# Python On Resonance (PyOR)

## Everybody can simulate NMR

## Version: Jeener

## Tutorial: Introduction to PyOR - NOE (Liouville Space - Exponential Propagation - Sparse Matrix)

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## Define the Path to PyOR source code, PythonOnResonance.py

In [1]:
```
pathSource = '/media/HD2/Vineeth/PostDoc_Simulations/Github/PyOR_V1/Source'
```

## Load Python packages

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 *
```

## Define Spin System (Two Spin Half)

In [3]:
```
Spin_list = [1/2, 1/2]
```

## Define the unit of Hamiltonian

hbarEQ1 is True, then unit of Hamiltonian is in angular frequency

In [4]:
```
hbarEQ1 = True
```

## Generate the spin operators: Sx, Sy and Sz

Sx [ i ], Sy [ i ] and Sz [ i ]

'i' is the index of the spin

In [5]:
```
System = PyOR.Numerical_MR(Spin_list,hbarEQ1)

Sx,Sy,Sz = System.SpinOperator()
```

## Generate the spin operators: S+ and S-

Sp [ i ] and Sm [ i ]

'i' is the index of the spin

In [6]:
```
Sp,Sm = System.PMoperators(Sx,Sy)
```

## Generating Zeeman Hamiltonian (Lab and Rotating Frame)

In [7]:
```
# Gyromagnetic Ratio
Gamma = [System.gammaH1,System.gammaH1]
```

In [8]:
```
# B0 Field in Tesla, Static Magnetic field (B0) along Z
B0 = 9.4
```

In [9]:
```
# Rotating Frame Frequency
OmegaRF = [-System.gammaH1*B0,-System.gammaH1*B0]
```

In [10]:
```
# Offset Frequency in rotating frame (Hz)
Offset = [10.0,20.0]
```

In [11]:
```
# generate Larmor Frequencies
LarmorF = System.LarmorFrequency(Gamma,B0,Offset)
```

```
Larmor Frequency in MHz:  [-400.22802765 -400.22803765]
```

In [12]:
```
# Lab Frame Hamiltonian
Hz_lab = System.Zeeman(LarmorF,Sz)
```

In [13]:
```
# Rotating Frame Hamiltonian
Hz = System.Zeeman_RotFrame(LarmorF,Sz,OmegaRF)
```

## Zeeman Hamiltonian in Liouville Space (Sparse Matrix)

Sparse: True (Default: False)

In [14]:
```
System.Sparse_Matrix(True)
Hz_L = System.CommutationSuperoperator(Hz)
print(Hz_L)
```

```
(1, 1)        (-125.66370630264282+0j)
(2, 2)        (-62.83185291290283+0j)
(3, 3)        (-188.49555921554565+0j)
(4, 4)        (125.66370630264282+0j)
(6, 6)        (62.83185338973999+0j)
(7, 7)        (-62.83185291290283+0j)
(8, 8)        (62.83185291290283+0j)
(9, 9)        (-62.83185338973999+0j)
(11, 11)      (-125.66370630264282+0j)
(12, 12)      (188.49555921554565+0j)
(13, 13)      (62.83185291290283+0j)
(14, 14)      (125.66370630264282+0j)
```

## Initialize Density Matrix

In [15]:

```
Thermal_DensMatrix = True

if Thermal_DensMatrix:
    # Spin temperature of individual spins (initial) Kelvin
    Tin = [300.0,300.0]

    # Spin temperature of individual spins (equlibrium) Kelvin
    Tfi = [300.0,300.0]

    # High Temperature
    HT_approx = False

    # Initial Density Matrix
    rho_in = System.EqulibriumDensityMatrix_Advance(LarmorF,Sz,Tin,HT_approx)

    # Equlibrium Density Matrix
    rhoeq = System.EqulibriumDensityMatrix_Advance(LarmorF,Sz,Tfi,HT_approx)
else:
    rho_in = np.sum(Sz,axis=0)
    rhoeq = np.sum(Sz,axis=0)
```

```
Trace of density metrix =  1.0
Trace of density metrix =  1.0
```

## Converting initial and equlibrium density matrix into Liouvillian

In [16]:

```
rho_in_L = System.Vector_L(rho_in)
rhoeq_L = System.Vector_L(rhoeq)
```

## Pulse (Liouville Space)

In [17]:

```
flip_angle1 = 0.0
flip_angle2 = 180.0

rho_L = System.Rotate_L(rho_in_L,flip_angle1,Sy[0])
rho_L = System.Rotate_L(rho_L,flip_angle2,Sy[1])
```

## Relaxation in Liouville Space

In [18]:

```
R = None
Rprocess = "Auto-correlated Dipolar Homonuclear"
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)
```

In [19]:

```
print(R_L)
```

```
 (0, 0)        (0.15958496611406095+0j)
 (5, 0)        (-0.026631091045127824+0j)
 (6, 0)        (-0.026631091045127824+0j)
 (9, 0)        (-0.026631091045127824+0j)
 (10, 0)       (-0.026631091045127824+0j)
 (15, 0)       (-0.10632278402380532+0j)
 (1, 1)        (0.15083679390706045+0j)
 (2, 1)        (0.06216166689049526+0j)
 (7, 1)        (0.026631091045127824+0j)
 (11, 1)       (0.026631091045127824+0j)
 (1, 2)        (0.06216166689049526+0j)
 (2, 2)        (0.15083679390706045+0j)
 (7, 2)        (0.026631091045127824+0j)
 (11, 2)       (0.026631091045127824+0j)
 (3, 3)        (0.15958496611406095+0j)
 (4, 4)        (0.15083679390706045+0j)
 (8, 4)        (0.06216166689049526+0j)
 (13, 4)       (0.026631091045127824+0j)
 (14, 4)       (0.026631091045127824+0j)
 (0, 5)        (-0.026631091045127824+0j)
 (5, 5)        (0.07102747001221649+0j)
 (6, 5)        (0.026631091045127824+0j)
 (9, 5)        (0.026631091045127824+0j)
 (10, 5)       (-0.01776528792196085+0j)
 (15, 5)       (-0.026631091045127824+0j)
 :     :
 (0, 10)       (-0.026631091045127824+0j)
 (5, 10)       (-0.01776528792196085+0j)
 (6, 10)       (0.026631091045127824+0j)
 (9, 10)       (0.026631091045127824+0j)
 (10, 10)      (0.07102747001221649+0j)
 (15, 10)      (-0.026631091045127824+0j)
 (1, 11)       (0.026631091045127824+0j)
 (2, 11)       (0.026631091045127824+0j)
 (7, 11)       (0.06216166689049526+0j)
 (11, 11)      (0.15083679390706045+0j)
 (12, 12)      (0.15958496611406095+0j)
 (4, 13)       (0.026631091045127824+0j)
 (8, 13)       (0.026631091045127824+0j)
 (13, 13)      (0.15083679390706045+0j)
 (14, 13)      (0.06216166689049526+0j)
 (4, 14)       (0.026631091045127824+0j)
 (8, 14)       (0.026631091045127824+0j)
 (13, 14)      (0.06216166689049526+0j)
 (14, 14)      (0.15083679390706045+0j)
 (0, 15)       (-0.10632278402380532+0j)
 (5, 15)       (-0.026631091045127824+0j)
 (6, 15)       (-0.026631091045127824+0j)
 (9, 15)       (-0.026631091045127824+0j)
 (10, 15)      (-0.026631091045127824+0j)
 (15, 15)      (0.15958496611406095+0j)
```

# Evolution of Density Matrix Liouville Space

In [20]:

```
dt = 0.0001
AQ = 50.0
Npoints = int(AQ/dt)
```

```
method = "Relaxation Sparse"
System.ODE_Method('DOP853')

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

```
Total time = 2.959740161895752 seconds
```

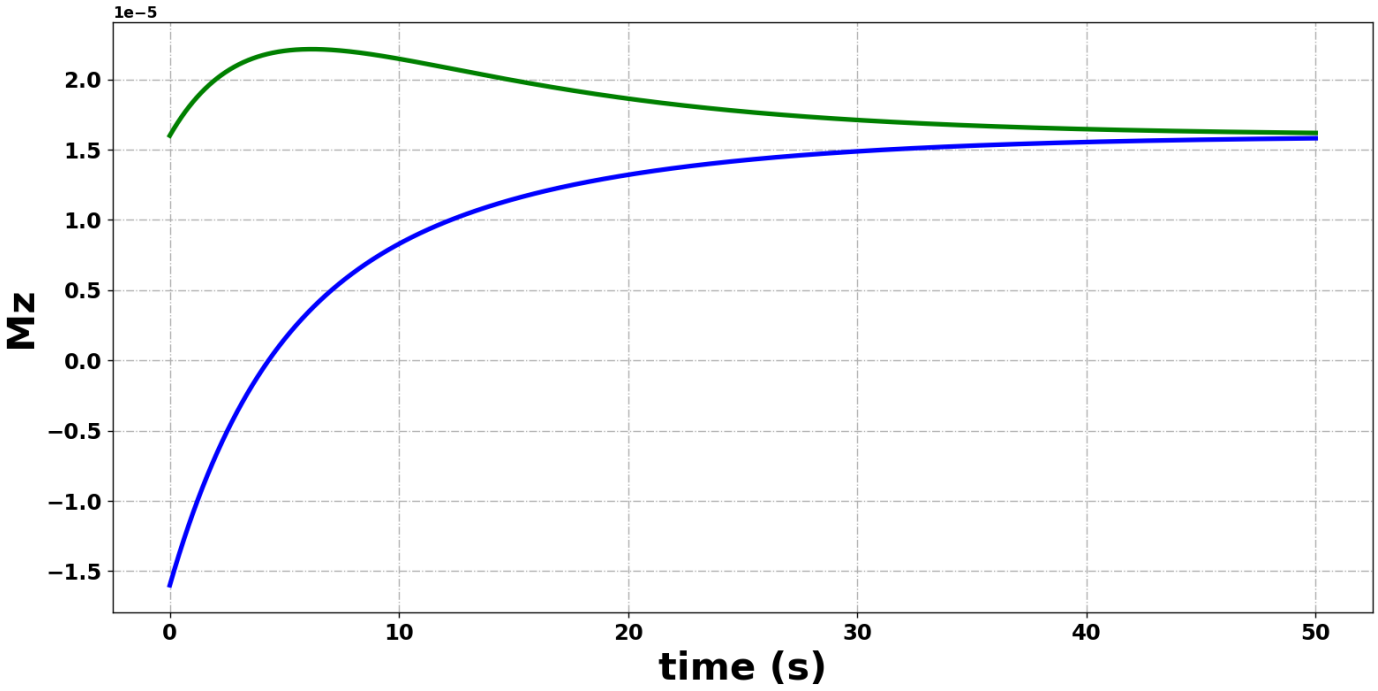
# Expectation value (Liouville Space)

In [21]:
```
det_Z1 = Sz[0]
det_Z2 = Sz[1]

LEXP_Z1 = System.Detection_L(det_Z1)
LEXP_Z2 = System.Detection_L(det_Z2)
```

In [22]:
```
t, MZ_1 = System.Expectation_L(rho_t,LEXP_Z1,dt,Npoints)
t, MZ_2 = System.Expectation_L(rho_t,LEXP_Z2,dt,Npoints)
```

In [23]:
```
System.PlottingMulti(4,[t,t],[MZ_1,MZ_2],"time (s)","Mz",["green","blue"])
```




```
/opt/anaconda3/lib/python3.9/site-packages/numpy/core/_asarray.py:102: ComplexWarning: Cas
ting 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: Cas
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.
```

# Remarks

If you see something is wrong, please write to me.

Any suggestion? write to me

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