

$$E_n = \frac{1}{2}mv^2$$

Using these expressions,  $e^{i2kL}$  close to resonance can be re-written as:

$$e^{i2kL} \sim e^{i \frac{\Delta E}{\hbar} \frac{2L}{v}}$$

Defining  $\tau = \frac{2L}{v}$ ,  $e^{i2kL}$  becomes:

$$e^{i2kL} \sim e^{i \frac{\Delta E}{\hbar \tau}}$$

Because  $\Delta E$  is a small number compared to  $\hbar/\tau$ ,  $e^{i2kL}$  can be expanded by using Taylor series:

$$e^{i2kL} \sim 1 + i \frac{\Delta E}{(\hbar/\tau)}$$

Then the denominator of  $T$  can be simplified to:

$$|1 - e^{i2kL} + \frac{|t_1|^2 + |t_2|^2}{2} e^{i2kL}|^2 \sim -i \frac{\Delta E}{\hbar \tau} + \frac{|t_1|^2 + |t_2|^2}{2}$$

Thus  $T$  can be expressed as:

$$T \approx \frac{|t_1|^2 |t_2|^2}{|-i \frac{\Delta E}{(\hbar \tau)} + \frac{|t_1|^2 + |t_2|^2}{2}|^2} \approx \frac{\Gamma_1 \Gamma_2}{(E - E_n)^2 + (\frac{\Gamma_1 + \Gamma_2}{2})^2}$$

where we define  $\Gamma_1 = \frac{\hbar}{\tau} |t_1|^2$  and  $\Gamma_2 = \frac{\hbar}{\tau} |t_2|^2$ .

### Part(a)

According the the text book chapter 10,

$$\Gamma_1 = \frac{\hbar}{\tau} |t_1|^2$$

$$\Gamma_2 = \frac{\hbar}{\tau} |t_2|^2$$

where  $\tau = \frac{2L}{v} = \frac{2Lm}{\hbar k}$ . Then  $\Gamma_1$  and  $\Gamma_2$  can be written as:

$$\Gamma_1 = \frac{\hbar}{\tau} |t_1|^2 = \frac{\hbar^2 k}{2Lm} |t_1|^2$$

$$\Gamma_2 = \frac{\hbar}{\tau} |t_2|^2 = \frac{\hbar^2 k}{2Lm} |t_2|^2$$

The units of  $\Gamma_1$  and  $\Gamma_2$  have a form of  $\frac{J^2 s^2 m^{-2}}{kg}$  which can be further simplified to  $\frac{J^2}{kg m^2 / s^2}$ . Thus, the units of  $\Gamma_1$  and  $\Gamma_2$  are  $J$ , which represents strength of coupling to the left and right semi-infinite regions.

### Part(b)

$$\frac{\hbar}{\Gamma_1 + \Gamma_2} = \frac{\tau}{|t_1|^2 + |t_2|^2}$$

The unit of this is  $s$ , which represents a time.  $\tau$  is the time required for a free particle to traverse the quantum well twice (back and forth).

### Part(c)

At energies close to resonance where  $kL = n\pi$  or  $E = E_n = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2$ , the maximum transmission probability is:

$$T_{max} = \frac{\Gamma_1 \Gamma_2}{\left(\frac{\Gamma_1 + \Gamma_2}{2}\right)^2}$$

When  $\Gamma_1 = \Gamma_2$ , which implies the two barriers are identical, the maximum transmission probability  $T_{max}$  is equal to 1. For example, when barrier width of the left barrier and the right barrier are equal  $L_{B,left} = L_{B,right} = 1nm$ , and the barrier height are also equal  $U_{o,left} = U_{o,right} = 0.5eV$ , we can achieve the highest transmission probability ( $T_{max} = 1$ ) at these resonance energy.

### Chapter-11 P1 :

Derive expressions for energy levels and wave functions for a particle of effective mass  $M$  on an infinitesimally thin cylindrical shell (an example is an ultrathin aluminum foil rolled up as a cylinder) with radius  $R$  and length  $L$ . The potential energy of the particle on the cylinder is a constant  $U_o$ . The potential energy outside the cylinder is infinity.

### Answer:

Based on the description of the problem, we can rewrite the  $H$  in a cylindrical coordinate:

$$H = -\frac{\hbar^2}{2m_c} \frac{1}{R^2} \frac{d^2}{d\theta^2} - \frac{\hbar^2}{2m_c} \frac{d^2}{dz^2} + U(\theta, z)$$

where

$$U(\theta, z) = \begin{cases} U_o & 0 < z < L \\ \infty & \text{Otherwise} \end{cases}$$

The wavefunction  $\psi$  in  $H\psi(\theta, z) = E\psi(\theta, z)$  can be expressed as  $\psi(\theta, z) = \Theta(\theta)Z(z)$ , where

$$-\frac{\hbar^2}{2m_c} \frac{d^2}{dz^2} = \epsilon_3 Z(z)$$

with potential being zero for  $0 < z < L$  and  $\infty$  outside. The  $Z(z)$  can be solved as:

$$Z(z) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} z\right) \quad \text{and} \quad \epsilon_3 = \frac{\hbar^2}{2m_c} \left(\frac{n\pi}{L}\right)^2$$

The general solution for  $\Theta(\theta)$  is:

$$\Theta(\theta) = e^{ik_1 R\theta}$$

Since  $\Theta(\theta)$  has a boundary condition  $e^{ik_1 \theta R} = e^{ik_1 (\theta+2\pi)R}$ . Then we will have

$$e^{ik_1 2\pi R} = 1$$

$$k_1 = \frac{2\pi}{2\pi R} l = \frac{l}{R} \quad l = 0, \pm 1, \pm 2$$

Then  $\psi$  is:

$$\psi(\theta, z) = e^{il\theta} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} z\right), \quad l = 0, \pm 1, \pm 2$$

The energy level in the conduction band is :

$$E = E_c + \frac{\hbar^2}{2m_c} \left(\frac{n\pi}{L}\right)^2, \quad n = 0, \pm 1, \pm 2$$

Similarly, the energy level in the valence band is :

$$E = E_v - \frac{\hbar^2}{2m_v} \left(\frac{n\pi}{L}\right)^2, \quad n = 0, \pm 1, \pm 2$$

### Chapter-11 P4 :

Consider a Gallium Arsenide nanowire with a square cross section.

(a) Plot the bandgap as a function of the edge dimension  $L$ . Vary  $L$  from  $1\text{nm}$  to  $15\text{nm}$  in increments of  $1\text{nm}$ . In the y-axis of the plot, indicate both the numerical value of the bandgap and the wavelength/color of light that the bandgap corresponds to.

(b) Write down the wave functions and plot the energy bands for the two lowest sub-band energies in the conduction band and the two highest sub-band energies in the valence band. Use  $L = 2nm$ .

Assume that the effective mass of electrons and holes are  $0.067m_o$  and  $0.47m_o$ , respectively, where  $m_o$  is the free electron mass.

### Answer

(a)

The bandgap of the bulk GaAs is 1.42eV. In a nano-wire structure, the bandgap is

$$Bandgap(NW) = Bandgap(Bulk) = \frac{\hbar^2}{2} \left( \frac{1}{m_c} + \frac{1}{m_v} \right) \left[ \left( \frac{\pi}{L_1} \right)^2 + \left( \frac{\pi}{L_2} \right)^2 \right]$$

Then by using the given number in this problem ( $Bandgap(Bulk) = 1.42eV$ ), we can plot the bandgap as a function of the edge dimension  $L$ . The code and the figure are shown below:

