

Python On Resonance (PyOR)

Everybody can simulate NMR

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Tutorial 12: Heteronuclear Nuclear Overhauser effect (NOE)

In this tutorial you will see Heteronuclear Nuclear Overhauser effect (NOE) of two spin half system (H1 and C13). We will evolve the density matrix in Liouville Space. Correlation time 10 pico second.

Load Python packages and define path to the source file "PythonOnResonance.py"

```
In [1]: pathSource = '/media/HD2/Vineeth/PostDoc_Simulations/Github/PyOR_G/Source'
```

```
In [2]: from IPython.display import display, HTML
display(HTML("<style>.container { width:100% !important; }</style>"))
import sys
sys.path.append(pathSource)

import PythonOnResonance as PyOR

import time
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import rc
%matplotlib notebook
import sympy as sp
from sympy import *
```

Generating Spin System

```
In [3]: """
Define Spin quantum numbers of your spins in "Slist1".
Slist1[0] is spin of first particle and Slist1[1] is spin of second particle.
""";

Slist1 = [1/2, 1/2]
```

```
In [4]: """
Define Planck constant equals 1.
Because NMR spectroscopists are more interested to write Energy in frequency units.
if False then hbarEQ1 = hbar
""";

hbarEQ1 = True
```

```
In [5]: """
Generate Spin Operators
""";

System = PyOR.Numerical_MR(Slist1,hbarEQ1)

"""
Sx, Sy and Sz Operators
""";
Sx,Sy,Sz = System.SpinOperator()

"""
S+ and S- Operators
""";
Sp,Sm = System.PMoperators(Sx,Sy)
```

Zeeman Hamiltonian in Lab Frame

```
In [6]: """
Gyromagnetic Ratio
Gamma = [Gyromagnetic Ratio spin 1, Gyromagnetic Ratio spin 1, ...]
""";
Gamma = [System.gammaH1,System.gammaC13]

"""
Define the field of the spectrometer, B0 in Tesla.
""";
B0 = 11.4

"""
Define the chemical Shift of individual spins
Offset = [chemical Shift spin 1, chemical Shift spin 1, ..]
""";
Offset = [0,0] # Offset frequency in Hz

"""
Function "LarmorF" give the list Larmor frequencies of individual spins in lab frame
""";
LarmorF = System.LarmorFrequency(Gamma,B0,Offset)

Hz = System.Zeeman(LarmorF,Sz)
```

Larmor Frequency in MHz: [-485.38291502 -122.07564834]

Initialize Density Matrix

```
In [7]: """
We will generate Initial Density Matrix in two ways:
First we will generate a density matrix as we prefer say, Sz.
Second we will create density matrix at thermal equilibrium

First Case
""";

Thermal_DensMatrix = True

if Thermal_DensMatrix:
    Hz_EnUnit = System.Convert_FreqUnitsTOEnergy(Hz)
    HT_approx = False # High Temperature Approximation is False
    T = 300 # Temperature in Kelvin
    rho_in = System.EquilibriumDensityMatrix(Hz_EnUnit,T,HT_approx)
```

```

rhoeq = rho_in.copy()
else:
    rho_in = np.sum(Sz,axis=0) # Initial Density Matrix
    rhoeq = np.sum(Sz,axis=0) # Equilibrium Density Matrix
    print("Trace of density metrix = ", np.trace(rho_in))

```

Trace of density metrix = 1.0

```

In [8]: """
Equilibrium population of Carbon and Proton
"""
print("Equilibrium Population of H1 = ", np.trace(Sz[0] @ rhoeq).real)
print("Equilibrium Population of C13 = ", np.trace(Sz[1] @ rhoeq).real)

```

Equilibrium Population of H1 = 1.9410853512036308e-05
Equilibrium Population of C13 = 4.88190345199202e-06

In []:

Zeeman Halitonian in Rotating Frame

```

In [9]: OmegaRF = [-System.gammaH1*B0, -System.gammaC13*B0]
Hzr = System.Zeeman_RotFrame(LarmorF, Sz, OmegaRF)

```

J Coupling Hamiltonian

```

In [10]: '''
Define J couplings between individual spins
'''
Jlist = np.zeros((len(Slist1),len(Slist1)))
Jlist[0][1] = 15.0
Hj = System.Jcoupling_Weak(Jlist,Sz)

```

Converting to Liouvillian

```

In [11]: Hz_L = System.CommutationSuperoperator(Hz)
Hzr_L = System.CommutationSuperoperator(Hzr)
Hj_L = System.CommutationSuperoperator(Hj)
rho_in_L = System.Vector_L(rho_in)
rhoeq_L = System.Vector_L(rhoeq)

```

Pulse

```

In [12]: """
Selective Pulse on Spin 1
"""
pulse_angle = 180.0
rho_L = System.Rotate_L(rho_in_L,pulse_angle,Sx[0])

```

Relaxation Constant

```

In [13]: """

```

```
Options: "No Relaxation", "Phenomenological", "Auto-correlated Dipolar Homonuclear", Auto-
""";
R = None
Rprocess = "Auto-correlated Dipolar Hetrnuclear"
tau = 10.0e-12
bIS = 30.0e3
System.Relaxation_Parameters(LarmorF, OmegaRF, tau, bIS)
R_L = System.Relaxation_L(Rprocess, R, Sx, Sy, Sz, Sp, Sm)
```

Evolution of Density Matrix

In [14]:

```
dt = 0.0005
AQ = 60.0
Npoints = int(AQ/dt)
print("Number of points in the simulation", Npoints)

"""
option for solver, "method": "Unitary Propagator", "Relaxation" or "ODE Solver"
"""
method = "Relaxation"

start_time = time.time()
t, rho_t = System.Evolution_L(rhoeq_L, rho_L, Sx, Sy, Hxr_L + Hj_L - 1j * R_L, dt, Npoints, method)
end_time = time.time()
timetaken = end_time - start_time
print("Total time = %s seconds " % (timetaken))
```

Number of points in the simulation 120000
Total time = 0.33464813232421875 seconds

Expectation value

In [15]:

```
EXP_Z1 = Sz[0]
EXP_Z2 = Sz[1]

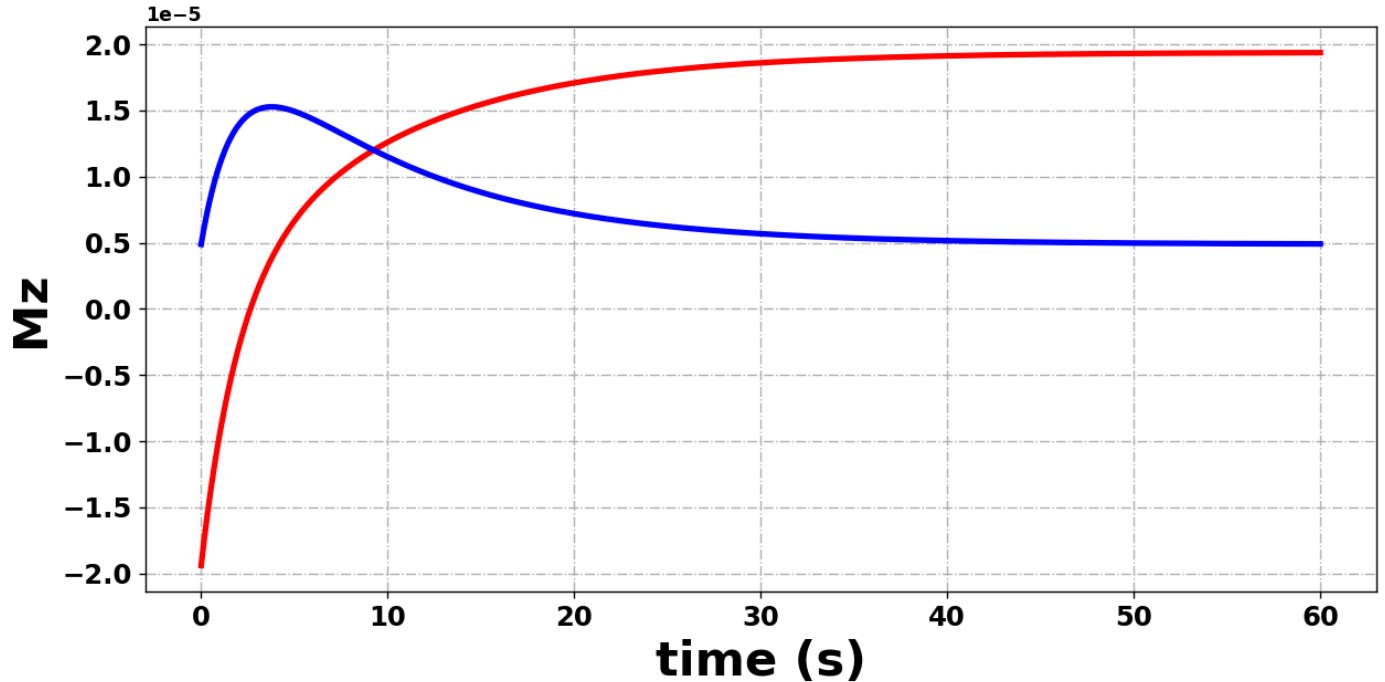
LEXP_Z1 = System.Detection_L(EXP_Z1)
LEXP_Z2 = System.Detection_L(EXP_Z2)

t, Mz1 = System.Expectation_L(rho_t, LEXP_Z1, dt, Npoints)
t, Mz2 = System.Expectation_L(rho_t, LEXP_Z2, dt, Npoints)
```

In [16]:

```
"""
Mz1: Red
Mz2: Blue
"""

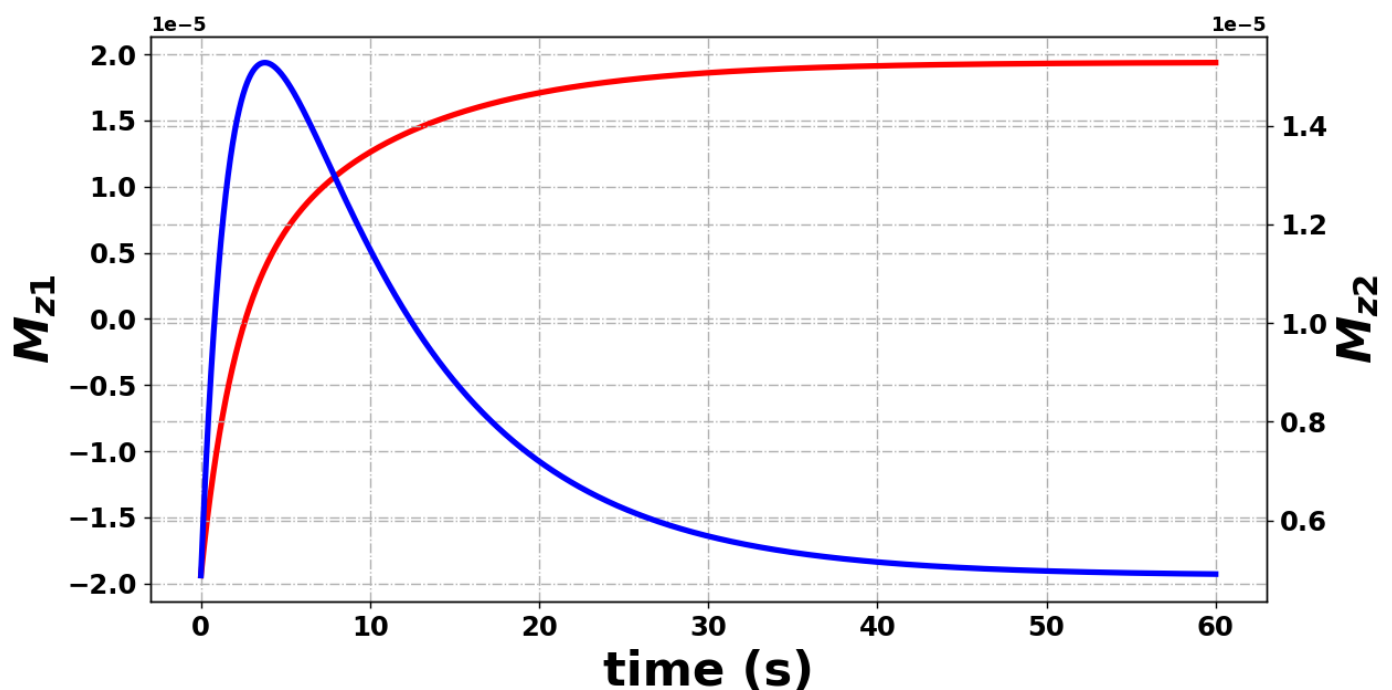
System.PlottingMulti(4, [t, t], [Mz1, Mz2], "time (s)", "Mz", ["red", "blue"])
```



```
/opt/anaconda3/lib/python3.9/site-packages/numpy/core/_asarray.py:102: ComplexWarning: Casting complex values to real discards the imaginary part
  return array(a, dtype, copy=False, order=order)
/opt/anaconda3/lib/python3.9/site-packages/numpy/core/_asarray.py:102: ComplexWarning: Casting complex values to real discards the imaginary part
  return array(a, dtype, copy=False, order=order)
No handles with labels found to put in legend.
```

In [17]:

```
"""
Mz1: Red
Mz2: Blue
"""
System.PlottingTwin(5,t,Mz1,Mz2,"time (s)",r"$M_{z1}$",r"$M_{z2}$","red","Blue")
```



```
/opt/anaconda3/lib/python3.9/site-packages/numpy/core/_asarray.py:102: ComplexWarning: Casting complex values to real discards the imaginary part
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```

```
ting complex values to real discards the imaginary part
    return array(a, dtype, copy=False, order=order)
No handles with labels found to put in legend.
```

Any suggestion? write to me

If you see something is wrong please write to me, so that the PyOR can be error free.

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In []: