Python On Resonance (PyOR)

Author: Vineeth Thalakottoor \ Email: vineethfrancis.physics@gmail.com

Tutorial 10: Correlation Spectroscopy (COSY) Part 2 J Coupling

In this tutorial we consider Two H1 spins (Homonuclear)

Reference book - "NMR: The Toolkit, How Pulse Sequences Work" by P.J Hore, J.A. Jones and S. Wimperis

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 *
from IPython.display import display, Math, Latex
```

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.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 = [150, 200] # 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:  [-400.22816765 -400.22821765]
```

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 = Sz[0] # 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]:

```
'''
Operator Basis
Option: 'Cartesian spin half' and 'PMZ spin half'
All the 16 operator basis are loaded in the matrix, 'B_car'
''';
Basis = 'Cartesian spin half'
B_car = System.TwoSpinOP(Sx,Sy,Sz,Sp,Sm,Basis)
```

Basis: $\frac{1}{2}E$,I_x,I_y,I_z,S_x,S_y,S_z,$2I_xS_z$,$2I_yS_z$,$2I_zS_x$,$2I_zS_y$,$2I_zS_z$,$2I_xS_x$,$2I_xS_y$,$2I_yS_x$,$2I_yS_y$

In [9]:

```
'''
B_car[0] = B0 = 1/2 E,
B_car[1] = B1 = Ix,
so on...
Hope you understand.
'''
System.OperatorBasis('Cartesian')
```

Basis: B0 = $\frac{1}{2}E$, B1 = I_x, B2 = I_y, B3 = I_z, B4 = S_x, B5 = S_y, B6 = S_z, B7 = $2I_xS_z$, B8 = $2I_yS_z$, B9 = $2I_zS_x$, B10 = $2I_zS_y$, B11 = $2I_zS_z$, B12 = $2I_xS_x$, B13 = $2I_xS_y$, B14 = $2I_yS_x$, B15 = $2I_yS_y$

In [10]:

```
'''
A density matrix (rho) can be written as:
rho = a B0 + b B1 + c B2 + ...
where B0, B1,... are operator basis.

Components of initial density matrix in cartesian basis
''';
Matrix(System.DensityMatrix_Components(B_car,rho_in))
```

Out[10]:

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

Zeeman Halitonian in Rotating Frame

In [11]:
```
OmegaRF = [-System.gammaH1*B0,-System.gammaH1*B0,-System.gammaH1*B0]
Hz = System.Zeeman_RotFrame(LarmorF, Sz, OmegaRF)
```

J Coupling Hamiltonian

In [12]:
```
'''
Define J couplings between individual spins
'''
Jlist = np.zeros((len(Slist1),len(Slist1)))
Jlist[0][1] = 10.5
Hj = System.Jcoupling_Weak(Jlist,Sz)
```

Total Hamiltonian

In [13]:
```
Htotal = Hz + Hj
```

Relaxation Constant

In [14]:
```
# Define longitudinal and transverse Relaxation
R1 = 0
R2 = 5
System.Relaxation_Constants(R1,R2)
Rprocess = "Phenomenological"
```

90 deg on spin 1

In [15]:
```
rho = System.Rotate_H(rho_in,90,Sx[0])
```

In [16]:
```
# Components of density matrix in cartesian basis
Matrix(System.DensityMatrix_Components(B_car,rho))
```

Out[16]:

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

Evolution

In [17]:

```
dt = 0.0005 #50e-6
delay = 1/(3 * Jlist[0][1]) # 1/2J
Dpoints = int(delay/dt)
print("Npoints = ", Dpoints)
method = "ODE Solver"

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

```
Npoints =  63
Total time = 0.29392361640930176 seconds
```

In [18]:

```
# Components of density matrix in cartesian basis
Matrix(System.DensityMatrix_Components(B_car,rho_t[-1]))
```

Out[18]:

$$\begin{bmatrix} 0 \\ 0.462846956633725 \\ 0.073307756649634 \\ 0 \\ 0 \\ 0 \\ 0 \\ -0.124625897122948 \\ 0.786856950563665 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

90 deg Pulse on all spins

In [19]:
```
rho1 = System.Rotate_H(rho_t[-1],90,np.sum(Sx,axis=0))
```

In [20]:
```
# Components of density matrix in cartesian basis
Matrix(System.DensityMatrix_Components(B_car,rho1))
```

Out[20]:
$$\begin{bmatrix} 0 \\ 0.462846956633725 \\ 0 \\ 0.073307756649634 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -0.786856950563665 \\ 0 \\ 0 \\ 0.124625897122948 \\ 0 \\ 0 \end{bmatrix}$$

Detection

In [21]:
```
AQ = 3.0
Npoints = int(AQ/dt)
print("Npoints = ", Npoints)
```

```
method = "ODE Solver"

start_time = time.time()
t1, rho_t1 = System.Evolution_H(rhoeq,rho1,Sx,Sy,Sz,Sp,Sm,Htotal,dt,Npoints,method,Rproces
end_time = time.time()
timetaken = end_time - start_time
print("Total time = %s seconds " % (timetaken))
```

```
Npoints =  6000
Total time = 17.94357991218567 seconds
```

In [22]:

```
# Components of density matrix in cartesian basis
Matrix(System.DensityMatrix_Components(B_car,rho_t1[-1]))
```

Out[22]:

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0.073307756649634 \\ -0.000435179297731539 \\ 0 \\ 0 \\ 0 \\ -0.000255991385522562 \\ 0 \\ 0 \\ 0 \\ 0 \\ 6.8888772156073 \cdot 10^{-5} \\ 0 \\ 0 \end{bmatrix}$$

Expectation Value

In [23]:

```
det1 = (B_car[1] + B_car[4]) + 1j * (B_car[2] + B_car[5])
det2 = B_car[7] + 1j * B_car[8]
det3 = B_car[13]
```

In [24]:

```
t1, Ex_det1 = System.Expectation_H(rho_t1,det1,dt,Npoints)
t1, Ex_det2 = System.Expectation_H(rho_t1,det2,dt,Npoints)
t1, Ex_det3 = System.Expectation_H(rho_t1,det3,dt,Npoints)
```

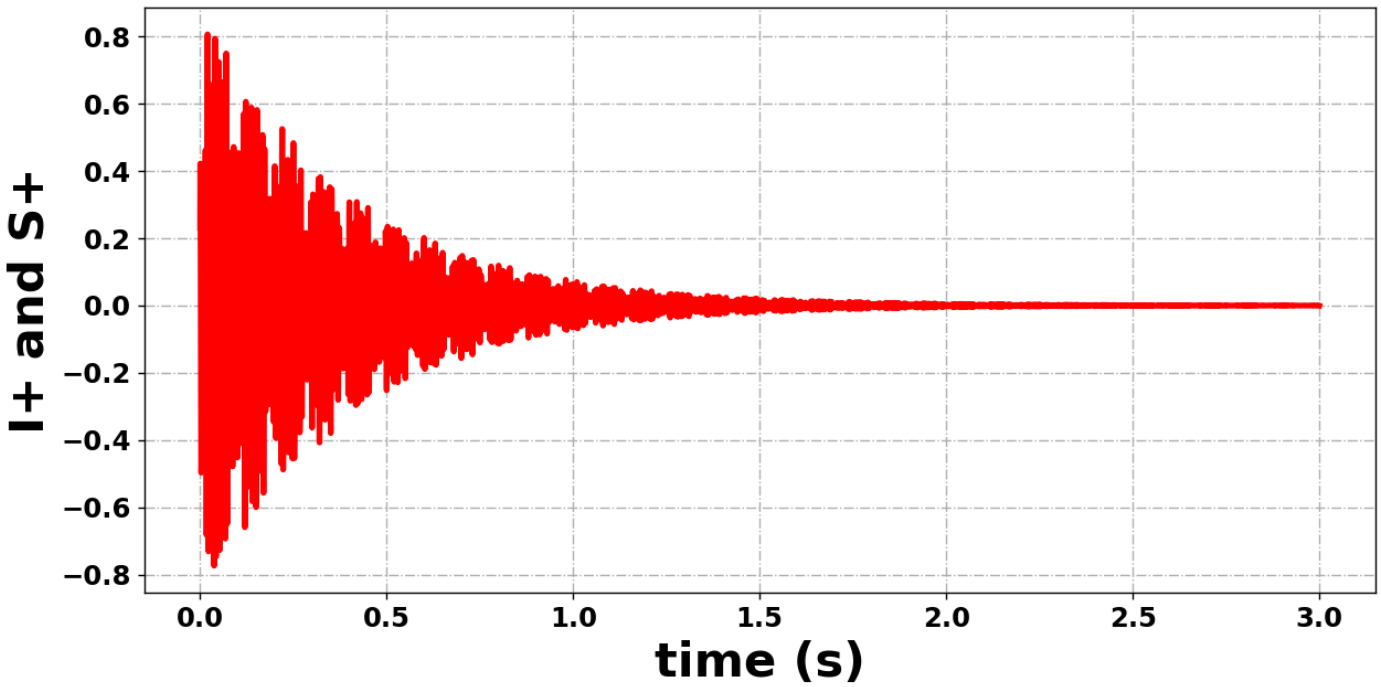
Fourier Transform

In [25]:

```
fs = 1.0/dt
freq, spectrum1 = System.FourierTransform(Ex_det1,fs,5)
freq, spectrum2 = System.FourierTransform(Ex_det2,fs,5)
freq, spectrum3 = System.FourierTransform(Ex_det3,fs,5)
```

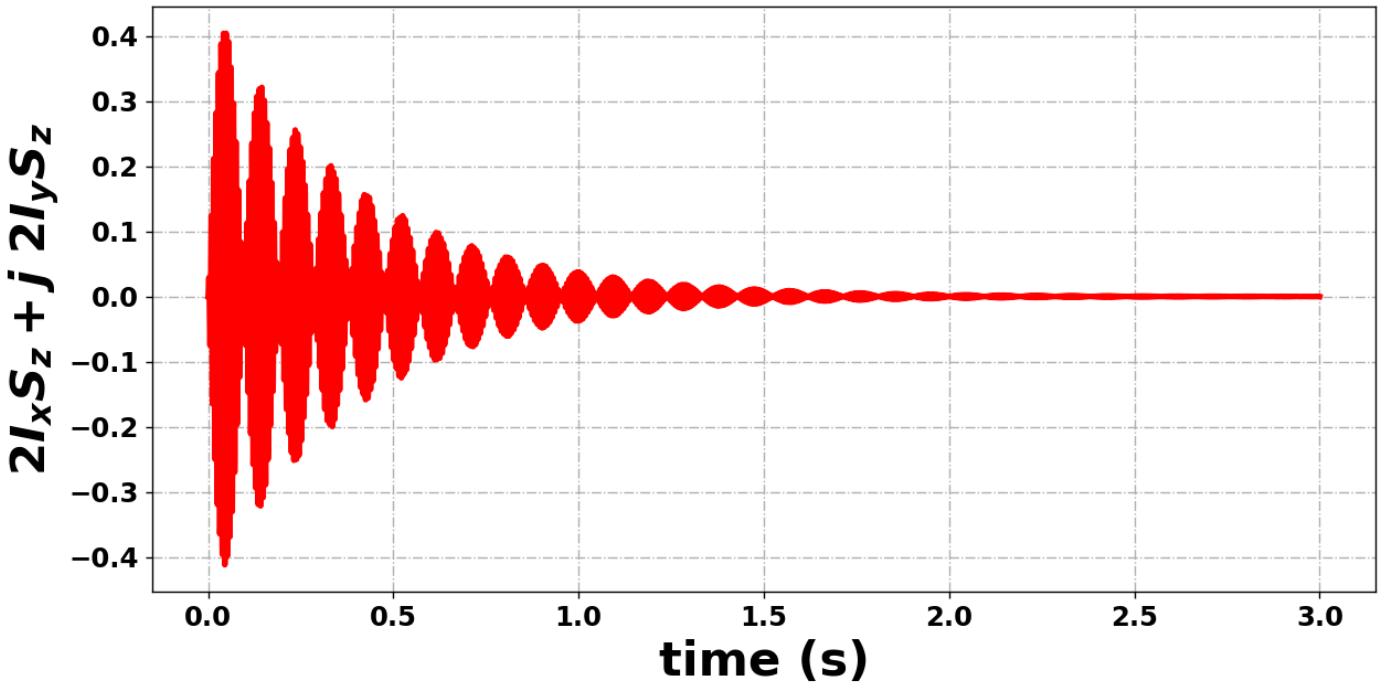
Ploting

In [26]:
```
System.Plotting(1,t1,Ex_det1,"time (s)","I+ and S+","red")
```



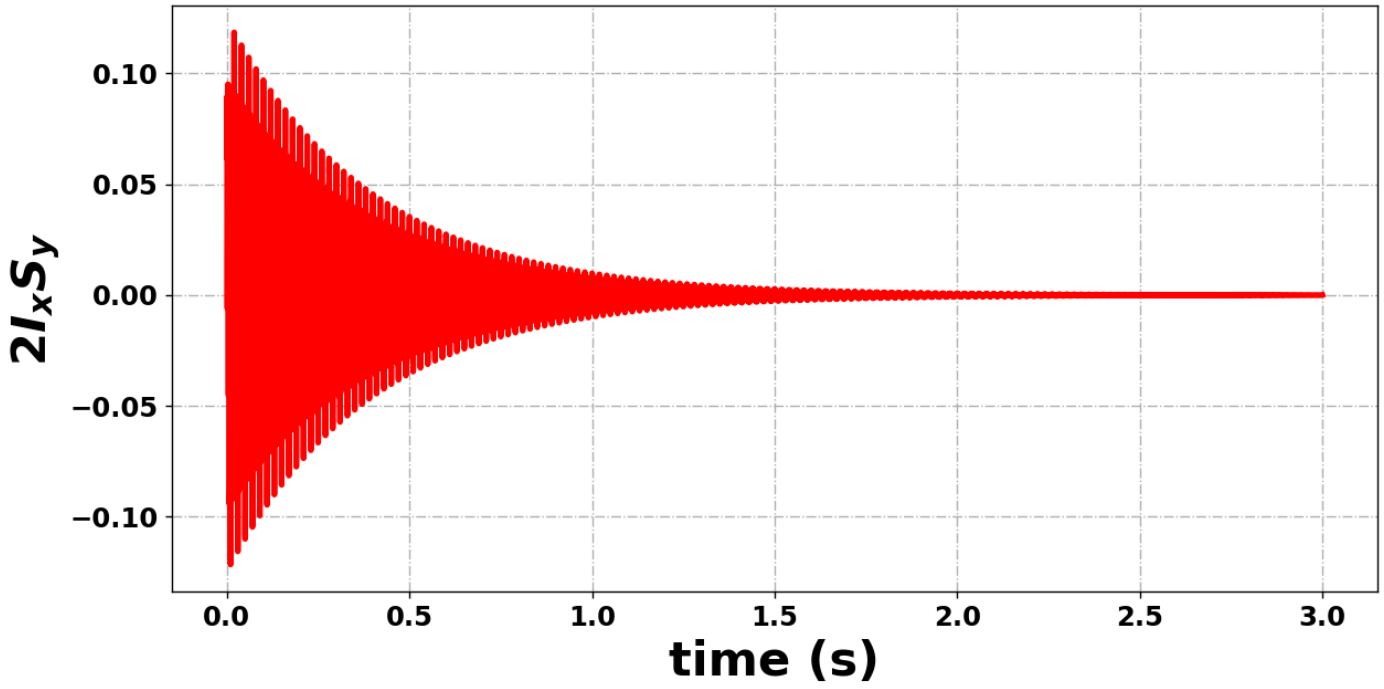

```
/opt/anaconda3/lib/python3.9/site-packages/numpy/core/_asarray.py:102: ComplexWarning: Cas
ting complex values to real discards the imaginary part
  return array(a, dtype, copy=False, order=order)
No handles with labels found to put in legend.
```

In [27]:
```
System.Plotting(2,t1,Ex_det2,"time (s)",r"$2I_{x}S_{z} + j \ 2I_{y}S_{z}$","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.
```

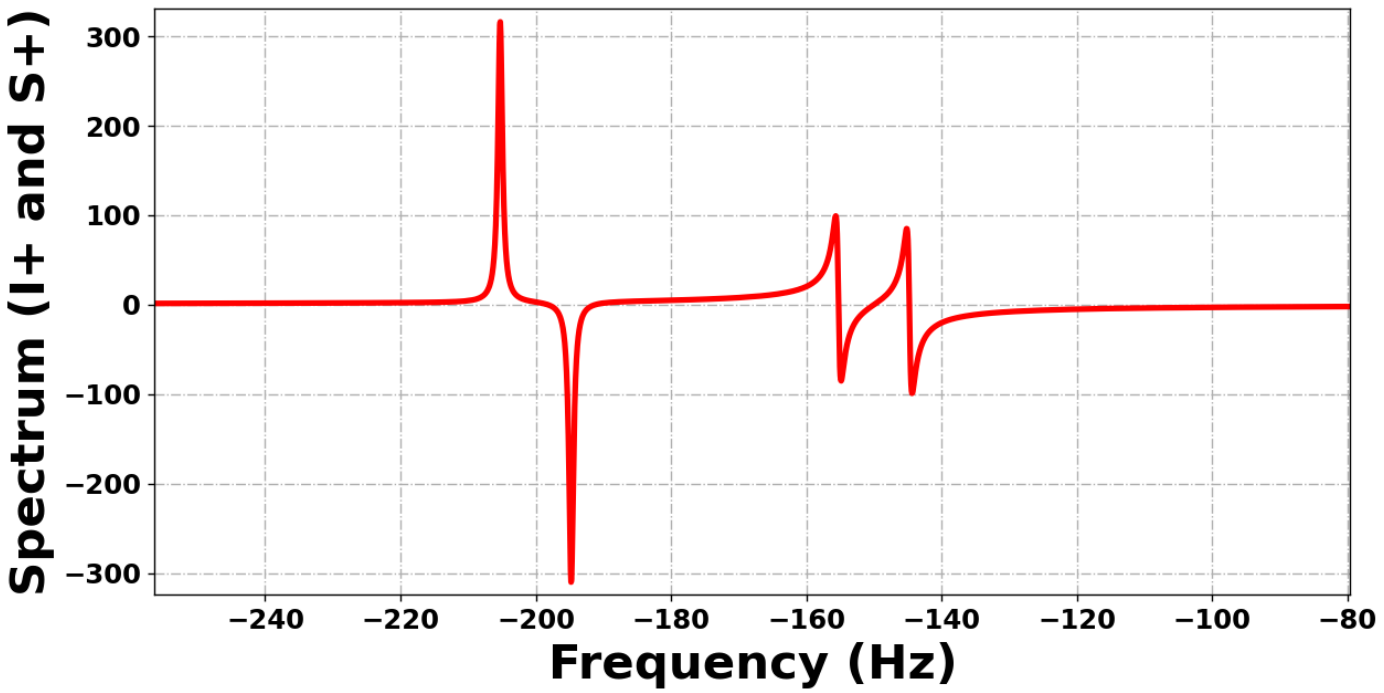
In [28]:
```
System.Plotting(3,t1,Ex_det3,"time (s)",r"$2I_{x}S_{y}$","red")
```




```
/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 [32]:

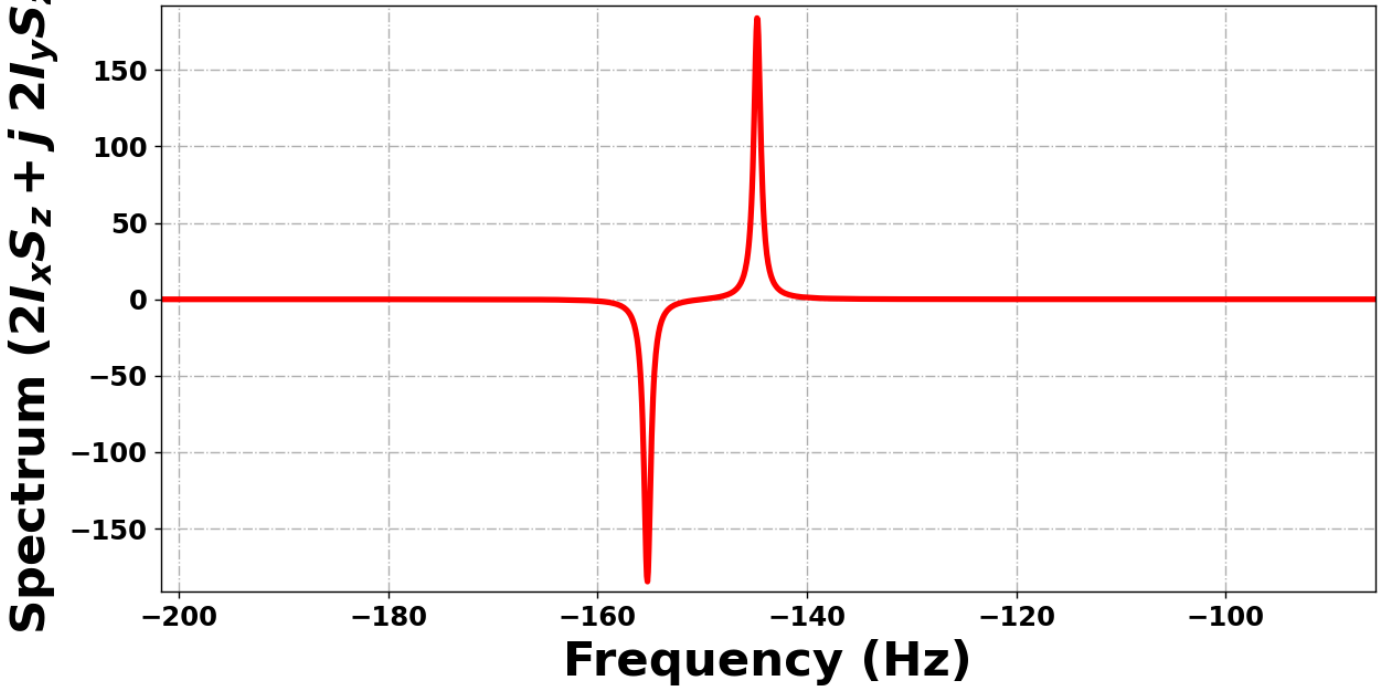
```
PH0 = -45.0
spectrum_PH0 = System.PhaseAdjust_PH0(spectrum1,PH0)
System.Plotting(4,freq,spectrum_PH0.real,"Frequency (Hz)",r"Spectrum (I+ and S+)","red")
```




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

In [33]:

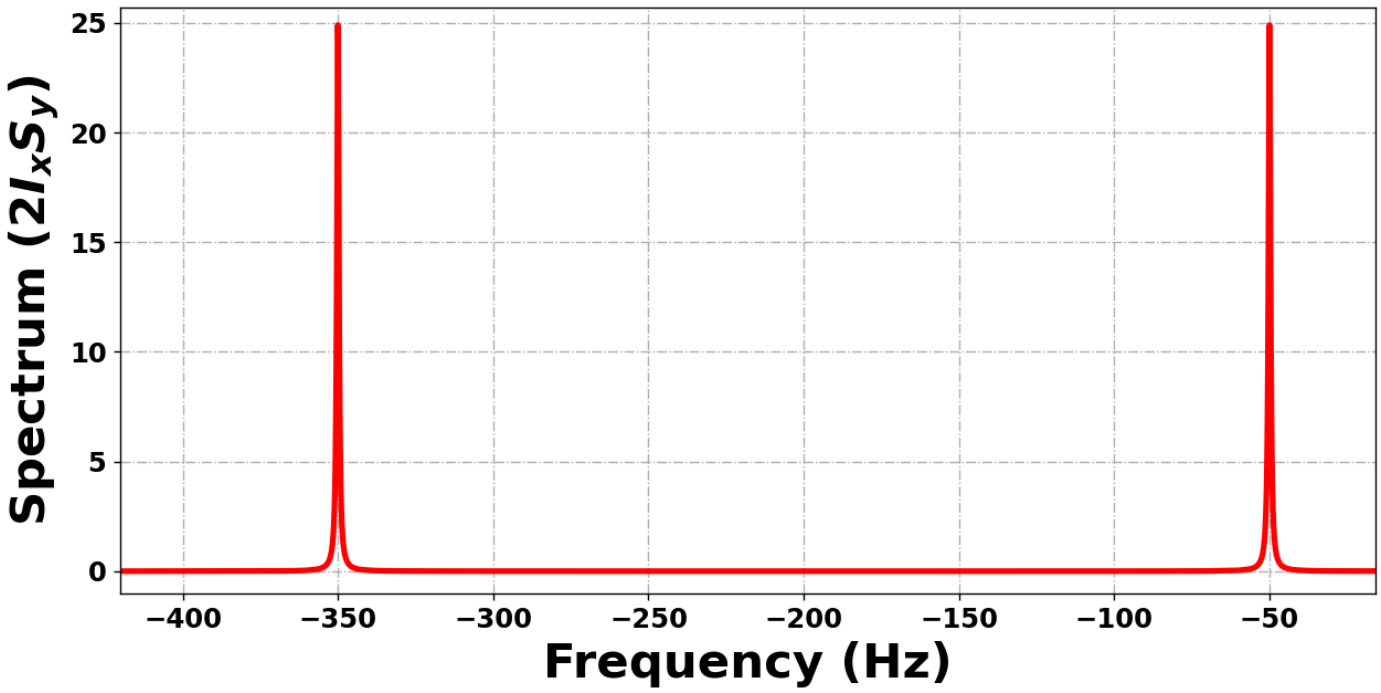
```
PH0 =0.0
spectrum_PH0 = System.PhaseAdjust_PH0(spectrum2,PH0)
System.Plotting(5,freq,spectrum_PH0.real,"Frequency (Hz)",r"Spectrum ($2I_{x}S_{z} + j \ 2
```




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

In [34]:

```
PH0 = 0.0
spectrum_PH0 = System.PhaseAdjust_PH0(spectrum3,PH0)
System.Plotting(64,freq,spectrum_PH0.real,"Frequency (Hz)",r"Spectrum ($2I_{x}S_{y}$)","re
```




```
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.

vineethfrancis.physics@gmail.com