In [9]:

```

eta = 6.63e-34/2/np.pi #Reduced Plank constant in eV.s
c=3e8
q = 1.6e-19
mo = 9.11e-31
mc=0.067*mo
mv=0.47*mo
BG_bulk=1.42*q #bandgap of the bulk semiconductor

L1end=15e-9
dL=1e-2*1e-9
L=np.arange(1e-9,L1end,dL)

BG_nw=BG_bulk+eta**2/2*(1/mc+1/mv)*((np.pi/L)**2+(np.pi/L)**2)
wavelength=eta*2*np.pi*c/BG_nw

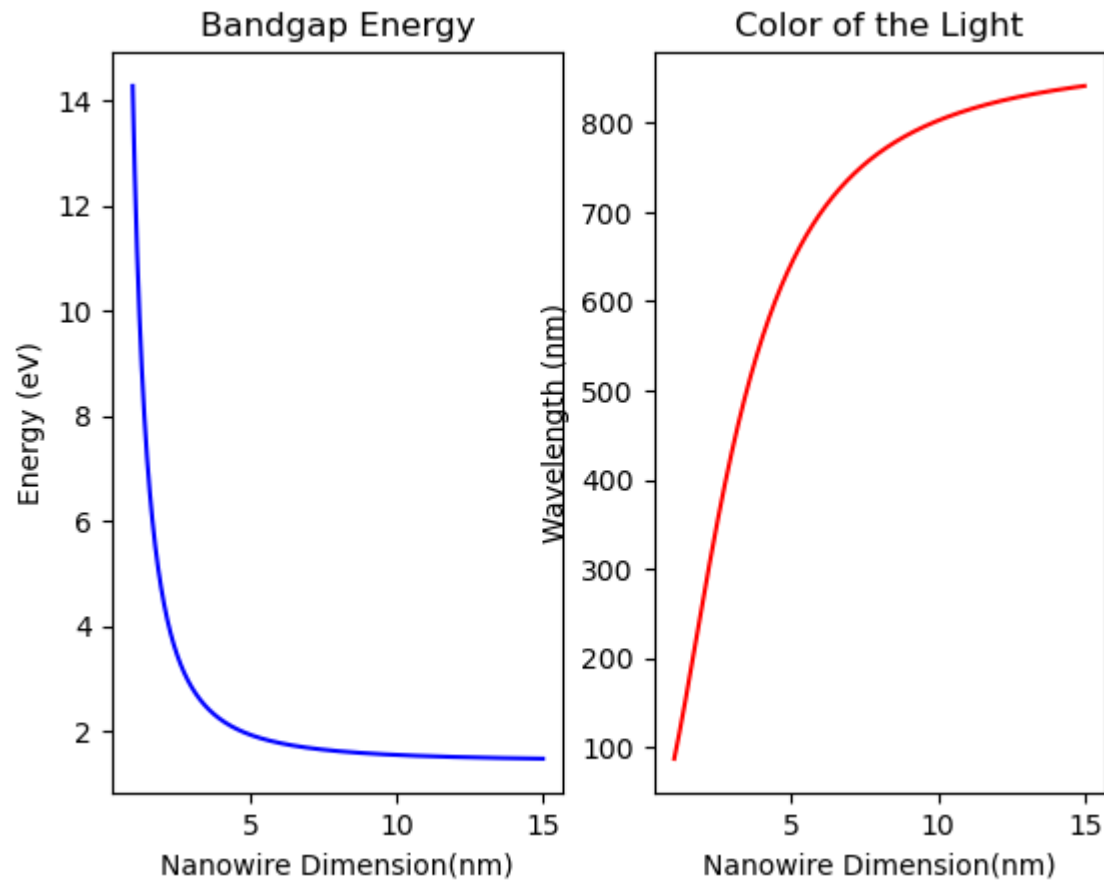
fig, (ax1, ax2) = plt.subplots(1,2)

plt.sca(ax1)
plt.title('Bandgap Energy')
plt.plot(L/1e-9, BG_nw/q, color='b', ls='--')
plt.xlabel('Nanowire Dimension(nm)')
plt.ylabel('Energy (eV)')

plt.sca(ax2)
plt.title('Color of the Light')
plt.plot(L/1e-9, wavelength/1e-9, color='r', ls='--')
plt.xlabel('Nanowire Dimension(nm)')
plt.ylabel('Wavelength (nm)')

```

Out[9]: Text(0, 0.5, 'Wavelength (nm)')



From the right figure, we can see the wavelength changes from 100nm to 800nm when increasing the nanowire dimension from 1nm to 15nm. The color of the emitted light change from ultraviolet to infrared during the process.

**(b)**

In this part, we consider the two lowest subband in the conduction band where  $(l, m) = (1, 1)$  and  $(l, m) = (1, 2)$  or  $(2, 1)$ . The corresponding expression of the wavefunctions in the conduction band are:

$$\psi_{1,1,k}(x, y, z) = A \sin\left(\frac{\pi}{L_1} x\right) \sin\left(\frac{\pi}{L_2} y\right) e^{ik_z z}$$

$$\psi_{1,2,k}(x, y, z) = A \sin\left(\frac{\pi}{L_1} x\right) \sin\left(\frac{2\pi}{L_2} y\right) e^{ik_z z}$$

$$\psi_{2,1,k}(x, y, z) = A \sin\left(\frac{2\pi}{L_1}x\right) \sin\left(\frac{\pi}{L_2}y\right) e^{ik_z z}$$

where  $L_1 = L_2 = L = 2nm$  in this problem. And the subband energies are:

$$E_{c1,1,k} = E_c + \frac{\hbar^2}{2m_c} \left(\frac{\pi}{L}\right)^2 + \frac{\hbar^2}{2m_c} \left(\frac{\pi}{L}\right)^2 + \frac{\hbar^2 k_z^2}{2m_c} = E_c + \frac{\hbar^2}{m_c} \left(\frac{\pi}{L}\right)^2 + \frac{\hbar^2 k_z^2}{2m_c}$$

$$E_{c1,2,k} = E_{c2,1,k} = E_c + \frac{\hbar^2}{2m_c} \left(\frac{2\pi}{L}\right)^2 + \frac{\hbar^2}{2m_c} \left(\frac{\pi}{L}\right)^2 + \frac{\hbar^2 k_z^2}{2m_c} = E_c + \frac{5\hbar^2}{2m_c} \left(\frac{\pi}{L}\right)^2 + \frac{\hbar^2 k_z^2}{2m_c}$$

Similarly, in the valence band, we have

$$\psi_{1,1,k}(x, y, z) = A \sin\left(\frac{\pi}{L_1}x\right) \sin\left(\frac{\pi}{L_2}y\right) e^{ik_z z}$$

$$\psi_{1,2,k}(x, y, z) = A \sin\left(\frac{\pi}{L_1}x\right) \sin\left(\frac{2\pi}{L_2}y\right) e^{ik_z z}$$

$$\psi_{2,1,k}(x, y, z) = A \sin\left(\frac{2\pi}{L_1}x\right) \sin\left(\frac{\pi}{L_2}y\right) e^{ik_z z}$$

And the subband energies are:

$$E_{v1,1,k} = E_v - \frac{\hbar^2}{2m_v} \left(\frac{\pi}{L}\right)^2 - \frac{\hbar^2}{2m_v} \left(\frac{\pi}{L}\right)^2 - \frac{\hbar^2 k_z^2}{2m_v} = E_v - \frac{\hbar^2}{m_v} \left(\frac{\pi}{L}\right)^2 - \frac{\hbar^2 k_z^2}{2m_v}$$

$$E_{v1,2,k} = E_{v2,1,k} = E_v - \frac{\hbar^2}{2m_v} \left(\frac{2\pi}{L}\right)^2 - \frac{\hbar^2}{2m_v} \left(\frac{\pi}{L}\right)^2 - \frac{\hbar^2 k_z^2}{2m_v} = E_v - \frac{5\hbar^2}{2m_v} \left(\frac{\pi}{L}\right)^2 - \frac{\hbar^2 k_z^2}{2m_v}$$

The energy bands for the two lowest sub-band energies in the conduction band and the two highest sub-band energies in the valence band described above will be plotted using the following codes.

```

In [10]: eta = 6.63e-34/2/np.pi #Reduced Plank constant in eV.s
c=3e8
q = 1.6e-19
mo = 9.11e-31
mc=0.067*mo
mv=0.47*mo
BG_bulk=1.42*q #bandgap of the bulk semiconductor
Ec0=0
Ev0=Ec0-BG_bulk

L2=2e-9

kzb=6e9
dkz=kzb/10e3
kz=np.arange(-kzb,kzb,dkz)

Ec11=Ec0+eta**2/(2*mc)*(1*np.pi/L2)**2+eta**2/(2*mc)*(1*np.pi/L2)**2+eta**2*kz**2/(2*mc)
Ec12=Ec0+eta**2/(2*mc)*(1*np.pi/L2)**2+eta**2/(2*mc)*(2*np.pi/L2)**2+eta**2*kz**2/(2*mc)
Ec21=Ec12

Ev11=Ev0-eta**2/(2*mv)*(1*np.pi/L2)**2-eta**2/(2*mv)*(1*np.pi/L2)**2-eta**2*kz**2/(2*mv)
Ev12=Ev0-eta**2/(2*mv)*(1*np.pi/L2)**2-eta**2/(2*mv)*(2*np.pi/L2)**2-eta**2*kz**2/(2*mv)
Ev21=Ev12

plt.figure()
plt.plot(kz*1e-9, Ec11/q, color='b', ls='--')
plt.plot(kz*1e-9, Ec12/q, color='g', ls='--')
plt.plot(kz*1e-9, Ev11/q, color='r', ls='--')
plt.plot(kz*1e-9, Ev12/q, color='m', ls='--')

plt.legend(['Ec11', 'Ec12&Ec21', 'Ev11', 'Ev12&Ev21'])
plt.title('Energy band in GaAs nanowire')
plt.xlabel('k(1/nm)')
plt.ylabel('Energy(eV)')
plt.xlim(-kzb*1e-9, kzb*1e-9)

```

Out[10]: (-6.0, 6.0)



