# Katha\_Computational\_Physics\_01

#### September 16, 2024

```
[1]: import numpy as np
    import matplotlib.pyplot as plt
    # Constants
    hbar = 1.0 # Assume hbar = 1 for simplicity
    dt = 0.01 # Time step
    t max = 10 # Maximum time
    n_steps = int(t_max / dt) # Number of time steps
    gamma_values = np.linspace(0.01, 1.01, 5) # Gamma values from 0.01 to 1.01
    # Set up subplots
    fig, axs = plt.subplots(len(gamma_values), 4, figsize=(18, 12))
    fig.suptitle('Time Evolution and FFT for Varying Gamma Values (1 and 2)', __
      →fontsize=16)
     # Loop over gamma values
    for idx, gamma in enumerate(gamma_values):
         # Define the initial wavefunction (start in state |0>)
        psi_0 = np.array([1 + 0j, 0 + 0j]) # Initial wavefunction [psi_0, psi_1]
        # Define the Hamiltonian matrix
        H = np.array([[1j * gamma, -1], [-1, -1j*gamma]])
        # Arrays to store the wavefunction components over time
        psi_0_t = np.zeros(n_steps, dtype=complex) # For 1(t)
        psi_1_t = np.zeros(n_steps, dtype=complex) # For 2(t)
         # Set initial condition
        psi_0_t[0] = psi_0[0]
        psi_1t[0] = psi_0[1]
        # Euler-Cromer method loop
        for i in range(1, n_steps):
             # Compute the derivative of the wavefunction
             dpsi_dt = -1j * np.dot(H, psi_0)
```

```
# Update the wavefunction using Euler-Cromer method
      psi_0 += dt * dpsi_dt # Update both components
      # Store the wavefunction components for plotting
      psi_0_t[i] = psi_0[0] # 1(t)
      psi_1_t[i] = psi_0[1] # 2(t)
  # Time array
  tlist = np.linspace(0, t_max, n_steps)
  # Perform FFT on both 1 and 2
  fft_psi_0 = np.fft.fft(psi_0_t)
  fft_psi_1 = np.fft.fft(psi_1_t)
  fft_freqs = np.fft.fftfreq(n_steps, dt)
  # Shift the FFT and frequencies for proper negative/positive plotting
  fft_psi_0_shifted = np.fft.fftshift(fft_psi_0)
  fft_psi_1_shifted = np.fft.fftshift(fft_psi_1)
  fft_freqs_shifted = np.fft.fftshift(fft_freqs)
  # Plot time-domain |1(t)|^2
  axs[idx, 0].plot(tlist, np.abs(psi_0_t)**2, label=f'|1(t)|^2, Gamma =_U
axs[idx, 0].set_xlabel('Time')
  axs[idx, 0].set_ylabel(r'$|\psi_1(t)|^2$')
  axs[idx, 0].legend()
  axs[idx, 0].grid(True)
  # Plot time-domain |2(t)|^2
  axs[idx, 1].plot(tlist, np.abs(psi_1_t)**2, label=f'|2(t)|^2, Gamma = ___

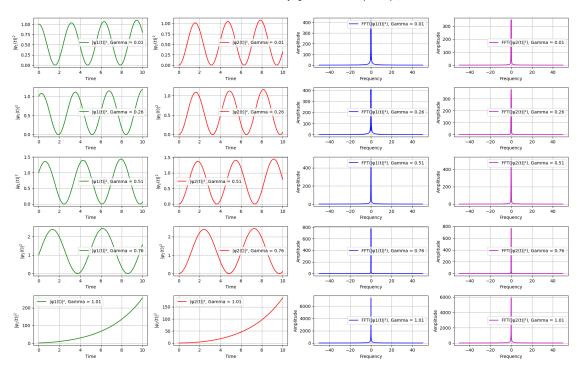
√{gamma:.2f}', color='r')

  axs[idx, 1].set xlabel('Time')
  axs[idx, 1].set_ylabel(r'$|\psi_2(t)|^2$')
  axs[idx, 1].legend()
  axs[idx, 1].grid(True)
  # Plot FFT of |1(t)| (with negative and positive frequencies)
  axs[idx, 2].plot(fft_freqs_shifted, np.abs(fft_psi_0_shifted),__
\Rightarrowlabel=f'FFT(|1(t)|2), Gamma = {gamma:.2f}', color='b')
  axs[idx, 2].set xlabel('Frequency')
  axs[idx, 2].set_ylabel('Amplitude')
  axs[idx, 2].legend()
  axs[idx, 2].grid(True)
  # Plot FFT of |2(t)| (with negative and positive frequencies)
  axs[idx, 3].plot(fft_freqs_shifted, np.abs(fft_psi_1_shifted),__
\Rightarrowlabel=f'FFT(|2(t)|2), Gamma = {gamma:.2f}', color='m')
```

```
axs[idx, 3].set_xlabel('Frequency')
axs[idx, 3].set_ylabel('Amplitude')
axs[idx, 3].legend()
axs[idx, 3].grid(True)

plt.tight_layout(rect=[0, 0, 1, 0.96])
plt.show()
```

Time Evolution and FFT for Varying Gamma Values ( $\psi 1$  and  $\psi 2$ )



# 1 Solve $\psi_1$ & $\psi_2$ , Plot ${\psi_1}^2$ & ${\psi_2}^2$ in Time and Frequency Domain:

```
[11]: import numpy as np
import matplotlib.pyplot as plt

# Constants
hbar = 1.0  # Assume hbar = 1 for simplicity
dt = 0.01  # Time step
t_max = 10  # Maximum time
n_steps = int(t_max / dt)  # Number of time steps
gamma_values = np.linspace(0.01, 1.01, 5)  # Gamma values from 0.01 to 1.01

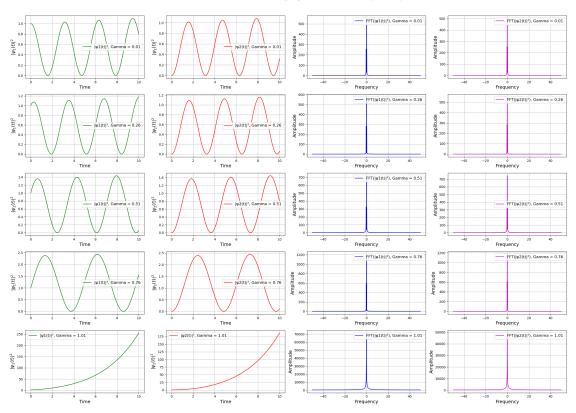
# Set up subplots with enlarged figure size
```

```
fig, axs = plt.subplots(len(gamma_values), 4, figsize=(24, 18)) # Increased_
 ⇔fiqsize for larger plots
fig.suptitle('Time Evolution and FFT for Varying Gamma Values (1 and 2)', u
⇔fontsize=24) # Larger title font size
# Loop over gamma values
for idx, gamma in enumerate(gamma_values):
    # Define the initial wavefunction (start in state |0>)
   psi_0 = np.array([1 + 0j, 0 + 0j]) # Initial wavefunction [psi_0, psi_1]
   # Define the Hamiltonian matrix
   H = np.array([[1j * gamma, -1], [-1, -1j*gamma]])
   # Arrays to store the wavefunction components over time
   psi_0_t = np.zeros(n_steps, dtype=complex) # For 1(t)
   psi_1_t = np.zeros(n_steps, dtype=complex) # For 2(t)
   # Set initial condition
   psi_0_t[0] = psi_0[0]
   psi_1t[0] = psi_0[1]
   # Euler-Cromer method loop
   for i in range(1, n_steps):
        # Compute the derivative of the wavefunction
       dpsi_dt = -1j * np.dot(H, psi_0)
        # Update the wavefunction using Euler-Cromer method
       psi_0 += dt * dpsi_dt # Update both components
       # Store the wavefunction components for plotting
       psi_0_t[i] = psi_0[0] # 1(t)
       psi_1_t[i] = psi_0[1] # 2(t)
    # Time array
   tlist = np.linspace(0, t_max, n_steps)
   # Perform FFT on both 1 and 2
   fft_psi_0 = np.fft.fft(abs(psi_0_t)**2)
   fft_psi_1 = np.fft.fft(abs(psi_1_t)**2)
   fft_freqs = np.fft.fftfreq(n_steps, dt)
   # Shift the FFT and frequencies for proper negative/positive plotting
   fft_psi_0_shifted = np.fft.fftshift(fft_psi_0)
   fft_psi_1_shifted = np.fft.fftshift(fft_psi_1)
   fft_freqs_shifted = np.fft.fftshift(fft_freqs)
```

```
# Find the frequency with the maximum amplitude for 1 and 2
    peak freq psi 0 = fft freqs_shifted[np.argmax(np.abs(fft_psi_0_shifted))]
    peak_freq_psi_1 = fft_freqs_shifted[np.argmax(np.abs(fft_psi_1_shifted))]
    # Print the peak frequencies for both 1 and 2
    print(f"Gamma = {gamma:.2f}: Peak frequency for 1 = {peak_freq_psi_0:.4f},__
 →Peak frequency for 2 = {peak_freq_psi_1:.4f}")
    # Plot time-domain | 1(t) | 2
    axs[idx, 0].plot(tlist, np.abs(psi_0_t)**2, label=f' \mid 1(t) \mid 2, Gamma =__
  axs[idx, 0].set xlabel('Time', fontsize=14)
    axs[idx, 0].set_ylabel(r'$|\psi_1(t)|^2$', fontsize=14)
    axs[idx, 0].legend(fontsize=12)
    axs[idx, 0].grid(True)
    # Plot time-domain /2(t)/2
    axs[idx, 1].plot(tlist, np.abs(psi_1_t)**2, label=f' \mid 2(t) \mid 2, Gamma =__
  axs[idx, 1].set_xlabel('Time', fontsize=14)
    axs[idx, 1].set_ylabel(r'$|\psi_2(t)|^2$', fontsize=14)
    axs[idx, 1].legend(fontsize=12)
    axs[idx, 1].grid(True)
    # Plot FFT of | 1(t) | (with negative and positive frequencies)
    axs[idx, 2].plot(fft_freqs_shifted, np.abs(fft_psi_0_shifted),__
  \hookrightarrowlabel=f'FFT(|1(t)|2), Gamma = {gamma:.2f}', color='b')
    axs[idx, 2].set_xlabel('Frequency', fontsize=14)
    axs[idx, 2].set_ylabel('Amplitude', fontsize=14)
    axs[idx, 2].legend(fontsize=12)
    axs[idx, 2].grid(True)
    # Plot FFT of | 2(t) | (with negative and positive frequencies)
    axs[idx, 3].plot(fft_freqs_shifted, np.abs(fft_psi_1_shifted),__
  \subseteqlabel=f'FFT(|2(t)|2), Gamma = {gamma:.2f}', color='m')
    axs[idx, 3].set_xlabel('Frequency', fontsize=14)
    axs[idx, 3].set_ylabel('Amplitude', fontsize=14)
    axs[idx, 3].legend(fontsize=12)
    axs[idx, 3].grid(True)
plt.tight_layout(rect=[0, 0, 1, 0.96])
plt.show()
Gamma = 0.01: Peak frequency for 1 = 0.0000, Peak frequency for 2 = 0.0000
Gamma = 0.26: Peak frequency for 1 = 0.0000, Peak frequency for 2 = 0.0000
Gamma = 0.51: Peak frequency for 1 = 0.0000, Peak frequency for 2 = 0.0000
Gamma = 0.76: Peak frequency for 1 = 0.0000, Peak frequency for 2 = 0.0000
```

Gamma = 1.01: Peak frequency for 1 = 0.0000, Peak frequency for 2 = 0.0000

Time Evolution and FFT for Varying Gamma Values (ψ1 and ψ2)



```
[16]: import numpy as np
  import matplotlib.pyplot as plt

# Constants
gamma = 0.5
hbar = 1.0 # Assume hbar = 1 for simplicity
dt = 0.01 # Time step
t_max = 10 # Maximum time
n_steps = int(t_max / dt) # Number of time steps

# Define the initial wavefunction (start in state |0>)
psi_0 = np.array([1 + 0j, 0 + 0j]) # Initial wavefunction [psi_0, psi_1]

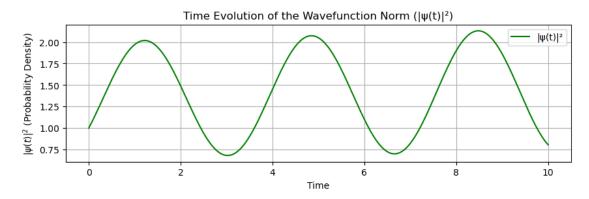
# Define the Hamiltonian matrix
H = np.array([[1j * gamma, -1], [-1, -1j*gamma]])

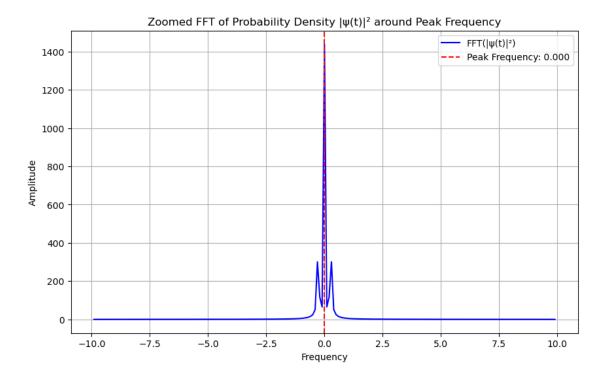
# Arrays to store the wavefunction components over time
psi_0_t = np.zeros(n_steps, dtype=complex)
psi_1_t = np.zeros(n_steps, dtype=complex)
```

```
psi_norm_t = np.zeros(n_steps) # Array to store |psi(t)|^2 (norm)
# Set initial condition
psi_0_t[0] = psi_0[0]
psi_1t[0] = psi_0[1]
psi_norm_t[0] = np.abs(psi_0[0])**2 + np.abs(psi_0[1])**2 # Initial norm
# Euler-Cromer method loop
for i in range(1, n steps):
   # Compute the derivative of the wavefunction
   dpsi_dt = -1j * np.dot(H, psi_0)
   # Update the wavefunction using Euler-Cromer method
   psi_0 += dt * dpsi_dt # Update both components
   # Store the wavefunction components for plotting
   psi_0_t[i] = psi_0[0]
   psi_1t[i] = psi_0[1]
    # Calculate and store the norm |psi(t)|^2 = |psi_0|^2 + |psi_1|^2
   psi_norm_t[i] = np.abs(psi_0[0])**2 + np.abs(psi_0[1])**2
# Time array
tlist = np.linspace(0, t max, n steps)
# Perform FFT on the norm |psi(t)|^2
fft_result = np.fft.fft(psi_norm_t)
fft_freqs = np.fft.fftfreq(n_steps, dt)
# Shift the FFT and frequencies for proper negative/positive plotting
fft_result_shifted = np.fft.fftshift(fft_result)
fft_freqs_shifted = np.fft.fftshift(fft_freqs)
# Plot the norm of the wavefunction |psi(t)|^2
plt.figure(figsize=(10, 6))
plt.subplot(2, 1, 1)
plt.plot(tlist, psi_norm_t, label="|(t)|2", color='g')
plt.xlabel('Time')
plt.ylabel(r'$|\psi(t)|^2$ (Probability Density)')
plt.title('Time Evolution of the Wavefunction Norm (|(t)|^2)')
plt.legend()
plt.grid(True)
# Assuming you already have the fft_result_shifted and fft_fregs_shifted arrays
# Define the range to zoom in around the peak
zoom_range = 10  # Adjust this value if you want to zoom more or less
```

```
# Find the index where the peak occurs
zoom_indices = np.where(np.abs(fft_freqs_shifted) < zoom_range)</pre>
# Find the frequency of the peak
peak_index = np.argmax(np.abs(fft_result_shifted[zoom_indices]))
peak_frequency = fft_freqs_shifted[zoom_indices][peak_index]
# Plot the zoomed-in FFT around the peak frequency
plt.figure(figsize=(10, 6))
plt.plot(fft_freqs_shifted[zoom_indices], np.
 \negabs(fft_result_shifted[zoom_indices]), label="FFT(|(t)|2)", color='b')
plt.axvline(peak_frequency, color='r', linestyle='--', label=f'Peak Frequency:

√{peak_frequency:.3f}')
plt.xlabel('Frequency')
plt.ylabel('Amplitude')
plt.title(f'Zoomed FFT of Probability Density | (t) | 2 around Peak Frequency')
plt.legend()
plt.grid(True)
plt.show()
print(f"The peak frequency is located at: {peak_frequency}")
```





The peak frequency is located at: 0.0

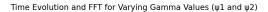
```
[14]: import numpy as np
      import matplotlib.pyplot as plt
      # Constants
      hbar = 1.0 # Assume hbar = 1 for simplicity
      dt = 0.01 # Time step
      t_max = 10 # Maximum time
      n_steps = int(t_max / dt) # Number of time steps
      gamma_values = np.linspace(0.01, 1.01, 5) # Gamma values from 0.01 to 1.01
      # Set up subplots with enlarged figure size
      fig, axs = plt.subplots(len(gamma_values), 4, figsize=(24, 18)) # Increased_
      → figsize for larger plots
      fig.suptitle('Time Evolution and FFT for Varying Gamma Values (1 and 2)', __
       ⇔fontsize=24) # Larger title font size
      # Loop over gamma values
      for idx, gamma in enumerate(gamma_values):
          # Define the initial wavefunction (start in state |0>)
         psi_0 = np.array([1 + 0j, 0 + 0j]) # Initial wavefunction [psi_0, psi_1]
```

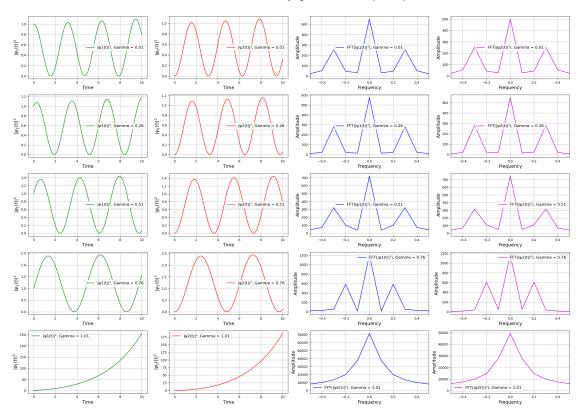
```
# Define the Hamiltonian matrix
  H = np.array([[1j * gamma, -1], [-1, -1j*gamma]])
  # Arrays to store the wavefunction components over time
  psi_0_t = np.zeros(n_steps, dtype=complex) # For 1(t)
  psi_1_t = np.zeros(n_steps, dtype=complex) # For 2(t)
  # Set initial condition
  psi_0_t[0] = psi_0[0]
  psi_1t[0] = psi_0[1]
  # Euler-Cromer method loop
  for i in range(1, n_steps):
      # Compute the derivative of the wavefunction
      dpsi_dt = -1; * np.dot(H, psi_0)
      # Update the wavefunction using Euler-Cromer method
      psi_0 += dt * dpsi_dt # Update both components
      # Store the wavefunction components for plotting
      psi_0_t[i] = psi_0[0] # 1(t)
      psi_1_t[i] = psi_0[1] # 2(t)
  # Time array
  tlist = np.linspace(0, t_max, n_steps)
  # Perform FFT on both 1 and 2
  fft_psi_0 = np.fft.fft(abs(psi_0_t)**2)
  fft_psi_1 = np.fft.fft(abs(psi_1_t)**2)
  fft_freqs = np.fft.fftfreq(n_steps, dt)
  # Shift the FFT and frequencies for proper negative/positive plotting
  fft_psi_0_shifted = np.fft.fftshift(fft_psi_0)
  fft_psi_1_shifted = np.fft.fftshift(fft_psi_1)
  fft_freqs_shifted = np.fft.fftshift(fft_freqs)
  # Find the frequency with the maximum amplitude for 1 and 2
  peak_freq_psi_0 = fft_freqs_shifted[np.argmax(np.abs(fft_psi_0_shifted))]
  peak_freq_psi_1 = fft_freqs_shifted[np.argmax(np.abs(fft_psi_1_shifted))]
  # Print the peak frequencies for both 1 and 2
  print(f"Gamma = {gamma:.2f}: Peak frequency for 1 = {peak_freq_psi_0:.4f},__
→Peak frequency for 2 = {peak_freq_psi_1:.4f}")
  # Plot time-domain |1(t)|^2
  axs[idx, 0].plot(tlist, np.abs(psi_0_t)**2, label=f'|1(t)|^2, Gamma = ___
```

```
axs[idx, 0].set_xlabel('Time', fontsize=14)
    axs[idx, 0].set_ylabel(r'$|\psi_1(t)|^2$', fontsize=14)
    axs[idx, 0].legend(fontsize=12)
    axs[idx, 0].grid(True)
    # Plot time-domain |2(t)|^2
    axs[idx, 1].plot(tlist, np.abs(psi_1_t)**2, label=f'|2(t)|^2, Gamma = ___

√{gamma:.2f}', color='r')

    axs[idx, 1].set_xlabel('Time', fontsize=14)
    axs[idx, 1].set_ylabel(r'$|\psi_2(t)|^2$', fontsize=14)
    axs[idx, 1].legend(fontsize=12)
    axs[idx, 1].grid(True)
    # Plot FFT of |1(t)| (with negative and positive frequencies)
    axs[idx, 2].plot(fft_freqs_shifted, np.abs(fft_psi_0_shifted),__
  \Rightarrowlabel=f'FFT(|1(t)|2), Gamma = {gamma:.2f}', color='b')
    axs[idx, 2].set_xlabel('Frequency', fontsize=14)
    axs[idx, 2].set_ylabel('Amplitude', fontsize=14)
    axs[idx, 2].legend(fontsize=12)
    axs[idx, 2].grid(True)
    # Zoom in around the peak frequency for 1
    zoom_range_psi_0 = 0.5  # Adjust this value to zoom in as needed
    axs[idx, 2].set_xlim(peak_freq_psi_0 - zoom_range_psi_0, peak_freq_psi_0 + __
  ⇒zoom_range_psi_0)
    # Plot FFT of | 2(t) | (with negative and positive frequencies)
    axs[idx, 3].plot(fft_freqs_shifted, np.abs(fft_psi_1_shifted),__
  \Rightarrowlabel=f'FFT(|2(t)|2), Gamma = {gamma:.2f}', color='m')
    axs[idx, 3].set_xlabel('Frequency', fontsize=14)
    axs[idx, 3].set_ylabel('Amplitude', fontsize=14)
    axs[idx, 3].legend(fontsize=12)
    axs[idx, 3].grid(True)
    # Zoom in around the peak frequency for 2
    zoom range psi 1 = 0.5 # Adjust this value to zoom in as needed
    axs[idx, 3].set_xlim(peak_freq_psi_1 - zoom_range_psi_1, peak_freq_psi_1 + __
 →zoom_range_psi_1)
plt.tight_layout(rect=[0, 0, 1, 0.96])
plt.show()
Gamma = 0.01: Peak frequency for 1 = 0.0000, Peak frequency for 2 = 0.0000
Gamma = 0.26: Peak frequency for 1 = 0.0000, Peak frequency for 2 = 0.0000
Gamma = 0.51: Peak frequency for 1 = 0.0000, Peak frequency for 2 = 0.0000
Gamma = 0.76: Peak frequency for 1 = 0.0000, Peak frequency for 2 = 0.0000
Gamma = 1.01: Peak frequency for 1 = 0.0000, Peak frequency for 2 = 0.0000
```





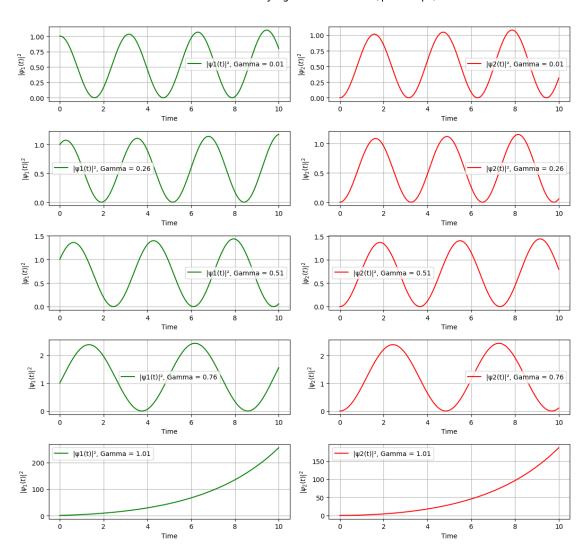
# 2 Q1. Eigenvalues and Eigenvectors for Different Values of $\gamma$ :

```
[17]: import numpy as np
      import matplotlib.pyplot as plt
      def dot_product_check(H):
          eigenvalues, eigenvectors = np.linalg.eig(H)
          # Dot product
          v1 = eigenvectors[:,0]
          v2 = eigenvectors[:,1]
         dot_product = np.dot(np.conjugate(v1), v2)
          if np.isclose(dot_product, 0):
              result = "Orthogonal"
          else:
              result = "Not orthogonal"
          return f"The eigenvectors are {result}", eigenvalues, eigenvectors
      # Constants
      dt = 0.01 # Time step
      t_max = 10 # Maximum time
```

```
n_steps = int(t_max / dt) # Number of time steps
gamma_values = np.linspace(0.01, 1.01, 5) # Gamma values from 0.01 to 1.01
# Set up subplots
fig, axs = plt.subplots(len(gamma_values), 2, figsize=(12, 12))
fig.suptitle('Time Evolution for Varying Gamma Values (1 and 2)', fontsize=16)
# Loop over gamma values
for idx, gamma in enumerate(gamma_values):
    # Define the Hamiltonian matrix
   H = np.array([[1j * gamma, -1], [-1, -1j*gamma]])
   # Orthogonality check and get eigenvalues and eigenvectors
   orthogonality_result, eigenvalues, eigenvectors = dot_product_check(H)
   # Print the eigenvalues and eigenvectors for this gamma
   print(f"Gamma = {gamma:.2f}: {orthogonality_result}")
   print(f"Eigenvalues: {eigenvalues}")
   print(f"Eigenvectors:\n{eigenvectors}\n")
   # Define the initial wavefunction (start in state |0>)
   psi_0 = np.array([1 + 0j, 0 + 0j]) # Initial wavefunction [psi_0, psi_1]
   # Arrays to store the wavefunction components over time
   psi_0_t = np.zeros(n_steps, dtype=complex) # For 1(t)
   psi_1_t = np.zeros(n_steps, dtype=complex) # For 2(t)
    # Set initial condition
   psi_0_t[0] = psi_0[0]
   psi_1t[0] = psi_0[1]
   # Euler-Cromer method loop
   for i in range(1, n_steps):
        # Compute the derivative of the wavefunction
       dpsi_dt = -1j * np.dot(H, psi_0)
        # Update the wavefunction using Euler-Cromer method
       psi_0 += dt * dpsi_dt # Update both components
        # Store the wavefunction components for plotting
       psi_0_t[i] = psi_0[0] # 1(t)
       psi_1_t[i] = psi_0[1] # 2(t)
    # Time array
   tlist = np.linspace(0, t_max, n_steps)
```

```
# Plot time-domain | 1(t) | 2
    axs[idx, 0].plot(tlist, np.abs(psi_0_t)**2, label=f'|1(t)|^2, Gamma =_U
  axs[idx, 0].set xlabel('Time')
    axs[idx, 0].set_ylabel(r'$|\psi_1(t)|^2$')
    axs[idx, 0].legend()
    axs[idx, 0].grid(True)
    # Plot time-domain |2(t)|^2
    axs[idx, 1].plot(tlist, np.abs(psi_1_t)**2, label=f'|2(t)|^2, Gamma = ___
  axs[idx, 1].set xlabel('Time')
    axs[idx, 1].set_ylabel(r'$|\psi_2(t)|^2$')
    axs[idx, 1].legend()
    axs[idx, 1].grid(True)
plt.tight_layout(rect=[0, 0, 1, 0.96])
plt.show()
Gamma = 0.01: The eigenvectors are Not orthogonal
Eigenvalues: [ 0.99995-1.73472348e-18j -0.99995+2.16840434e-18j]
Eigenvectors:
[[-0.70707142-0.00707107j 0.70710678+0.j
 [ 0.70710678+0.j
                          0.70707142+0.00707107j]]
Gamma = 0.26: The eigenvectors are Not orthogonal
Eigenvalues: [ 0.96560862+0.00000000e+00j -0.96560862-3.12250226e-17j]
Eigenvectors:
[[ 0.70710678+0.j
                          0.6827884 -0.18384776j]
 [-0.6827884 +0.18384776j 0.70710678+0.j
                                                ]]
Gamma = 0.51: The eigenvectors are Not orthogonal
Eigenvalues: [ 0.8601744+2.93160153e-17j -0.8601744-1.81971681e-16j]
Eigenvectors:
[[-0.60823515-0.36062446j 0.60823515-0.36062446j]
 [ 0.70710678+0.j
                          0.70710678+0.j
                                                ]]
Gamma = 0.76: The eigenvectors are Not orthogonal
Eigenvalues: [ 0.64992307-2.49433278e-16j -0.64992307+2.73886730e-17j]
Eigenvectors:
[[ 0.70710678+0.j
                          0.70710678+0.j
 [-0.45956501+0.53740115j 0.45956501+0.53740115j]]
Gamma = 1.01: The eigenvectors are Not orthogonal
Eigenvalues: [-8.32667268e-17+0.14177447j -9.92956938e-17-0.14177447j]
Eigenvectors:
[[7.55106205e-01+0.j
                          5.63724021e-17-0.65560249j]
```

#### Time Evolution for Varying Gamma Values ( $\psi$ 1 and $\psi$ 2)



# 3 Q2. Orthogonality Check of Eigenvectors:

```
[21]: import numpy as np
import matplotlib.pyplot as plt

def dot_product_check(H):
    eigenvalues, eigenvectors = np.linalg.eig(H)
    # Dot product
    v1 = eigenvectors[:,0]
```

```
v2 = eigenvectors[:,1]
   dot_product = np.dot(np.conjugate(v1), v2)
   if np.isclose(dot_product, 0):
       result = "Orthogonal"
   else:
       result = "Not orthogonal"
   return f"The eigenvectors are {result}"
# Constants
dt = 0.01 # Time step
t max = 10 # Maximum time
n_steps = int(t_max / dt) # Number of time steps
gamma_values = np.linspace(0.01, 1.01, 5) # Gamma values from 0.01 to 1.01
# Set up subplots
fig, axs = plt.subplots(len(gamma_values), 2, figsize=(12, 12))
fig.suptitle('Time Evolution for Varying Gamma Values (1 and 2)', fontsize=16)
# Loop over gamma values
for idx, gamma in enumerate(gamma_values):
    # Define the Hamiltonian matrix
   H = np.array([[1j * gamma, -1], [-1, -1j*gamma]])
    # Orthogonality check
   orthogonality_result = dot_product_check(H)
   print(f"Gamma = {gamma:.2f}: {orthogonality_result}")
    # Define the initial wavefunction (start in state |0>)
   psi_0 = np.array([1 + 0j, 0 + 0j]) # Initial wavefunction [psi_0, psi_1]
    # Arrays to store the wavefunction components over time
   psi_0_t = np.zeros(n_steps, dtype=complex) # For 1(t)
   psi_1_t = np.zeros(n_steps, dtype=complex) # For 2(t)
    # Set initial condition
   psi_0_t[0] = psi_0[0]
   psi_1t[0] = psi_0[1]
   # Euler-Cromer method loop
   for i in range(1, n steps):
        # Compute the derivative of the wavefunction
       dpsi_dt = -1j * np.dot(H, psi_0)
        # Update the wavefunction using Euler-Cromer method
       psi_0 += dt * dpsi_dt # Update both components
```

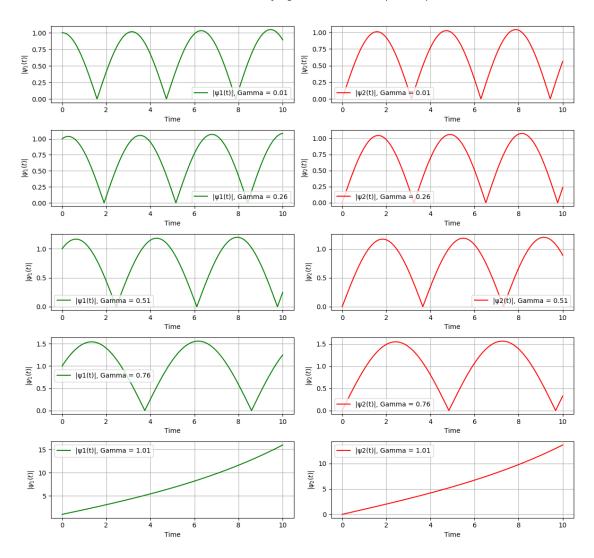
```
# Store the wavefunction components for plotting
       psi_0_t[i] = psi_0[0] # 1(t)
       psi_1_t[i] = psi_0[1] # 2(t)
   # Time array
   tlist = np.linspace(0, t_max, n_steps)
    # Plot time-domain |1(t)|^2
   axs[idx, 0].plot(tlist, np.abs(psi_0_t), label=f'|1(t)|, Gamma = {gamma:.
 axs[idx, 0].set_xlabel('Time')
   axs[idx, 0].set_ylabel(r'$|\psi_1(t)|$')
   axs[idx, 0].legend()
   axs[idx, 0].grid(True)
    # Plot time-domain /2(t)/2
   axs[idx, 1].plot(tlist, np.abs(psi_1_t), label=f'|2(t)|, Gamma = {gamma:.

⇔2f}', color='r')

   axs[idx, 1].set_xlabel('Time')
   axs[idx, 1].set_ylabel(r'$|\psi_2(t)|$')
   axs[idx, 1].legend()
   axs[idx, 1].grid(True)
plt.tight_layout(rect=[0, 0, 1, 0.96])
plt.show()
```

```
Gamma = 0.01: The eigenvectors are Not orthogonal Gamma = 0.26: The eigenvectors are Not orthogonal Gamma = 0.51: The eigenvectors are Not orthogonal Gamma = 0.76: The eigenvectors are Not orthogonal Gamma = 1.01: The eigenvectors are Not orthogonal
```

#### Time Evolution for Varying Gamma Values ( $\psi$ 1 and $\psi$ 2)



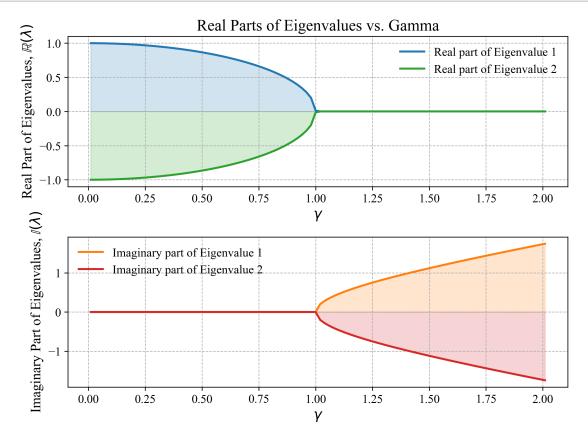
```
[50]: import numpy as np
  import matplotlib.pyplot as plt

# Use LaTeX-style fonts and publication-quality settings
plt.rcParams.update({
       "font.family": "serif",
       "font.serif": ["Times New Roman"],
       "font.size": 14,
       "axes.titlesize": 16,
       "axes.labelsize": 14,
       "legend.fontsize": 12,
       "xtick.labelsize": 12,
       "ytick.labelsize": 12,
```

```
"figure.dpi": 300, # High DPI for publication
    "lines.linewidth": 2,
    "text.usetex": False, # Can be switched to True if LaTeX is available
})
# Constants
gamma_values = np.linspace(0.01, 2.01, 100) # Gamma values from 0.01 to 2.01
# Arrays to store eigenvalues
real_parts = np.zeros((len(gamma_values), 2)) # Real parts of the eigenvalues
imaginary_parts = np.zeros((len(gamma_values), 2)) # Imaginary parts of the
⇔eigenvalues
# Loop over gamma values and calculate eigenvalues
for idx, gamma in enumerate(gamma_values):
    # Define the Hamiltonian matrix for given gamma
   H = np.array([[1j * gamma, -1], [-1, -1j * gamma]])
   # Compute the eigenvalues of the Hamiltonian
   eigvals = np.linalg.eigvals(H)
   # Store the real and imaginary parts of the eigenvalues
   real_parts[idx] = np.real(eigvals)
   imaginary_parts[idx] = np.imag(eigvals)
# Plot the real and imaginary parts of the eigenvalues
fig, ax = plt.subplots(2, 1, figsize=(8, 6))
# Define colors that are visually distinct, colorblind-friendly, and \Box
 ⇔print-friendly
real_colors = ['#1f77b4', '#2ca02c'] # Blue and Green for real parts
imaginary_colors = ['#ff7f0e', '#d62728'] # Orange and Red for imaginary parts
shade_alpha = 0.2 # Transparency for shading
# Plot real parts of eigenvalues with shading
ax[0].plot(gamma_values, real_parts[:, 0], label='Real part of Eigenvalue 1',

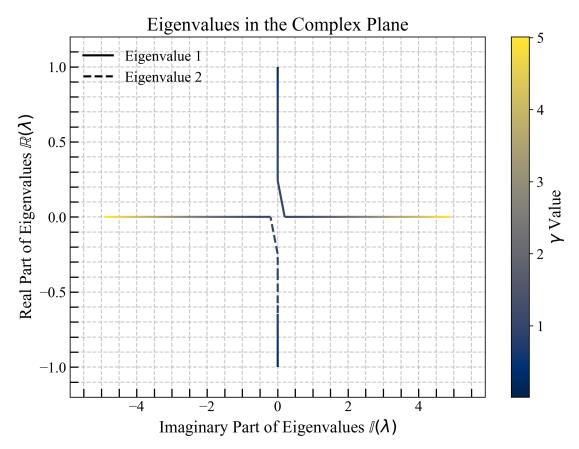
¬color=real_colors[0], linewidth=2)
ax[0].plot(gamma_values, real_parts[:, 1], label='Real part of Eigenvalue 2', __
⇔color=real_colors[1], linewidth=2)
ax[0].fill_between(gamma_values, real_parts[:, 0], color=real_colors[0],__
 →alpha=shade_alpha)
ax[0].fill_between(gamma_values, real_parts[:, 1], color=real_colors[1],
⇒alpha=shade_alpha)
ax[0].set_title('Real Parts of Eigenvalues vs. Gamma', fontsize=16)
ax[0].set_xlabel('$\gamma$', fontsize=14)
ax[0].set_ylabel(r'Real Part of Eigenvalues, $\mathbb{R}(\lambda)$')
```

```
ax[0].legend(frameon=False)
ax[0].grid(True, linestyle='--', linewidth=0.7)
# Plot imaginary parts of eigenvalues with shading
ax[1].plot(gamma_values, imaginary_parts[:, 0], label='Imaginary part of_u
 → Eigenvalue 1', color=imaginary_colors[0], linewidth=2)
ax[1].plot(gamma_values, imaginary_parts[:, 1], label='Imaginary part of_
 → Eigenvalue 2', color=imaginary colors[1], linewidth=2)
ax[1].fill_between(gamma_values, imaginary_parts[:, 0],__
 ⇔color=imaginary_colors[0], alpha=shade_alpha)
ax[1].fill_between(gamma_values, imaginary_parts[:, 1],__
 ⇔color=imaginary_colors[1], alpha=shade_alpha)
ax[1].set_ylabel(r'Imaginary Part of Eigenvalues, $\mathbb{I}(\lambda)$')
ax[1].set_xlabel('$\gamma$', fontsize=14)
ax[1].set_ylabel(r'Imaginary Part of Eigenvalues, $\mathbb{I}(\lambda)$')
ax[1].legend(frameon=False)
ax[1].grid(True, linestyle='--', linewidth=0.7)
# Adjust layout for better spacing
plt.tight_layout()
# Show the plot
plt.show()
```



```
[49]: import numpy as np
      import matplotlib.pyplot as plt
      from matplotlib.collections import LineCollection
      from matplotlib import cm
      # Use LaTeX-style fonts for scientific publications
      plt.rcParams.update({
          "font.family": "serif",
          "font.serif": ["Times New Roman"],
          "font.size": 16,
          "axes.titlesize": 18,
          "axes.labelsize": 16,
          "legend.fontsize": 14,
          "xtick.labelsize": 14,
          "ytick.labelsize": 14,
          "figure.dpi": 300, # High DPI for publication
          "text.usetex": False, # You can switch to True if LaTeX is available
      })
      # Constants
      gamma_values = np.linspace(0.01, 5.01, 100) # Gamma values from 0.01 to 5.01
      # Arrays to store eigenvalues
      real_parts = np.zeros((len(gamma_values), 2)) # To store the real parts of the_
      imaginary_parts = np.zeros((len(gamma_values), 2)) # To store the imaginary_
       ⇔parts of the eigenvalues
      # Loop over gamma values and calculate eigenvalues
      for idx, gamma in enumerate(gamma_values):
          # Define the Hamiltonian matrix for given gamma
          H = np.array([[1j * gamma, -1], [-1, -1j * gamma]])
          # Compute the eigenvalues of the Hamiltonian
          eigvals = np.linalg.eigvals(H)
          # Store the real and imaginary parts of the eigenvalues
          real_parts[idx] = np.real(eigvals)
          imaginary_parts[idx] = np.imag(eigvals)
      # Helper function to create fading line plots
      def plot_fading_lines(x, y, gamma_values, ax, label, line_style):
          points = np.array([x, y]).T.reshape(-1, 1, 2)
```

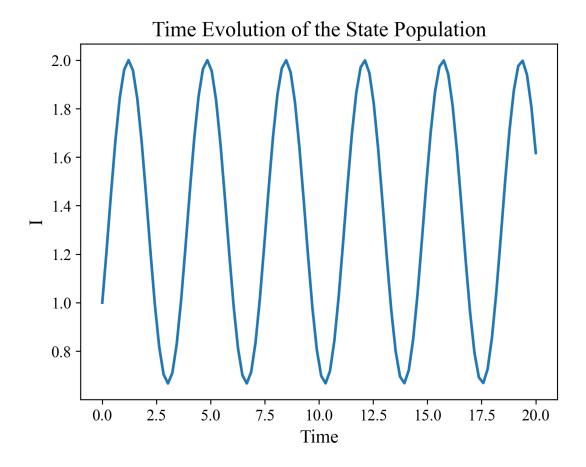
```
segments = np.concatenate([points[:-1], points[1:]], axis=1)
    # Create a colormap that varies with gamma values
   norm = plt.Normalize(gamma_values.min(), gamma_values.max())
   lc = LineCollection(segments, cmap='cividis', norm=norm) # Use a__
 ⇔colorblind-friendly colormap
   lc.set array(gamma values)
   lc.set_linewidth(2.0) # Adjust line width for publication quality
   lc.set_linestyle(line_style) # Set the line style
    # Add the fading lines to the plot
   ax.add_collection(lc)
# Create the figure and axis
fig, ax = plt.subplots(figsize=(8, 6)) # Larger figure for better clarity
# Plot the eigenvalues with a fading effect for both branches
plot_fading_lines(imaginary_parts[:, 0], real_parts[:, 0], gamma_values, ax, __
 ⇔'Eigenvalue 1', '-')
plot_fading_lines(imaginary_parts[:, 1], real_parts[:, 1], gamma_values, ax, u
 ⇔'Eigenvalue 2', '--')
# Add colorbar to show gamma values
cbar = plt.colorbar(cm.ScalarMappable(cmap='cividis', norm=plt.
 →Normalize(gamma_values.min(), gamma_values.max())), ax=ax)
cbar.set_label(r'$\gamma$ Value', fontsize=16) # Use math text for Greek_
 ⇔symbols
cbar.ax.tick_params(labelsize=14) # Increase font size of colorbar ticks
# Add labels and title
ax.set_title('Eigenvalues in the Complex Plane', fontsize=18)
ax.set_xlabel(r'Imaginary Part of Eigenvalues $\mathbb{I}(\lambda)$',__
ax.set_ylabel(r'Real Part of Eigenvalues $\mathbb{R}(\lambda)$', fontsize=16)
# Set axis limits with a buffer
x_buffer = (np.max(imaginary_parts) - np.min(imaginary_parts)) * 0.1
y_buffer = (np.max(real_parts) - np.min(real_parts)) * 0.1
ax.set_xlim(np.min(imaginary_parts) - x_buffer, np.max(imaginary_parts) +_u
 →x_buffer)
ax.set_ylim(np.min(real_parts) - y_buffer, np.max(real_parts) + y_buffer)
# Add a fine grid and light ticks
ax.grid(True, which='both', linestyle='--', linewidth=1.0, alpha=0.7)
ax.minorticks_on() # Minor ticks for precision
```



# 4 Using Evolution Operator:

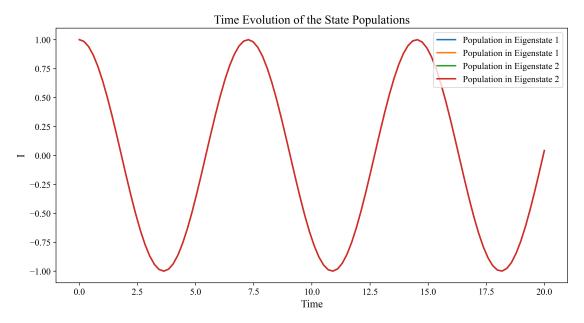
```
[56]: import numpy as np
import scipy.linalg
import matplotlib.pyplot as plt
from qutip import *
```

```
# Parameters
N = 100
psi0 = basis(2, 0) # Initial state
t = np.linspace(0, 20, N, endpoint=True) # Time steps
gamma = 0.5
# Hamiltonian as defined earlier
sigmaaa = tensor(basis(2, 0) * basis(2, 0).dag())
sigmabb = tensor(basis(2, 1) * basis(2, 1).dag())
sigmaab = tensor(basis(2, 0) * basis(2, 1).dag())
sigmaba = sigmaab.dag()
H = 1j * gamma * sigmaaa - 1j *gamma* sigmabb - sigmaab - sigmaba # Hamiltonian
# Initialize arrays to store results
I = np.zeros(len(t))
# Time evolution loop
for i in range(len(t)):
   U = scipy.linalg.expm(-1j * H.full() * t[i]) # Time evolution operator
   psi_t = Qobj(U @ psi0.full()) # Apply evolution to the initial state
   I[i] = np.real((psi_t.dag() * psi_t).full()) # Compute the population of__
 →the state
# Plotting the results
plt.plot(t, I)
plt.xlabel('Time')
plt.ylabel('I')
plt.title('Time Evolution of the State Population')
plt.show()
```



```
[63]: import numpy as np
      import scipy.linalg
      import matplotlib.pyplot as plt
      from qutip import *
      # Parameters
      N = 100
      t = np.linspace(0, 20, N, endpoint=True) # Time steps
      gamma = 0.5
      # Basis states
      basis_0 = basis(2, 0)
      basis_1 = basis(2, 1)
      # Hamiltonian
      sigmaaa = tensor(basis_0 * basis_0.dag())
      sigmabb = tensor(basis_1 * basis_1.dag())
      sigmaab = tensor(basis_0 * basis_1.dag())
      sigmaba = sigmaab.dag()
```

```
H = 1j * gamma * sigmaaa - 1j * gamma * sigmabb - sigmaab - sigmaba #<math>_{\sqcup}
 \hookrightarrow Hamiltonian
# Compute eigenstates and eigenvalues
eigenvalues, eigenstates = H.eigenstates()
# Initialize arrays to store results
I = np.zeros((len(t), len(eigenstates)))
# Time evolution loop
for i in range(len(t)):
    U = scipy.linalg.expm(-1j * H.full() * t[i]) # Time evolution operator
    for j, eigenstate in enumerate(eigenstates):
        psi_t = Qobj(U @ eigenstate.full()) # Apply evolution to the eigenstate
        I[i, j] = np.real((psi_t.dag() * eigenstate).full()) # Compute the__
 →population in the eigenstate
# Plotting the results
plt.figure(figsize=(12, 6))
for j in range(len(eigenstates)):
    plt.plot(t, I[:, j], label=f'Population in Eigenstate {j+1}')
plt.xlabel('Time')
plt.ylabel('I')
plt.title('Time Evolution of the State Populations')
plt.legend()
plt.show()
```



[]: