

# **Quantum Electronics and Photonics**

## **Assignment 2**

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February 18, 2013

## Contents

<b>Problem 1</b>	<b>3</b>
(b) . . . . .	3
(c) . . . . .	4
(c) . . . . .	4
<b>Problem 2</b>	<b>4</b>
(a) . . . . .	4
(b) . . . . .	8
(c) . . . . .	8
<b>Problem 3</b>	<b>9</b>
(a) . . . . .	9
(b) . . . . .	10
(c) . . . . .	10
(d) . . . . .	10
<b>Problem 4</b>	<b>11</b>
(a) . . . . .	11
(b) . . . . .	11
(c) . . . . .	12
(d) . . . . .	12
(e) . . . . .	12
<b>Problem 5</b>	<b>12</b>
(a) . . . . .	13
(b) . . . . .	13
(c) . . . . .	16
<b>Appendix</b>	<b>18</b>

## Problem 1

(a) If the the state  $|\Psi\rangle$  is a normalized linear combination of two basis as

$$|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

then the normalization condition is translated as:

$$\langle\Psi|\Psi\rangle = \begin{pmatrix} \alpha \\ \alpha \end{pmatrix}^\dagger \begin{pmatrix} \alpha \\ \alpha \end{pmatrix} = |\alpha|^2 + |\beta|^2 = 1 \quad (1)$$

where  $\dagger$  is *transpose conjugate* operator. So  $\alpha$  and  $\beta$  are related to each other by:

$$|\alpha|^2 + |\beta|^2 = 1 \quad (2)$$

(b)

The Hamiltonian of the system is represented by the following matrix:

$$\hat{H} = \begin{pmatrix} a & b \\ b & a \end{pmatrix} \quad (3)$$

Time independent Schrödinger equation in the abstract space is:

$$H|\Psi\rangle = E|\Psi\rangle \quad (4)$$

This abstract equation can be represented in  $\mathbb{C}^2$  space as the following eigenvalue problem:

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \implies \begin{pmatrix} a-E & b \\ b & a-E \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \quad (5)$$

Putting the determinant the matrix of the coefficients equal to zero ensures us to have non-trivial solutions:

$$\det \begin{pmatrix} a-E & b \\ b & a-E \end{pmatrix} = 0 \implies (a-E)^2 = b^2 \implies E = a \pm b \quad (6)$$

and the associated eigenvectors are:

$$E_1 = a + b \implies \begin{pmatrix} a & b \\ b & a \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = (a+b) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \implies \alpha = \beta \quad (7)$$

$$E_2 = a - b \implies \begin{pmatrix} a & b \\ b & a \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = (a-b) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \implies \alpha = -\beta \quad (8)$$

So two orthonormal eigenstates are:

$$E = a + b \implies |\Psi_1\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle) \quad (9)$$

$$E = a - b \implies |\Psi_2\rangle = \frac{1}{\sqrt{2}} (|1\rangle - |2\rangle) \quad (10)$$

(c)

Time-dependent solution to the schrödinger equation can be obtained just by applying the time evolution operator on an arbitrary state:

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = H|\Psi\rangle \implies |\Psi(t)\rangle = \exp\left(\frac{-iHt}{\hbar}\right) |\Psi(t=0)\rangle \quad (11)$$

By decomposing  $|\Psi(t=0)\rangle = \alpha|1\rangle + \beta|2\rangle$  to the energy eigenstates we get:

$$|\Psi(t)\rangle = \exp\left(\frac{-iHt}{\hbar}\right) \left\{ \sum_n |\Psi_n\rangle \langle \Psi_n| \right\} |\Psi(t=0)\rangle = \sum_n \exp\left(\frac{-iE_n t}{\hbar}\right) |\Psi_n\rangle \langle \Psi_n| \Psi(t=0)\rangle \quad (12)$$

Hence:

$$|\Psi(t)\rangle = \frac{1}{2}(\alpha + \beta) \exp\left(\frac{-i(a+b)t}{\hbar}\right) (|1\rangle + |2\rangle) + \frac{1}{2}(\alpha - \beta) \exp\left(\frac{-i(a-b)t}{\hbar}\right) (|1\rangle - |2\rangle) \quad (13)$$

(c)

If the system starts out at  $t = 0$  in state  $|0\rangle$ , the state after time  $t$  can be predicted by (13). By putting  $\alpha = 1$  and  $\beta = 0$  we obtain:

$$\begin{aligned} |\Psi(t)\rangle &= \frac{1}{2} \exp\left(\frac{-iat}{\hbar}\right) \left\{ \exp\left(\frac{-ibt}{\hbar}\right) (|1\rangle + |2\rangle) + \exp\left(\frac{+ibt}{\hbar}\right) (|1\rangle - |2\rangle) \right\} \\ &= \exp\left(\frac{-iat}{\hbar}\right) \left\{ \cos\left(\frac{bt}{\hbar}\right) |1\rangle - i \sin\left(\frac{bt}{\hbar}\right) |2\rangle \right\} \end{aligned} \quad (14)$$

## Problem 2

(a)

To find the possible values of energy providing electron bound state inside the MQW, the conventional *Transfer Matrix Method* is employed. Figure 1 shows eight cascaded quantum well which can be locally treated as a periodic structure.

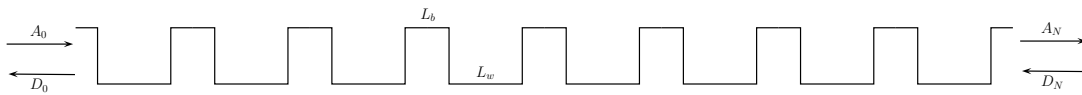


Figure 1: MQW composed of eight cascaded quantum wells

Suppose that the transfer matrix  $\mathbf{M}_t$  relates  $A_0$  and  $D_0$  to  $A_N$  and  $D_N$  as:

$$\begin{bmatrix} A_0 \\ D_0 \end{bmatrix} = \begin{bmatrix} M_{t11} & M_{t12} \\ M_{t21} & M_{t22} \end{bmatrix} \begin{bmatrix} A_N \\ D_N \end{bmatrix} \quad (1)$$

To have bound states  $A_0$  and  $D_N$  should be zero, that is, the outgoing part of the wavefunction outside of the MQW should vanish. This condition is translated as:

$$M_{t11} = 0 \quad (2)$$

This equation is actually the characteristic equation which determines possible energies providing bound states inside the structure. To construct  $\mathbf{M}_t$  we should first work on the transfer matrix associated with

each unit cell. Figure 2 shows a unite cell of the structure. The transfer matrix assocoited with this unite cell can be calculated by multiplying  $\mathbf{M}_b(L_b/2)$ ,  $\mathbf{M}_{bw}$ ,  $\mathbf{M}_w(L_w)$  and  $\mathbf{M}_{wb}$  as follows:

$$\mathbf{M}_{cell} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} = \mathbf{M}_b(L_b/2)\mathbf{M}_{bw}\mathbf{M}_w(L_w)\mathbf{M}_{wb}\mathbf{M}_b(L_b/2) \quad (3)$$

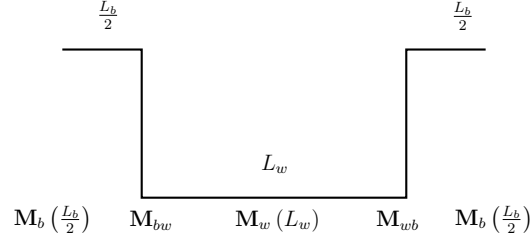


Figure 2: a unit cell of the MQW structure

where

$$\mathbf{M}_b(L_b/2) = \begin{bmatrix} \exp(k_b L_b/2) & 0 \\ 0 & \exp(k_b L_b/2) \end{bmatrix} \quad (4)$$

$$\mathbf{M}_{bw} = \frac{1}{2} \begin{bmatrix} 1 - i \frac{k_w}{k_b} & 1 + i \frac{k_w}{k_b} \\ 1 + i \frac{k_w}{k_b} & 1 - i \frac{k_w}{k_b} \end{bmatrix} \quad (5)$$

$$\mathbf{M}_w(L_w) = \begin{bmatrix} \exp(-ik_w L_w) & 0 \\ 0 & \exp(ik_w L_w) \end{bmatrix} \quad (6)$$

$$\mathbf{M}_{wb} = \frac{1}{2} \begin{bmatrix} 1 + i \frac{k_b}{k_w} & 1 - i \frac{k_b}{k_w} \\ 1 - i \frac{k_b}{k_w} & 1 + i \frac{k_b}{k_w} \end{bmatrix} \quad (7)$$

In above equations  $k_w$  and  $k_b$  are the wavenumber in the wells and the barriers respectively:

$$k_w = \sqrt{\frac{2m_{eff}E}{\hbar^2}}$$

$$k_b = \sqrt{\frac{2m_{eff}(V_0 - E)}{\hbar^2}}$$

By insering (4)-(7) into (3) we obtain:

$$m_{11} = \exp(k_b L_b) \left[ \cos(k_w L_w) - 0.5 \left( \frac{k_w}{k_b} - \frac{k_b}{k_w} \right) \sin(k_w L_w) \right] \quad (8)$$

$$m_{12} = -0.5 \exp(k_b L_b) \left( \frac{k_w}{k_b} + \frac{k_b}{k_w} \right) \sin(k_w L_w) \quad (9)$$

$$m_{21} = 0.5 \exp(k_b L_b) \left( \frac{k_w}{k_b} + \frac{k_b}{k_w} \right) \sin(k_w L_w) \quad (10)$$

$$m_{22} = \exp(-k_b L_b) \left[ \cos(k_w L_w) + 0.5 \left( \frac{k_w}{k_b} - \frac{k_b}{k_w} \right) \sin(k_w L_w) \right] \quad (11)$$

Now we can calculate  $\mathbf{M}_t$  by mmultiplying a series of transfer matrices of each unite cell:

$$\mathbf{M}_t = \mathbf{M}_{cell}^8 \quad (12)$$

Based on the lecture the possible discrete energy eigenvalues for the bound state can be calculated by considering the possible continuous energy bands for the infinite structure. In fact it is shown that the possible solutions satisfy the following condition:

$$U = \frac{1}{2} (m_{11} + m_{22}) \leq 1 \quad (13)$$

By evaluating  $U$  as a function of  $E$  allowable energy bands can be determined. Figure 3 shows the continuous energy bands for the infinite chain of wells. As explained previously to find discrete energy eigenfunctions

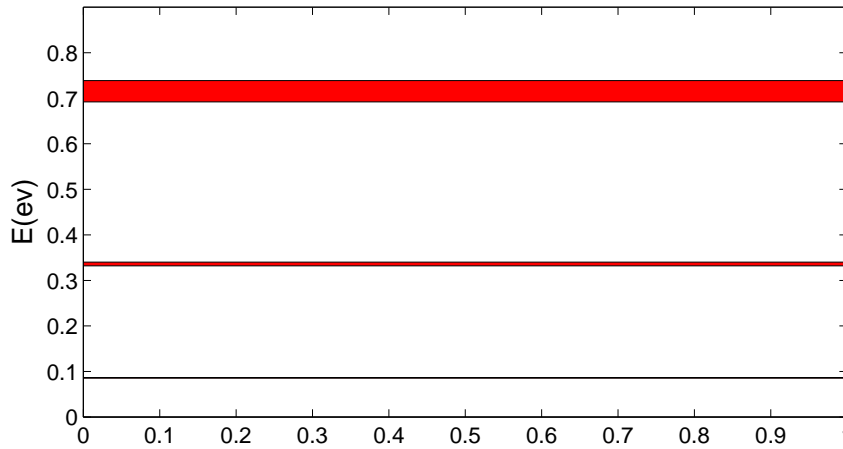
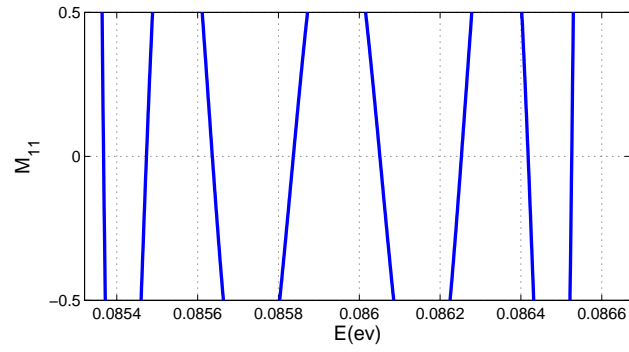


Figure 3: continuous energy bands for MQW

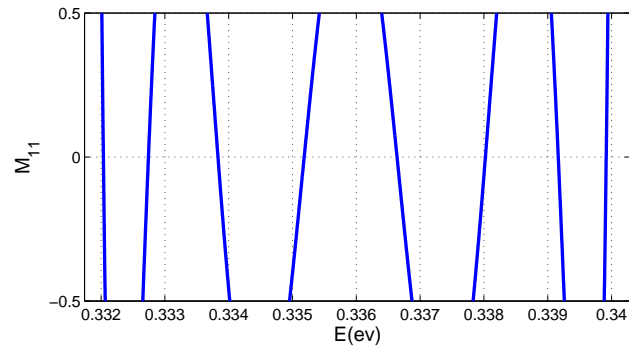
for the bound states we should find the solutions of (2). However  $M_{t11}$  fluctuations are so striking and this makes our job difficult. In fact very fine meshes have to be used to find all zeros. To avoid computational complexity we have used the notion of continuous band structures:

1. Find continuous energy band using coarse meshes.(figure 3)
2. Search for the roots of  $M_{t11}$  inside each continuous energy bands. It's expected that 8 zeros (solutions) can be found inside each band. In this stage we should use more fine meshes.
3. Refine your meshes near each approximate solution to get more precise solutions.

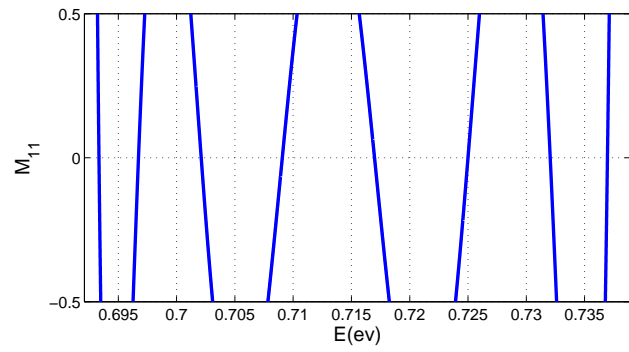
Figure 4 shows three  $M_{t11}$  inside three allowable energy bands. As it was expected in each region we have 8 solutions (correspond to eight QW).



(a)



(b)



(c)

Figure 4:  $M_{t11}$  in three energy bands (a) first band (b) second band and (c) third band

Possible energy eigenvalues are given in table 1.

Table 1: Energy eigenvalues for three bands (eV)

8	7	6	5	4	3	2	1	n
0.0865	0.0864	0.0863	0.0861	0.0858	0.0856	0.0855	0.0854	1st band
0.3399	0.3392	0.3380	0.3366	0.3352	0.3338	0.3327	0.3320	2nd band
0.7370	0.7321	0.7250	0.7170	0.7091	0.7021	0.6967	0.6933	3rd band

(b)

As it's shown in figure 3 there are two forbidden energy band inside first seventeen energy eigenvalues. Energy bands are shown in table 2

Table 2: Energy bands (eV)

0.0854-0.0866	1st band
0.3318-0.3402	2nd band
0.6922-0.7388	3rd band

(c)

To find the wave function for each energy eigenvalue we can utilize transfer matrices given in (4)-(7). Form the solution of the Schrödinger equation the wave function inside each region is:

$$\Psi_n^b(x) = A_n^{(b)} \exp[-k_b(x - b_n)] + D_n^{(b)} \exp[k_b(x - b_n)] \quad (14)$$

$$\Psi_n^w(x) = A_n^{(w)} \exp[ik_w(x - w_n)] + D_n^{(w)} \exp[-ik_w(x - w_n)] \quad (15)$$

In above equations  $\Psi_n^b(x)$  and  $\Psi_n^w(x)$  are the wavefunction inside the nth barrier and nth well respectively.  $b_n$  is the position of the center nth barrier and  $w_n$  is the center of the nth well. to plot the wave function we follow the steps given below:

1. select  $A_1^{(b)} = 1$  and  $D_1^{(b)} = 0$ .
2. use the transfer matrices to find  $A_n^{(b)}$  and  $D_n^{(b)}$  in term of  $A_n^{(w)}$  and  $D_n^{(w)}$  :

$$\begin{bmatrix} A_n^{(w)} \\ D_n^{(w)} \end{bmatrix} = \mathbf{M}_w(L_w/2) \mathbf{M}_{bw} \mathbf{M}_b(L_b/2) \begin{bmatrix} A_n^{(b)} \\ D_n^{(b)} \end{bmatrix}$$

3. evaluate  $A_{n+1}^{(b)}$  and  $D_{n+1}^{(b)}$ :

$$\begin{bmatrix} A_{n+1}^{(b)} \\ D_{n+1}^{(b)} \end{bmatrix} = \mathbf{M}_b(L_b/2) \mathbf{M}_{bw} \mathbf{M}_w(L_w/2) \begin{bmatrix} A_n^{(b)} \\ D_n^{(b)} \end{bmatrix}$$

4. Normalize the wave function.

The wavefunctions for two energy eigenvalues are plotted in figures 5 and 6. The computer program is given in the appendix.



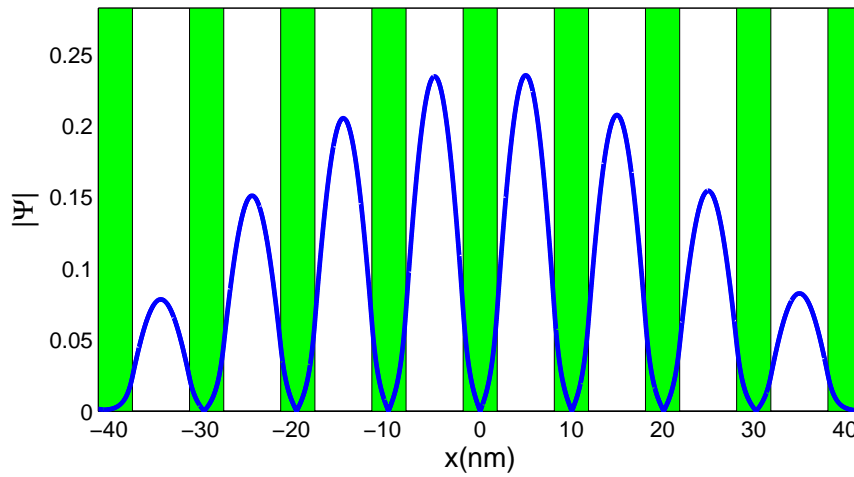


Figure 5: 8th energy eigenfunction

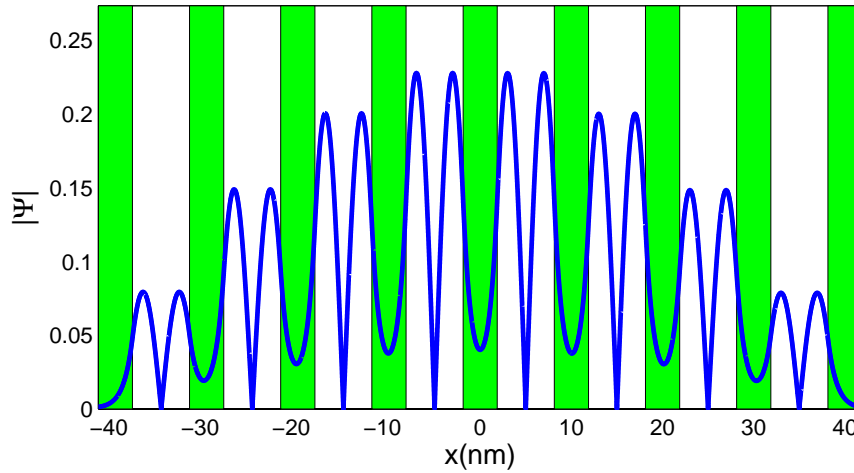


Figure 6: 9th energy eigenfunction

### Problem 3

(a)

A simple harmonic oscillator is initially in a state described by a wavefunction  $|\Psi\rangle$  as:

$$|\Psi\rangle = A \sum_{n=0}^{\infty} c^n |\psi_n\rangle \quad (1)$$

where  $|\psi_n\rangle$  are normalized energy eigenfunctions of SHO. The normalization constant  $A$  can be calculated as a function of  $c$ . Using orthogonality of eigenfunctions we can write:

$$\langle\Psi|\Psi\rangle = |A|^2 \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} c^n c^{*m} \langle\psi_m|\psi_n\rangle = |A|^2 \sum_{n=0}^{\infty} |c|^{2n} = 1 \quad (2)$$

From (2) we can write:

$$|A|^2 = \frac{1}{\sum_{n=0}^{\infty} |c|^{2n}} = 1 - |c|^2 \implies A = \sqrt{1 - |c|^2} \quad (3)$$

**(b)**

The wavefunction of the system at a later time  $t$  can be determined by applying time evolution operator:

$$|\Psi(t)\rangle = \exp\left(\frac{-iHt}{\hbar}\right) |\Psi(0)\rangle = \sqrt{1 - |c|^2} \sum_{n=0}^{\infty} c^n \exp\left(-\frac{iE_n t}{\hbar}\right) |\psi_n\rangle \quad (4)$$

From the lecture the energy eigenvalues of SHO are

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega_0$$

so:

$$|\Psi(t)\rangle = \sqrt{1 - |c|^2} \sum_{n=0}^{\infty} c^n \exp\left[-i\left(n + \frac{1}{2}\right)\omega_0 t\right] |\psi_n\rangle \quad (5)$$

**(c)**

The probability of finding the system again in its initial state at a later time  $t$  can be simply calculated as below:

$$P = |\langle\Psi(t=0)|\Psi(t)\rangle|^2 = \left| \left(1 - |c|^2\right) \sum_{n=0}^{\infty} |c|^{2n} \exp\left[\left(n + \frac{1}{2}\right)\omega_0 t\right] \right|^2 = \left| \frac{1 - |c|^2}{1 - |c|^2 e^{-i\omega_0 t}} \right|^2 \quad (6)$$

This expression can be simplified more:

$$P = \frac{1 + |c|^4 - 2|c|^2}{1 + |c|^4 - 2\cos(\omega_0 t)|c|^2} \quad (7)$$

**(d)**

The expectation value of the total energy of the system is:

$$\langle H \rangle_t = \langle \Psi(t) | H | \Psi(t) \rangle \quad (8)$$

Note that energy is a *constant of motion* and consequently expectation value of the total energy is independent of time. So  $H$  can be calculated at the initial state:

$$\langle H \rangle_t = \langle H \rangle_{t=0} = \langle \Psi(t=0) | H | \Psi(t=0) \rangle \quad (9)$$

Using

$$H|\psi_n\rangle = \left(n + \frac{1}{2}\right) \hbar\omega_0 |\psi_n\rangle$$

we obtain:

$$\langle H \rangle = \left(1 - |c|^2\right) \sum_{n=0}^{\infty} \left(n + \frac{1}{2}\right) \hbar\omega_0 |c|^{2n} \quad (10)$$

To evaluate this series we first prove the following equality:

$$\sum_{n=0}^{\infty} nq^n = \frac{q}{(1-q)^2} \quad |q| \leq 1 \quad (11)$$

Proof:

$$\sum_{n=0}^{\infty} nq^n = \lim_{N \rightarrow \infty} q \frac{\partial}{\partial q} \sum_{n=0}^N q^{n+1} = q \frac{\partial}{\partial q} \frac{q}{1-q} = \frac{q}{(1-q)^2} \quad (12)$$

Using (12) and after some simple algebraic manipulations we get:

$$\langle H \rangle = \hbar\omega_0 (1 - |c|^2) \left\{ \frac{|c|^2}{(1 - |c|^2)^2} + \frac{1}{2} \frac{1}{1 - |c|^2} \right\} = \frac{\hbar\omega}{2} \frac{1 + |c|^2}{1 - |c|^2} \quad (13)$$

## Problem 4

We first prove the following identity:

$$[A, BC] = B[A, C] + [A, B]C \quad (1)$$

Proof: If we expand the right hand side of (1) we get:

$$B[A, C] + [A, B]C = B(AC - CA) + (AB - BA)C = -BCA + ABC = [A, BC] \quad (2)$$

We have used the associative axiom of multiplication

(a)

$$[\hat{x}^2, \hat{p}] = \hat{x}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{x} = 2i\hbar\hat{x} \quad (3)$$

(b)

We define:

$$\mathcal{A}_n = [\hat{x}^n, \hat{p}] \quad (4)$$

Using (1), we can draw a recursive expression for  $\mathcal{A}_n$

$$\mathcal{A}_n = [\hat{x}^n, \hat{p}] = [\hat{x}\hat{x}^{n-1}, \hat{p}] = \hat{x}[\hat{x}^{n-1}, \hat{p}] + [\hat{x}, \hat{p}]\hat{x}^{n-1} = \hat{x}\mathcal{A}_{n-1} + i\hbar\hat{x}^{n-1} \quad (5)$$

So:

$$\mathcal{A}_n = \hat{x}\mathcal{A}_{n-1} + i\hbar\hat{x}^{n-1}, \quad \mathcal{A}_1 = i\hbar \quad (6)$$

We claim that:

$$\mathcal{A}_n = in\hbar\hat{x}^{n-1} \quad (7)$$

Proof by induction:

1. The theory works for  $n = 1$ :

$$\mathcal{A}_1 = i\hbar\hat{x}^0$$

2. Assume (7) works for  $N = n$ , that is,  $\mathcal{A}_n = in\hbar\hat{x}^{n-1}$  we show it also works for  $N = n + 1$

$$\mathcal{A}_{n+1} = \hat{x}\mathcal{A}_n + i\hbar\hat{x}^n = \hat{x}in\hbar\hat{x}^{n-1} + i\hbar\hat{x}^n = i(n+1)\hbar\hat{x}^n$$

(c)

It's assumed that  $g(\hat{x})$  is a well-defined function of position and we can expand this function as the power series of  $\hat{x}$  as:

$$g(\hat{x}) = \sum_{n=0}^{\infty} g_n \hat{x}^n \quad (8)$$

As a matter of the fact power series representation is the natural way of representing any function of an operator. So we obtain:

$$[g(\hat{x}), \hat{p}] = \left[ \sum_{n=0}^{\infty} g_n \hat{x}^n, \hat{p} \right] = \sum_{n=0}^{\infty} g_n [\hat{x}^n, \hat{p}] \quad (9)$$

From part (c) we have:

$$[g(\hat{x}), \hat{p}] = \sum_{n=0}^{\infty} i n \hbar g_n \hat{x}^{n-1} = i \hbar \left. \frac{dg(\zeta)}{d\zeta} \right|_{\zeta=\hat{x}} \quad (10)$$

(d)

$$[\hat{x}, H] = \left[ \hat{x}, \frac{\hat{p}^2}{2m} + V(\hat{x}) \right] = \frac{1}{2m} [\hat{x}, \hat{p}^2] + [\hat{x}, V(\hat{x})] \quad (11)$$

$\hat{x}$  and  $V(\hat{x})$  commute and the second term on the right hand side of (11) vanishes and just the first term remains. Using (1) we obtain:

$$[\hat{x}, \hat{p}^2] = [\hat{x}, \hat{p}] \hat{p} + \hat{p} [\hat{x}, \hat{p}] = 2i\hbar \hat{p} \quad (12)$$

At the end of the day:

$$[\hat{x}, H] = \frac{i\hbar}{m} \hat{p} \quad (13)$$

(e)

$$[\hat{p}, H] = \left[ \hat{p}, \frac{\hat{p}^2}{2m} + V(\hat{x}) \right] = \frac{1}{2m} [\hat{p}, \hat{p}^2] + [\hat{p}, V(\hat{x})] \quad (14)$$

$\hat{p}$  and  $\hat{p}^2$  commute and just the second term on the right hand side of (14) remains. Using the result of part (c) we get:

$$[\hat{p}, H] = [\hat{p}, V(\hat{x})] = -[V(\hat{x}), \hat{p}] = -i\hbar \left. \frac{dV(\zeta)}{d\zeta} \right|_{\zeta=\hat{x}} \quad (15)$$

## Problem 5

Three identical atoms at the corner of an equilateral triangle can be considered as a graphen unite cell. Assume that each atom contributes one electron. By neglecting electron -electron interaction Matrix representation of the Hamiltonian for each electron in the localized basis is:

$$\hat{H}_0 = \begin{pmatrix} E_0 & -a & -a \\ -a & E_0 & -a \\ -a & -a & E_0 \end{pmatrix} \quad (1)$$

where  $E_0$  is the self energy of the electron shared by each atom.  $a$  describes nondiagonal terms originate from adjacent site wave function overlap. In this representation expanding basis functions which are designated by  $|1\rangle$ ,  $|2\rangle$  and  $|3\rangle$  are the states vectors describing each atom at its own site.

(a)

To calculate energy eigenvalues of the system we have to solve the following eigen value problem:

$$\hat{H}_0 \Psi = E \Psi \implies \begin{pmatrix} E_0 & -a & -a \\ -a & E_0 & -a \\ -a & -a & E_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} \quad (2)$$

where  $\Psi$  is the matrix representation (isomorphism) of the state

$$|\Psi\rangle = \psi_1|1\rangle + \psi_2|2\rangle + \psi_3|3\rangle$$

So we have:

$$\det \begin{pmatrix} E_0 - E & -a & -a \\ -a & E_0 - E & -a \\ -a & -a & E_0 - E \end{pmatrix} = 0 \implies \begin{cases} E_1 = E_0 - 2a \\ E_2 = E_0 + a \\ E_3 = E_0 + a \end{cases} \quad (3)$$

$E_1$ ,  $E_2$  and  $E_3$  are three energy eigenvalues.  $E_1$  corresponds to the ground state of the system. As we can see  $E_2 = E_3$  so there is a two-fold degeneracy in this eigen value problem. The associated eigenvectors are:

$$E = E_1 \implies \begin{pmatrix} 2a & -a & -a \\ -a & 2a & -a \\ -a & -a & 2a \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = 0 \implies \Psi_1 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad (4)$$

Since two other eigenvalues are degenerate we have a kind of freedom in selecting two other eigenstates. As a matter of the fact we have to just find two orthonormal vectors which both lie in  $\psi_1 + \psi_2 + \psi_3 = 0$  plane:

$$E = E_2, E_3 \implies \begin{pmatrix} -a & -a & -a \\ -a & -a & -a \\ -a & -a & -a \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = 0 \implies \psi_1 + \psi_2 + \psi_3 = 0 \quad (5)$$

we just choose:

$$\Psi_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \quad \Psi_3 = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix} \quad (6)$$

Since now  $|\Psi_1\rangle$ ,  $|\Psi_2\rangle$  and  $|\Psi_3\rangle$  are abstract state kets correspond to  $\Psi_1$ ,  $\Psi_2$  and  $\Psi_3$  respectively.

(b)

Suppose a static electrical field is applied to the system such that potential energy of the electron on the top of the triangle is lowered by  $V_0$  which is assumed it's so smaller than  $a$ . Actually this electrical field perturbs the Hamiltonian. From the primary assumptions we have:

$$\hat{H} = \hat{H}_0 + \gamma \hat{H}_1 = \begin{pmatrix} E_0 - V_0 & -a & -a \\ -a & E_0 & -a \\ -a & -a & E_0 \end{pmatrix} \quad (7)$$

where  $\gamma$  is dimensionless parameter and is defined as

$$\gamma = \frac{V_0}{a} \quad (8)$$

and  $H_1$  is the perturbing Hamiltonian

$$\hat{H}_1 = \begin{pmatrix} -a & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (9)$$

To evaluate the new energy eigenvalues and associated eigenstates the direct diagonalization procedure is given at first and then the general formulation of *time independent perturbation theory* is applied to give a better insight about energy shift and break of degeneracy.

In order to diagonalize the new Hamiltonian the following eigenvalue problem should be solved:

$$H|\Psi\rangle = \lambda|\Psi\rangle \quad (10)$$

If we take a look at matrix representation of  $H$  it can be seen that  $H$  can be rewritten as below:

$$\hat{H} = E_0 \mathbf{I}_{3 \times 3} - a \begin{pmatrix} \gamma & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \quad (11)$$

where  $\mathbf{I}_{3 \times 3}$  is 3 unity matrix. for every eigenvalue we have  $\lambda = E_0 - a\lambda_1$  where  $\lambda_1$  is eigenvalue of the second matrix in the right hand side of (11). So we have to just work on the second matrix.

$$\det \begin{pmatrix} \gamma - \lambda_1 & 1 & 1 \\ 1 & -\lambda_1 & 1 \\ 1 & 1 & -\lambda_1 \end{pmatrix} = 0 \implies (\gamma - \lambda_1)(\lambda_1^2 - 1) + 2(\lambda_1 + 1) = 0 \quad (12)$$

Note that since  $V_0 \ll a$  then  $\gamma \ll 1$ . Therefore:

$$\begin{cases} \lambda_1 = \frac{1+\gamma}{2} + \sqrt{\frac{(1+\gamma)^2}{4} + 2 - \gamma} \implies E_1 \approx E_0 - a \left(2 + \frac{\gamma}{3}\right) = E_0 - 2a - \frac{1}{3}V_0 \\ \lambda_1 = \frac{1+\gamma}{2} - \sqrt{\frac{(1+\gamma)^2}{4} + 2 - \gamma} \implies E_2 \approx E_0 - a \left(-1 + \frac{2}{3}\gamma\right) = E_0 + a - \frac{2}{3}V_0 \\ \lambda_1 = 1 \implies E_3 = E_0 + a \end{cases} \quad (13)$$

First order approximation has been applied to get the final results. Applied electrical fields breaks the symmetry and removes the degeneracy. The formulation of the problem based on time independent perturbation theory is developed in continue.

Let us assume that we have found the eigen value and the complete set of normalized eigenfunctions for a Hamiltonian  $H_0$ ,

$$H_0|\Psi_n\rangle = E_n^{(0)}|\Psi_n\rangle \quad (14)$$

We now ask to solve

$$(H_0 + \gamma H_1)|\Phi_n\rangle = E_n|\Phi_n\rangle \quad (15)$$

In general we may view the Hamiltonian as a matrix, we can write:

$$\hat{H}_{mn} = \langle \Psi_m | H | \Psi_n \rangle = E_m^{(0)} \delta_{mn} + \langle \Psi_m | \gamma H_1 | \Psi_n \rangle \quad (16)$$

We will express the desired quantities as a power series in  $\gamma$ . and we will assume that as  $\gamma \rightarrow 0$ ,  $E_n \rightarrow E_n^{(0)}$ . Since  $|\Psi_n\rangle$  form a complete set, we may expand  $|\Phi_n\rangle$  in series involving  $|\Psi_n\rangle$ ,

$$|\Phi_n\rangle = N(\gamma) \left\{ |\Psi_n\rangle + \sum_{k \neq n} C_{nk}(\gamma) |\Psi_k\rangle \right\} \quad (17)$$

The factor  $N(\gamma)$  is the normalization coefficient guarating  $\langle \Phi_n | \Phi_n \rangle = 1$ . Note that if  $\gamma = 0$  then we should have:

$$N(0) = 1 \quad C_{nk}(0) = 0 \quad E_n(0) = E_n^{(0)} \quad (18)$$

This allows us to expanse  $C_{nk}(\gamma)$  and  $E_n(\gamma)$  as a power series of  $\gamma$  :

$$C_{nk}(\gamma) = \gamma C_{nk}^{(1)} + \gamma^2 C_{nk}^{(2)} + \dots \quad (19)$$

$$E_n(\gamma) = E_n^{(0)} + \gamma E_n^{(1)} + \gamma^2 E_n^{(2)} + \dots \quad (20)$$

Inserting (19) and (20) into (15) leads to a set of equations. Identifying powers of  $\gamma$  yields a series of equations. The first one is:

$$H_0 \sum_{k \neq n} C_{nk}^{(1)} |\Psi_k\rangle + H_1 |\Psi_n\rangle = E_n^{(0)} \sum_{k \neq n} C_{nk}^{(1)} |\Psi_k\rangle + E_n^{(1)} |\Psi_n\rangle \quad (21)$$

Multiplying both sides of (21) by  $\langle \Psi_n |$  and using orthogonality condition we obtain

$$\gamma E_n^{(1)} = \langle \Psi_n | \gamma H_1 | \Psi_n \rangle \quad (22)$$

This shows the first order energy shift in the energy levels. Similarly if we multiply both sides of (21) by  $\langle \Psi_m |$  we obtain:

$$\gamma C_{nm} = \frac{\langle \Psi_m | H_1 | \Psi_n \rangle}{E_n^{(0)} - E_m^{(0)}} \quad (23)$$

The numerator is the matrix elements of  $\gamma H_1$  in basis of states in which  $H_0$  is diagonal. First order energy shift and the coefficients of the other basis expanding new eigenstates of the perturbed Hamiltonian were given. In deriving (23) it's assumed that there is no degeneracy i.e.  $E_n^{(0)} \neq E_k^{(0)}$  for  $k \neq n$ . Quite generally assume a subspace made of some orthogonal eigen states of original Hamiltonian is a degenerate subspace, i.e. the expectation value of the original Hamiltonian evaluated on every state vector in this subspace is constant. Suppose that a unitary operator acts only on this subspace and rotates orthogonal basis functions. Definitely Hamiltonian in the rotated states is still diagonal. Now we can rotate the subspace to diagonalize  $\gamma H_1$  without affecting the states outside of this subspace. In this case diagonalized perturbing Hamiltonian directly shifts energy levels in the first order. Clearly diagonalizing  $H_1$  in the degenerate subspace leads to the determination of proper eigen states.

Now we can apply this theory to our original problem. First we can readily evaluate the first order (in term of  $\gamma$ ) energy shift for the ground state. Since the ground state is not a degenerate state we can use ordinary perturbation theory. From (22) we have:

$$\gamma E_1^{(1)} = \langle \Psi_1 | \gamma H_1 | \Psi_1 \rangle = \gamma \Psi_1^\dagger \hat{H} \Psi_1 = \frac{-V_0}{3} (\langle 1 | + \langle 2 | + \langle 3 |) | 1 \rangle \langle 1 | (\langle 1 | + \langle 2 | + \langle 3 |) = -\frac{V_0}{3} \quad (24)$$

If we use (23) then:

$$\gamma C_{12} = \gamma \frac{\Psi_2^\dagger \hat{H}_1 \Psi_1}{(E_0 - 2a) - (E_0 + a)} = -\frac{\gamma}{3\sqrt{6}} \quad (25)$$

$$\gamma C_{13} = \gamma \frac{\Psi_3^\dagger \hat{H}_1 \Psi_1}{(E_0 - 2a) - (E_0 + a)} = -\frac{\gamma}{9\sqrt{2}} \quad (26)$$

So we have:

$$c|\Phi_1\rangle = \left(1 - \frac{2\gamma}{9}\right) |1\rangle + \left(1 + \frac{\gamma}{9}\right) |2\rangle + \left(1 + \frac{\gamma}{9}\right) |3\rangle \quad (27)$$

To evaluate energy shift in the degenerate states we should first represent  $H_1$  in  $|\Psi_i\rangle$  basis:

$$\hat{H}'_1 = -V_0 \begin{pmatrix} \frac{1}{3} & \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} \\ \frac{1}{\sqrt{6}} & \frac{1}{2} & \frac{1}{2\sqrt{3}} \\ \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{3}} & \frac{1}{6} \end{pmatrix} \quad (28)$$

At this stage we should diagonalize the 2 block matrix the lower corner of  $\hat{H}'_1$ :

$$-V_0 \begin{pmatrix} \frac{1}{2} & \frac{1}{2\sqrt{3}} \\ \frac{1}{2\sqrt{3}} & \frac{1}{6} \end{pmatrix} \Phi' = \lambda \Phi' \implies \begin{cases} \lambda = 0 & \Phi'_2 = \frac{1}{2} (1 \quad -\sqrt{3})^T \\ \lambda = -\frac{2V_0}{3} & \Phi'_3 = \frac{1}{2} (\sqrt{3} \quad 1)^T \end{cases} \quad (29)$$

New eigenstates can be represented in the old basis as:

$$|\Phi_2\rangle = \frac{1}{2}|\Psi_2\rangle - \frac{\sqrt{3}}{2}|\Psi_3\rangle = -\frac{1}{\sqrt{2}}|2\rangle + \frac{1}{\sqrt{2}}|3\rangle \quad (30)$$

$$|\Phi_3\rangle = \frac{\sqrt{3}}{2}|\Psi_2\rangle + \frac{1}{2}|\Psi_3\rangle = \sqrt{\frac{2}{3}}|1\rangle - \frac{1}{\sqrt{6}}|2\rangle + \frac{1}{\sqrt{6}}|3\rangle \quad (31)$$

The result of our analysis is shown in the figure 7.

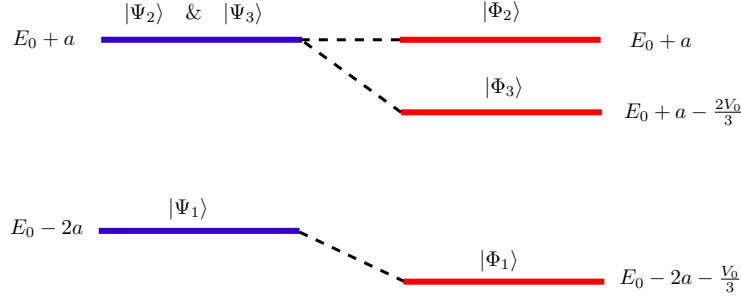


Figure 7: First order energy shift

(c)

It's assumed that initially electron is in the ground level of the system ,that is,  $|\Phi_1\rangle$  suddenly the field is rotated 120 dgrees and points toward one of the atomes on basis of the triangle (give it the second atom!). In this case the new Hamiltonian is:

$$\hat{H}_{new} = \hat{H}_0 + \gamma \hat{H}_2 = \begin{pmatrix} E_0 & -a & -a \\ -a & E_0 - V_0 & -a \\ -a & -a & -E_0 \end{pmatrix} \quad (32)$$

The probability for the electron to remainin the ground state can be readily evaluated by calculating squar of the inner product of the ground states of two Hamiltonians (before and after the field rotation). Generally those eigenstates are very complicated function of  $\gamma$  . The exact value of the eigenfunctions based numerical analysis is plotted in figure 8.

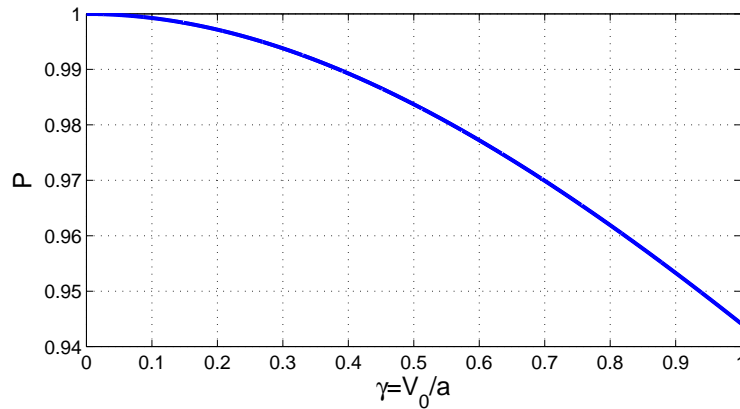


Figure 8: Exact probability of emaining in the ground state



If we take a look at (7) we can clearly see that both Hamiltonian are the same and we should just swap  $|1\rangle$   $|2\rangle$  that is those states should be mutually exchanged in our formulation If we represents the ground state of the new Hamiltonian as  $|\Omega_1\rangle$  then from (27) we have:

$$c|\Omega_1\rangle = \left(1 - \frac{2\gamma}{9}\right) |2\rangle + \left(1 + \frac{\gamma}{9}\right) |1\rangle + \left(1 + \frac{\gamma}{9}\right) |3\rangle \quad (33)$$

The probability for the electron to remain in the ground state is:

$$P = |\langle\Omega_1|\Phi_1\rangle|^2 \approx \left[ \frac{2 \left(1 - \frac{2\gamma}{9}\right) \left(1 + \frac{\gamma}{9}\right) + \left(1 + \frac{\gamma}{9}\right)^2}{\left(1 - \frac{2\gamma}{9}\right)^2 + \left(1 + \frac{\gamma}{9}\right)^2 + \left(1 + \frac{\gamma}{9}\right)^2} \right]^2 \quad (34)$$

## Appendix

```

clc
clear all
close all

N=8;           %Number of QW
level=8;       % number of desired mode
%-----
Lw=6.25;
Lb=3.75;
V0=0.9;
%---constants-----
c=300;         %light speed
h=0.65;        % reduced plank constant
Meff=0.07*(0.511* 10^6)/c^2; % electron effective mass

%-----Determination of the Energybands (coarse root searching)-----
DE=V0/10^4;
E=[DE:DE:V0-DE];
kw=sqrt(2*Meff*E/h^2);
kb=sqrt(2*Meff*(V0-E)/h^2);
M11=exp(kb*Lb).*(cos(kw*Lw)-0.5*(kw./kb-kb./kw).*sin(kw*Lw));
M22=exp(-kb*Lb).*(cos(kw*Lw)+0.5*(kw./kb-kb./kw).*sin(kw*Lw));
U=abs(0.5*(M11+M22))>1;
n=length(E);
Eg=[]; % Eg is the vector of the edges of the allowable enrgy bands
swich=1;
for j=2:n
    if(U(j)==0 && swich==1)
        Eg=[Eg E(j)];
        swich=0;
    end
    if(U(j)==1 && swich==0)
        Eg=[Eg E(j)];
        swich=1;
    end
end

end
%-----
Neb=length(Eg)/2;
Ox=[];
Oy=[];
for u=1:Neb
    Ox=[Ox 0 1 1 0];
    Oy=[Oy Eg(2*u-1) Eg(2*u) Eg(2*u) Eg(2*u)];
end

```

```

figure
fill(0x,0y,'r')
Xlim([0 1]);
Ylim([0 V0]);
Ylabel('E(ev)','fontsize',15) % plots energy bands
%-----Determination of the Energy Eigenvalues-----
dE=DE/10^2;
Z=[];
for n=1:Neb
    El=Eg(2*n-1)-DE;
    Eh=Eg(2*n)+DE;
    n
    R=[];
    c=0;
    EE=[El:dE:Eh];
    for E0=El:dE:Eh
        c=c+1;
        k1=sqrt(2*Meff*E0/h^2);
        k2=sqrt(2*Meff*(V0-E0)/h^2);
        M11=exp(k2*Lb).*(cos(k1*Lw)-0.5*(k1./k2-k2./k1).*sin(k1*Lw));
        M22=exp(-k2*Lb).*(cos(k1*Lw)+0.5*(k1./k2-k2./k1).*sin(k1*Lw));
        M12=-0.5*exp(k2*Lb).*(k1./k2+k2./k1).*sin(k1*Lw);
        M21=0.5*exp(-k2*Lb).*(k1./k2+k2./k1).*sin(k1*Lw);
        M=[M11 M12;M21 M22];
        Mt=M^N;
        R=[R Mt(1,1)];

%-----

if(R(end)==0)
    Z=[Z E0];
elseif(c==1)
elseif(R(end)*R(end-1)<0)
    Z=[Z E0-dE/2];
end

%-----
end
figure
plot(EE,R,'linewidth',2.5);
Ylim([-0.5 0.5]);
Xlim([El Eh]);
Xlabel('E(ev)','fontsize',15)
Ylabel('M_{11}','fontsize',15)
end

%----- Part C- Wavefunction Determination -----
Ed=Z(level);
U2=0;

```

```

for E0=Ed-dE:dE/100:Ed+dE
k1=sqrt(2*Meff*E0/h^2);
k2=sqrt(2*Meff*(V0-E0)/h^2);
M11=exp(k2*Lb).*(cos(k1*Lw)-0.5*(k1./k2-k2./k1).*sin(k1*Lw));
M22=exp(-k2*Lb).*(cos(k1*Lw)+0.5*(k1./k2-k2./k1).*sin(k1*Lw));
M12=-0.5*exp(k2*Lb).*(k1./k2+k2./k1).*sin(k1*Lw);
M21=0.5*exp(-k2*Lb).*(k1./k2+k2./k1).*sin(k1*Lw);
M=[M11 M12;M21 M22];
Mt=M^N;

%-----

U1=Mt(1,1);
if(U1==0)
    Ed=E0;
    break
elseif(U1*U2<0)
    Ed=E0-dE/2;
    break
end

U2=U1;
end

%-----

%-----Mb-----
Mb=zeros(2);
kw=sqrt(2*Meff*Ed/h^2);
q=sqrt(2*Meff*(V0-Ed)/h^2);
Mb(1,1)=exp(q*Lb);
Mb(2,2)=exp(-q*Lb);
%-----Mwb-----
Mwb=zeros(2,2);
Mwb(1,1)=1+1i*q/kw;
Mwb(2,2)=Mwb(1,1);
Mwb(1,2)=1-1i*q/kw;
Mwb(2,1)=Mwb(1,2);
Mwb=0.5*Mwb;
%-----Mw-----
Mw=zeros(2);
Mw(1,1)=exp(-1i*kw*Lw);
Mw(2,2)=exp(+1i*kw*Lw);
%-----Mbw-----
Mbw=zeros(2);
Mbw(1,1)=1-1i*kw/q;
Mbw(1,2)=1+1i*kw/q;
Mbw(2,1)=Mbw(1,2);
Mbw(2,2)=Mbw(1,1);

```

```

Mbw=0.5*Mbw;
%-----
V1=[1;0];
delta=0.001;
zb=[delta:delta:Lb];
zw=[delta:delta:Lw];
Fb=[exp(-q*zb);exp(+q*zb)];
Fw=[exp(1i*k*zw);exp(-1i*k*zw)];
%-----
z=[];
Y=[];
for(n=1:N)
    if(n~=1)
V1=Mb*Mbw*V2;
        end
z=[zb z];
Y=[V1.'*Fb Y];
z=[zw z+Lw];
V2=Mw*Mwb*V1;
Y=[V2.'*Fw Y];
z=z+Lb;
end
V1=Mb*Mbw*V2;
z=[zb z];
Y=[V1.'*Fb Y];
L=max(z);
x=z-L/2;
figure
Nor=sqrt(trapz(x,abs(Y.^2)));
Max=max(abs(Y)/Nor);

y1=0;
y2=1.2*Max;
Oy=[];
Ox=[];
x1=x(1);
for(m=1:N+1)
    Ox=[Ox x1 x1 x1+Lb x1+Lb];
    Oy=[Oy y1 y2 y2 y1];
    x1=x1+Lb+Lw;
end
fill(Ox,Oy,'g')
Xlim([x(1) x(end)]);
Ylim([0 1.2*Max]);
hold on
plot(x,abs(Y)/Nor,'linewidth',2.5)
Xlabel('x(nm)','fontsize',15)
Ylabel('|Psi|','fontsize',15)

```

