HW-7

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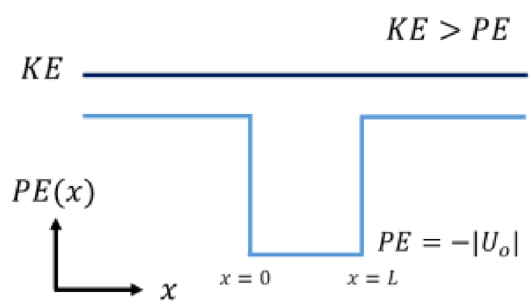
A) Xichen Li: I did HW7 independently.

Chapter-10 P3 :

Assume an electron is moving to the right from $x < 0$, and it is facing a potential trough witha depth of $-|U_o|$, That is, $PE = -|U_o|$.
(a) Show that there will be a reflection at the trough and calculate the reflection (R) and transmission (T) coefficients.
(b) Plot the reflection and transmission probabilities in terms of $KE/|U_o|$, where KE is the kinetic energy of the incident electron.
Note that this problem is like the case of a potential barrier when $KE > PE$, discussed in this chapter. The only difference is that you can simply replace U_o with $-|U_o|$ in the corresponding equations for T and R.



Answer

(a) According to the definition of R and T:

$$R = |\frac{B}{A}|^2$$
$$T = |\frac{F}{A}|^2$$

Since $KE > PE$, the boundary condition needs to be re-written as:

$$A + B = C + D$$
$$ik(A - B) = \alpha(C - D)$$
$$Ce^{\alpha L} + De^{-\alpha L} = Fe^{i\beta L}$$
$$\alpha(Ce^{\alpha L} - De^{-\alpha L}) = i\beta e^{i\beta L}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$
$$\alpha = \sqrt{\frac{2m(-|U_o| - E)}{\hbar^2}}$$
$$\beta = \sqrt{\frac{2mE}{\hbar^2}}$$

Note α is an imaginary number.

Then we can solve for B/A and F/A: And we also have :

$$\frac{B}{A} = \frac{(\alpha + i\beta)(\alpha - ik)e^{-\alpha L} - (\alpha - i\beta)(\alpha + ik)e^{\alpha L}}{(\alpha + i\beta)(\alpha + ik)e^{-\alpha L} - (\alpha - i\beta)(\alpha - ik)e^{\alpha L}} e^{-i\beta L}$$
$$\frac{F}{A} = \frac{-4i\alpha k}{(\alpha + i\beta)(\alpha + ik)e^{-\alpha L} - (\alpha - i\beta)(\alpha - ik)e^{\alpha L}} e^{-i\beta L}$$

Because $\beta = k$, then B/A and F/A can be re-written as :

$$\frac{B}{A} = \frac{(\alpha^2 + k^2)(e^{-\alpha L} + e^{\alpha L})}{(\alpha + ik)^2 e^{-\alpha L} - (\alpha - ik)^2 e^{\alpha L}} e^{-ikL}$$
$$\frac{F}{A} = \frac{-4i\alpha k}{(\alpha + ik)^2 e^{-\alpha L} - (\alpha - ik)^2 e^{\alpha L}} e^{-ikL}$$

Then T and R coefficients are:

$$R = |\frac{B}{A}|^2 = |\frac{(\alpha^2 + k^2)(e^{-\alpha L} + e^{\alpha L})}{(\alpha + ik)^2 e^{-\alpha L} - (\alpha - ik)^2 e^{\alpha L}} e^{-ikL}|^2$$
$$T = |\frac{F}{A}|^2 = |\frac{-4i\alpha k}{(\alpha + ik)^2 e^{-\alpha L} - (\alpha - ik)^2 e^{\alpha L}} e^{-ikL}|^2$$

As you can see from the expressions for R and T, there will still be reflection at the trough.

