**T1 and T2 NMR Python**

For this lab, we could write a Python component to analyze the data collected from the NMR experiment and fit the relaxation times (T₁ and T₂) using the appropriate mathematical models. The Python script will plot the data, perform curve fitting, and calculate the relaxation times from the collected NMR data.

Here’s a Python script that takes data (signal intensity vs. time), fits it to the exponential decay equations for T₁ and T₂, and extracts the relaxation times.

**Python Code for NMR Data Analysis:**

**import** numpy as np  
**import** matplotlib.pyplot as plt  
**from** scipy.optimize **import** curve\_fit  
  
# Define the exponential decay models **for** T1 **and** T2  
# T1 relaxation model: Mz = M0 \* (1 - 2 \* exp(-t/T1))  
def T1\_relaxation(t, M0, T1):  
 **return** M0 \* (1 - 2 \* np.exp(-t / T1))  
  
# T2 relaxation model: Mxy = M0 \* exp(-t/T2)  
def T2\_relaxation(t, M0, T2):  
 **return** M0 \* np.exp(-t / T2)  
  
# Example data (replace with your experimental data)  
time\_T1 = np.array([0, 0.5, 1, 2, 5, 10, 20]) # time points **for** T1 measurements  
intensity\_T1 = np.array([0, 0.3, 0.5, 0.7, 0.9, 0.95, 1]) # signal intensity **for** T1  
  
time\_T2 = np.array([0, 0.1, 0.2, 0.5, 1, 2, 5]) # time points **for** T2 measurements  
intensity\_T2 = np.array([1, 0.8, 0.6, 0.4, 0.3, 0.2, 0.1]) # signal intensity **for** T2  
  
# Fit T1 relaxation data  
params\_T1, \_ = curve\_fit(T1\_relaxation, time\_T1, intensity\_T1)  
M0\_T1, T1\_value = params\_T1  
  
# Fit T2 relaxation data  
params\_T2, \_ = curve\_fit(T2\_relaxation, time\_T2, intensity\_T2)  
M0\_T2, T2\_value = params\_T2  
  
# Print the results  
print(f"T1 Relaxation Time: {T1\_value:.3f} seconds")  
print(f"T2 Relaxation Time: {T2\_value:.3f} seconds")  
  
# Plotting T1 relaxation  
plt.figure(figsize=(10, 5))  
plt.subplot(1, 2, 1)  
plt.scatter(time\_T1, intensity\_T1, color='blue', label='Experimental Data')  
plt.plot(time\_T1, T1\_relaxation(time\_T1, M0\_T1, T1\_value), color='red', label=f'Fit: T1 = {T1\_value:.3f} s')  
plt.title("T1 Relaxation")  
plt.xlabel("Time (s)")  
plt.ylabel("Signal Intensity")  
plt.legend()  
  
# Plotting T2 relaxation  
plt.subplot(1, 2, 2)  
plt.scatter(time\_T2, intensity\_T2, color='green', label='Experimental Data')  
plt.plot(time\_T2, T2\_relaxation(time\_T2, M0\_T2, T2\_value), color='orange', label=f'Fit: T2 = {T2\_value:.3f} s')  
plt.title("T2 Relaxation")  
plt.xlabel("Time (s)")  
plt.ylabel("Signal Intensity")  
plt.legend()  
  
plt.tight\_layout()  
plt.show()

**Steps of the Script:**

1. **Define Relaxation Models:**
   * The model for T₁ relaxation is Mz=M0(1−2e−tT1)M\_z = M\_0 \left(1 - 2e^{-\frac{t}{T\_1}}\right)Mz​=M0​(1−2e−T1​t​).
   * The model for T₂ relaxation is Mxy=M0e−tT2M\_{xy} = M\_0 e^{-\frac{t}{T\_2}}Mxy​=M0​e−T2​t​.
2. **Data Input:**
   * time\_T1 and intensity\_T1 are arrays of time points and corresponding signal intensities for T₁ measurements.
   * time\_T2 and intensity\_T2 are arrays of time points and signal intensities for T₂ measurements.
3. **Curve Fitting:**
   * The curve\_fit function from scipy.optimize is used to fit the experimental data to the T₁ and T₂ models, extracting the values of T1T\_1T1​ and T2T\_2T2​.
4. **Plotting Results:**
   * The experimental data is plotted along with the fitted exponential decay curve to visualize how well the model fits the data.
   * The calculated T₁ and T₂ values are displayed on the plot.

**Input Your Data:**

Replace the example time\_T1, intensity\_T1, time\_T2, and intensity\_T2 arrays with your actual experimental data collected from the NMR measurements.

**Output:**

The script will output the calculated T₁ and T₂ relaxation times and show plots comparing the experimental data with the fitted relaxation curves.

Question 1

What is the purpose of using the curve\_fit function in the analysis of the NMR data, and what information does it provide?

Question 2

In the context of T₁ and T₂ relaxation, explain why different mathematical models are used for T₁ and T₂ decay. How do these models reflect the physical processes occurring during NMR relaxation?

Question 3

After running the Python script, the values of T₁ and T₂ are extracted. How do these values relate to the physical properties of the sample, and what factors might influence their magnitudes?

Question 4

The Python script generates plots comparing the experimental data with the fitted models. What features would you look for in the plot to determine if the curve fitting was successful? What might cause poor fitting of the data?

Question 5

If the curve\_fit function fails to converge to a solution or gives unexpected results, what steps would you take to troubleshoot the issue? What modifications could you make to the script or the experimental procedure to improve data quality and fitting?

Here is a sample dataset for T₁ and T₂ relaxation times for a different molecule, **ethanol**:

**Experimental Data for Ethanol**

|  |  |  |
| --- | --- | --- |
| **Time (ms)** | **Signal Amplitude for T₁** | **Signal Amplitude for T₂** |
| 0 | 0.00 | 100.00 |
| 10 | 12.50 | 93.10 |
| 20 | 23.30 | 86.60 |
| 30 | 31.80 | 80.60 |
| 40 | 39.00 | 75.10 |
| 50 | 44.90 | 70.10 |
| 60 | 49.70 | 65.50 |
| 70 | 53.50 | 61.30 |
| 80 | 56.40 | 57.30 |
| 90 | 58.60 | 53.70 |
| 100 | 60.20 | 50.40 |
| 120 | 62.00 | 44.30 |
| 140 | 63.20 | 39.20 |
| 160 | 64.00 | 34.90 |
| 180 | 64.50 | 31.10 |
| 200 | 64.80 | 27.70 |
| 250 | 65.10 | 20.20 |
| 300 | 65.20 | 14.80 |
| 350 | 65.30 | 10.80 |
| 400 | 65.40 | 7.80 |
| 450 | 65.50 | 5.60 |
| 500 | 65.50 | 4.00 |

Question 6

Write a Python function that imports the provided dataset for ethanol T₁ and T₂ relaxation times from a CSV file. How would you visualize the signal amplitudes for T₁ and T₂ over time using Matplotlib?

Question 7

Use the curve\_fit function from the SciPy library to fit an exponential decay function to the signal amplitudes for T₁ and T₂. What are the fitted parameters for both T₁ and T₂, and how do they relate to the relaxation times?

Question 8

After fitting the data, calculate the T₁ and T₂ relaxation times based on the fitted parameters. What are the estimated relaxation times, and how do they compare to literature values for ethanol?

Question 9

Implement a method to calculate the residuals between the experimental signal amplitudes and the fitted exponential curve for T₁ and T₂. How can you evaluate the goodness of fit using metrics like the Root Mean Square Error (RMSE)?

Question 10

Analyze how the T₁ and T₂ relaxation times change with respect to increasing time based on your fitted model. What conclusions can you draw about the molecular dynamics of ethanol based on these relaxation times, and how might these findings differ from those of the molecule you are analyzing experimentally?