Bloch\_Equations\_1D\_SEXY

We will describe how to use the SEXY script and simulate SEXY experiment.

% here is an example of simulations of 1D NMR spectrum using Bloch class

% 90y - FID

clear all

close all

p = LoadPath() ;

% System parameters

System = SPINS\_Systems(1) ; % 1 = AB, 2 = ABC

[T1,T2,C,Wz,K] = Load\_SPINS\_Systems(System) ;

% Declaration of spins

M = SPINS(T1,T2,C) ;

Spec.time2relax = 1000 ; % this is to let system to reach steady state

Spec.time\_mix = linspace(0,1,20)' ;

% sepctral parameters

Spec.LB = 2 ; % Linebroadening [Hz]

Spec.Fs = 2000 ; % Sampling frequency

Spec.L = 2^13 ; % Length of signal

Spec.time = (0:Spec.L-1)'/Spec.Fs ; % Time vector for acquisition

Spec.AQ = Spec.time(end) ; % Total acquisition time

Spec.d1 = 10 ; % Time before total acquisition time

Spec.selective\_excitation = [1] ; % Excite with selective excitation spin 1

Spec.Integral\_width = 40 ; % Hz this is the integration width

Spec.DS = 8 ; % Dummy scans

% Simulation of SEXY experiment

[Spec, M] = M.SEXY(Spec,Wz,K) ; % Calculate sexy sequence

M.Plot\_Spectra(Spec) ; Plot spectra of sexy experiment

%% plot and save SEXY integrals

figure("color","white")

plot(Spec.time\_mix,Spec.Integrals,"o") ;

Spec.Legends = {"1","2","3","4","5"} ;

legend(Spec.Legends{1:M.N})

ylabel("integral")

xlabel("time mix (s)")

out = [Spec.time\_mix,Spec.Integrals/max(Spec.Integrals)] ;

%save("integrals.txt","out","-ASCII")

First Step: % System parameters

Define the system of spins to simulate either 2 spins (1) AB or 3 spins (2) ABC.

The function: **LOAD\_SPINS\_Systems:** will return T1, T2, concentration of the spins, Frequency and exchange rate so therefore you need to set the right values.

Define:

* T1 and T2 for your spins
* Wz : frequency of each spin (rad/s)
* k : exchange rate (s-1). NB: make sure that the sum of column is zero
* C : Concentration of each spin in the system

Second Step: % Declaration of spins

Define in:

* Spec.time2relax: the time to reach the steady state
* Spec.time\_mix: the vector of the list for the mixing time

Ex: linspace(0,1,20)' : 20 points between 0 and 1s

Third Step: % sepctral parameters

Define;

* all the parameters of the spectra ( LB,Fs, L,time, AQ)
* d1 is the delay between 2 consecutives experiments.
* Selective\_excitation either 1, 2 or 3 : Select which spin to excite
* DS : number of dummy scans before the real acquisition
* Integral\_width : this is the width of the peak to integrate.

Forth Step: % Simulation of SEXY experiment

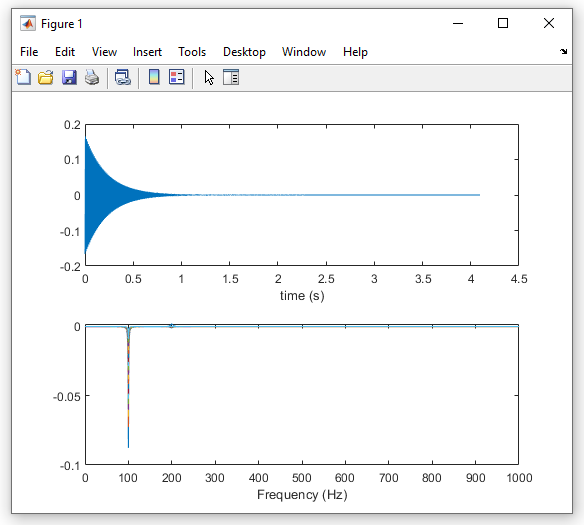
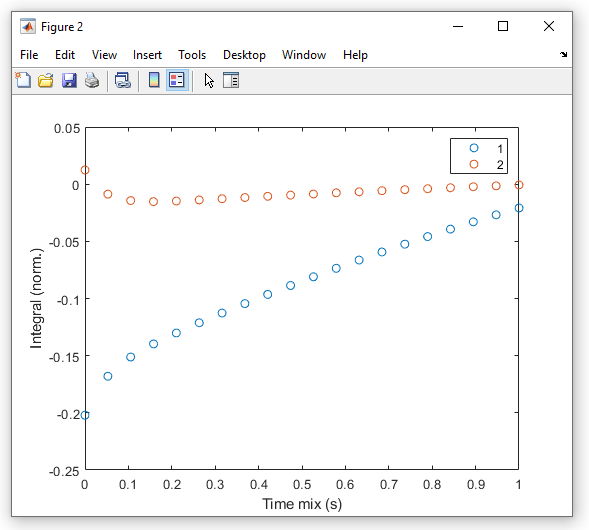
In this section we will simulate our SEXY experiment

The function **SEXY** will run dummy scans then makes the real scan

Fifth Step: %% plot and save SEXY integrals

Figure 1: Plotting of the Fid and all the spectra for the several times mixing

Figure 2: Plotting of the Integrals of each spin in function of the mixing time



BlochEquations\_2D\_EXSY

tic

clear all

close all

p = LoadPath() ; % system parameters

System = SPINS\_Systems(1) ; % 1 = AB, 2 = ABC

[T1,T2,C,Wz,K] = Load\_SPINS\_Systems(System) ;

%declaration of spins

M = SPINS(T1,T2,C) ;

% evolution during timeFID

% spectral parameters: direct dimension

Spec.Fs = 1000 ; % Sampling frequency

Spec.L = 2^10 ; % Length of signal

Spec.time = (0:Spec.L-1)'/Spec.Fs ;% Time vector

% spectral parameters: idirect dimension

Spec.Fs1 = 1000 ; % Sampling frequency

Spec.L1 = 2^10 ;% Length of signal

Spec.D0 = (0:Spec.L1-1)'/Spec.Fs1 ; % Time vector

% additional sequence parameters

Spec.D1 = 10 ; Time before total acquisition time

Spec.D8 = 0.1 ;% mixing time

Spec.DS = 32 ; % dummy scans

% calculate experiment

[Spec, M] = M.noesyph(Spec,Wz,K) ; % Calculate EXSY sequence

toc

%% Plot 2D spectrum

Spec.LB = 10 ; % linebroadening [Hz]

Spec.LB1 = 10 ; % linebroadening [Hz]

Spec = M.Spectrum2D(Spec) ;

M.Plot\_Spectrum2D(Spec) ;

%% analyze integrals

Spec.Integral\_width = 50 ; % half width for the spectrum integration Hz

Spec.Peaks = Wz/(2\*pi) ; % this peaks we will integrate

[Is,Maxs] = D2\_integrals(Spec.FRQ,Spec.FRQ1,abs(Spec.Spectrum),Spec.Peaks,Spec.Integral\_width); % specify your integrations area

Same steps as for SEXY.

Section: %% analyze integrals

This section will provide the Exchange rate matrix Is

Is =

0.0544 0.0476

0.0474 0.0187

