Project3

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A) Xichen Li: I worked on project-3 all independently.

Consider a 1-D problem with potential energy:

$$U(x) = \begin{cases} \infty & for \quad x < 0 \\ \infty & for \quad x > L \\ 0 & for \quad 0 < x < L \end{cases}$$

The eigenfunction corresponding to quantum number n is, $\psi_n = A_n sin(\frac{n\pi}{L}x)$, where A_n is the normalization constant. Find the expectation value of the position operator for an electron in the state:

- (i) ψ_2
- (ii) $(\frac{3}{\sqrt{2}}\psi_1 - \frac{3}{\sqrt{2}}\psi_2 + 4\psi_3)/5$ at $t = 0$
- (iii) Recalculate (ii) by including the time dependent part of the wave function. Derive an expression. Plot this as a function of time.
- (iv) By using the mass of the particle is $9.1 * 10^{-31} kg$ and the length of the box is 3nm, plot the expectation value of position as a function of time.

Answer

- **(i)** At t=0, the expectation of the position is:

$$< x >= \int_0^L A_2 sin(\frac{2\pi}{L}x) x A_2 sin(\frac{2\pi}{L}x)\, dx$$

Where $A_n = \sqrt{\frac{2}{L}}$. And this integraal can be calculated using trigonometruc identity:

$$< x >= \frac{2}{L}\int_0^L \frac{x}{2}\, dx + \frac{2}{L}\int_0^L \frac{-x}{2} cos(\frac{4\pi x}{L})\, dx$$

The second term is equal to zero and $< x >= \frac{L}{2}$

- **(ii)** At t=0, the expectation of the position is:

$$< x >= \int_0^L A_n(\frac{3}{5\sqrt{2}} sin(\frac{\pi}{L}x) - \frac{3}{5\sqrt{2}} sin(\frac{2\pi}{L}x) + \frac{4}{5} sin(\frac{3\pi}{L}x)) x A_n(\frac{3}{5\sqrt{2}} sin(\frac{\pi}{L}x) - \frac{3}{5\sqrt{2}} sin(\frac{2\pi}{L}x) + \frac{4}{5} sin(\frac{3\pi}{L}x))\, dx$$

$$< x >= \frac{2}{L}\int_0^L x[\frac{9}{50} sin^2(\frac{\pi}{L}x) + \frac{9}{50} sin^2(\frac{2\pi}{L}x) + \frac{16}{25} sin^2(\frac{3\pi}{L}x) - \frac{18}{50} sin(\frac{\pi}{L}x) sin(\frac{2\pi}{L}x) + \frac{24}{25\sqrt{2}} sin(\frac{\pi}{L}x) sin(\frac{3\pi}{L}x)$$

$$- \frac{24}{25\sqrt{2}} sin(\frac{2\pi}{L}x) sin(\frac{3\pi}{L}x)]\, dx$$

$$< x >= \frac{L}{2}\frac{9}{50} + \frac{L}{2}\frac{9}{50} + \frac{L}{2}\frac{16}{25} + a + 0 + b \approx 0.697L$$

- **(iii)** Include the time dependent part, the expression becomes:

$$< x >= \int_0^L A_n(e^{\frac{iE_1 t}{\hbar}} \frac{3}{5\sqrt{2}} sin(\frac{\pi}{L}x) - e^{\frac{iE_2 t}{\hbar}} \frac{3}{5\sqrt{2}} sin(\frac{2\pi}{L}x) + e^{\frac{iE_3 t}{\hbar}} \frac{4}{5} sin(\frac{3\pi}{L}x)) x A_n(e^{\frac{-iE_1 t}{\hbar}} \frac{3}{5\sqrt{2}} sin(\frac{\pi}{L}x) - e^{\frac{-iE_2 t}{\hbar}} \frac{3}{5\sqrt{2}} sin(\frac{2\pi}{L}x)$$

$$+ e^{\frac{-iE_3 t}{\hbar}} \frac{4}{5} sin(\frac{3\pi}{L}x))\, dx$$

Where $E_n = \frac{\hbar^2}{2m}(\frac{n\pi}{L})^2$ As we can see from the expression which include some additional cosine term for each interference between the three eigenfunctions.
Use the code below to calculate the expression of $< x >$ as a function of time. A normalized mass and charge and $\hbar$ are used in the code below for part (iii).

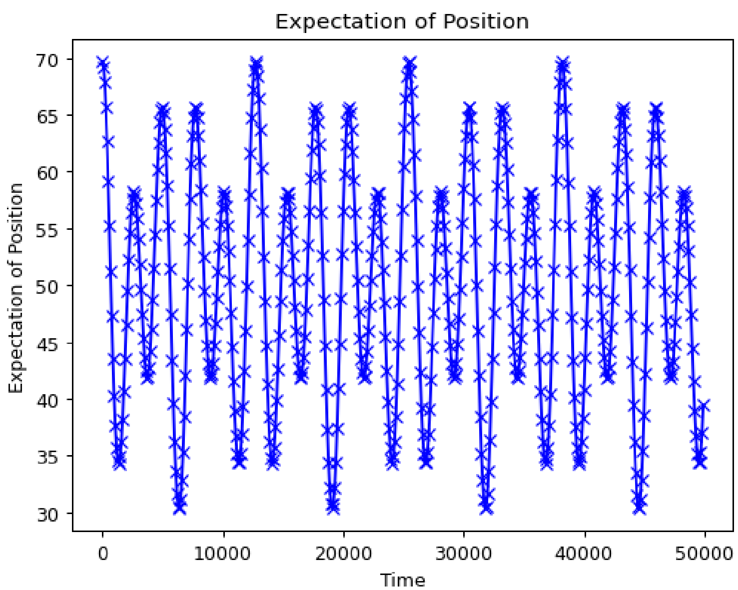
In [113]:
```
import numpy as np
#import numpy.pi as pi
%matplotlib notebook
import matplotlib.pyplot as plt
import scipy.integrate as spi

eta = 1
m = 1
q = 1
L=100
T0=50e3
dt=100
```

