Python On Resonance (PyOR)

Everybody can simulate NMR

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Tutorial 5: Evolution of Density Matrix in Hilbert Space Part 2

In previous tutorial, we try to evolve the density matrix in time by solving Liouville-Von Neumann equation in Hilbert Space for a single spin half system. In this tutorial we will see two spin half system with out coupling.

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

In [51]:
```
pathSource = '/media/HD2/Vineeth/PostDoc_Simulations/Github/PyOR_G/Source'
```

In [52]:
```
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 [53]:
```
"""
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 [54]:
```
"""
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 [55]:
```
"""
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 [56]:
```
"""
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 = [20,40] # 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:  [-400.22803765 -400.22805765]
```

Initialize Density Matrix

In [57]:
```
"""
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))
```

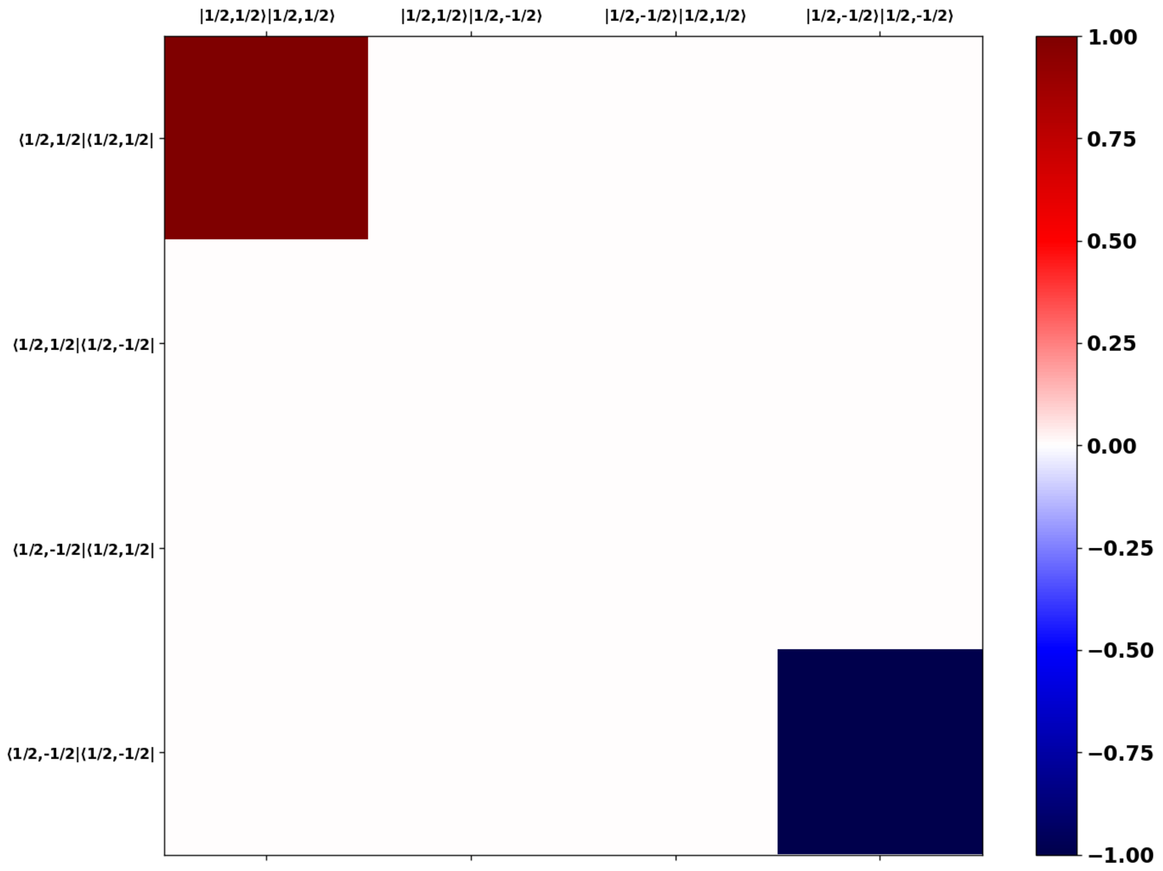
```
Trace of density metrix =  0j
```

In [58]:
```
Matrix(rho_in)
```

Out[58]:

$$\begin{bmatrix} 1.0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1.0 \end{bmatrix}$$

In [59]:
```
System.MatrixPlot(1,rho_in.real)
```



```
/media/HD2/Vineeth/PostDoc_Simulations/Github/PyOR_G/Source/PythonOnResonance.py:669: User
Warning: FixedFormatter should only be used together with FixedLocator
  ax.set_xticklabels([''] + labelx,fontsize=10)
/media/HD2/Vineeth/PostDoc_Simulations/Github/PyOR_G/Source/PythonOnResonance.py:670: User
Warning: FixedFormatter should only be used together with FixedLocator
  ax.set_yticklabels([''] + labely,fontsize=10)
```

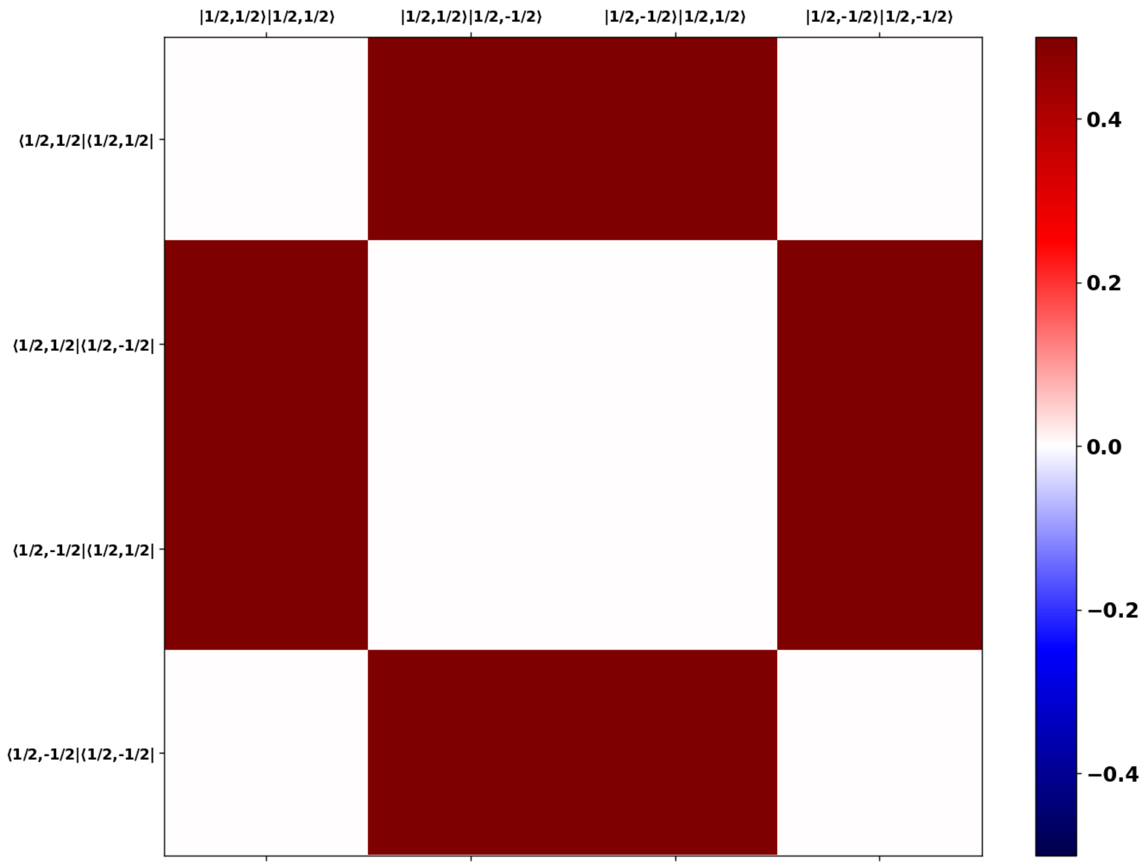
Zeeman Halitonian in Rotating Frame

In [60]:
```
OmegaRF = [-System.gammaH1*B0,-System.gammaH1*B0]
Hzr = System.Zeeman_RotFrame(LarmorF, Sz, OmegaRF)
```

Pulse

In [61]:
```
"""
Rotate the magnetization about Y-axis, by an angle theta.
""";
pulse_angle = 90.0
rho = System.Rotate_H(rho_in,pulse_angle,np.sum(Sy,axis=0))
```

In [62]:
```
System.MatrixPlot(2,rho.real)
```



Relaxation Constant

In [63]:
```
'''
Define longitudinal (R1) and transverse Relaxation (R2)
R1 = [R1 of first spin, R1 of second spin,...]
R2 = [R2 of first spin, R2 of second spin,...]
''';

R1 = np.asarray([0,0])
R2 = np.asarray([0,0])
System.Relaxation_Constants(R1,R2)
```

```
'''
Options for "Rprocess": "No Relaxation" or "Phenomenological"
                         or "Random Field Fluxtuation" or "Dipolar"
''';
Rprocess = "No Relaxation"
```

Evolution of Density Matrix

In [64]:
```
"""
Samplling Rate, fs = n * Highest_Larmor_Frequency; minimum value of n = 2 (Nyquist-Shannon
Dwell time, dt = 1/fs
Acquisition time, AQ is time for which we evolve the density matrix, in seconds.
Number of points in the simulation, Npoints
""";
Highest_Larmor_Frequency = 40.0
fs = 4 * Highest_Larmor_Frequency
dt = 1.0/fs
AQ = 5.0
Npoints = int(AQ/dt)
print("Number of points in the simulation", Npoints)

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

start_time = time.time()
t, rho_t = System.Evolution_H(rhoeq,rho,Sx,Sy,Sz,Sp,Sm,Hzr,dt,Npoints,method,Rprocess)
end_time = time.time()
timetaken = end_time - start_time
print("Total time = %s seconds " % (timetaken))
```

```
Number of points in the simulation 800
Total time = 0.010149955749511719 seconds
```

Expectation value

In [65]:
```
"""
Basis Operators in plus minus Z
""";
Basis = "PMZ spin half"
B_PMZ = System.TwoSpinOP(Sx,Sy,Sz,Sp,Sm,Basis)
```

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

In [66]:
```
"""
Lets see the expectation value of I+ and S+
""";

t, Mp = System.Expectation_H(rho_t,B_PMZ[1] + B_PMZ[4],dt,Npoints)
```

Windowing

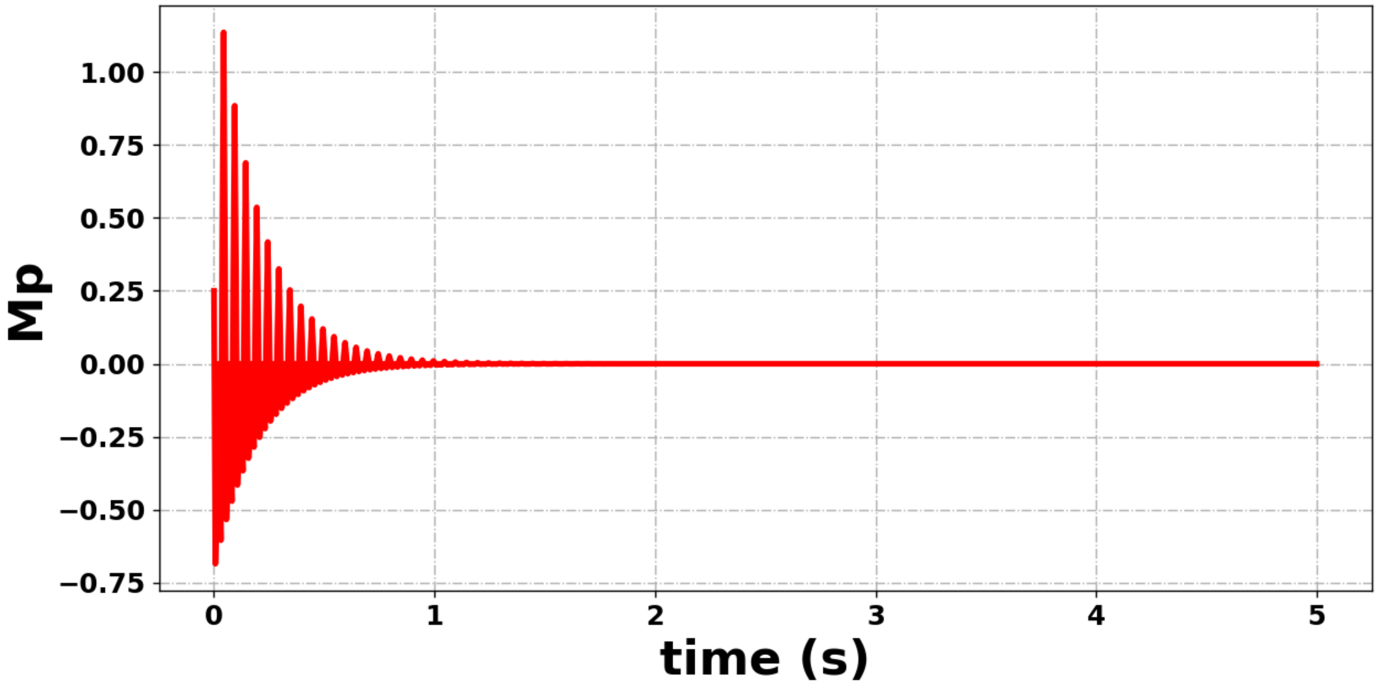
In [67]:
```
Mp = System.WindowFunction(t,Mp,5.0)
```

Fourier Transform

In [68]:
```
fs = 1.0/dt
freq, spectrum = System.FourierTransform(Mp,fs,5)
```

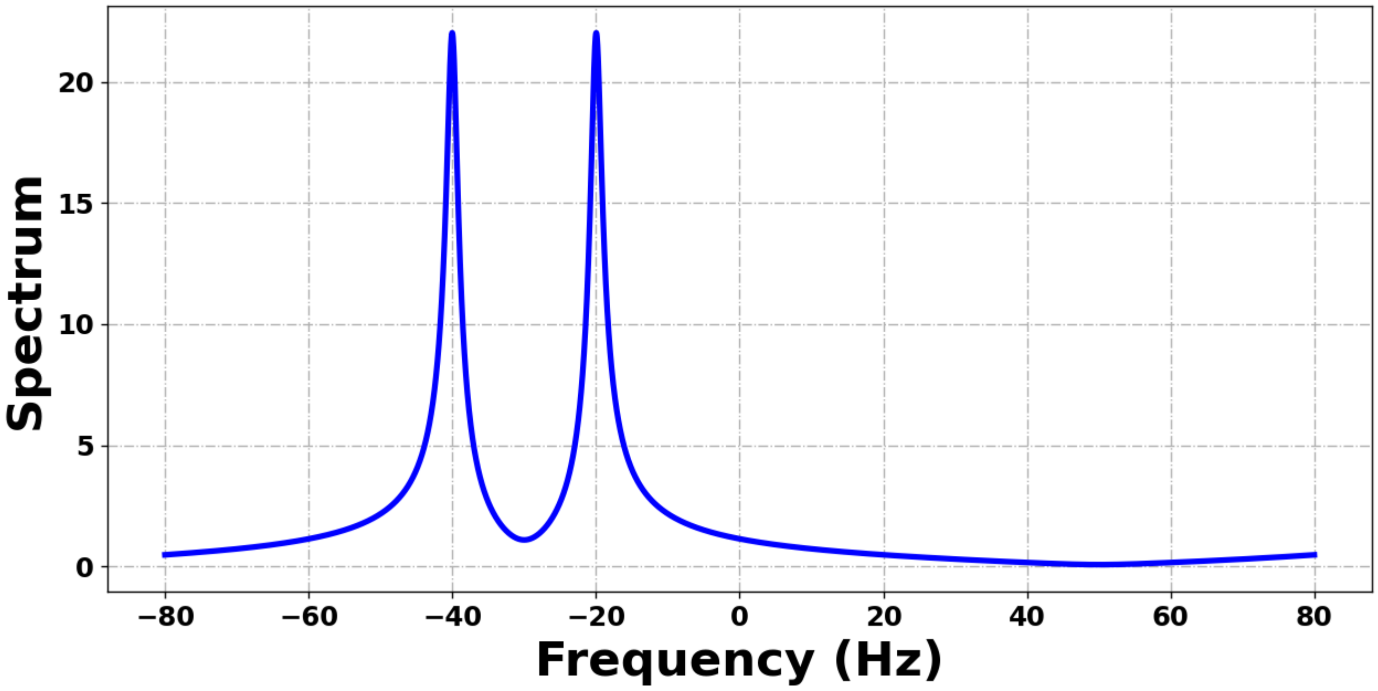
Plotting

In [69]:
```
System.Plotting(3,t,Mp,"time (s)","Mp","red")
```



```
/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 [71]:
```
System.Plotting(4,freq,np.absolute(spectrum),"Frequency (Hz)","Spectrum","blue")
```



```
No handles with labels found to put in legend.
```

Next tutorial: Evolution of Density Matrix in Hilbert Space Part 3

In this lecture you will see how to evolve the desnity matrix in time by solving Liouville-Von Neumann equation in Hilbert Space of 6 spin half system (ethanol).

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 [ ]:

```

```