(b)Plot the reflection and transmission probabilities in terms of $E/|U_o|$

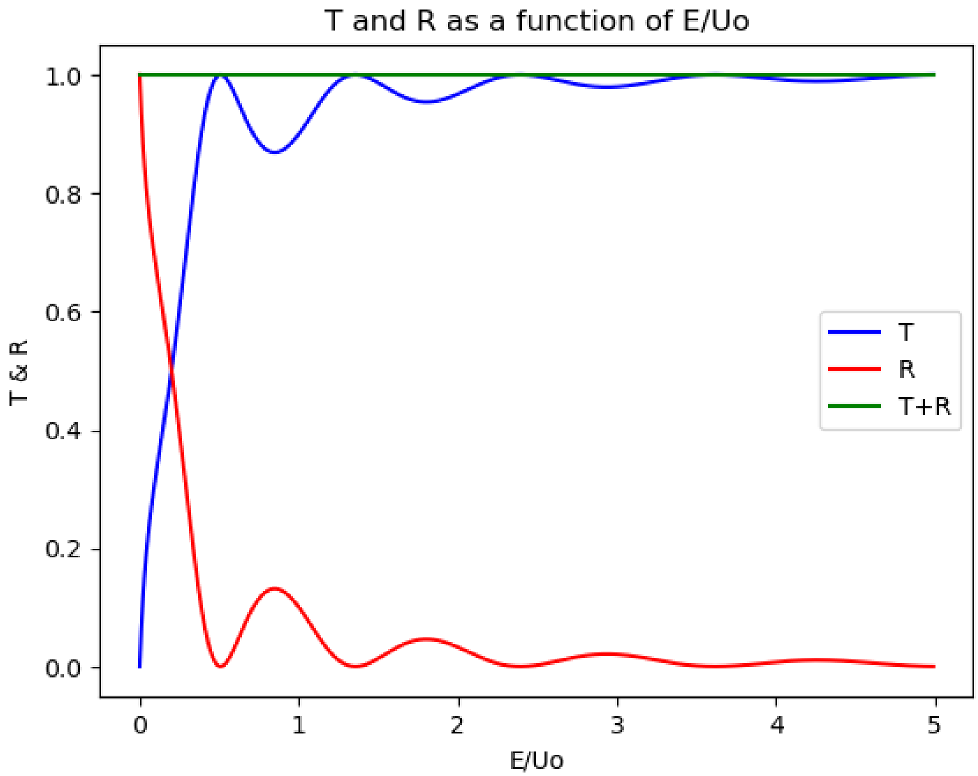
Because α is an imaginary number, thus we can define $\alpha = ia$ to simplify the calculation where $a = \sqrt{\frac{2m(|U_o|+E)}{\hbar^2}}$. Then R and T can be re-written as:

$$R = |\frac{B}{A}|^2 = |\frac{(-a^2 + k^2)(e^{-iaL} + e^{iaL})}{-(a + k)^2 e^{-iaL} + (a - k)^2 e^{iaL}} e^{-ikL}|^2$$
$$T = |\frac{F}{A}|^2 = |\frac{4ak}{-(a + k)^2 e^{-iaL} + (a - k)^2 e^{iaL}} e^{-ikL}|^2$$

The R and T are plotted in Plot package in Python:

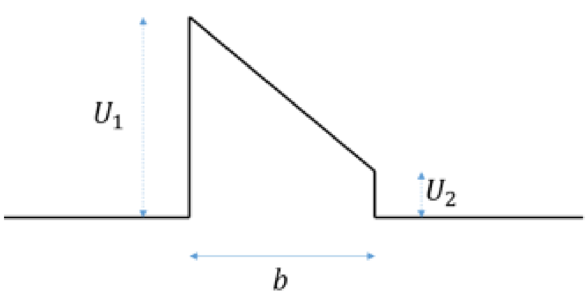
In [140]:
```
import numpy as np
%matplotlib inline
import matplotlib.pyplot as plt
eta = 6.63e-34/2/np.pi #Reduced Plank constant in eV.s
q = 1.6e-19
L=2e-9
m = 9.11e-31   #Assuming the particle mass is equal to a free electron

Uo=q
N=100
E1=5*q
dE=1e-2*q
E=np.arange(0,E1,dE)
k=np.sqrt(2*m*E/(eta**2))
a=np.sqrt(2*m*(E+Uo)/(eta**2))

#print(k)
#print(a)

#print(np.exp(1j*np.pi))

FdA=4*a*k/(-(a+k)**2*np.exp(-1j*a*L)+(a-k)**2*np.exp(1j*a*L))*np.exp(-1j*k*L)
T=abs(FdA)**2
R=1-T

plt.figure()
plt.plot(E/Uo, T, color='b', ls='-')
plt.plot(E/Uo, R, color='r', ls='-')
plt.plot(E/Uo, T+R, color='g', ls='-')
plt.legend(['T', 'R','T+R'])
plt.title('T and R as a function of E/Uo')
plt.xlabel('E/Uo')
plt.ylabel('T & R')
```

Out[140]:
```
Text(0, 0.5, 'T & R')
```



Chapter-10 P9 :

Calculate the transmission probability of a triangular barrier as shown in the figure below for energies between $10meV$ and $1eV$. The values of the parameters are $b = 5nm$, $U_1 = 800meV$ and $U_2 = 200meV$.
(You may want to break this down into many rectangular barriers with varying width and heights.)



Answer

According to the 10.7 in the textbook, the scattering matrix M of a transmission through a system consisting of multiple barriers can be broken into small piece of barriers:

$$M = M_1 M_2 ... M_n$$

where M_n can be written as:

$$M_n = \frac{1}{2ik}\begin{pmatrix} ik+\alpha & ik-\alpha \\ ik-\alpha & ik+\alpha \end{pmatrix} \frac{1}{2\alpha}\begin{pmatrix} (\alpha+i\beta)e^{-\alpha L_n} & (\alpha-i\beta)e^{-\alpha L_n} \\ (\alpha-i\beta)e^{+\alpha L_n} & (\alpha+i\beta)e^{+\alpha L_n} \end{pmatrix}$$

where k, α, and β is related to the shape of the rectangular barrier at any specific location x:

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\alpha = \sqrt{\frac{2m(qU(x)-E)}{\hbar^2}}$$

$$\beta = \sqrt{\frac{2mE}{\hbar^2}}$$

The transmission probablity can be calculated from the cascaded matrix:

$$T = |\frac{1}{M_{11}}|^2$$

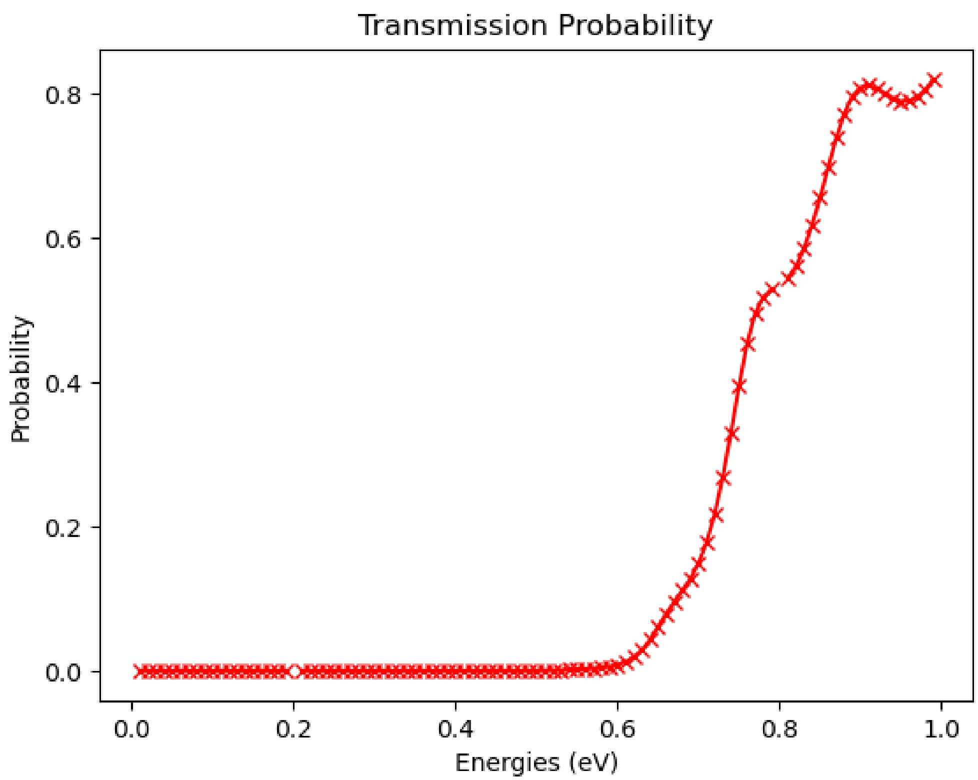
This problem will be solved in Python code below.

In [141]:
```
q=1.6e-19
b=5e-9
U1=0.8*q
U2=0.2*q
m=9.1e-31
eta = 6.63e-34/2/np.pi #Reduced Plank constant in eV.s

Num=400;
Ux=np.linspace(U1,U2,Num)
#print(Ux)
Ln=b/(Num-1)

Ta=[]
Ra=[]
Ein=np.arange(10e-3*q,1000e-3*q,10e-3*q)
#Ein=[10e-3*q, 1000e-3*q]
#E=10e-3*q
for E in Ein:
    k=np.sqrt(2*m*E/(eta**2))
    alphax=np.sqrt(2*m*(Ux-E)/(eta**2)+0j)
    beta=k
    Cx=1/(2*1j*k)*1/(2*alphax)
    M=np.eye(2)
    for i in range(Num):
        A11=1j*k+alphax[i]
        A12=1j*k-alphax[i]
        A21=1j*k-alphax[i]
        A22=1j*k+alphax[i]
        A=np.array([[A11, A12], [A21, A22]])
        B11=(alphax[i]+1j*beta)*np.exp(-alphax[i]*Ln)
        B12=(alphax[i]-1j*beta)*np.exp(-alphax[i]*Ln)
        B21=(alphax[i]-1j*beta)*np.exp(alphax[i]*Ln)
        B22=(alphax[i]+1j*beta)*np.exp(alphax[i]*Ln)
        B=np.array([[B11, B12], [B21, B22]])
        Mn=Cx[i]*A @ B
        M = M @ Mn
        T=abs(1/M[0,0])**2
        R=abs(M[1,0]/M[0,0])**2

    Ta=Ta+[T]
    Ra=Ra+[R]


plt.figure()
plt.plot(Ein/q, Ta, color='r', ls='-', marker='x')
#plt.plot(Ein/q, Ra, color='b', ls='-', marker='x')
#plt.legend(['Transmission Probability', 'Reflection Probability'])
plt.title('Transmission Probability')
plt.xlabel('Energies (eV)')
```

```
plt.ylabel('Probability')
```

```
C:\Users\lixic\AppData\Local\Temp\ipykernel_5372\3281876816.py:22: RuntimeWarning: divide by zero encountered in divide
  Cx=1/(2*1j*k)*1/(2*alphax)
C:\Users\lixic\AppData\Local\Temp\ipykernel_5372\3281876816.py:22: RuntimeWarning: invalid value encountered in divide
  Cx=1/(2*1j*k)*1/(2*alphax)
C:\Users\lixic\AppData\Local\Temp\ipykernel_5372\3281876816.py:35: RuntimeWarning: invalid value encountered in multiply
  Mn=Cx[i]*A @ B
C:\Users\lixic\AppData\Local\Temp\ipykernel_5372\3281876816.py:37: RuntimeWarning: invalid value encountered in cdouble_scalars
  T=abs(1/M[0,0])**2
C:\Users\lixic\AppData\Local\Temp\ipykernel_5372\3281876816.py:38: RuntimeWarning: invalid value encountered in cdouble_scalars
  R=abs(M[1,0]/M[0,0])**2
```

Out[141]: `Text(0, 0.5, 'Probability')`



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:

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

where

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

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

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

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

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

The euqation related to $\Theta(\theta)$ is

$$-\frac{\Theta''}{\Theta} = C$$

with a periodicity of 2π, $\Theta(0) = \Theta(2\pi)$. The Θ can be solved as:

$$\Theta(\theta) = Ae^{il\theta} + Be^{-il\theta}, \quad l = 0, \pm 1, \pm 2$$

The euqation related to $R(r)$ can be rearranged into:

$$R'' + \frac{1}{r}R' + (\frac{2m_c\epsilon}{\hbar^2} - \frac{l}{r^2})R = 0$$

with $\epsilon = E - \epsilon_3 = E - \frac{\hbar^2}{2m_c}(\frac{n\pi}{L})^2$. The solution of $R(r)$ are well defined by the Bessel functions:

$$R(r) = aJ_l(\sqrt{\frac{2m_c\epsilon}{\hbar^2}}r) + bY_l(\sqrt{\frac{2m_c\epsilon}{\hbar^2}}r)$$

where a and b are constants. Since Y_l doesn't converge to zero, b must be zero. Then $\psi(r,\theta,z)$ is:

$$\psi(r,\theta,z) = aJ_l(\sqrt{\frac{2m_c\epsilon}{\hbar^2}}r)(Ae^{il\theta} + Be^{-il\theta})\sqrt{\frac{2}{L}} sin(\frac{n\pi}{L}z)$$

The energy level expression is :

$$E = \frac{\hbar^2}{2m_c}(\frac{n\pi}{L})^2 + \frac{\hbar^2}{2m_c}(\frac{\alpha_{n,l}}{R})^2$$

where $\alpha_{n,l}$ are the roots in Bessel functions.

Chapter-11 P3 :

You have a bulk semiconductor with a bandgap of $0.7eV$. Assume that the effective mass of both electrons and holes is $9.1 \times 10^{-31}kg$. Furthermore, this semiconductor is known to be a poor emitter of light both at 500 nm and 8000 nm. How would you engineer this structure so that it emits light with a wavelength of (a) $500nm$ and (b) $8000nm$? Find the nanostructure dimensions to achieve (a) and (b). Your design can be based on quantum wells, dots or nanowires.

Answer

(a) For $\lambda = 500nm$, we can caculate a required bandgap energy from

$$E = \hbar\omega = hf = \frac{hc}{\lambda} = \frac{6.626 * 10^{-34} * 3 * 10^8}{500 * 10^{-9}} = 3.9756 * 10^{-19}J = 2.485eV$$

In a bulk semiconductor, at the bottom of the band, we have:

$$E_c - E_v = 0.7eV$$

In aquantum dot structure, at the bottom of the band, we have

$$E_{c,qd} - E_{v,qd} = 0.7 + \frac{\hbar^2}{2}(\frac{1}{m_c} + \frac{1}{m_v})[(\frac{\pi}{L_1})^2 + (\frac{\pi}{L_2})^2 + (\frac{\pi}{L_3})^2]$$

In order to emit light with a wavelength of $500nm$, L_1, L_2, and L_3 in a quantom dot needs to satisfy:

$$\frac{\hbar^2}{2}(\frac{1}{m_c} + \frac{1}{m_v})[(\frac{\pi}{L_1})^2 + (\frac{\pi}{L_2})^2 + (\frac{\pi}{L_3})^2] = (2.485 - 0.7)eV$$

By solving the equation above, we can find $L_1 = L_2 = L_3 \approx 0.95nm$ can meet the requirement.

(b) For $\lambda = 8000nm$, we can caculate a required bandgap energy from

$$E = \hbar\omega = hf = \frac{hc}{\lambda} = \frac{6.626 * 10^{-34} * 3 * 10^8}{8000 * 10^{-9}} = 2.485 * 10^{-20}J = 0.155eV$$

In a bulk semiconductor, at the bottom of the band, we have:

$$E_c - E_v = 0.7eV$$

The required bandgap energy is less than the energy in a bulk semiconductor. Thus, in this case, the energy difference between two conduction bands need to be used to emit light with a wavelength of 8000nm. I will still choose to use a quantum dot toachieve this. Assuming $L_1 = L_2 = L_3 = L$, the energy difference between the $E_{1,1,1}$ and $E_{2,1,1}$ should be equal to $0.155eV$:

$$\frac{\hbar^2}{2}\frac{1}{m_c}(\frac{\pi}{L})^2 = 0.155eV$$

Then by solving the equation above, we can find $L_1 = L_2 = L_3 \approx 1.56nm$ can meet the requirement.

In [ ]: