Python On Resonance (PyOR)

Everybody can simulate NMR

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Tutorial 12: Homonuclear Nuclear Overhauser effect (NOE)

In this tutorial you will see Homonuclear Nuclear Overhauser effect (NOE) of two spin half system. 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]:
```python
pathSource = '/media/HD2/Vineeth/PostDoc_Simulations/Github/PyOR_G/Source'
```

In [2]:
```python
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]:
```python
"""
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]:
```python
"""
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.gammaH1]

           """
           Define the field of the spectromter, B0 in Tesla.
           """
           B0 = 9.4

           """
           Define the chemical Shift of individual spins
           Offset = [chemical Shift spin 1, chemical Shift spin 1, ..]
           """
           Offset = [100,500] # 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:  [-400.22811765 -400.22851765]
```

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 equlibrium

           First Case
           """;

           Thermal_DensMatrix = False

           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.EqulibriumDensityMatrix(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)  # Equlibrium Density Matrix
        print("Trace of density metrix = ", np.trace(rho_in))
```

Trace of density metrix = 0j

In [8]:
```
Basis = 'PMZ spin half'
B_car = System.TwoSpinOP(Sx,Sy,Sz,Sp,Sm,Basis)
```

Basis: $\frac{1}{2}E, \frac{1}{\sqrt{2}}I_+, \frac{1}{\sqrt{2}}I_-, \frac{1}{\sqrt{2}}I_z, \frac{1}{\sqrt{2}}S_+, \frac{1}{\sqrt{2}}S_-, S_z, \sqrt{2}I_xS_z, \sqrt{2}I_yS_z, \sqrt{2}I_zS_x, \sqrt{2}I_zS_y, 2I_zS_z, I_+S_+, I_+S_-, I_-S_+, I_-S_-$

Zeeman Halitonian in Rotating Frame

In [9]:
```
OmegaRF = [-System.gammaH1*B0,-System.gammaH1*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] = 10.5
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", "Dipolar"
""";
R = None
Rprocess = "Dipolar"
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 [14]:
```
R_redkite, Basis_L = System.Transform_Redkite(R_L,Sp,Sm,Sz)
```

$S_-I_-, S_-I_z, S_zI_-, S_-, I_-, S_-I_+, S_+I_-, S_zI_z, I_z, S_z, E, S_+I_z, S_zI_+, S_+, I_+, S_+I_+$

## Eigen Values of Commutation Hamiltonian superoperator

In [15]:
```
"""
Zero Quantum index: 0-5
Singel Quantum index: 6-13
Double Quantum index: 14-15
"""

index_basis = 15
print("Eigen Values (MHz): ", np.dot(Hz_L@Basis_L[:,index_basis],Basis_L[:,index_basis]).r
```

```
Eigen Values (MHz):  -800.4566352936044
```

Plotting the Redkite

In [16]:
```
System.PlotLabel_Hilbert = False
System.Redkite_Label_SpinDynamica = True
System.MatrixPlot(1,R_redkite.real)
```
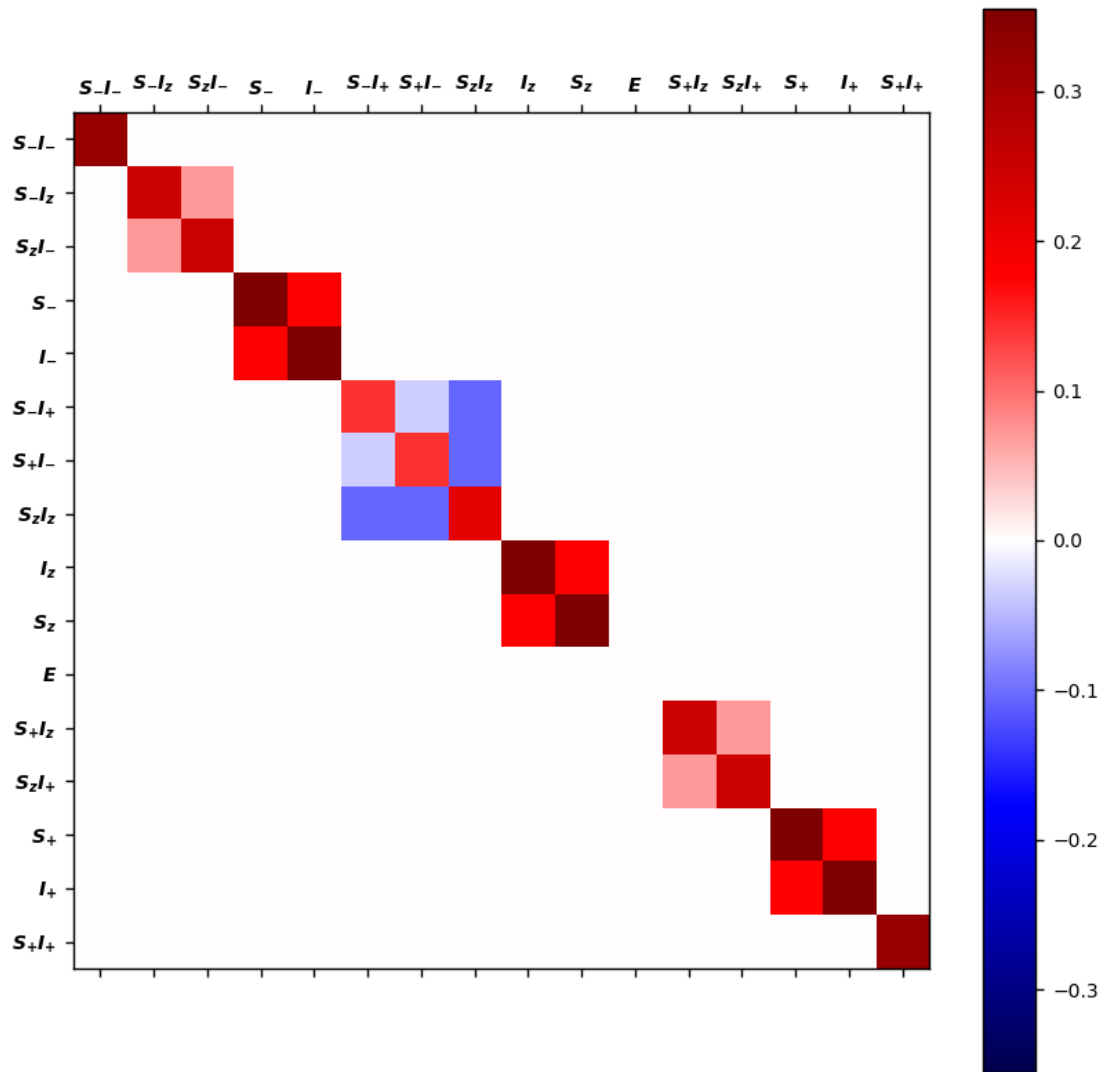
Evolution of Density Matrix

In [17]:
```python
dt = 0.0005
AQ = 30.0
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,Hzr_L + Hj_L - 1j * R_L,dt,Npoints,methc
end_time = time.time()
timetaken = end_time - start_time
print("Total time = %s seconds " % (timetaken))
```

Number of points in the simulation 60000

```
Total time = 0.19527482986450195 seconds
```
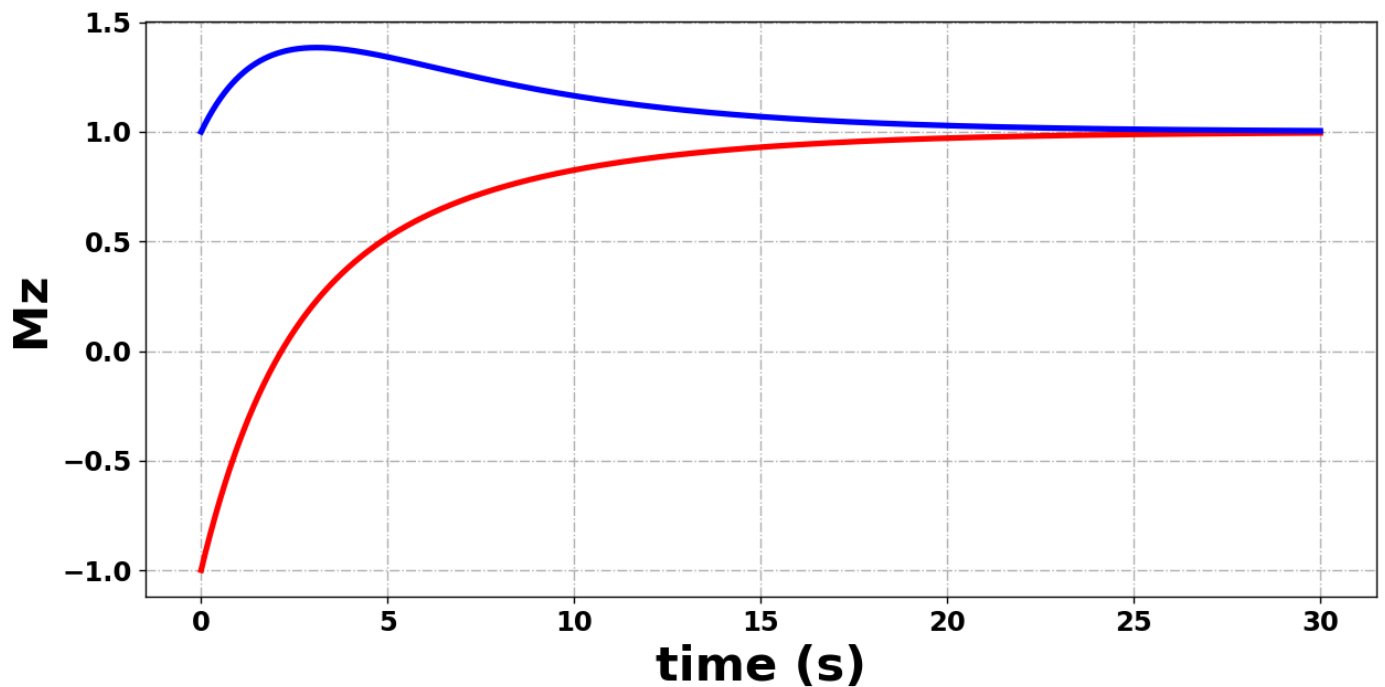
Expectation value

