Winter 2011- EE482

Solutions to HW1:

1(a): 1ev is the energy gained by an electron falling through a 1V potential difference. 1Joule is the energy gained by a 1C charge accelerated through a 1V potential difference.

$$\Rightarrow 2ev = 2\times(1.6\times10^{-19})CV = 3.2\times10^{-19}J$$

1(b):

$$m_{electron} = 9.1\times10^{-31}kg$$

$$q = 1.6\times10^{-19}C$$

$$E = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mE}$$

$$p = \frac{h}{\lambda} \Rightarrow \lambda = \frac{h}{p}$$

(i):

$$E = 0.04ev \Rightarrow p = \sqrt{2\times9.1\times10^{-31}\times0.04\times1.6\times10^{-19}} = 1.08\times10^{-25}$$

$$\lambda = \frac{(6.63\times10^{-34})}{1.08\times10^{-25}} = 6.14nm$$

(ii):

$$E = hf \Rightarrow f = \frac{1.2\times1.6\times10^{-19}}{6.63\times10^{-34}} = 2.9\times10^{14}Hz$$

$$C = f\lambda \Rightarrow \lambda = \frac{C}{f} = \frac{3\times10^{8}ms^{-1}}{2.9\times10^{14}s^{-1}} = 1.03\times10^{-6}m = 1.03\mu m$$

(iii):

$$145grams = 0.145kg$$

$$Momentum = mv = 0.145\times45 = 6.525kgms^{-1}$$

$$\lambda = \frac{h}{p} = \frac{6.63\times10^{-34}}{6.525} = 1.02\times10^{-34}m$$

2(a): For a particle in a 1-D infinite well, the Schrödinger equation is:

$$\frac{\partial^2\psi}{\partial x^2}+\frac{2mE}{\hbar^2}\psi(x)=0$$

-We know that $\psi(x)$ would be of the form of:

$$\psi(x)=A_1\cos kx+A_2\sin kx$$

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

-We also know that @ x=0 and x=a, $\psi(x)$=0 (This is boundary condition)

$$\psi(0)=0\Rightarrow A_1=0$$

$$\psi(a)=0\Rightarrow A_2\sin ka=0\Rightarrow ka=n\pi$$

-Using the fact that the probability of finding an electron in the well is 1,

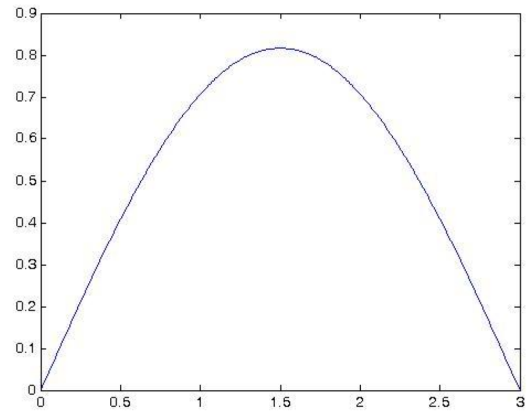
$$\int_0^a\psi^2(x)dx=1=A_2^{\,2}\int_0^a\sin^2 kxdx=1$$

$$A_2=\pm\sqrt{\frac{2}{a}}$$

(The sign of A_2 has no physical meaning)

Therefore, $\psi(x)=\sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$.

n=1: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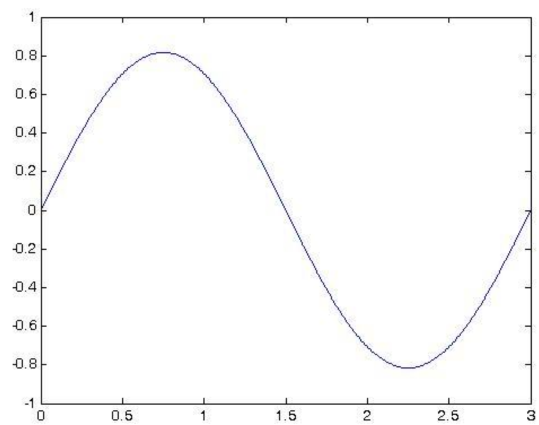
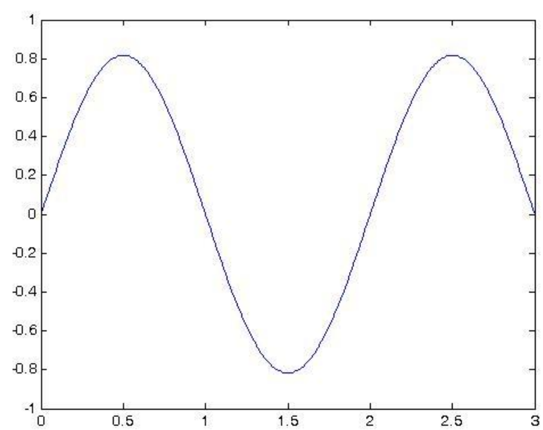
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.5
1
1.5
2
2.5
3

n=2:


1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
0.5
1
1.5
2
2.5
3

n=3:


1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
0.5
1
1.5
2
2.5
3

2(a) Expected value of x:

$$\langle X\rangle = \int_0^a \psi^*(x)\psi(x)x dx = \int_0^a \left[\sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})\right]^2 x dx = \frac{a}{2}$$

This makes sense. We would expect the "average" position to be in the middle.

Expected value of p:

$$\langle P\rangle = \int_0^a \psi^*(x)\frac{\hbar}{j}\frac{\partial}{\partial x}\psi(x)dx$$

$$= \frac{\hbar}{j}\frac{2}{a}\int_0^a \sin(\frac{n\pi x}{a})\frac{\partial \sin(\frac{n\pi x}{a})}{\partial x}dx$$

$$= \frac{\hbar}{j}\frac{2n\pi}{a^2}\int_0^a \sin(\frac{n\pi x}{a})\cos(\frac{n\pi x}{a})dx = 0$$

Makes sense, too! It is a closed system.

Energy: $E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2(\frac{n\pi}{a})^2}{2m}$

Substituting values:

$$E_1 = \frac{3.76\times10^{-19}}{a^2}ev$$

$$E_2 = \frac{1.5\times10^{-18}}{a^2}ev$$

$$E_3 = \frac{3.38\times10^{-18}}{a^2}ev$$

2(b): Given that:

$$\langle \Delta X\rangle = \sqrt{\langle X^2\rangle - \langle X\rangle^2}$$

$$\langle \Delta P\rangle = \sqrt{\langle P^2\rangle - \langle P\rangle^2}$$

-From 2(a), we already know $\langle X\rangle$ and $\langle P\rangle$.

-Need to find $\langle X^2\rangle$ and $\langle P^2\rangle$ to get $\langle \Delta X\rangle$ and $\langle \Delta P\rangle$.

$$\langle X^2\rangle = \int_0^a \left[\sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})\right]^2 x^2 dx = \frac{2}{a}\left[\frac{x^3}{6} - \frac{x\cos(2kx)}{4k^2} - \frac{(-1+2k^2x^2)\sin(2kx)}{8k^3}\right]_0^a$$

$$= \frac{2}{a}\left[\frac{a^3}{6} - \frac{a}{4}\frac{a^2}{n^2\pi^2}\right] = \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}$$

2(b)

$$\left\langle P^2 \right\rangle = \int_0^a \psi^*(x) - \hbar^2 \frac{\partial^2}{\partial x^2}\psi(x)dx$$

$$= \frac{2k^2\hbar^2}{a}\int_0^a \sin^2(kx)dx$$

$$= \frac{2k^2\hbar^2}{a}\left[\frac{x}{2} - \frac{\sin 2kx}{4k}\right]_0^a$$

$$= \frac{n^2\pi^2\hbar^2}{a^2}$$

So,

$$\left\langle \Delta X \right\rangle = \sqrt{\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} - \frac{a^2}{4}}$$

$$\left\langle \Delta P \right\rangle = \sqrt{\frac{n^2\pi^2\hbar^2}{a^2} - 0} = \frac{n\pi\hbar}{a}$$

For n=1, $\left\langle \Delta X \right\rangle \left\langle \Delta P \right\rangle = 0.568\hbar > \frac{\hbar}{2}$

Uncertainty Principle holds.

3(a):

$$\frac{\partial E}{\partial kx} = 2Akx - 12Bkx^3 = 0 \Rightarrow kx = \begin{cases} 0 \\ \pm\sqrt{\frac{A}{6B}} \end{cases}$$

$$\frac{\partial E}{\partial ky} = 4Aky - 4Bky^3 = 0 \Rightarrow ky = \begin{cases} 0 \\ \pm\sqrt{\frac{A}{B}} \end{cases}$$

To find the max and min, we need to use the second derivative of E:

$$\frac{\partial^2 E}{\partial kx^2} = 2A - 36Bkx^2$$

$$\frac{\partial^2 E}{\partial ky^2} = 4A - 12Bky^2$$

$$\frac{\partial^2 E}{\partial kx \partial ky} = 0$$

Using the 2nd partial derivative test,

$$M = \frac{\partial^2 E}{\partial kx^2}\frac{\partial^2 E}{\partial ky^2} - \left(\frac{\partial^2 E}{\partial kx \partial ky}\right)^2$$

If M>0 and $\frac{\partial^2 E}{\partial kx^2}$ >0 $\rightarrow$ min.

If M>0 and $\frac{\partial^2 E}{\partial kx^2} < 0 \rightarrow$ max.
M<0 $\rightarrow$ saddle.
M=0 $\rightarrow$ inconclusive.

This gives:
(0,0) $\rightarrow$ local minima.
$(\pm\sqrt{\frac{A}{6B}}, \pm\sqrt{\frac{A}{B}}) \rightarrow$ local maxima.
$(0, \pm\sqrt{\frac{A}{B}})$ and $(\pm\sqrt{\frac{A}{6B}}, 0) \rightarrow$ saddle points.
Sketches can be done in Matlab or by hand.

3(b):

$$M^{-1} = \frac{1}{\hbar^2}\begin{bmatrix} \frac{\partial^2 E}{\partial kx^2} & \frac{\partial^2 E}{\partial kx \partial ky} \\ \frac{\partial^2 E}{\partial kx \partial ky} & \frac{\partial^2 E}{\partial ky^2} \end{bmatrix} = \frac{1}{\hbar^2}\begin{bmatrix} 2A - 36Bkx^2 & 0 \\ 0 & 4A - 12Bky^2 \end{bmatrix}$$

@ (0,0), $M^{-1} = \frac{1}{\hbar^2}\begin{bmatrix} 2A & 0 \\ 0 & 4A \end{bmatrix} \Rightarrow e^-$ (Positive effective mass)

@ $(\pm\sqrt{\frac{A}{6B}}, \pm\sqrt{\frac{A}{B}})$, $M^{-1} = \frac{1}{\hbar^2}\begin{bmatrix} -4A & 0 \\ 0 & -8A \end{bmatrix} \Rightarrow hole$ (Negative effective mass)

@ $(0, \pm\sqrt{\frac{A}{B}})$, $M^{-1} = \frac{1}{\hbar^2}\begin{bmatrix} 2A & 0 \\ 0 & -8A \end{bmatrix} \Rightarrow neither$

@ $(\pm\sqrt{\frac{A}{6B}}, 0)$, $M^{-1} = \frac{1}{\hbar^2}\begin{bmatrix} -4A & 0 \\ 0 & 4A \end{bmatrix} \Rightarrow neither$

3(c):

k= (0,0), F=[1,1]

$$\vec{a} = M^{-1}\vec{F} = \frac{1}{\hbar^2}\begin{bmatrix} 2A & 0 \\ 0 & 4A \end{bmatrix}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{2A}{\hbar^2}\begin{bmatrix} 1 \\ 2 \end{bmatrix} \leftarrow \text{direction}$$

3(d):

$$k = \left(\pm\sqrt{\frac{A}{6B}}, \pm\sqrt{\frac{A}{B}}\right)$$

$$\vec{a} = M^{-1}\vec{F} = \frac{1}{\hbar^2}\begin{bmatrix} -4A & 0 \\ 0 & -8A \end{bmatrix}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{-4A}{\hbar^2}\begin{bmatrix} 1 \\ 2 \end{bmatrix}$$