In [114]:
```
#t = np.linspace(0,T0,num=N)
#t=0
E1=eta**2/(2*m)*(np.pi/L)**2
E2=eta**2/(2*m)*(2*np.pi/L)**2
E3=eta**2/(2*m)*(3*np.pi/L)**2
An=np.sqrt(2/L)
x0 = 0
x1 = L

x_avg=[]
tr=np.arange(0,T0,dt)
for t in tr:
    integrand = lambda x : An*(3/(5*np.sqrt(2))*np.exp(1j*E1*t/eta)*np.sin(np.pi/L*x)-3/(5*np.sqrt(2))*np.exp(1j*E2*t/eta)*np.sin(2*np.pi/L*x)+
        4/(5)*np.exp(1j*E3*t/eta)*np.sin(3*np.pi/L*x))*x*An*(3/(5*np.sqrt(2))*np.exp(-1j*E1*t/eta)*np.sin(np.pi/L*x)
        -3/(5*np.sqrt(2))*np.exp(-1j*E2*t/eta)*np.sin(2*np.pi/L*x)+4/(5)*np.exp(-1j*E3*t/eta)*np.sin(3*np.pi/L*x))
    result, error = spi.quad(integrand, x0, x1)
    x_avg=x_avg+[result]

print(x_avg[0])
```

```
69.69014298960704
```

In [115]:
```
plt.figure()
plt.plot(tr, x_avg, color='b', ls='-', marker='x')
plt.title('Expectation of Position')
plt.xlabel('Time')
plt.ylabel('Expectation of Position')
```

Figure 1



Out[115]: Text(0, 0.5, 'Expectation of Position')

- (iv) By using the mass of the particle is $9.1 * 10^{-31} kg$ and the length of the box is 3nm, plot the expectation value of position as a function of time.

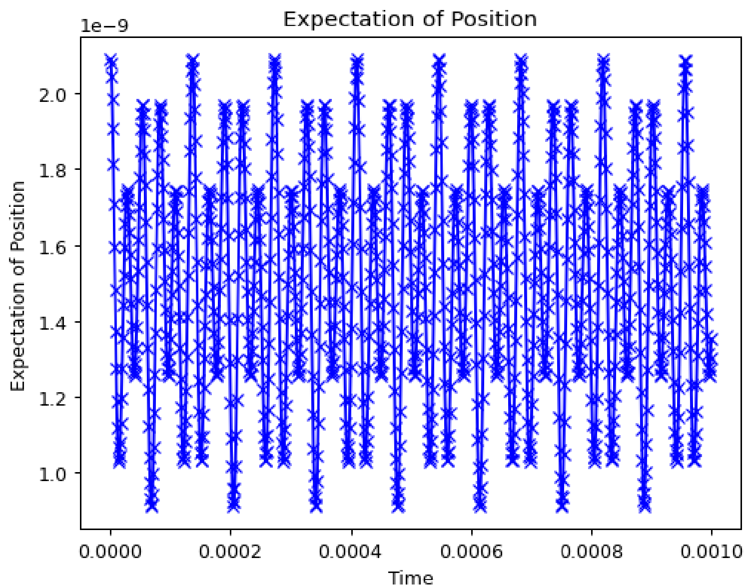
In [116]:

```
eta = 6.63e-34/2/np.pi #Reduced Plank constant in eV.s
m = 9.11e-31   #Assuming the particle mass is equal to a free electron
q = 1.6e-19
L=3e-9
T0=1e-3
dt=1e-6

#t = np.linspace(0,T0,num=N)
#t=0
E1=eta**2/(2*m)*(np.pi/L)**2
E2=eta**2/(2*m)*(2*np.pi/L)**2
E3=eta**2/(2*m)*(3*np.pi/L)**2
An=np.sqrt(2/L)
x0 = 0
x1 = L

x_avg=[]
tr=np.arange(0,T0,dt)
for t in tr:
    integrand = lambda x : An*(3/(5*np.sqrt(2))*np.exp(1j*E1*t/eta)*np.sin(np.pi/L*x)-3/(5*np.sqrt(2))*np.exp(1j*E2*t/eta)*np.sin(2*np.pi/L*x)+
        4/(5)*np.exp(1j*E3*t/eta)*np.sin(3*np.pi/L*x))*x*An*(3/(5*np.sqrt(2))*np.exp(-1j*E1*t/eta)*np.sin(np.pi/L*x)
        -3/(5*np.sqrt(2))*np.exp(-1j*E2*t/eta)*np.sin(2*np.pi/L*x)+4/(5)*np.exp(-1j*E3*t/eta)*np.sin(3*np.pi/L*x))
    result, error = spi.quad(integrand, x0, x1)
    x_avg=x_avg+[result]

print(x_avg[0])
```

```
2.090704289688212e-09
```

In [117]:
```
plt.figure()
plt.plot(tr, x_avg, color='b', ls='-', marker='x')
plt.title('Expectation of Position')
plt.xlabel('Time')
plt.ylabel('Expectation of Position')
```

Figure 2



Out[117]: Text(0, 0.5, 'Expectation of Position')

In [ ]:

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