In [18]:
```python
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 [19]:
```python
"""
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: 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.
```

In [20]:
```python
"""
Mz1: Red
Mz2: Blue
"""
System.PlottingTwin(5,t,Mz1,Mz2,"time (s)",r"$M_{z1}$",r"$M_{z2}$","red","Blue")
```
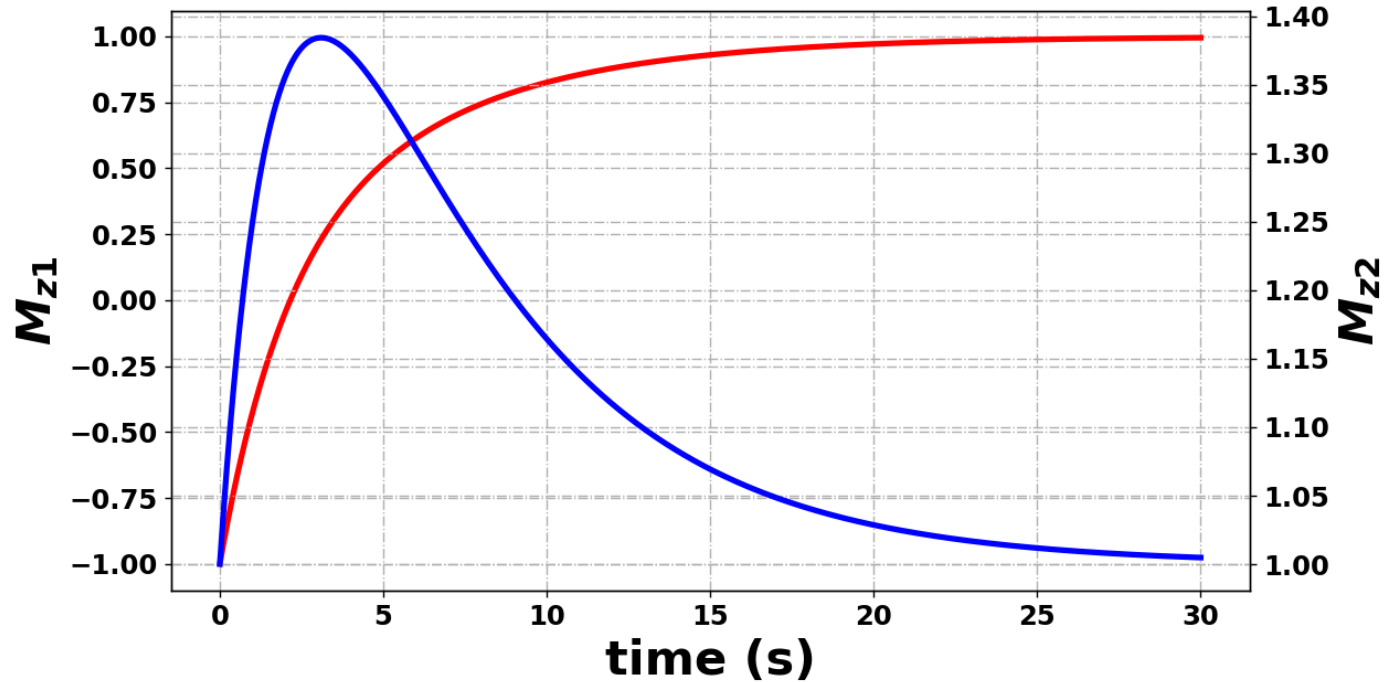
```
/opt/anaconda3/lib/python3.9/site-packages/numpy/core/_asarray.py:102: ComplexWarning: Cas
ting complex values to real discards the imaginary part
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/opt/anaconda3/lib/python3.9/site-packages/numpy/core/_asarray.py:102: ComplexWarning: Cas
ting complex values to real discards the imaginary part
  return array(a, dtype, copy=False, order=order)
No handles with labels found to put in legend.
```

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 [ ]: