# Physics 245 Homework #1

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**Problem 1.a.**

Since the given equation doesn't have a phase factor or anything, I will assume that the instantaneous velocity of the string at $t = 0$ is zero everywhere. Then we can decompose $y(x, 0)$ into a sum of sines and cosines:

$$y(x,0) = \sum_{n=0}^{\infty} \left( A_n \sin\left(\frac{n\pi x}{L}\right) + B_n \cos\left(\frac{n\pi x}{L}\right)\right).$$

The differential equation is linear, so we can solve the differential equation term by term, then put the terms back in the sum, to obtain

$$y(x,t) = \sum_{n=0}^{\infty} \left( A_n \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi v}{L} t + \varphi\right) + B_n \cos\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi v}{L} t + \phi\right)\right).$$

Because we assumed $\frac{\partial}{\partial t} y(x,t) = 0$, the phase factors $\varphi$ and $\phi$ must both be zero. Using our boundary condition that $y(0,t) = 0$ for all $t$, we also see that every $B_n$ must be zero. Lastly, $A_0$ may as well be zero because $\sin(0) = 0$. Now the equation can be simplified to

$$y(x,t) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi v}{L} t\right).$$

**Problem 1.b.**

The coefficients $A_n$ are given by the Fourier transform, which we can evaluate using integration by parts.

$$\begin{aligned}
A_n &= \frac{2}{L}\int_{x=0}^{L} \sin\left(\frac{n\pi x}{L}\right) y(x,0)\mathrm{d}x \\
&= \frac{2}{L}\int_{x=0}^{L/2} \sin\left(\frac{n\pi x}{L}\right) \frac{2xd}{L}\mathrm{d}x + \frac{2}{L}\int_{x=L/2}^{L} \sin\left(\frac{n\pi x}{L}\right) \frac{2d(L-x)}{L}\mathrm{d}x \\
&= \frac{2}{L}\left(\left[\frac{2xd}{L}\cdot\left(-\frac{L}{n\pi}\cos\left(\frac{n\pi x}{L}\right)\right)\right]_{x=0}^{L/2} - \int_{x=0}^{L/2}\frac{2d}{L}\cdot\left(-\frac{L}{n\pi}\cos\left(\frac{n\pi x}{L}\right)\right)\mathrm{d}x\right) + \frac{2}{L}\int_{x=L/2}^{L} \sin\left(\frac{n\pi x}{L}\right) \frac{2d(L-x)}{L}\mathrm{d}x \\
&= \frac{4d}{Ln\pi}\left(\left[-x\cos\left(\frac{n\pi x}{L}\right)\right]_{x=0}^{L/2} + \left[\frac{L}{n\pi}\sin\left(\frac{n\pi x}{L}\right)\right]_{x=0}^{L/2}\right) + \frac{2}{L}\int_{x=L/2}^{L} \sin\left(\frac{n\pi x}{L}\right) \frac{2d(L-x)}{L}\mathrm{d}x \\
&= \frac{4d}{Ln\pi}\left(\frac{L}{2}\cos\left(\frac{n\pi}{2}\right) + \frac{L}{n\pi}\sin\left(\frac{n\pi}{2}\right)\right) + \frac{4d}{L}\int_{x=L/2}^{L}\sin\left(\frac{n\pi x}{L}\right)\mathrm{d}x - \frac{4d}{L^2}\int_{x=L/2}^{L} x\sin\left(\frac{n\pi x}{L}\right)\mathrm{d}x \\
&= \frac{4d}{Ln\pi}\left(\frac{L}{2}\cos\left(\frac{n\pi}{2}\right) + \frac{L}{n\pi}\sin\left(\frac{n\pi}{2}\right)\right) + \frac{4d}{L}\left[-\frac{L}{n\pi}\cos\left(\frac{n\pi x}{L}\right)\right]_{x=L/2}^{L} - \frac{4d}{L^2}\int_{x=L/2}^{L} x\sin\left(\frac{n\pi x}{L}\right)\mathrm{d}x \\
&= \frac{4d}{Ln\pi}\left(\frac{L}{2}\cos\left(\frac{n\pi}{2}\right) + \frac{L}{n\pi}\sin\left(\frac{n\pi}{2}\right) - L\cos(n\pi) + L\cos\left(\frac{n\pi}{2}\right)\right) - \frac{4d}{L^2}\int_{x=L/2}^{L} x\sin\left(\frac{n\pi x}{L}\right)\mathrm{d}x \\
&= \frac{4d}{Ln\pi}\left(\frac{L}{2}\cos\left(\frac{n\pi}{2}\right) + \frac{L}{n\pi}\sin\left(\frac{n\pi}{2}\right) - L(-1)^n\right) + \frac{4d}{L^2}\left(\left[x\frac{L}{n\pi}\cos\left(\frac{n\pi x}{L}\right)\right]_{x=L/2}^{L} + \int_{x=L/2}^{L}\left(-\frac{L}{n\pi}\cos\left(\frac{n\pi x}{L}\right)\right)\mathrm{d}x\right) \\
&= \frac{4d}{Ln\pi}\left(\frac{L}{2}\cos\left(\frac{n\pi}{2}\right) + \frac{L}{n\pi}\sin\left(\frac{n\pi}{2}\right) - L(-1)^n + \left[x\cos\left(\frac{n\pi x}{L}\right)\right]_{x=L/2}^{L} + \int_{x=L/2}^{L}\left(-\cos\left(\frac{n\pi x}{L}\right)\right)\mathrm{d}x\right) \\
&= \frac{4d}{Ln\pi}\left(\frac{L}{2}\cos\left(\frac{n\pi}{2}\right) + \frac{L}{n\pi}\sin\left(\frac{n\pi}{2}\right) - L(-1)^n + L(-1)^n - \frac{L}{2}\cos\left(\frac{n\pi}{2}\right) + \left[-\frac{L}{n\pi}\sin\left(\frac{n\pi x}{L}\right)\right]_{x=L/2}^{L}\right) \\
&= \frac{4d}{Ln\pi}\cdot\frac{2L}{n\pi}\sin\left(\frac{n\pi}{2}\right) \\
&= \frac{8d}{n^2\pi^2}\sin\left(\frac{n\pi}{2}\right)
\end{aligned}$$

