

2022 Spring ECE606 - Homework 2 Solutions

Problem 1 (a)

$$\mu_{i-f} = \frac{2A}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{(n_{initial} + 1)\pi(x + L/2)}{L}\right) \cdot x \cdot \sin\left(\frac{(n_{final} + 1)\pi(x + L/2)}{L}\right) dx \quad (1)$$

Change the interval of integration and let $(n_{initial} + 1) = i$ and $(n_{final} + 1) = f$. The equation can be written as:

$$\mu_{i-f} = \frac{2A}{L} \int_0^L x \sin\left(\frac{f\pi x}{L}\right) \sin\left(\frac{i\pi x}{L}\right) dx \quad (2)$$

Calculate the integral by using the product-to-sum formulas:

$$\mu_{i-f} = \frac{A}{L} \left[\int_0^L x \cos\left(\frac{(f-i)\pi x}{L}\right) dx - \int_0^L x \cos\left(\frac{(i+f)\pi x}{L}\right) dx \right] \quad (3)$$

$$= \frac{A}{L} \left(\frac{L}{\pi}\right)^2 \left[\frac{1}{(f-i)^2} (\cos((f-i)\pi) - 1) - \frac{1}{(i+f)^2} (\cos((i+f)\pi) - 1) \right] \quad (4)$$

$$+ \frac{1}{(f-i)} \sin((f-i)\pi) - \frac{1}{(i+f)} \sin((i+f)\pi) \quad (5)$$

If i and f are both even or both odd integers then μ_{i-f} is 0. If i is an odd integer and f is an even integer or vice versa, we have

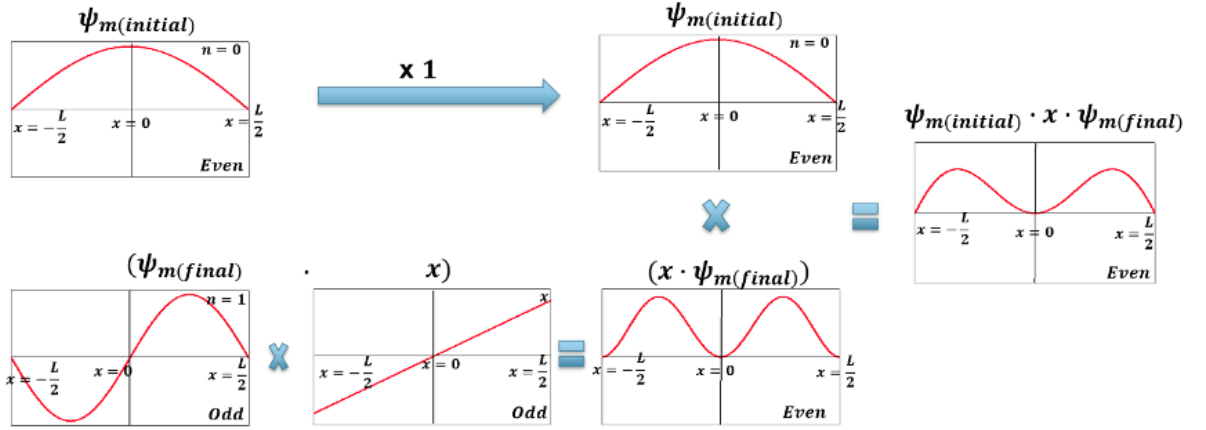
$$\mu_{i-f} = \frac{2AL}{\pi^2} \left[\frac{1}{(i+f)^2} - \frac{1}{(f-i)^2} \right] \quad (6)$$

$$\mu_{i-f} = \begin{cases} \frac{2AL}{\pi^2} \left[\frac{1}{(i+f)^2} - \frac{1}{(f-i)^2} \right] & \text{if } f-i = \text{odd} \\ 0 & \text{if } f-i = \text{even} \end{cases} \quad (7)$$

Problem 1 (b)

Let's consider the products of $\psi_i \cdot x \cdot \psi_f$ graphically. For $0 \rightarrow 1$:

$0 \Rightarrow 1$

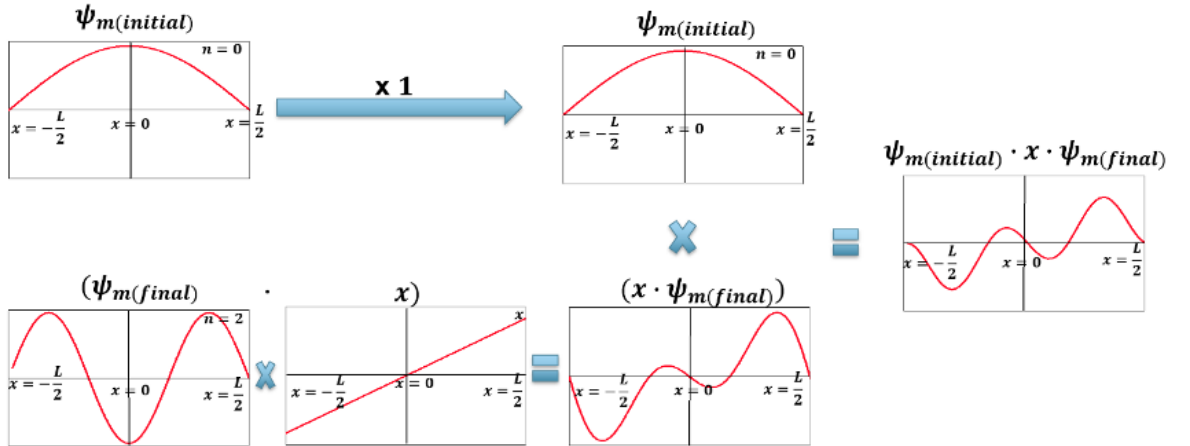


The $\psi_i(x)x\psi_f(x)$ is even, this means the integral does have a finite integral solution. Optical matrix elements have a finite value.

Let's consider symmetry about the $x = 0$ point. Three functions are multiplied inside the integral. The functions' symmetries are *even*, *odd*, and *odd* about the $x = 0$ point. Note here that the integral of functions of type (*even* $\times$ *odd* $\times$ *odd*) is an integral of a function of type (*even*), which results in a non-zero integral value.

For $0 \rightarrow 2$:

$0 \Rightarrow 2$



The $\psi_i(x)x\psi_f(x)$ is odd, this means the integral does have a finite integral solution. Optical matrix elements are zero in this case.

Let's consider again the symmetry about the $x = 0$ point. Three functions are multiplied inside the integral. The functions' symmetries are *even*, *odd*, and *even* about the $x = 0$ point. Note here that the integral of functions of type (*even* $\times$ *odd* $\times$ *even*) is an integral of a function of type *odd*, which results in a zero integral value.

Given that the optical matrix operator x is an *odd* function it can by symmetry only connect an *even* and an *odd* function, which means that the quantum number difference between the initial and final state ($f - i$) must be *odd* to obtain a non-zero matrix element by simple symmetry arguments.

Problem 1 (c)

The odd functions having integral values to be zero are called as forbidden transitions or “verboten”. The table summarizes the transitions. The U stands for upper transitions (higher final state), D stands for down transition (Lower final state). The “-” indicate that these transitions do not occur, which means they are forbidden.

I \ F	0	1	2	3	4	5	6	7
0	-	U	-	U	-	U	-	U
1	D	-	U	-	U	-	U	
2	-	D	-	U	-	U	-	U
3	D	-	D	-	U	-	U	-
4	-	D	-	D	-	U	-	U
5	D	--	D	-	D	-	U	-
6	-	D	-	D	-	D	-	U
7	D	-	D	-	D	-	D	-

Problem 2 (a)

Similar to problem 1 (a) but now we need to integrate over x , y , and z :

$$\mu_x = \frac{2A}{L_x} \int_{-\frac{L_x}{2}}^{\frac{L_x}{2}} \sin\left(\frac{(n_x^{initial} + 1)\pi(x + L_x/2)}{L_x}\right) \cdot x \cdot \sin\left(\frac{(n_x^{final} + 1)\pi(x + L_x/2)}{L_x}\right) dx \quad (8)$$

$$\cdot \frac{2}{L_y} \int_{-\frac{L_y}{2}}^{\frac{L_y}{2}} \sin\left(\frac{(n_y^{initial} + 1)\pi(y + L_y/2)}{L_y}\right) \sin\left(\frac{(n_y^{final} + 1)\pi(y + L_y/2)}{L_y}\right) dy \quad (9)$$

$$\cdot \frac{2}{L_z} \int_{-\frac{L_z}{2}}^{\frac{L_z}{2}} \sin\left(\frac{(n_z^{initial} + 1)\pi(z + L_z/2)}{L_z}\right) \sin\left(\frac{(n_z^{final} + 1)\pi(z + L_z/2)}{L_z}\right) dz \quad (10)$$

The last two terms in the integral can be combined together as a constant C_1 . Therefore, we have:

$$\mu_x = \frac{2AC_1}{L_x} \int_{-\frac{L_x}{2}}^{\frac{L_x}{2}} \sin\left(\frac{(n_x^{initial} + 1)\pi(x + L_x/2)}{L_x}\right) \cdot x \cdot \sin\left(\frac{(n_x^{final} + 1)\pi(x + L_x/2)}{L_x}\right) dx \quad (11)$$

Similarly we can change the interval of integration and let $(n_x^{initial} + 1) = i_x$ and $(n_x^{final} + 1) = f_x$. If i_x and f_x are both even or both odd integers then μ_x is 0. If i_x is an odd integer and f_x is an even integer or vice versa, μ_x is a finite integral:

$$\mu_x = \frac{2AC_1 L_x}{\pi^2} \left[\frac{1}{(i_x + f_x)^2} - \frac{1}{(f_x - i_x)^2} \right] \quad (12)$$

We can get the expressions for μ_y and μ_z in the same fashion. If i_y (or i_z) and f_y (or f_z) are both even or both odd integers then $\mu_y = 0$ and $\mu_z = 0$. If i_y (or i_z) is an odd integer and f_y (or f_z) is an even integer or vice versa, we have:

$$\mu_y = \frac{2AC_2L_y}{\pi^2} \left[\frac{1}{(i_y + f_y)^2} - \frac{1}{(f_y - i_y)^2} \right] \quad (13)$$

$$\mu_z = \frac{2AC_3L_z}{\pi^2} \left[\frac{1}{(i_z + f_z)^2} - \frac{1}{(f_z - i_z)^2} \right] \quad (14)$$

where C_2 and C_3 are just a constant, and $(n_y^{initial} + 1) = i_y$, $(n_z^{initial} + 1) = i_z$, $(n_y^{final} + 1) = f_y$, and $(n_z^{final} + 1) = f_z$.

Problem 2 (b)

$$E_{n_x, n_y, n_z} = \frac{\pi^2 \hbar^2}{2m^*} \left[\left(\frac{n_x}{L_x} \right)^2 + \left(\frac{n_y}{L_y} \right)^2 + \left(\frac{n_z}{L_z} \right)^2 \right] \quad (15)$$

$$n_x, n_y, n_z = 1, 2, 3 \dots \quad (16)$$

$$E_{n_x, n_y, n_z} = \frac{\pi^2 \hbar^2}{2m^*} \left[\left(\frac{n_x}{6L_z} \right)^2 + \left(\frac{n_y}{4L_z} \right)^2 + \left(\frac{n_z}{L_z} \right)^2 \right] = \frac{\pi^2 \hbar^2}{2m^* L_z} \left(\frac{n_x^2}{36} + \frac{n_y^2}{16} + \frac{n_z^2}{1} \right) \quad (17)$$

$$\Delta E_{f-i} = E_{n_{x,f}, n_{y,f}, n_{z,f}} - E_{n_{x,i}, n_{y,i}, n_{z,i}} = E_{norm} \left[\frac{n_{x,f}^2 - n_{x,i}^2}{36} + \frac{n_{y,f}^2 - n_{y,i}^2}{16} + (n_{z,f}^2 - n_{z,i}^2) \right] \quad (18)$$

The energy cost to raise an x -quantum number change is 36 times lower than a z -quantum number change. x excitations are a factor of $36/6 = 2.25$ lower cost than y excitations.

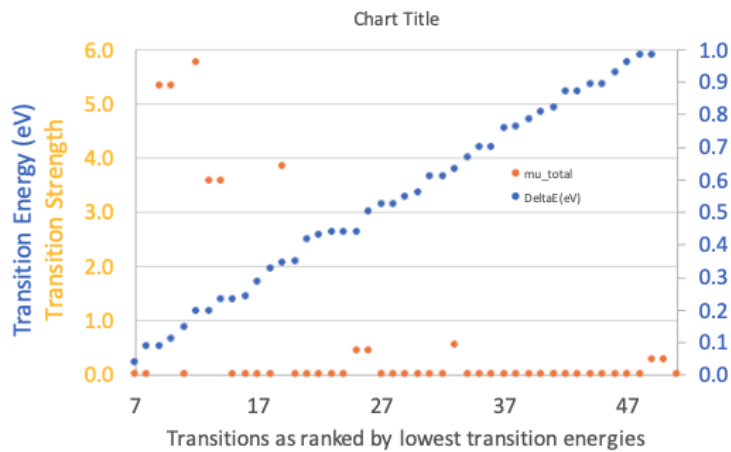
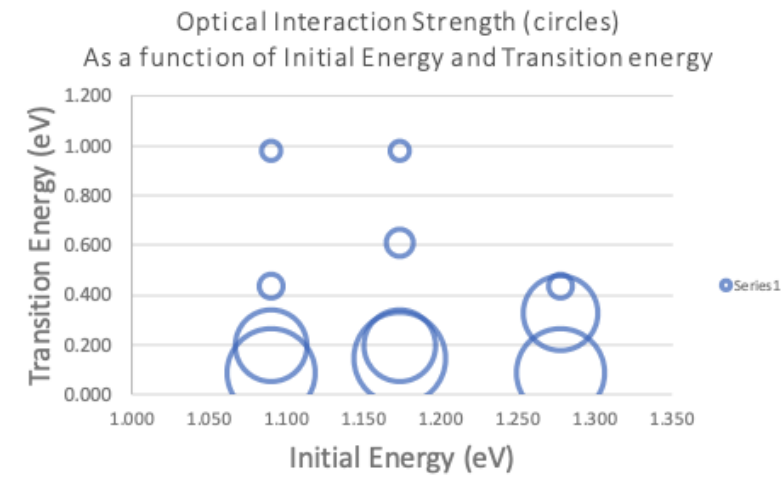
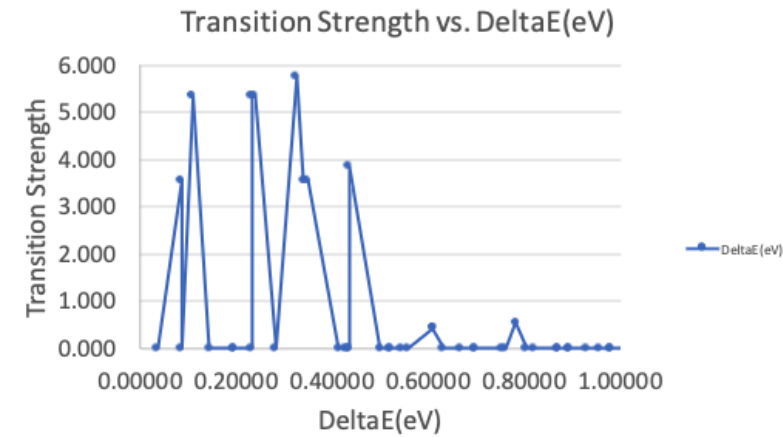
Problem 2 (c)

Ei (allowed)	deltaE (allowed)	mu_x+mu_y+mu_z	nx _i	ny _i	nz _i	nx _f	ny _f	nz _f
0	0	0	0	1	0	2	0	0
1.09027778	0.08703952	5.33335333	0	0	0	1	0	0
1.27777778	0.08703952	5.33335333	0	1	0	1	1	0
0	0	0	1	0	0	0	1	0
1.17361111	0.14506587	5.76002	1	0	0	2	0	0
1.09027778	0.19583892	3.55557556	0	0	0	0	1	0
1.17361111	0.19583892	3.55557556	1	0	0	1	1	0
0	0	0	0	0	0	2	0	0
0	0	0	0	1	0	2	1	0
0	0	0	0	1	0	3	0	0
0	0	0	0	0	0	1	1	0
1.27777778	0.32639821	3.84002	0	1	0	0	2	0
0	0	0	1	0	0	2	1	0
0	0	0	1	0	0	3	0	0
0	0	0	0	1	0	1	2	0
0	0	0	0	0	0	2	1	0
0	0	0	1	0	0	0	2	0
1.09027778	0.43519761	0.42668667	0	0	0	3	0	0
1.27777778	0.43519761	0.42668667	0	1	0	3	1	0
0	0	0	0	1	0	4	0	0
0	0	0	0	0	0	0	2	0
0	0	0	1	0	0	1	2	0
0	0	0	1	0	0	3	1	0
0	0	0	0	1	0	2	2	0
0	0	0	0	0	0	1	2	0
1.17361111	0.60927665	0.54423769	1	0	0	4	0	0
0	0	0	0	0	0	3	1	0
0	0	0	1	0	0	2	2	0
0	0	0	0	0	0	4	0	0
0	0	0	0	1	0	4	1	0
0	0	0	0	0	0	2	2	0
0	0	0	0	1	0	3	2	0
0	0	0	0	1	0	0	3	0
0	0	0	1	0	0	4	1	0
0	0	0	0	1	0	5	0	0
0	0	0	0	1	0	1	3	0
0	0	0	1	0	0	3	2	0
0	0	0	1	0	0	0	3	0
0	0	0	0	0	0	4	1	0
0	0	0	1	0	0	5	0	0
0	0	0	0	0	0	3	2	0
1.09027778	0.97919462	0.28446444	0	0	0	0	3	0
1.17361111	0.97919462	0.28446444	1	0	0	1	3	0

total transitions in considered energy range	Allowed optical matrix elements for considered transitions (1200 total)	Total allowed optical matrix elements in considered energy range
43	34	11

Even for this small system thousands of possible transitions exist (1,200). Only 43 are in the energy range of interest ($43/1200 = 3.6\%$). Only $34/1200 = 2.8\%$ are allowed for the considered transitions. Therefore, only $11/1200 = 0.9\%$ are allowed and in the energy range.

Optical absorptions can happen at the peaks where transition strength = 1.



Problem 2 (d)

Classes of optical matrix elements that are zero in value are so by underlying symmetry of the wavefunction and the operator. Problem 1b visualizes this. The physical operator "x" cannot be changed conceptually, as it represents the oscillating electric field.

However, the wavefunction symmetry of say the $n = 0$ and $n = 1$ states can be changed by the confinement. In the most simple case here we consider a FLAT potential well at the bottom of the quantum well. What if the the potential were tilted in the x direction, say lower on the left than the right? The wavefunctions would be distorted and be "leaning" more to the left and therefore breaking the perfect left/right symmetry of the system.

What are the physical effects that can lead to such a potential distortion:

- 1) an electrostatic potential
 - imposed by an external gate
 - or some external charge sheets (confined by other heterostructures)
- 2) a strain field that is created by dissimilar materials in a heterostructure
- 3) Crystal symmetry that is not perfectly left/right symmetric in the quantum well

Problem 3 (a)

$$\mu_z = \frac{2A}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{(n_i + 1)\pi(z + L/2)}{L}\right) \cdot z \cdot \sin\left(\frac{(n_f + 1)\pi(z + L/2)}{L}\right) dz \quad (19)$$

$$\cdot \int_{-\infty}^{\infty} \exp(ik_{x,f}x) \cdot \exp(-ik_{x,i}x) dx \cdot \int_{-\infty}^{\infty} \exp(ik_{y,f}y) \cdot \exp(-ik_{y,i}y) dy \quad (20)$$

$$= \frac{2A}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{(n_i + 1)\pi(z + L/2)}{L}\right) \cdot z \cdot \sin\left(\frac{(n_f + 1)\pi(z + L/2)}{L}\right) dz \quad (21)$$

$$\cdot \int_{-\infty}^{\infty} \exp(i(k_{x,f} - k_{x,i})x) dx \cdot \int_{-\infty}^{\infty} \exp(i(k_{y,f} - k_{y,i})y) dy \quad (22)$$

We know that

$$\delta(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(ikx) dx \quad (23)$$

so the exponential integration term can be written as:

$$\int_{-\infty}^{\infty} \exp(i(k_{x,f} - k_{x,i})x) dx \cdot \int_{-\infty}^{\infty} \exp(i(k_{y,f} - k_{y,i})y) dy = 4\pi^2 \delta(k_{x,f} - k_{x,i}) \cdot \delta(k_{y,f} - k_{y,i}) \quad (24)$$

According to problem 1 (a), we can easily know the final expression of μ_z :

$$\mu_z = \frac{2AL}{\pi^2} \left[\frac{1}{(n_i + n_f + 2)^2} - \frac{1}{(n_f - n_i)^2} \right] 4\pi^2 \delta(k_{x,f} - k_{x,i}) \delta(k_{y,f} - k_{y,i}) \quad (25)$$

$$= 8AL \left[\frac{1}{(n_i + n_f + 2)^2} - \frac{1}{(n_f - n_i)^2} \right] \delta(k_{x,f} - k_{x,i}) \delta(k_{y,f} - k_{y,i}) \quad (26)$$

If n_i is an odd integer and n_f is an even integer or vice versa. If n_i and n_f are both even or both odd integers then $\mu_z = 0$. For μ_x and μ_y :

$$\mu_x = \frac{2A}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{(n_i+1)\pi(z+L/2)}{L}\right) \cdot \sin\left(\frac{(n_f+1)\pi(z+L/2)}{L}\right) dz \quad (27)$$

$$\cdot \int_{-\infty}^{\infty} \exp(ik_{x,f}x) \cdot x \cdot \exp(-ik_{x,i}x) dx \cdot \int_{-\infty}^{\infty} \exp(ik_{y,f}y) \cdot \exp(-ik_{y,i}y) dy = 0 \quad (28)$$

and

$$\mu_y = \frac{2A}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{(n_i+1)\pi(z+L/2)}{L}\right) \cdot \sin\left(\frac{(n_f+1)\pi(z+L/2)}{L}\right) dz \quad (29)$$

$$\cdot \int_{-\infty}^{\infty} \exp(ik_{x,f}x) \cdot \exp(-ik_{x,i}x) dx \cdot \int_{-\infty}^{\infty} \exp(ik_{y,f}y) \cdot y \cdot \exp(-ik_{y,i}y) dy = 0 \quad (30)$$

since we can assume $k_f = k_i$

$$\int_{-\infty}^{\infty} \exp(ik_fx) \cdot x \cdot \exp(-ik_ix) dx = \int_{-\infty}^{\infty} x dx = 0 \quad (31)$$

Problem 3 (b)

The technical implication is that there is NO light absorption or emission in the z direction, since the electric field is either in the x or the y direction and the matrix elements are zero. This is a serious challenge for planar devices to get them to emit or detect light. The light has to be "turned" through diffractive methods. Quantum dots on the other hand can absorb and emit light in any direction due to their 3D properties.

Problem 3 (c) Bonus

Propagating wave is normalized to a nominal volume

$$\psi(x) = \frac{1}{\sqrt{L}} e^{ikx} \quad (32)$$

for arbitrary L , that is

$$\int_{-L/2}^{L/2} |\psi(x)|^2 dx \equiv 1 \quad (33)$$

optical matrix elements with

$$\begin{aligned} \psi_i(x) &= \frac{1}{\sqrt{L}} e^{ik_i x} \\ \psi_f(x) &= \frac{1}{\sqrt{L}} e^{ik_f x} \end{aligned} \quad (34)$$

is expressed as

$$\begin{aligned}
\mu_x &= \int_{-L/2}^{L/2} dx \psi_i(x) x \psi_f^*(x) \\
&= \int_{-L/2}^{L/2} dx x e^{i(k_i - k_f)x} \\
&= \int_{-L/2}^{L/2} dx x e^{i\Delta k x}
\end{aligned} \tag{35}$$

where $\Delta k = k_i - k_f$.
When $\Delta k = 0$,

$$\mu_x(\Delta k = 0) = \frac{1}{L} \int_{-L/2}^{L/2} dx x e^{0} = 0 \tag{36}$$

otherwise,

$$\begin{aligned}
\mu_x(\Delta k, L) &= \frac{1}{L} \int_{-L/2}^{L/2} dx x e^{i\Delta k x} \\
&= \frac{1}{L} \int_{-L/2}^{L/2} dx x (\cos(\Delta k x) + i \sin(\Delta k x)) \\
&= \frac{1}{L} \left[\int_{-L/2}^{L/2} dx x \cos(\Delta k x) + i \int_{-L/2}^{L/2} dx x \sin(\Delta k x) \right]
\end{aligned} \tag{37}$$

$x \cos(\Delta k x)$ is an odd function, and thus the integral equals 0. Solving the second integral using integration by parts by letting

$$\begin{aligned}
v &= x, dv = dx \\
du &= \sin(\Delta k x) dx, u = -\frac{1}{\Delta k} \cos(\Delta k x)
\end{aligned} \tag{38}$$

and

$$\begin{aligned}
\mu_x(\Delta k, L) &= \frac{i}{L} \int v du = \frac{i}{L} (uv - \int u dv) \\
&= \frac{i}{L} \left[\left[-x \frac{1}{\Delta k} \cos(\Delta k x) \right]_{-L/2}^{L/2} - \int_{-L/2}^{L/2} -\frac{1}{\Delta k} \cos(\Delta k x) dx \right] \\
&= \frac{i}{L} \left[-2 \frac{L}{2} \frac{1}{\Delta k} \cos(\Delta k \frac{L}{2}) + \left[\frac{1}{\Delta k^2} \sin(\Delta k x) \right]_{-L/2}^{L/2} \right] \\
&= \frac{i}{L} \left(\frac{L}{\Delta k} \cos(\Delta k \frac{L}{2}) - \frac{2}{\Delta k^2} \sin(\Delta k \frac{L}{2}) \right) \\
&= -\frac{i}{\Delta k} \cos(\Delta k \frac{L}{2}) + \frac{2i}{L \Delta k^2} \sin(\Delta k \frac{L}{2})
\end{aligned} \tag{39}$$

Let's explore the limits of the expression by assuming L being large and $\Delta k \rightarrow 0$ ($\Delta k = \frac{C}{L}$ as $C \rightarrow 0$), (39) becomes

$$\begin{aligned}
\mu &= -\frac{i}{\Delta k} \cos(\Delta k \frac{L}{2}) + \frac{2i}{L \Delta k^2} \sin(\Delta k \frac{L}{2}) \\
&= -\frac{iL}{C} \cos(\frac{C}{2}) + \frac{2iL}{C^2} \sin(\frac{C}{2})
\end{aligned} \tag{40}$$

Taylor Expand the trig functions for small C :

$$\begin{aligned}
\cos(\frac{C}{2}) &= 1 - \text{small} \\
\sin(\frac{C}{2}) &= \frac{C}{2} - \text{small}
\end{aligned} \tag{41}$$

and μ becomes

$$\mu = -\frac{iL}{C} \cdot 1 + \frac{2iL}{C^2} \cdot \frac{C}{2} = 0 \quad (42)$$

If we assume Δk to be finite, and let $L \rightarrow \infty$, (39) becomes

$$\begin{aligned} \mu &= -\frac{i}{\Delta k} \cos(\Delta k \frac{L}{2}) + \lim_{L \rightarrow \infty} \left(\frac{2i}{L \Delta k^2} \sin(\Delta k \frac{L}{2}) \right) \\ &= -\frac{i}{\Delta k} \cos(\Delta k \frac{L}{2}) + 0 \end{aligned} \quad (43)$$

μ is now a finite imaginary value.

Problem 4 (a)

The wavefunctions and eigen energies of a 1D infinite potential square well can be written as

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad (44)$$

$$E_n = \frac{\hbar^2 k_n^2}{2m^*} \quad (45)$$

where $k_n = n\pi/L$. So the first 10 eigen energies are ($\frac{\hbar^2 \pi^2}{2m_0} = 0.376 \text{ eV nm}^2$)

$$E_1 = \frac{\hbar^2 \pi^2}{2m_0} \frac{1}{m_e L^2} \approx 0.376 \frac{1}{0.067 \times 10^2} = 0.05612 \text{ eV} \quad (46)$$

$$E_2 = E_1 \times 2^2 = 0.2245 \text{ eV} \quad (47)$$

$$E_3 = E_1 \times 3^2 = 0.5051 \text{ eV} \quad (48)$$

$$E_4 = E_1 \times 4^2 = 0.8979 \text{ eV} \quad (49)$$

$$E_5 = E_1 \times 5^2 = 1.403 \text{ eV} \quad (50)$$

$$E_6 = E_1 \times 6^2 = 2.0203 \text{ eV} \quad (51)$$

$$E_7 = E_1 \times 7^2 = 2.75 \text{ eV} \quad (52)$$

$$E_8 = E_1 \times 8^2 = 3.5917 \text{ eV} \quad (53)$$

$$E_9 = E_1 \times 9^2 = 4.5457 \text{ eV} \quad (54)$$

$$E_{10} = E_1 \times 10^2 = 5.612 \text{ eV} \quad (55)$$

Problem 4 (b)

There are three wavefunctions confined in the well. The corresponding eigen energies are 0.03578 eV, 0.1402 eV, and 0.2996 eV.

Problem 4 (c)

The ground (lowest) confined state energies of 0.1 eV, 0.2 eV, 0.4 eV, 0.8 eV, 1.6 eV, and 3.2 eV are 0.0246 eV, 0.0305 eV, 0.0358 eV, 0.0403 eV, 0.0439 eV, and 0.0468 eV respectively.

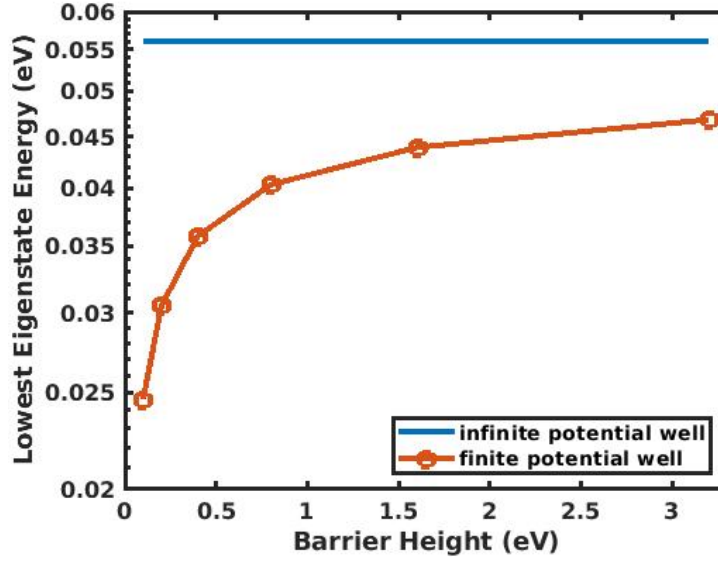


Figure 1: Lowest eigenstate energy vs Barrier height

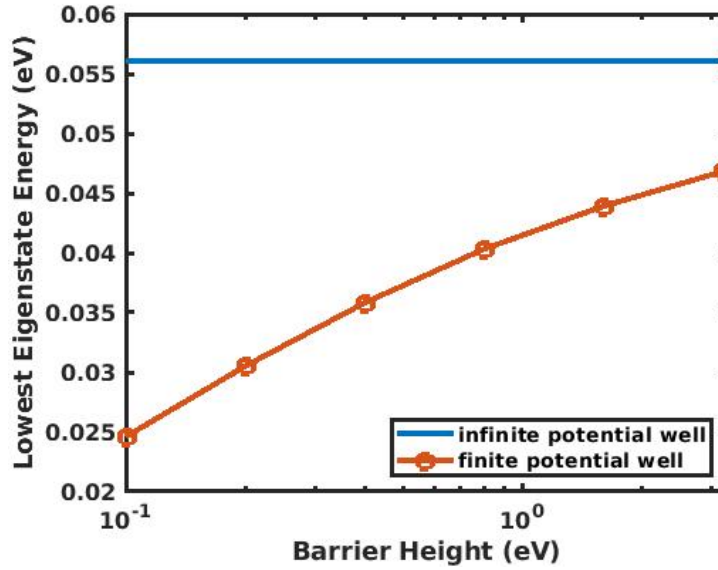


Figure 2: Lowest eigenstate energy vs Barrier height (Semi-log scale)

Because of the confinement effect, the lowest eigenstate energy is increasing as the total potential barrier becomes higher. In the semi-log scale plot, the overall trend remains the same - ground state energy is getting higher while the barrier is increasing.

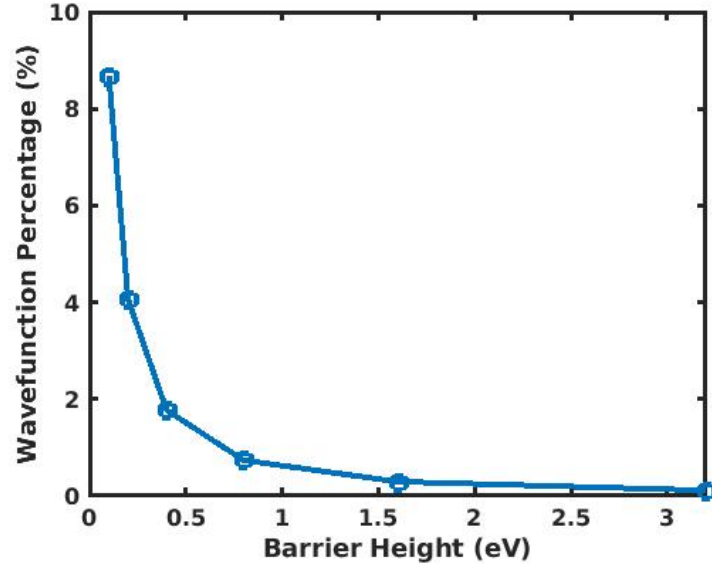


Figure 3: Wavefunction Percentage vs Barrier height

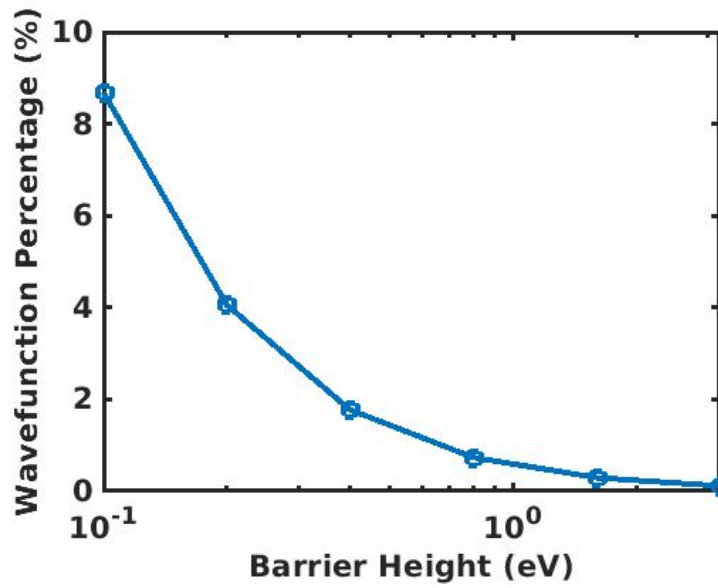
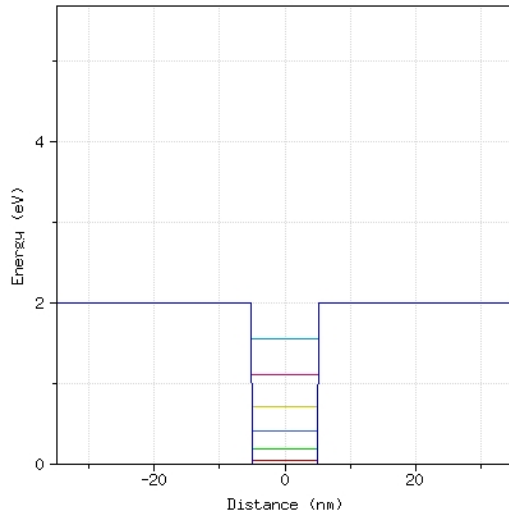


Figure 4: Wavefunction Percentage vs Barrier height (Semi-log scale)

Indeed, all the ground state wavefunctions are normalized to 1. The MATLAB code for the wavefunction integration is attached at the end of this file. Also, it's pretty straightforward that electron has lower chance to penetrate into higher potential barriers. Therefore, as can be seen in fig 4, the wavefunction percentage is getting smaller when the barrier height increases. Ultimately, the wavefunction percentage will be zero when the barrier height is infinite, which means electron is totally confined to the well. That's why the analytical expression is a sine function.

Problem 4 (d)

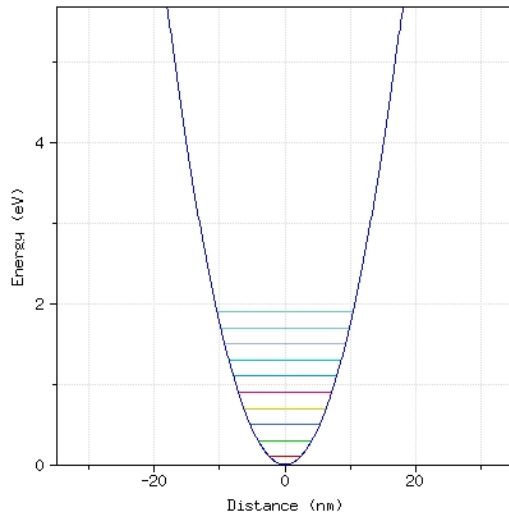


(a) PotentialvsDistance.jpg

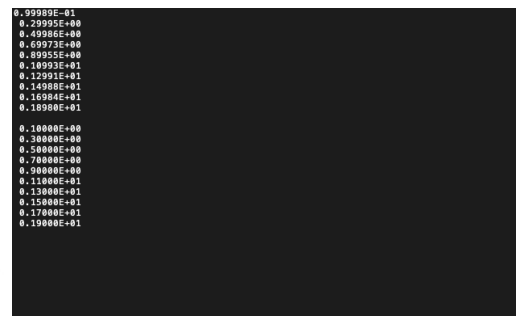


(b) energiestxt.txt

Figure 5: Square Well

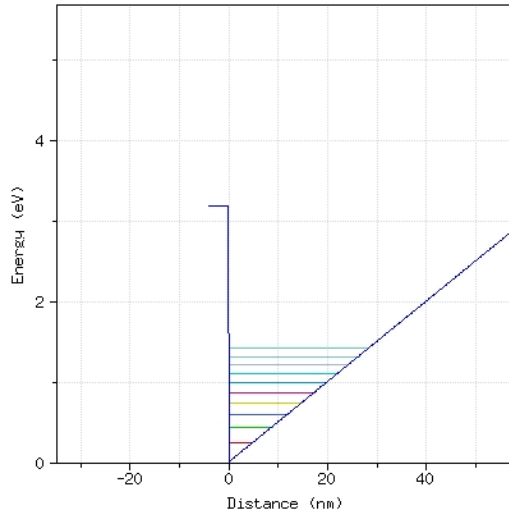


(a) PotentialvsDistance.jpg



(b) energiestxt.txt

Figure 6: Parabolic Well

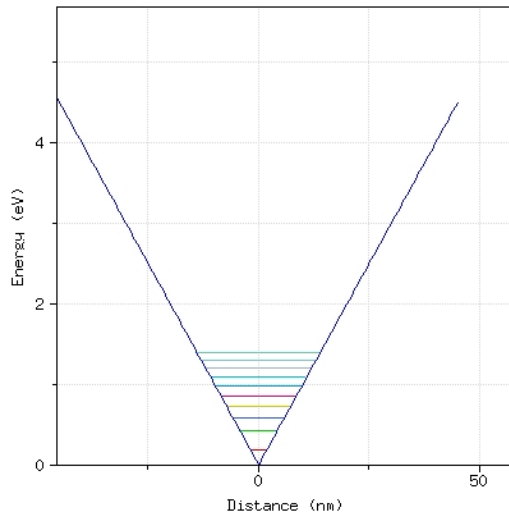


(a) PotentialvsDistance.jpg

```
0.24592E+00
0.44230E+00
0.60300E+00
0.74497E+00
0.87470E+00
0.99554E+00
0.11095E+01
0.12179E+01
0.13217E+01
0.14210E+01
0.20800E+00
0.45891E+00
0.62829E+00
0.76276E+00
0.89290E+00
0.10143E+01
0.11207E+01
0.12376E+01
0.13419E+01
0.14422E+01
```

(b) energiestxt.txt

Figure 7: Triangular Well



(a) PotentialvsDistance.jpg

```
0.18020E+00
0.45890E+00
0.57683E+00
0.72572E+00
0.85452E+00
0.97813E+00
0.10900E+01
0.12004E+01
0.13026E+01
0.14020E+01
```

(b) energiestxt.txt

Figure 8: V-Shaped Well

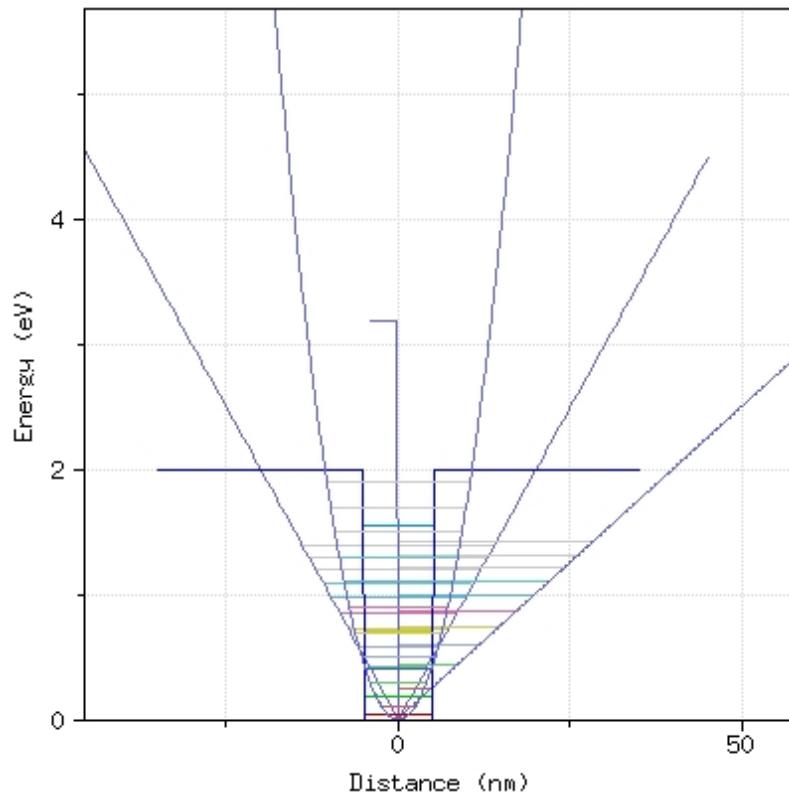


Figure 9: Potential vs. Distance (all)

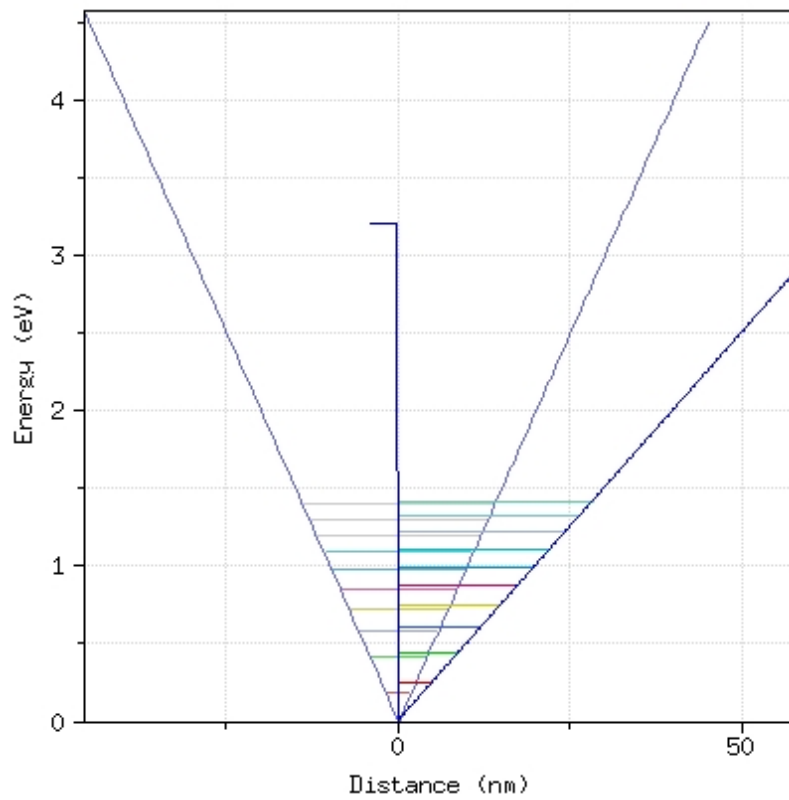


Figure 10: Potential vs. Distance (Triangular and V-Shaped)

Both the triangular potential well and the V-shaped well have 10 eigenstates. But electron has lower degree of freedom to move in the Triangular well (the confinement effect is stronger), so all

the eigenstate energies are slightly higher than the ones of the V-shaped well.

Problem 4 (e)

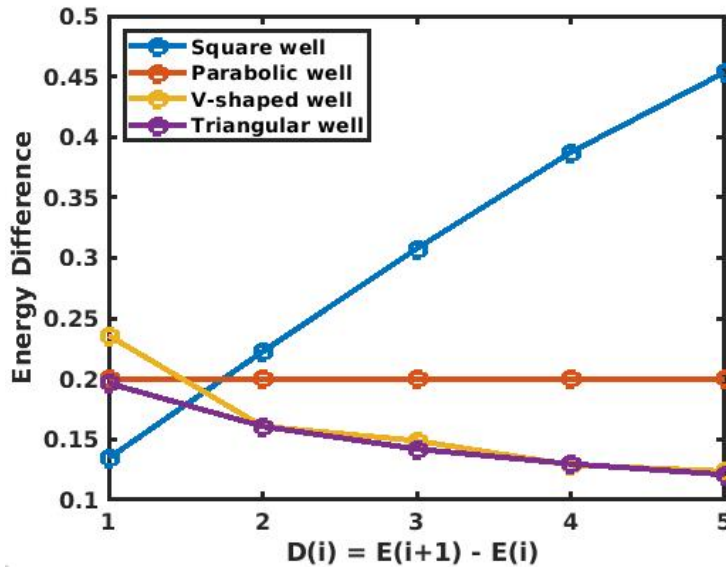


Figure 11: Energy Difference Comparison

For the parabolic case, the energy separations between two consecutive levels are identical. However, the energy differences of square well become larger and larger as the index i increases, and the ones of V-shaped well and triangular well have a similar trend - decreasing with higher i .

MATLAB Code

```
clear all

barrier_height = [0.1, 0.2, 0.4, 0.8, 1.6, 3.2];
lowest_eigen_energy = [0.0246, 0.0305, 0.0358, 0.0403, 0.0439, 0.0468];
lowest_eigen_energy_analytic = 0.05612;
%
FIG = figure(1)
hold on
set(gca,'FontWeight','bold','FontSize',16)
set(gca,'LineWidth',2)
xlabel('Barrier Height (eV)','FontWeight','bold','FontSize',16)
ylabel('Lowest Eigenstate Energy (eV)','FontWeight','bold','FontSize',16)
xt=get(gca, 'XTick');
set(gca, 'FontSize', 12)
plot(barrier_height,lowest_eigen_energy_analytic*ones(size(barrier_height)),'LineWidth',3)
plot(barrier_height,lowest_eigen_energy,'-o','LineWidth',3,'MarkerSize',8)
%set(gca,'YScale','log')
legend('infinite potential well','finite potential well','Location','southeast')
xlim([0 3.3])
ylim([0.02 0.06])
box on
hold off
%}
%
wvsq_in_barrier = [];
```

```

for ii = 1:1:6
    load_name = append('magsqrd_wavefunction_vs_distancetxt_', num2str(barrier_height(ii)), '.txt')
    wvsq_vs_dist = load(load_name);
    [num_x num_e] = size(wvsq_vs_dist);
    dx = abs(wvsq_vs_dist(1,1) - wvsq_vs_dist(num_x,1))/(num_x - 1);

    probability = 0;
    wvsqr_in_barrier_sum = 0;
    for xi = 1:1:num_x
        probability = probability + wvsq_vs_dist(xi,2)*dx;
        if (wvsq_vs_dist(xi,1) < -5 || wvsq_vs_dist(xi,1) > 5)
            wvsqr_in_barrier_sum = wvsqr_in_barrier_sum + wvsq_vs_dist(xi,2)*dx;
        end

    end
    probability
    wvsqr_in_barrier_sum
    wvsq_in_barrier = [wvsq_in_barrier, wvsqr_in_barrier_sum];

end
wvsq_in_barrier = wvsq_in_barrier*100;

FIG = figure(2)
hold on
set(gca, 'FontWeight', 'bold', 'FontSize', 16)
set(gca, 'LineWidth', 2)
xlabel('Barrier Height (eV)', 'FontWeight', 'bold', 'FontSize', 16)
ylabel('Wavefunction Percentage (%)', 'FontWeight', 'bold', 'FontSize', 16)
xt=get(gca, 'XTick');
%set(gca, 'FontSize', 12)
plot(barrier_height, wvsq_in_barrier, '-o', 'LineWidth', 3, 'MarkerSize', 8)
set(gca, 'YScale', 'log')
ylim([0 1e1])
box on
hold off
%}

eigen_sq = load('energiestxt_sq.txt');
eigen_para = load('energiestxt_para.txt');
eigen_tri = load('energiestxt_tri.txt');
eigen_v = load('energiestxt_v.txt');

diff_sq = [];
diff_para = [];
diff_tri = [];
diff_v = [];
for ii = 1:1:5
    diff_sq = [diff_sq, eigen_sq(ii+1,1)-eigen_sq(ii,1)];
    diff_para = [diff_para, eigen_para(ii+1,1)-eigen_para(ii,1)];
    diff_tri = [diff_tri, eigen_tri(ii+1,1)-eigen_tri(ii,1)];
    diff_v = [diff_v, eigen_v(ii+1,1)-eigen_v(ii,1)];
end

diff = linspace(1,5,5);
FIG = figure(3)
hold on
set(gca, 'FontWeight', 'bold', 'FontSize', 16)
set(gca, 'LineWidth', 2)

```

```

xlabel('D(i) = E(i+1) - E(i) ', 'FontWeight', 'bold', 'FontSize', 16)
ylabel('Energy Difference', 'FontWeight', 'bold', 'FontSize', 16)
xt=get(gca, 'XTick');
set(gca, 'FontSize', 12)
plot(diff, diff_sq, '-o', 'LineWidth', 3, 'MarkerSize', 8)
plot(diff, diff_para, '-o', 'LineWidth', 3, 'MarkerSize', 8)
plot(diff, diff_v, '-o', 'LineWidth', 3, 'MarkerSize', 8)
plot(diff, diff_tri, '-o', 'LineWidth', 3, 'MarkerSize', 8)
legend('Square well', 'Parabolic well', 'V-shaped well', 'Triangular well', 'Location', 'northwest')
box on
hold off
%}

```