Python On Resonance (PyOR)

Everybody can simulate NMR

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Tutorial 5: Evolution of Density Matrix in Hilbert Space Part 1

In previous tutorial, we saw how to generate initial density matrix for two spin system a electron and a proton at thermal equlibrium. In this 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

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

In [67]:

```
pathSource = '/media/HD2/Vineeth/PostDoc_Simulations/Github/PyOR_G/Source'
```

In [68]:

```
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 [69]:

```
"""
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]
```

In [70]:

```
"""
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 [71]:
```
"""
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 [72]:
```
"""
Gyromagnetic Ratio
Gamma = [Gyromagnetic Ratio spin 1, Gyromagnetic Ratio spin 1, ...]
""";
Gamma = [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] # 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]
```

Initialize Density Matrix

In [73]:
```
"""
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 [74]:

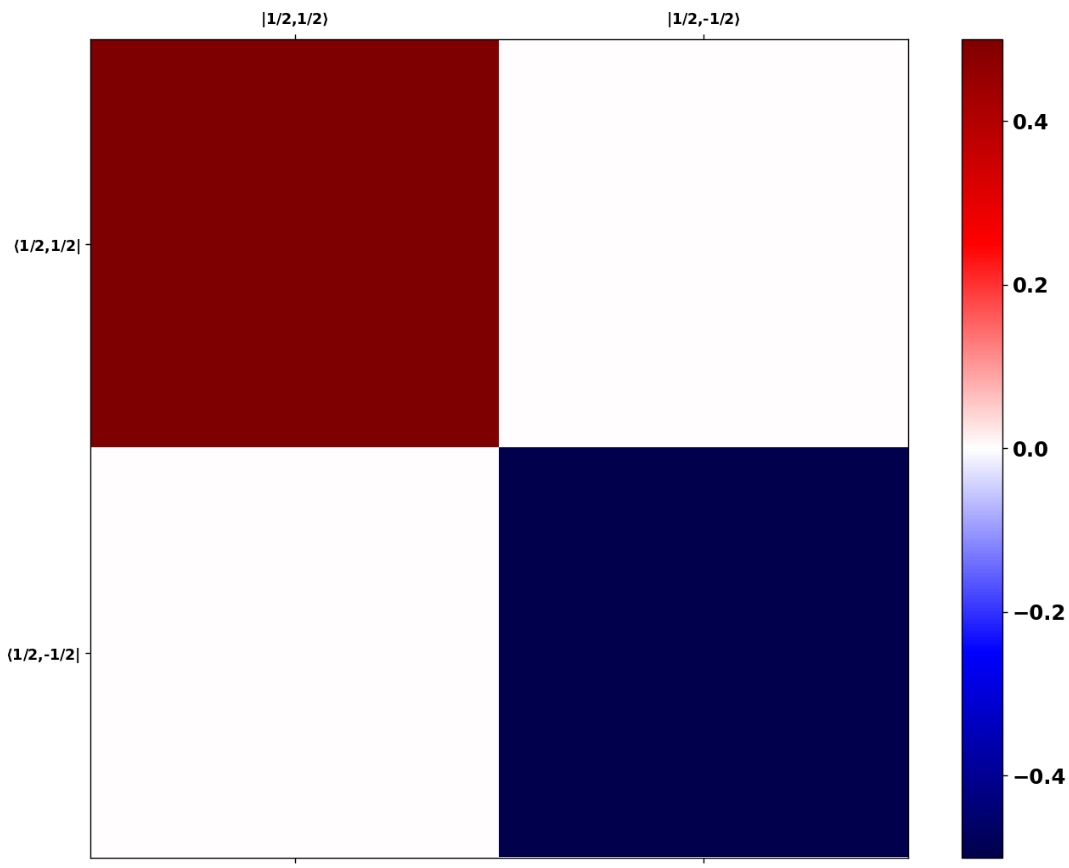
```
Matrix(rho_in)
```

Out[74]:

$$\begin{bmatrix} 0.5 & 0 \\ 0 & -0.5 \end{bmatrix}$$

In [75]:

```
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 [76]:

```
OmegaRF = [-System.gammaH1*B0]
```

```
Hzr = System.Zeeman_RotFrame(LarmorF, Sz, OmegaRF)
```

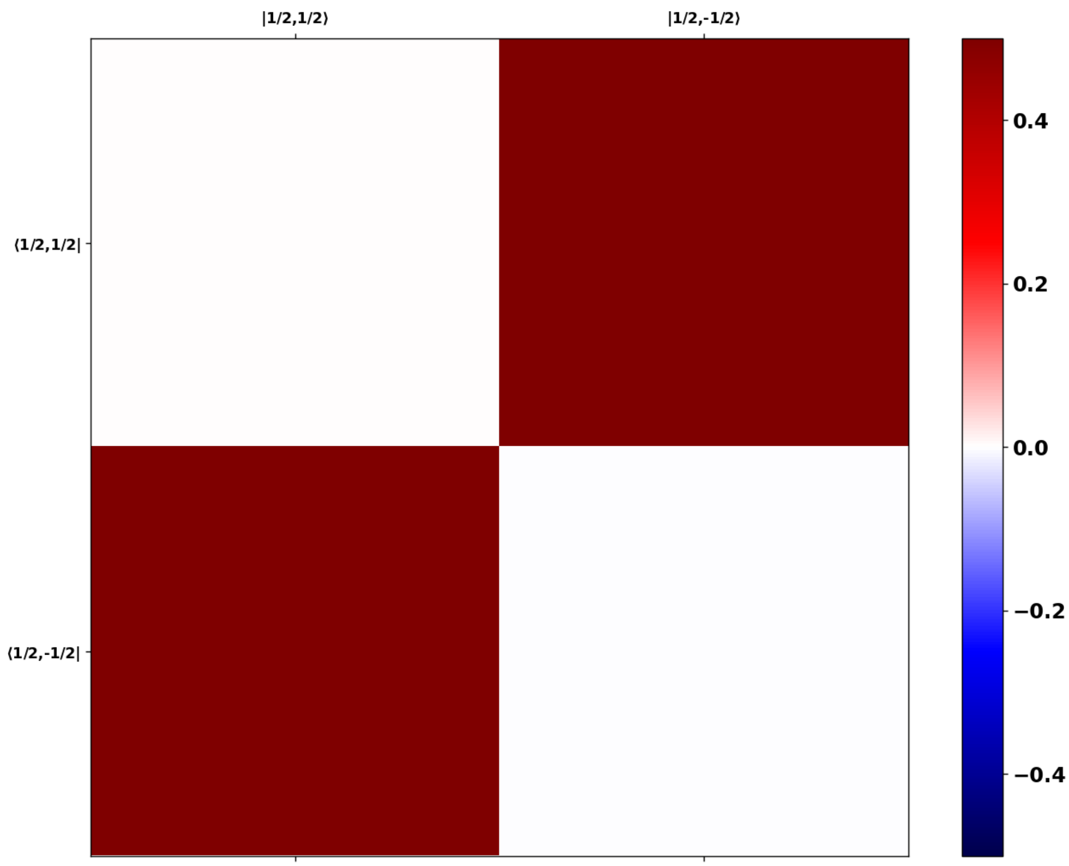
Pulse

In [77]:

```
"""
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 [78]:

```
System.MatrixPlot(2,rho.real)
```



Relaxation Constant

In [79]:

```
'''
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])
R2 = np.asarray([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 [80]:

```
"""
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 = 20.0
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 400
Total time = 0.003989934921264648 4 seconds
```

Expectation value

In [81]:

```
"""
Basis Operators in plus minus Z
""";
Basis = "PMZ spin half"
B_PMZ = System.SingleSpinOP(Sx,Sy,Sz,Sp,Sm,Basis)
```

Basis: $\frac{1}{\sqrt{2}}E,I_+,I_-,\sqrt{2}I_z$

In [82]:

```
"""
Lets see the expectation value of I+
""";

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

Windowing

In [83]:

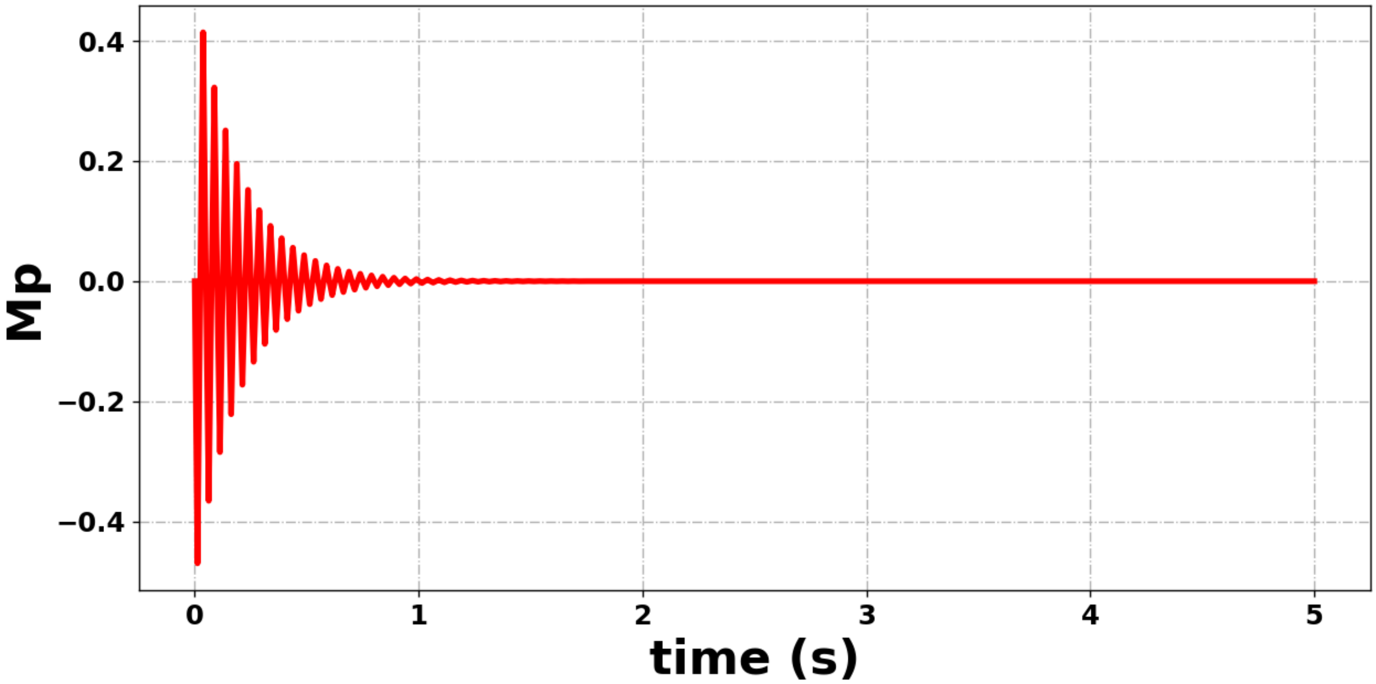
```
Mp = System.WindowFunction(t,Mp,5.0)
```

Fourier Transform

In [84]:
```
fs = 1.0/dt
freq, spectrum = System.FourierTransform(Mp,fs,5)
```

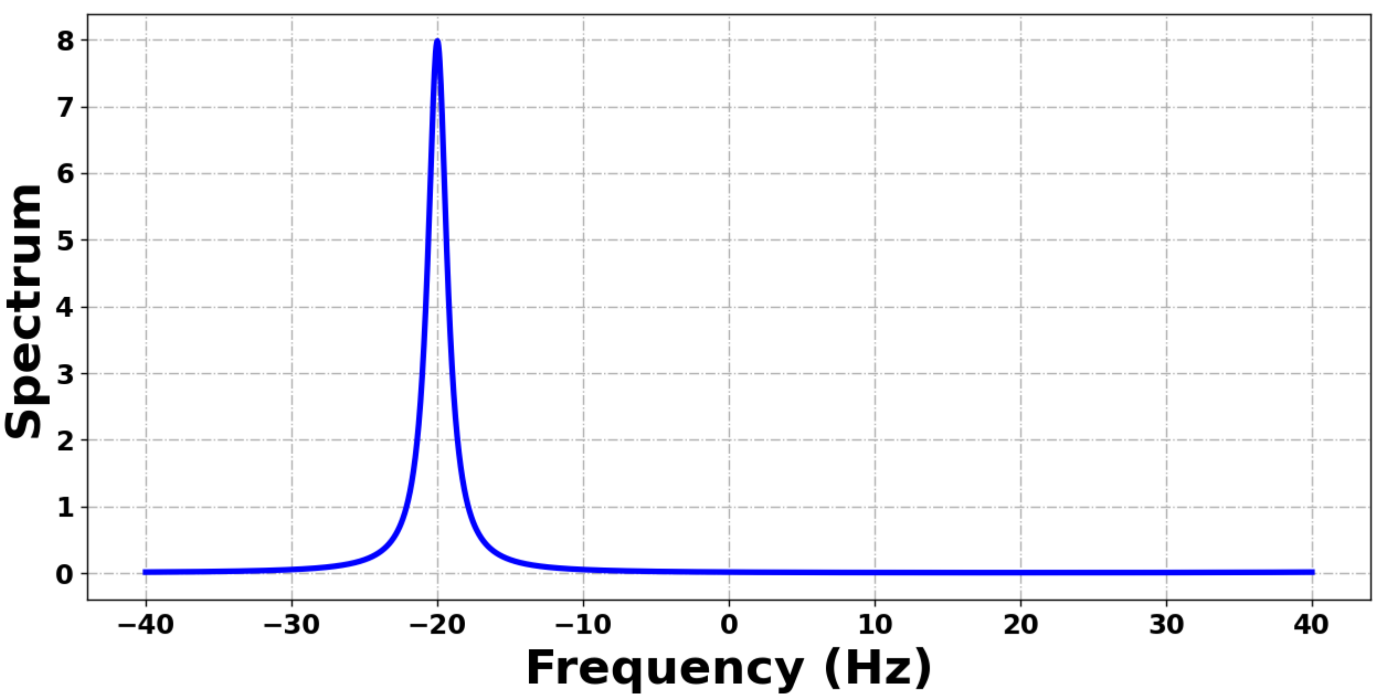
Plotting

In [85]:
```
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 [86]:
```
PH0 = 45.0
spectrum_PH0 = System.PhaseAdjust_PH0(spectrum,PH0)
System.Plotting(4,freq,spectrum_PH0,"Frequency (Hz)","Spectrum","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)
No handles with labels found to put in legend.
```

Next tutorial: Evolution of Density Matrix in Hilbert Space Part 2

In this lecture you will see how to evolve the desnity matrix in time by solving Liouville-Von Neumann equation in Hilbert Space for two spin half system.

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 [ ]:
```

```