Therefore the first nonzero coefficients are

$$\begin{aligned}
A_1 &= \frac{8d}{\pi^2} \\
A_3 &= -\frac{8d}{9\pi^2} \\
A_5 &= \frac{8d}{25\pi^2}
\end{aligned}$$

**Problem 1.c.**

The differential equation is linear, so each vibrational mode will not affect other vibrational modes. That means if we approximate the formula given in part (a) with a partial sum, that approximation will be just as valid at a later time.

**Problem 3.a.**

$$
\begin{aligned}
M &= \frac{\Omega}{4i\hbar}\sigma_x \\
\exp(Mt) &= \sum_{n=0}^{\infty} \frac{1}{n!}(Mt)^n \\
&= \left( I_2 + \frac{M^2t^2}{2!} + \frac{M^4t^4}{4!} + \cdots \right) + \left( Mt + \frac{M^3t^3}{3!} + \frac{M^5t^5}{5!} + \cdots \right) \\
&= \left( \sum_{n=0}^{\infty} \frac{1}{(2n)!} \left( \frac{\Omega t}{4i\hbar} \right)^{2n} \right) I_2 + \left( \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \left( \frac{\Omega t}{4i\hbar} \right)^{2n+1} \right) \sigma_x \\
&= \left( \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \left( \frac{\Omega t}{4\hbar} \right)^{2n} \right) I_2 - \left( \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} \left( \frac{\Omega t}{4\hbar} \right)^{2n+1} \right) i\sigma_x \\
&= \cos\left( \frac{\Omega}{4\hbar} t \right) I_2 - i \sin\left( \frac{\Omega}{4\hbar} t \right) \sigma_x \\
&= \begin{bmatrix} \cos\left(\frac{\Omega}{4\hbar}t\right) & -i\sin\left(\frac{\Omega}{4\hbar}t\right) \\ -i\sin\left(\frac{\Omega}{4\hbar}t\right) & \cos\left(\frac{\Omega}{4\hbar}t\right) \end{bmatrix}
\end{aligned}
$$

If we suppose that initially, $a_1 = 1$ and $a_2 = 0$, then the state after time $t$ is the first column of $\exp(Mt)$. Otherwise, the state after time $t$ is the initial state left-multiplied by $\exp(Mt)$.

## Problem 4.a.

The spatial function for the $n$th state is given by

$$
\Psi_n = \sqrt{\frac{2}{L}} \sin\left( \frac{n\pi x}{L} \right), 0 \le x \le L.
$$

Since this function has reflectional symmetry (about $x = L/2$), the expected value $\langle x \rangle$ must be $L/2$, and $\langle p \rangle$ must be zero.

## Problem 4.b.

$$
\begin{aligned}
\sigma_x^2 &= \left\langle x^2 \right\rangle - \langle x \rangle^2 \\
&= \left( \int_{x=0}^{L} \Psi_n^* x^2 \Psi_n \mathrm{d}x \right) - \frac{L^2}{4} \\
&= \left( \frac{2}{L} \int_{x=0}^{L} x^2 \sin^2\left(\frac{n\pi x}{L}\right) \mathrm{d}x \right) - \frac{L^2}{4} \\
&= \left( \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2} \right) - \frac{L^2}{4} \\
&= \frac{L^2}{12} - \frac{L^2}{2n^2\pi^2} \\
\sigma_x = \sqrt{\sigma_x^2} &= L\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}} \\
\sigma_p^2 &= \int_{x=0}^{L} \Psi_n^* (p - \langle p \rangle)^2 \Psi_n \mathrm{d}x \\
&= \frac{2}{L} \int_{x=0}^{L} \sin\left(\frac{n\pi x}{L}\right) \left(-\hbar^2 \frac{\partial^2}{\partial x}\right) \sin\left(\frac{n\pi x}{L}\right) \mathrm{d}x \\
&= \frac{2n^2\pi^2\hbar^2}{L^3} \int_{x=0}^{L} \sin^2\left(\frac{n\pi x}{L}\right) \mathrm{d}x \\
&= \frac{n^2\pi^2\hbar^2}{L^2} \\
\sigma_p = \sqrt{\sigma_p^2} &= \frac{n\pi\hbar}{L}
\end{aligned}
$$

These answers are reasonable because they satisfy the Heisenberg uncertainty principle, and because $\sigma_x$ and $\sigma_p$ both increase as $n$ increases.

$$
\begin{aligned}
\sigma_x \sigma_p &= n\pi\hbar\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}} \\
&\geq \pi\hbar\sqrt{\frac{1}{12} - \frac{1}{2\pi^2}} \geq \hbar\sqrt{\frac{\pi^2}{12} - \frac{1}{2}} \geq \hbar\sqrt{\frac{9-6}{12}} \geq \frac{\hbar}{2}.
\end{aligned}
$$

## Problem 5.a.

This state, $\left|s = \frac{1}{2}, m_s = \frac{1}{2}\right\rangle$, is an eigenstate of $S^2$ (with eigenvalue $\hbar^2 s(s+1)$) and an eigenstate of $S_z$ (with eigenvalue $\hbar m_s = \frac{\hbar}{2}$). Therefore, the uncertainties in $S^2$ and in $S_z$ are both zero. Since $|\Psi_1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} |+X\rangle - \frac{1}{\sqrt{2}} |-X\rangle$, where $|+X\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $|-X\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ are the eigenvectors of $S_x$, $S_x$ has a one half chance of being measured as $\frac{\hbar}{2}$ (the eigenvalue of $|+X\rangle$) and a one half chance of being $-\frac{\hbar}{2}$ (the eigenvalue of $|-X\rangle$), so the uncertainty in $S_x$ is $\frac{\hbar}{2}$.

## Problem 5.b.

By the same logic as in part (a), the uncertainty in $S^2$ and in $S_x$ are zero, but since $S_z$ has a half chance each of being measured as positive and negative $\frac{\hbar}{2}$, the uncertainty in $S_z$ is $\frac{\hbar}{2}$.

# notebook

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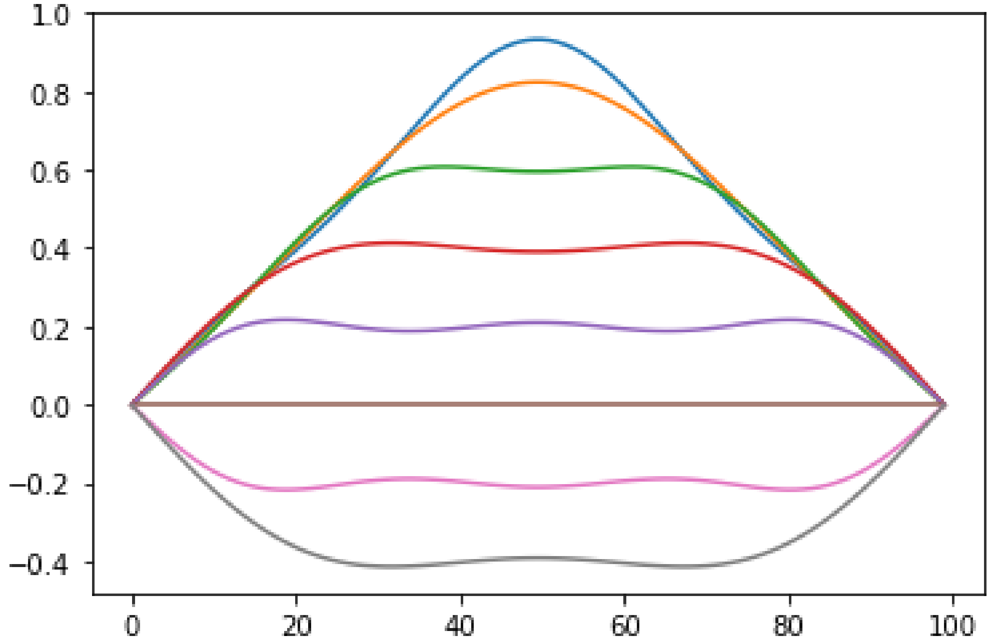
[1]:
```
# 1.b
import matplotlib.pyplot as plt
import numpy as np

L = 1
d = 1
v = 1
x = np.linspace(0, L, 100)

def y(x, t, A):
    sum = x*0
    for n in range(len(A)):
        sum += A[n] * np.sin(x * n * np.pi / L) * np.cos(n * np.pi * v * t / L)
    return sum

A = np.array([0, 1, 0, -1/9, 0, 1/25]) * 8 * d / np.pi**2

for t in [0, .1, .2, .3, .4, .5, .6, .7]:
    plt.plot(y(x, t, A))
plt.show()
```

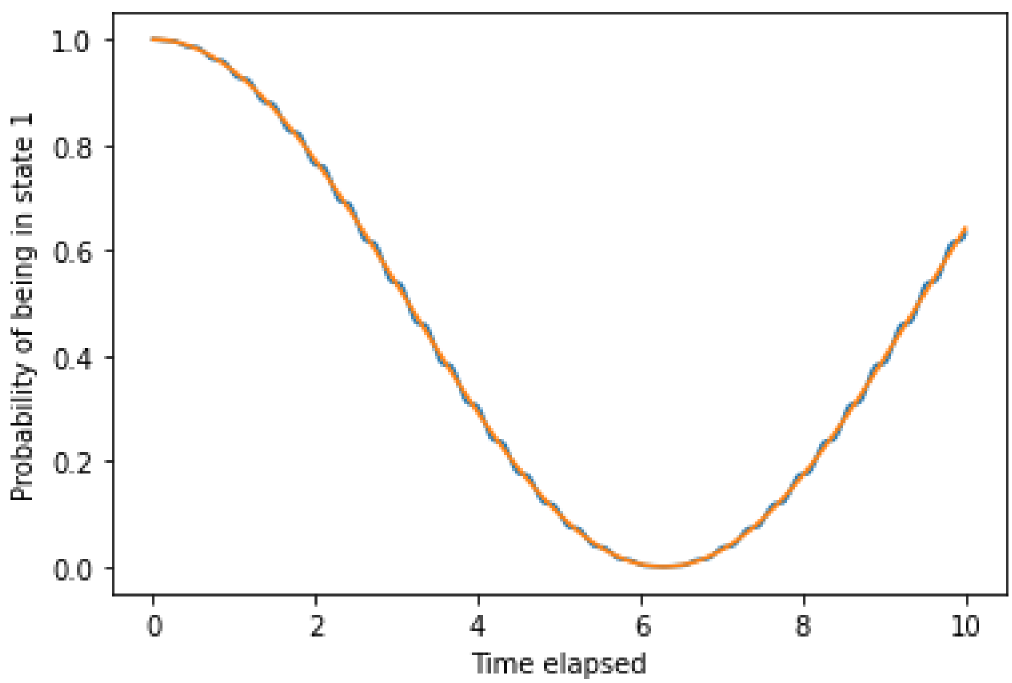



[2]:

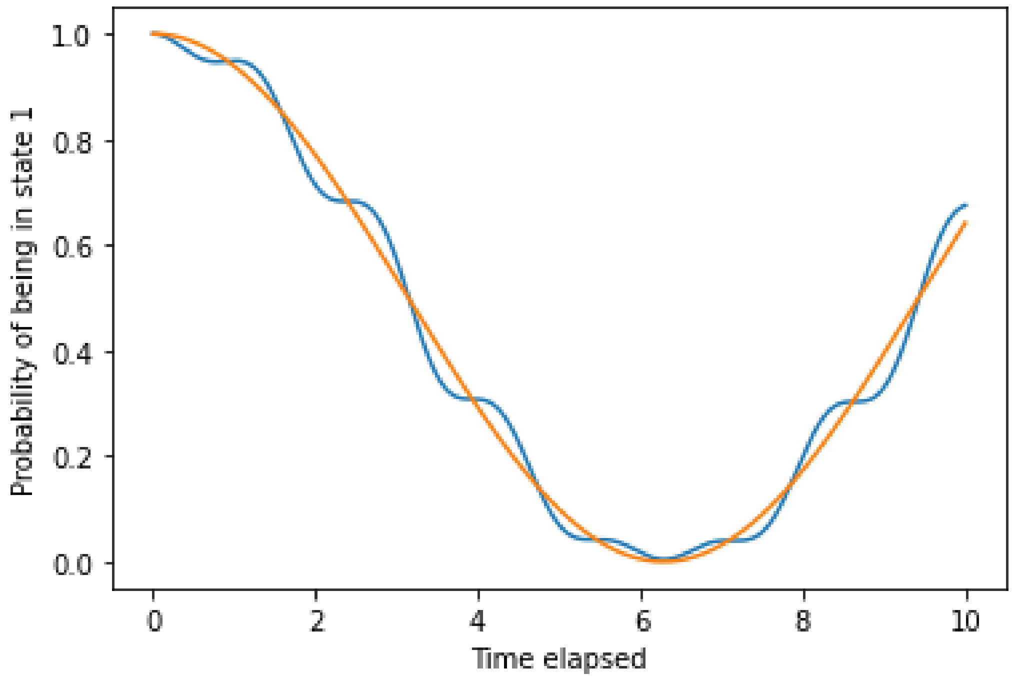
```
# 2 and 3
def plot(Omega_over_hbar, omega_1, time, time_step):
    state_1_probabilities = []
    a_1 = 1
    a_2 = 0
    times = np.arange(0, time, time_step)
    for t in times:
        # calculate derivatives
        d_1 = (Omega_over_hbar / 4) * a_2 * (1 + np.exp((0-2j) * t * omega_1)) /
 ↪ (0+1j)
        d_2 = (Omega_over_hbar / 4) * a_1 * (1 + np.exp((0+2j) * t * omega_1)) /
 ↪ (0+1j)
        a_1 += time_step * d_1
        a_2 += time_step * d_2
        t += time_step
        state_1_probabilities.append(np.abs(a_1) ** 2)
    plt.xlabel("Time elapsed")
    plt.ylabel("Probability of being in state 1")
    plt.plot(times, state_1_probabilities)
    plt.plot(times, np.cos(Omega_over_hbar * times / 4)**2)
    print(f"\n{Omega_over_hbar=} and {omega_1=}")
    print("The numerical solution is in blue and the rotating wave␣
 ↪approximation from question 3 is in orange.")
    plt.show()
```

```
time = 10
time_step = .001
plot(1, 10, time, time_step) # blue
plot(1, 2, time, time_step)  # orange
plot(2, 1, time, time_step)  # green

plt.show()
```

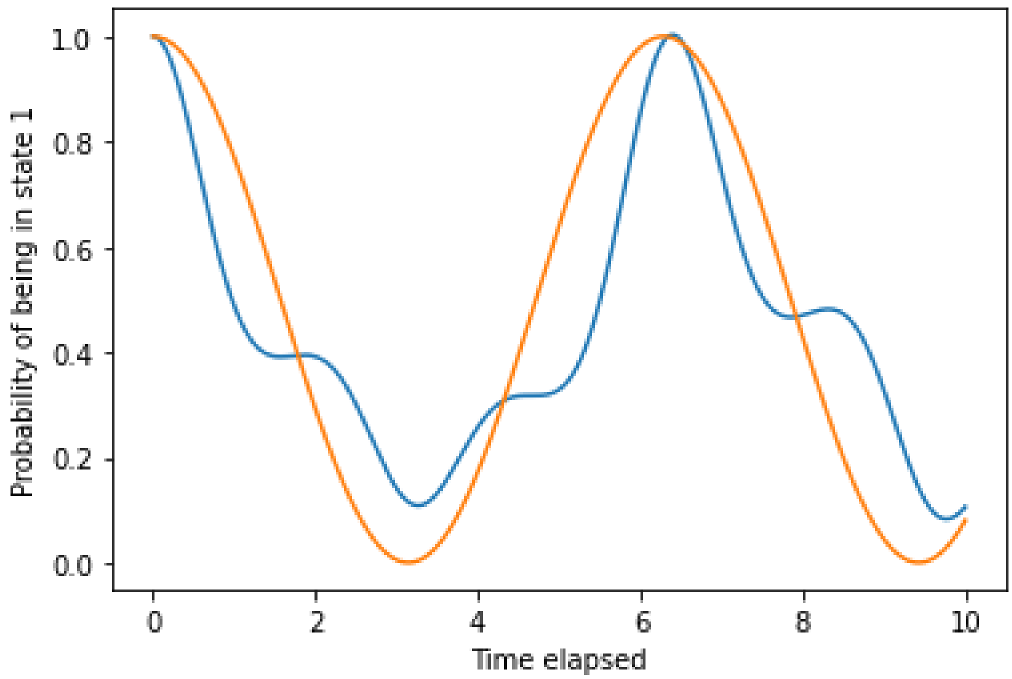
```
Omega_over_hbar=1 and omega_1=10
The numerical solution is in blue and the rotating wave approximation from
question 3 is in orange.
```




```
Omega_over_hbar=1 and omega_1=2
The numerical solution is in blue and the rotating wave approximation from
question 3 is in orange.
```




```
Omega_over_hbar=2 and omega_1=1
The numerical solution is in blue and the rotating wave approximation from
question 3 is in orange.
```



[3]:
```
!pip install qutip
```

```
Requirement already satisfied: qutip in
/home/nathan/anaconda3/lib/python3.9/site-packages (5.0.4)
Requirement already satisfied: packaging in
/home/nathan/anaconda3/lib/python3.9/site-packages (from qutip) (21.0)
Requirement already satisfied: scipy>=1.9 in
/home/nathan/anaconda3/lib/python3.9/site-packages (from qutip) (1.13.1)
Requirement already satisfied: numpy>=1.22 in
/home/nathan/anaconda3/lib/python3.9/site-packages (from qutip) (1.26.4)
Requirement already satisfied: pyparsing>=2.0.2 in
/home/nathan/anaconda3/lib/python3.9/site-packages (from packaging->qutip)
(3.0.4)
```

[4]:
```
# QUantum Toolbox In Python
import qutip as qt

def print_qobj(qutip_object):
    # Prints just the matrix data, without the other info
    assert isinstance(qt.sigmax(), qt.core.qobj.Qobj)
    print(qutip_object[:, :])
```

[5]:
```
# 6.a
# For convenience, assume hbar=1 throughout this course, so
# S = sigma / 2
S_x = qt.sigmax() / 2
S_y = qt.sigmay() / 2
S_z = qt.sigmaz() / 2
print_qobj(qt.sigmax())
print('\n')
print_qobj(qt.sigmay())
print('\n')
print_qobj(qt.sigmaz())
```

```
[[0.+0.j 1.+0.j]
 [1.+0.j 0.+0.j]]


[[0.+0.j 0.-1.j]
 [0.+1.j 0.+0.j]]


[[ 1.+0.j  0.+0.j]
 [ 0.+0.j -1.+0.j]]
```

[6]:
```
# 6.b
Psi_1 = qt.basis(2, 0)
print_qobj(Psi_1)
print('\n')
print(qt.expect(S_z, Psi_1))
```

```
[[1.+0.j]
 [0.+0.j]]


0.5
```

[7]:
```
# 6.c
Psi_2 = (qt.basis(2, 0) + qt.basis(2, 1)).unit()
print_qobj(Psi_2)
print('\n')
print(qt.expect(S_z, Psi_2))
```

```
[[0.70710678+0.j]
 [0.70710678+0.j]]


0.0
```

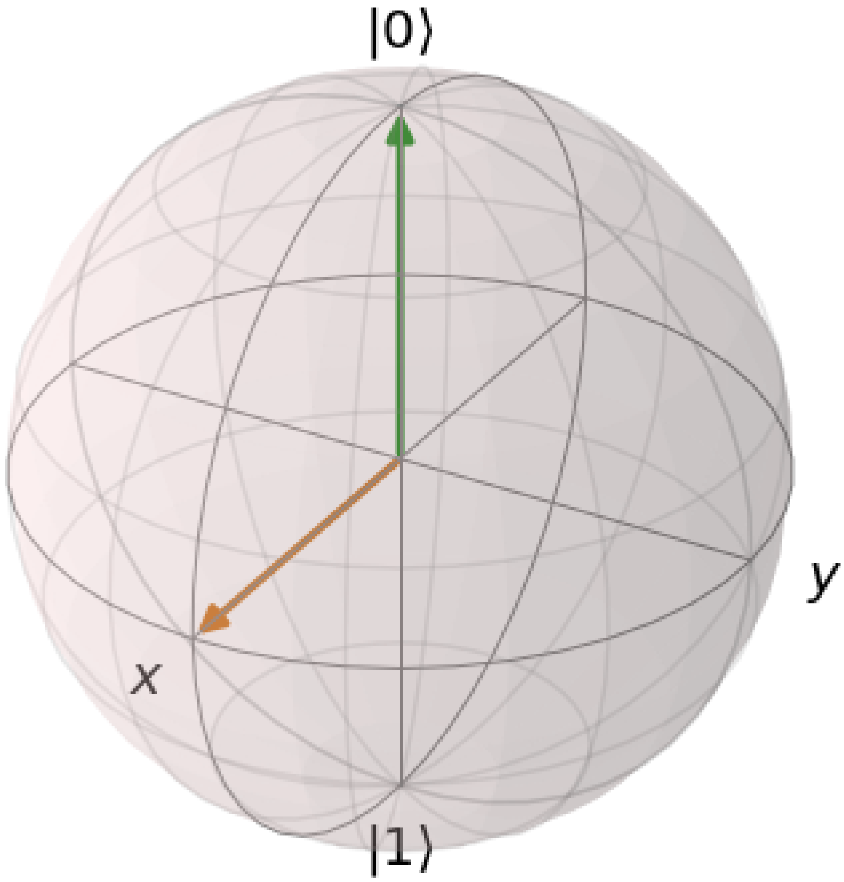
[8]:
```
# 6.d
def uncertainty(operator, state):
    return np.sqrt(qt.expect(operator * operator, state) - qt.expect(operator,␣
 ↪state) ** 2)

print(uncertainty(S_z, Psi_1))
```

```
0.0
```

[9]:
```
# 6.e
print(uncertainty(S_z, Psi_2))
```

```
0.49999999999999994
```

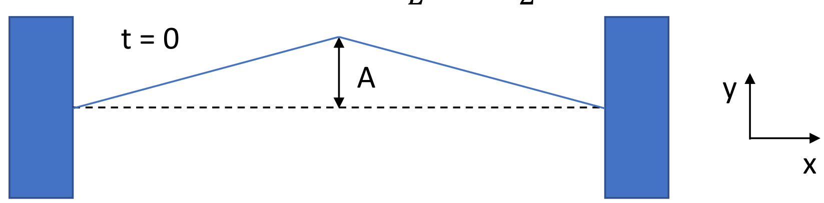
[10]:
```
# 6.f
b = qt.Bloch()
b.add_states(Psi_1) # plot in green
b.add_states(Psi_2) # plot in orange
b.show()
print("\n|+X> is Psi_2 because it is the eigenvector of S_x with eigenvalue +1.
 ↪")
```




```
|+X> is Psi_2 because it is the eigenvector of S_x with eigenvalue +1.
```

Phys 245 Quantum Computation
Homework 1

1. *[30] Quantization, basis sets, and so on aren't some uniquely quantum phenomena. They appear everywhere, as we'll see in this problem. Notice any similarities to the infinite square well?!* Suppose a string of length $L$ is stretched between two fixed endpoints (think guitar string). The classical wave equation that describes the strings vertical displacement, y, as a function of horizontal displacement, x, is:
$$\frac{\partial^2 y(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}$$
where $v$ is the speed of sound along the string.
   a. [10] Show that a general solution for a standing wave is:
$$y(x,t) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{n\pi v}{L}t\right),$$
   where the $A_n$ are constants that depend on the initial condition.
   b. [15] Suppose at t = 0 a string is plucked by pulling it's midpoint away from equilibrium by a distance $d$ and then releasing it, such that:
$$y(x,0) = \begin{cases} \dfrac{2dx}{L}, & 0 \le x \le \dfrac{L}{2} \\ \dfrac{2d(L-x)}{L}, & \dfrac{L}{2} \le x \le L \end{cases}$$




   Find the first three $A_n$ and use them to approximate $y(x,t)$. Plot $y(x,t)$ for a few times to show the evolution.
   c. [5] In words explain why we are able to use the expression in (a) to predict the behavior in (b).

2. *[30] Understanding the RWA.* In lecture, we studied an infinite 1D square well ($V = 0$ for $0 \le x \le L$ and infinite otherwise) that was perturbed by
$$V'(x,t) = \Omega\cos\left(\frac{\pi x}{L}\right)\cos\omega_1 t,$$
where $\hbar\omega_1 = E_2 - E_1$. Here, $E_n = \hbar^2 n^2\pi^2/(2mL^2)$ is the energy of the $n$th quantum state, $m$ is the particle mass, and $L$ is the width of the well. During this derivation, we found a set of equations for the evolution of the amplitudes in n = 1 ($a_1$) and n = 2 ($a_2$) as:
$$\frac{\Omega}{4}a_2(t)(1+e^{-2\imath\omega_1 t}) = \imath\hbar\dot{a}_1(t)$$
$$\frac{\Omega}{4}a_1(t)(1+e^{2\imath\omega_1 t}) = \imath\hbar\dot{a}_2(t)$$
which we approximated as

$$\frac{\Omega}{4}a_2(t) = \imath\hbar\dot{a}_1(t)$$
$$\frac{\Omega}{4}a_1(t) = \imath\hbar\dot{a}_2(t)$$

The reason for this approximation is that the exponential term oscillates quickly between positive and negative values and if $\omega_1 \gg \Omega$ then the term has no effect on the dynamics. As you'll learn, we make this approximation all of the time in the QST when dealing with time-dependent Hamiltonians and for historical reasons it is called the Rotating Wave Approximation or just the RWA. Let's see how good of an approximation this is. In this problem, use your favorite numerical integration tool (e.g. Mathematica or Python) to numerically solve the differential equations above and compare there results. Do the solution for the following parameters:

a.) [10] $\Omega/\hbar = 1$ and $\omega_1 = 10$.
b.) [10] $\Omega/\hbar = 1$ and $\omega_1 = 2$.
c.) [10] $\Omega/\hbar = 2$ and $\omega_1 = 1$.

3. *[20] Embracing the matrix exponential!* Continuing in the same situation as in problem 2 and as we discussed in class, our system of equations after the RWA equation was:

$$\frac{\Omega}{4}a_2(t) = \imath\hbar\dot{a}_1(t)$$
$$\frac{\Omega}{4}a_1(t) = \imath\hbar\dot{a}_2(t)$$

Can be written in matrix form as:

$$\dot{\vec{a}} = M\vec{a}$$

with

$$M = \begin{pmatrix} 0 & -\imath\frac{\Omega}{4\hbar} \\ -\imath\frac{\Omega}{4\hbar} & 0 \end{pmatrix}$$

As we'll see this quarter, and you've likely seen before, whenever $M$ is a constant matrix, as it is here, the solution of the differential equation is simply:

$$\vec{a}(t) = e^{Mt}\vec{a}(t=0)$$

where

$$e^{Mt} = \sum_{n=0}^{\infty}\frac{1}{n!}(Mt)^n$$

is the matrix exponential of $Mt$.

a.) [10] Find an analytic expression for $\vec{a}(t)$ by computing the matrix exponential. Hint: writing $M$ in terms of Pauli matrices can be useful.
b.) [10] Use the expression you found in 3(a) for the parameters of 2(a) and compare to the evolution you found from the two approaches (i.e plot them together).

4. *[20] Uncertainty principles in action.* For a particle trapped in a normal infinite square well, calculate:

a. [10] The expectation value of the position and momentum for the $n$th energy level.
b. [10] The uncertainty in position and momentum for the $n$th energy level. Do you results seem reasonable? Explain why.

5. *[20] Uncertainty principles in action again.* For a spin-1/2 particle do the following:
   a. For the state $|\psi_1\rangle = |\uparrow\rangle$
      i. [10] Calculate the uncertainty in the observables $\vec{S}^2$, $\vec{S}_z$, and $\vec{S}_x$
   b. For the state $|\psi_2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$
      i. [10] Calculate the uncertainty in the observables $\vec{S}^2$, $\vec{S}_z$, and $\vec{S}_x$

6. *[30] QuTip test drive.* Add the QuTip package to your Python installation and use a Jupyter notebook to do the following:
   a. [5] Show the three Pauli matrices
   b. [5] Create the state vector $|\psi_1\rangle = |\uparrow\rangle$ and calculate $\langle\vec{S}_z\rangle$
   c. [5] Create the state vector $|\psi_2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ and calculate $\langle\vec{S}_z\rangle$
   d. [5] Use QuTip to redo Problem 5 part a for $\vec{S}_z$ only.
   e. [5] Use Qutip to redo Problem 5 part b for $\vec{S}_z$ only.
   f. [5] Use QuTip to draw $|\psi_1\rangle$ and $|\psi_2\rangle$ on the Bloch sphere. Also, one of these states is commonly written as $|+X\rangle$. Which one do you think it is?