

ECE770 T14/QIC 885: Quantum Electronics & Photonics
Solution of Problem Set 2, University of Waterloo, Winter 2013

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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:

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

where \dagger is *transpose conjugate* operator. So α and β 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:

$$|\Psi_+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (9)$$

and

$$|\Psi_-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (10)$$

Now the initial qubit states can be written in terms of orthonormal eigenstates as:

$$|0\rangle = \frac{1}{\sqrt{2}} (|\Psi_+\rangle + |\Psi_-\rangle) \quad (11)$$

and

$$|1\rangle = \frac{1}{\sqrt{2}} (|\Psi_+\rangle - |\Psi_-\rangle) \quad (12)$$

c) Knowing the energy eigenstates, the time-dependent wave function as a result of solution to Schrodinger equation becomes:

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}} [e^{-i(a+b)t/\hbar} |\Psi_+\rangle + e^{-i(a-b)t/\hbar} |\Psi_-\rangle] \quad (13)$$

d) If the system starts out at $t = 0$ in state $|0\rangle$, the state after time t can be predicted by (??).

$$\begin{aligned} |\Psi(t)\rangle &= \frac{1}{\sqrt{2}} e^{-iat/\hbar} [e^{-ibt/\hbar} |\Psi_+\rangle + e^{ibt/\hbar} |\Psi_-\rangle] \\ &= e^{-iat/\hbar} \begin{pmatrix} \cos \frac{bt}{\hbar} \\ -i \sin \frac{bt}{\hbar} \end{pmatrix} \end{aligned} \quad (14)$$

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 wells which can be locally treated as a periodic structure.

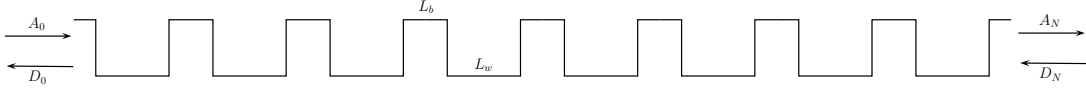


Figure 1: MQW composed of eight cascaded quantum wells

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

$$\begin{bmatrix} A_0 \\ D_0 \end{bmatrix} = \begin{bmatrix} M_{t11} & M_{t12} \\ M_{t21} & M_{t22} \end{bmatrix} \begin{bmatrix} A_N \\ D_N \end{bmatrix} \quad (15)$$

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

$$M_{t11} = 0 \quad (16)$$

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 assoicated with each unit cell. Figure 2 shows a unite cell of the structure. The transfer matrix assoicated 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:

$$\mathbf{M}_{cell} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} = \mathbf{M}_b(L_b/2)\mathbf{M}_{bw}\mathbf{M}_w(L_w)\mathbf{M}_{wb}\mathbf{M}_b(L_b/2) \quad (17)$$

where

$$\mathbf{M}_b(L_b/2) = \begin{bmatrix} \exp(k_b L_b/2) & 0 \\ 0 & \exp(k_b L_b/2) \end{bmatrix} \quad (18)$$

$$\mathbf{M}_{bw} = \frac{1}{2} \begin{bmatrix} 1 - i \frac{k_w}{k_b} & 1 + i \frac{k_w}{k_b} \\ 1 + i \frac{k_w}{k_b} & 1 - i \frac{k_w}{k_b} \end{bmatrix} \quad (19)$$

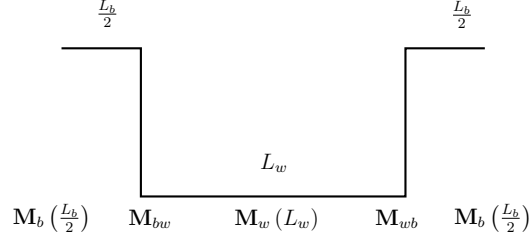


Figure 2: a unit cell of the MQW structure

$$\mathbf{M}_w(L_w) = \begin{bmatrix} \exp(-ik_w L_w) & 0 \\ 0 & \exp(ik_w L_w) \end{bmatrix} \quad (20)$$

$$\mathbf{M}_{wb} = \frac{1}{2} \begin{bmatrix} 1 + i \frac{k_b}{k_w} & 1 - i \frac{k_b}{k_w} \\ 1 - i \frac{k_b}{k_w} & 1 + i \frac{k_b}{k_w} \end{bmatrix} \quad (21)$$

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 (18)-(21) into (17) we obtain:

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

$$m_{12} = -0.5 \exp(k_b L_b) \left(\frac{k_w}{k_b} + \frac{k_b}{k_w} \right) \sin(k_w L_w) \quad (23)$$

$$m_{21} = 0.5 \exp(k_b L_b) \left(\frac{k_w}{k_b} + \frac{k_b}{k_w} \right) \sin(k_w L_w) \quad (24)$$

$$m_{22} = \exp(-k_b L_b) \left[\cos(k_w L_w) + 0.5 \left(\frac{k_w}{k_b} - \frac{k_b}{k_w} \right) \sin(k_w L_w) \right] \quad (25)$$

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

$$\mathbf{M}_t = \mathbf{M}_{cell}^8 \quad (26)$$

Based on the lecture the possible discrete energy eigenvalues for the bound state can be calculated by considering the possible continous energy bands for the infinite structure. In fact it is

shown that the possible solutions satisfy the following condition:

$$U = \frac{1}{2}(m_{11} + m_{22}) \leq 1 \quad (27)$$

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

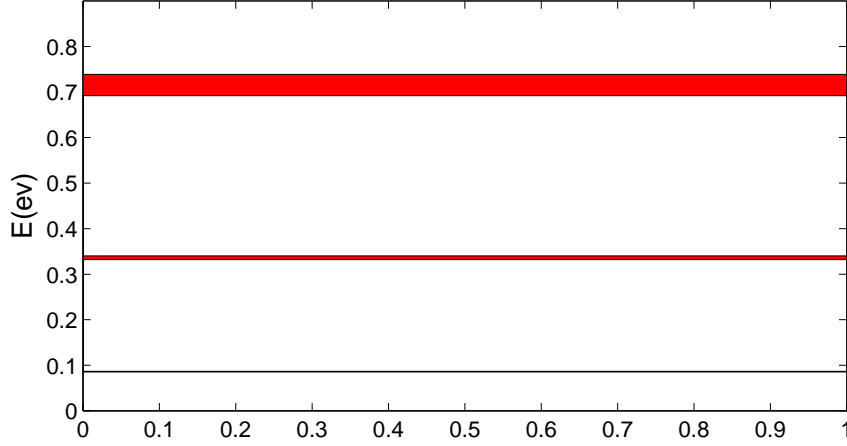
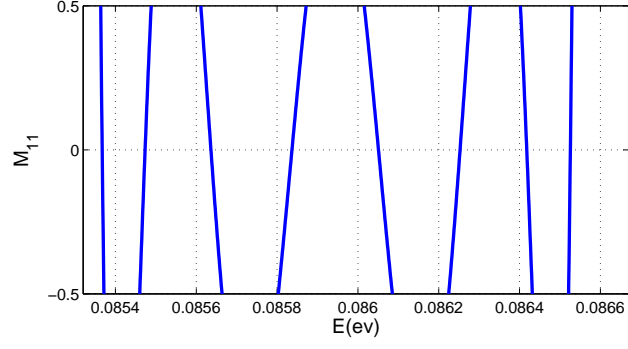


Figure 3: continuous energy bands for MQW

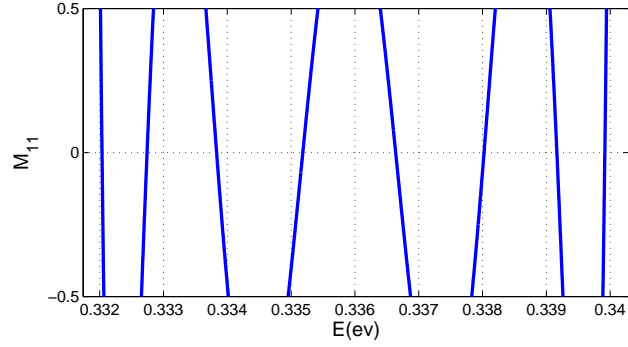
energy eigenfunctions for the bound states we should find the solutions of (31). However M_{t11} fluctuations are so striking and this makes our job difficult. In fact very fine meshes have to be used to find all zeros. To avoid computational complexity we have used the notion of continuous band structures:

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.

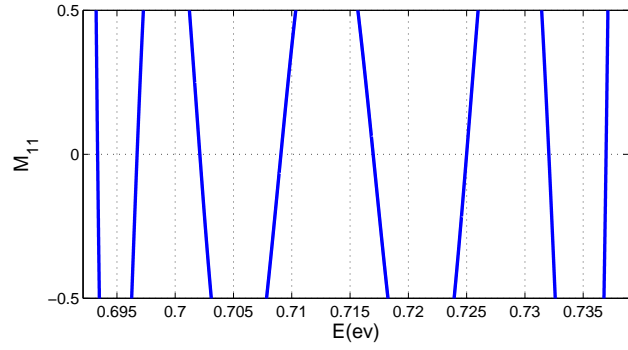
Figure 4 shows three M_{t11} inside three allowable energy bands. As it was expected in each region we have 8 solutions (correspond to eight QW).



(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.

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

c) To find the wave function for each energy eigenvalue we can utilize transfer matrices given

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

Table 2: Energy bands (eV)

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

in (18)-(21). Form the solution of the Schrödinger equation the wave function inside each region is:

$$\Psi_n^b(x) = A_n^{(b)} \exp[-k_b(x - b_n)] + D_n^{(b)} \exp[k_b(x - b_n)] \quad (28)$$

$$\Psi_n^w(x) = A_n^{(w)} \exp[ik_w(x - w_n)] + D_n^{(w)} \exp[-ik_w(x - w_n)] \quad (29)$$

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 centre 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.

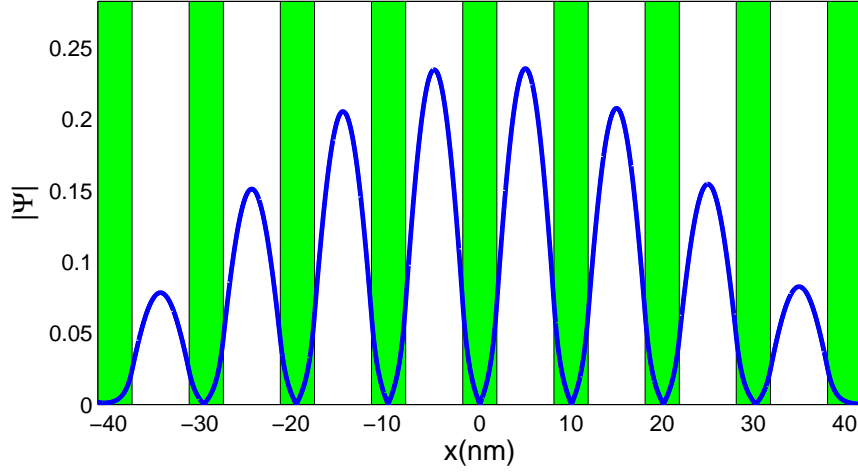


Figure 5: 8th energy eigenfunction

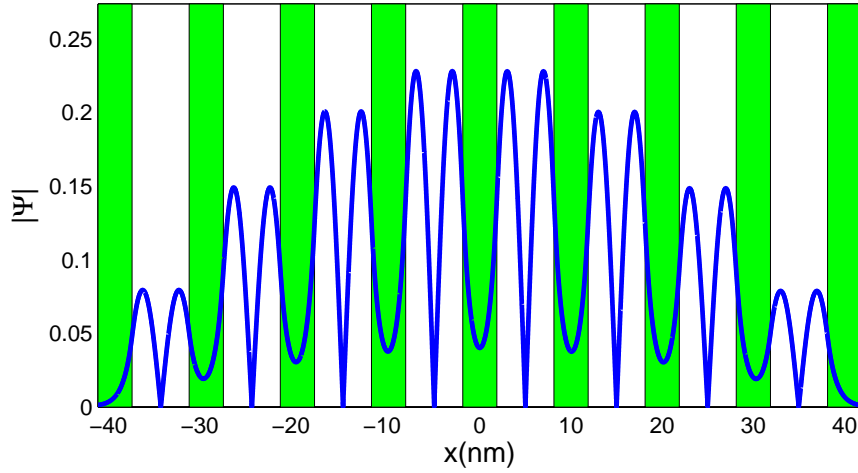


Figure 6: 9th energy eigenfunction

Problem 3-

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

$$|\Psi\rangle = A \sum_{n=0}^{\infty} c^n |\psi_n\rangle \quad (30)$$

where $|\psi_n\rangle$ are normalized energy eigenfunctions of SHO. The normalization constant A can be

calculated as a function of c . Using orthonormality of eigenfunctions we can write:

$$\langle \Psi | \Psi \rangle = |A|^2 \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} c^n c^{*m} \langle \psi_m | \psi_n \rangle = |A|^2 \sum_{n=0}^{\infty} |c|^{2n} = 1 \quad (31)$$

From (31) we can write:

$$|A|^2 = \frac{1}{\sum_{n=0}^{\infty} |c|^{2n}} = 1 - |c|^2 \implies A = \sqrt{1 - |c|^2} \quad (32)$$

b-

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

$$|\Psi(t)\rangle = \exp\left(\frac{-iHt}{\hbar}\right) |\Psi(0)\rangle = \sqrt{1 - |c|^2} \sum_{n=0}^{\infty} c^n \exp\left(-\frac{iE_n t}{\hbar}\right) |\psi_n\rangle \quad (33)$$

From the lecture the energy eigenvalues of SHO are

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

so:

$$|\Psi(t)\rangle = \sqrt{1 - |c|^2} \sum_{n=0}^{\infty} c^n \exp\left[-i\left(n + \frac{1}{2}\right) \omega_0 t\right] |\psi_n\rangle \quad (34)$$

c-

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

$$P = |\langle \Psi(t=0) | \Psi(t) \rangle|^2 = \left| \left(1 - |c|^2\right) \sum_{n=0}^{\infty} |c|^{2n} \exp\left[\left(n + \frac{1}{2}\right) \omega_0 t\right] \right|^2 = \left| \frac{1 - |c|^2}{1 - |c|^2 e^{-i\omega_0 t}} \right|^2 \quad (35)$$

This expression can be simplified to:

$$P = \frac{1 + |c|^4 - 2|c|^2}{1 + |c|^4 - 2\cos(\omega_0 t)|c|^2} \quad (36)$$

d-

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

$$\langle H \rangle_t = \langle \Psi(t) | H | \Psi(t) \rangle \quad (37)$$

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

$$\langle H \rangle_t = \langle H \rangle_{t=0} = \langle \Psi(t=0) | H | \Psi(t=0) \rangle \quad (38)$$

Using

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

we obtain:

$$\langle H \rangle = (1 - |c|^2) \sum_{n=0}^{\infty} \left(n + \frac{1}{2}\right) \hbar\omega_0 |c|^{2n} \quad (39)$$

To evaluate this series we first prove the following equality:

$$\sum_{n=0}^{\infty} nq^n = \frac{q}{(1-q)^2} \quad |q| \leq 1 \quad (40)$$

Proof:

$$\sum_{n=0}^{\infty} nq^n = \lim_{N \rightarrow \infty} q \frac{\partial}{\partial q} \sum_{n=0}^N q^{n+1} = q \frac{\partial}{\partial q} \frac{q}{1-q} = \frac{q}{(1-q)^2} \quad (41)$$

Using (41) and after some simple algebraic manipulations we get:

$$\langle H \rangle = \hbar\omega_0 (1 - |c|^2) \left\{ \frac{|c|^2}{(1 - |c|^2)^2} + \frac{1}{2} \frac{1}{1 - |c|^2} \right\} = \frac{\hbar\omega}{2} \frac{1 + |c|^2}{1 - |c|^2} \quad (42)$$

Problem 4-

a-

We first prove the following identity:

$$[A, BC] = B[A, C] + [A, B]C \quad (43)$$

Proof: If we expand the right hand side of (43) we get:

$$B[A, C] + [A, B]C = B(AC - CA) + (AB - BA)C = -BCA + ABC = [A, BC] \quad (44)$$

We have used the associative axiom of multiplication.

$$[\hat{x}^2, \hat{p}] = \hat{x}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{x} = 2i\hbar\hat{x} \quad (45)$$

b-

We define:

$$\mathcal{A}_n = [\hat{x}^n, \hat{p}] \quad (46)$$

Using (43), we can draw a recursive expersion for \mathcal{A}_n

$$\mathcal{A}_n = [\hat{x}^n, \hat{p}] = [\hat{x}\hat{x}^{n-1}, \hat{p}] = \hat{x} [\hat{x}^{n-1}, \hat{p}] + [\hat{x}, \hat{p}] \hat{x}^{n-1} = \hat{x}\mathcal{A}_{n-1} + i\hbar\hat{x}^{n-1} \quad (47)$$

So:

$$\mathcal{A}_n = \hat{x}\mathcal{A}_{n-1} + i\hbar\hat{x}^{n-1} \quad , \quad \mathcal{A}_1 = i\hbar \quad (48)$$

We claim that:

$$\mathcal{A}_n = in\hbar\hat{x}^{n-1} \quad (49)$$

Proof by induction:

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

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

2. Assume (49) 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:

$$g(\hat{x}) = \sum_{n=0}^{\infty} g_n \hat{x}^n \quad (50)$$

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

$$[g(\hat{x}), \hat{p}] = \left[\sum_{n=0}^{\infty} g_n \hat{x}^n, \hat{p} \right] = \sum_{n=0}^{\infty} g_n [\hat{x}^n, \hat{p}] \quad (51)$$

From part (c) we have:

$$[g(\hat{x}), \hat{p}] = \sum_{n=0}^{\infty} in\hbar g_n \hat{x}^{n-1} = i\hbar \left. \frac{dg(\zeta)}{d\zeta} \right|_{\zeta=\hat{x}} \quad (52)$$

d-

$$[\hat{x}, H] = \left[\hat{x}, \frac{\hat{p}^2}{2m} + V(\hat{x}) \right] = \frac{1}{2m} [\hat{x}, \hat{p}^2] + [\hat{x}, V(\hat{x})] \quad (53)$$

\hat{x} and $V(\hat{x})$ commute and the second term on the right hand side of (53) vanishes and just the first term remains. Using (43) we obtain:

$$[\hat{x}, \hat{p}^2] = [\hat{x}, \hat{p}] \hat{p} + \hat{p} [\hat{x}, \hat{p}] = 2i\hbar \hat{p} \quad (54)$$

At the end of the day:

$$[\hat{x}, H] = \frac{i\hbar}{m} \hat{p} \quad (55)$$

e-

$$[\hat{p}, H] = \left[\hat{p}, \frac{\hat{p}^2}{2m} + V(x) \right] = \frac{1}{2m} [\hat{p}, \hat{p}^2] + [\hat{p}, V(x)] \quad (56)$$

\hat{p} and \hat{p}^2 commute and just the second term on the right hand side of (56) remains. Using the result of part (c) we get:

$$[\hat{p}, H] = [\hat{p}, V(x)] = -[V(x), \hat{p}] = -i\hbar \frac{dV(x)}{dx} \quad (57)$$

Problem 5

Consider three identical atoms at the corner of an equilateral triangle as shown in Fig ?? . 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:

$$\hat{H}_0 = \begin{pmatrix} E_0 & -a & -a \\ -a & E_0 & -a \\ -a & -a & E_0 \end{pmatrix} \quad (58)$$

where E_0 is the self energy of the electron shared by each atom. a describes non-diagonal terms originating 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 state vectors describing each atom at its own site.

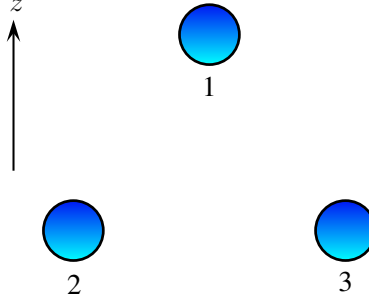


Figure 7: Atomic structure consisting of three identical atoms at the corners of an equilateral triangle

a-

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

$$\hat{H}_0 \Psi = E \Psi \implies \begin{pmatrix} E_0 & -a & -a \\ -a & E_0 & -a \\ -a & -a & E_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} \quad (59)$$

where Ψ 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:

$$\det \begin{pmatrix} E_0 - E & -a & -a \\ -a & E_0 - E & -a \\ -a & -a & E_0 - E \end{pmatrix} = 0 \implies \begin{cases} E_1 = E_0 - 2a \\ E_2 = E_0 + a \\ E_3 = E_0 + a \end{cases} \quad (60)$$

E_1 , E_2 and E_3 are three energy eigenvalues. E_1 corresponds to the ground state of the system and $E_2 = E_3$ are two-fold degenerate energy levels.

b-

After applying the electric field, the Hamiltonian of the system is:

$$\hat{H}_0 = \begin{pmatrix} E_0 - V_o & -a & -a \\ -a & E_0 & -a \\ -a & -a & E_0 \end{pmatrix} \quad (61)$$

The diagonalization gives the following energy levels:

$$E_1 = E_0 + a \quad (62)$$

$$E_2 = E_0 - \frac{a + V_o + \sqrt{(a - V_o)^2 + 8a^2}}{2} \quad (63)$$

$$E_3 = E_0 - \frac{a + V_o - \sqrt{(a - V_o)^2 + 8a^2}}{2} \quad (64)$$

E_2 has the lowest energy and corresponds to the ground state with the following wave function:

$$|\psi_0\rangle = \frac{1}{\sqrt{(E_0 - E_2 - a)^2 + 2a^2}} [E_0 - E_2 - a] |1\rangle + a|2\rangle + a|3\rangle \quad (65)$$

c-

After the rotation of the field the system has the same configuration as before but the sites are relabeled: $1 \rightarrow 2, 2 \rightarrow 3, 3 \rightarrow 1$. The new ground state is:

$$|\psi_0'\rangle = \frac{1}{\sqrt{(E_0 - E_2 - a)^2 + 2a^2}} [a|1\rangle + (E_0 - E_2 - a)|2\rangle + a|3\rangle] \quad (66)$$

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

$$|\langle\psi_0'|\psi_0\rangle|^2 = \left[\frac{2a(E_0 - E_2 - a) + a^2}{(E_0 - E_2 - a)^2 + a^2} \right]^2 \quad (67)$$