Python On Resonance (PyOR)

Everybody can simulate NMR

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Tutorial 3: Zeeman and B1 Hamiltonian Part 2

In previous tutorial, we saw how to generate Zeeman Hamiltonian (in lab and rotating frame) and B1 (RF field) Hamiltonian for a single spin half system. Now let us do the same for two spin half particle.

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 *
```

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

Let generate Hamiltonians

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 = [20, 35] # Offset frequency in Hz

"""
Function "LarmorF" give the list Larmor frequencies of individual spins in lab frame
"""
LarmorF = System.LarmorFrequency(Gamma,B0,Offset)
```

```
Larmor Frequency in MHz:  [-400.22803765 -400.22805265]
```

In [7]:
```
"""
Generate Zeeman Hamiltonian in Lab frame
""";
```

In [8]:
```
Hz = System.Zeeman(LarmorF,Sz)
```

In [9]:
```
"""
Now lets see how to get the eigen vectors of the Zeman Hamiltonian (lab frame)
""";
B_Z = System.ZBasis_H(Hz)
```

$|1/2,1/2\rangle|1/2,1/2\rangle,|1/2,1/2\rangle|1/2,-1/2\rangle,|1/2,-1/2\rangle|1/2,1/2\rangle,|1/2,-1/2\rangle|1/2,-1/2\rangle$

In [10]:
```
"""
```

```
Matrix representation of the eigen vectors
""";
Matrix(B_Z[0]) # First eigen vector
```

Out[10]:

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

In [11]:

```
Matrix(B_Z[1]) # Second eigen vector
```

Out[11]:

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

Zeeman Hamiltonian in Rotating Frame

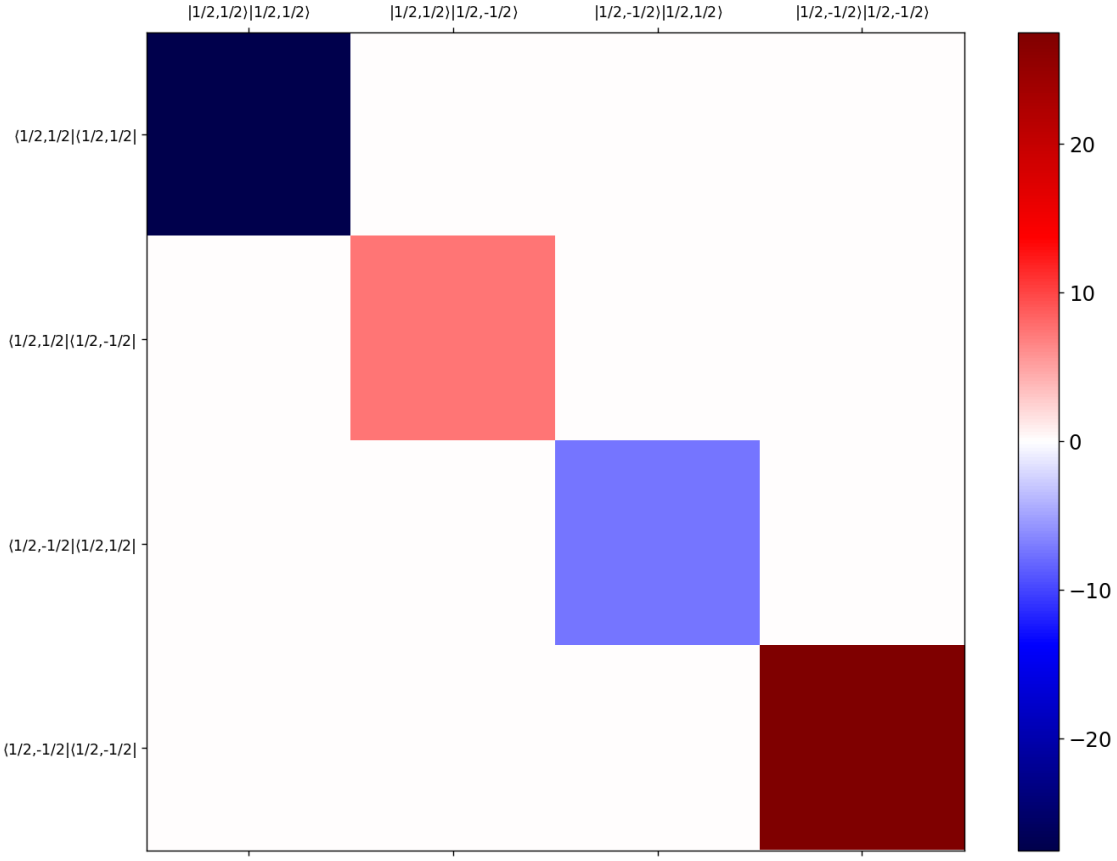
In [12]:

```
"""
"OmegaRF" is list of rotating frame frequencies
""";
OmegaRF = [-System.gammaH1*B0,-System.gammaH1*B0]

"""
Hamiltonian in the rotating frame
""";
Hzr = System.Zeeman_RotFrame(LarmorF, Sz, OmegaRF)
```

In [13]:

```
"""
Representation of Zeeman Hamiltonian in the rotating frame (Unit: Hz)
""";
System.MatrixPlot(1,Hzr.real/2.0/np.pi)
```




```
/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)
```

B1 Field Hamiltonian

In [14]:

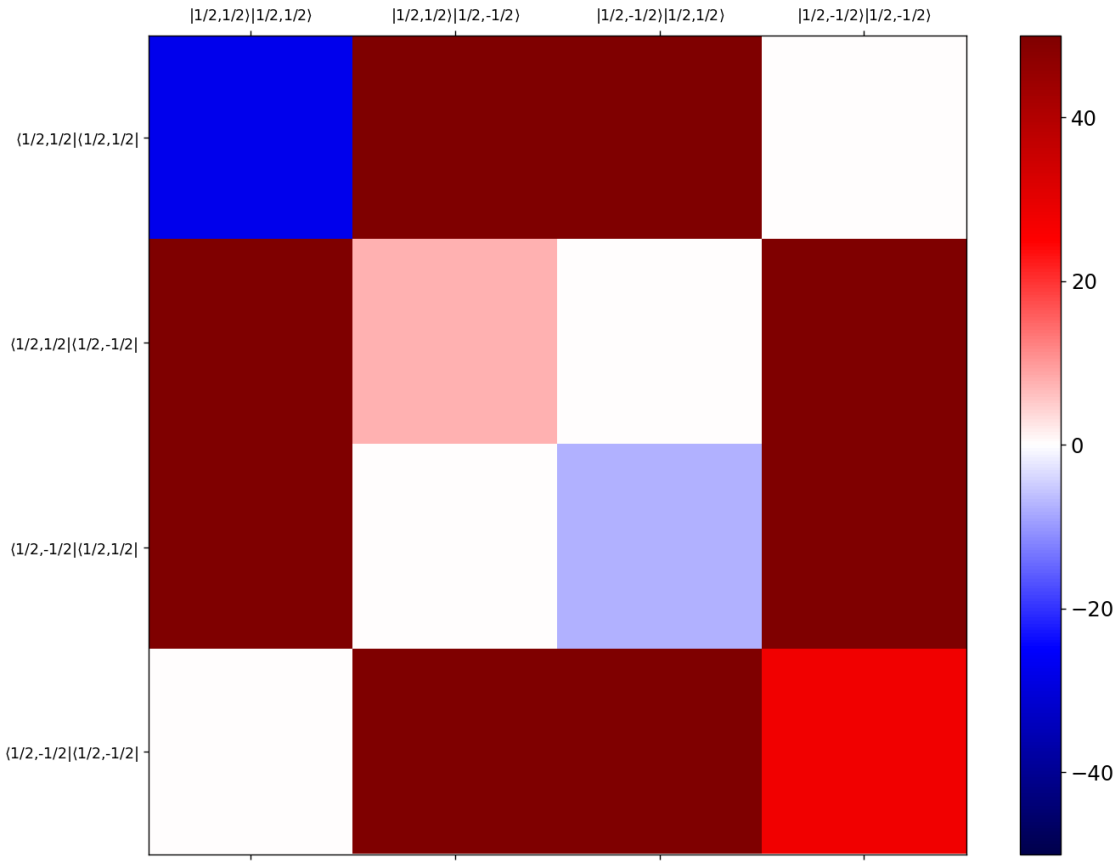
```
"""
So we have a spin half particle sitting at static magnetic field B0 along "Z" direction.
When a RF field is applied the magnetic dipole of the spin interact with the field and sta
The energy of the particle in this case is given by B1 Field Hamiltonian
""";

"""
List of RF amplitude (Hz) or Nutation frequency, "Omega1"
""";
Omega1 = [100,100] # Hz

"""
List of RF signal phase in degree
""";
Omega1Phase = [0,0] # deg

"""
B1 field hamiltonian
""";
HzB1 = System.Zeeman_B1(Sx,Sy,Omega1,Omega1Phase)
```

In [15]:
```
"""
Representation of Zeeman Hamiltonian and B1 Hamiltonian in the rotating frame (Unit: Hz)
""";
Htotal = Hzr + HzB1
System.MatrixPlot(2,Htotal.real/2.0/np.pi)
```



In [16]:
```
"""
From above picture we see that the Hamiltonian is not diagonal.
In some future tutorial we will look into it and find the eigen vectors of this Hamiltonia
""";
```

Basis Operators

Let us look into basis operators of spin half particle in cartesian and PMZ (plus minus Z)

In [17]:
```
"""
Basis Operators in Cartesian
""";
Basis = 'Cartesian spin half'
B_CarT = 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 [18]:
```
"""
Let us look the structure of "B_CarT"
```

```
"B_CarT" contain 16 (4x4) basis operator
""";
B_CarT.shape
```

Out[18]:
```
(16, 4, 4)
```

In [19]:
```
"""
We can call each basis operator by "B_CarT[i]", where 1=0,1,2,3
"""
B_CarT[0]
```

Out[19]:
```
array([[0.5+0.j, 0. +0.j, 0. +0.j, 0. +0.j],
       [0. +0.j, 0.5+0.j, 0. +0.j, 0. +0.j],
       [0. +0.j, 0. +0.j, 0.5+0.j, 0. +0.j],
       [0. +0.j, 0. +0.j, 0. +0.j, 0.5+0.j]], dtype=complex256)
```

In [20]:
```
"""
Basis Operators in PMZ
""";
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 [21]:
```
"""
We can call each basis operator by "B_PMZ[i]", where 1=0,1,2,3
"""
B_PMZ[0]
```

Out[21]:
```
array([[0.5+0.j, 0. +0.j, 0. +0.j, 0. +0.j],
       [0. +0.j, 0.5+0.j, 0. +0.j, 0. +0.j],
       [0. +0.j, 0. +0.j, 0.5+0.j, 0. +0.j],
       [0. +0.j, 0. +0.j, 0. +0.j, 0.5+0.j]], dtype=complex256)
```

Singlet Triplet state Basis

In [22]:
```
"""
Additional to Zeeman basis, for two spin half particles PyOR provides Singlet-Triplet Basi
""";
B_ST = System.STBasis(B_Z)
```

Basis: T_-, T_0, T_+, S_0

In [23]:
```
"""
Let us look the structure of "B_ST"
"B_ST" contain 4 (4x1) basis
""";
B_ST.shape
```

Out[23]:
```
(4, 4, 1)
```

In [24]:
```
"""
We can call each basis stater by "B_ST[i]", where 1=0,1,2,3
"""
B_ST[0] # Triplet -1
```

Out[24]:
```
array([[1.],
       [0.],
       [0.],
       [0.]])
```

In [25]:
```
B_ST[1] # Triplet 0
```

Out[25]:
```
array([[0.        ],
       [0.70710678],
       [0.70710678],
       [0.        ]])
```

In [26]:
```
B_ST[2] # Triplet +1
```

Out[26]:
```
array([[0.],
       [0.],
       [0.],
       [1.]])
```

In [27]:
```
B_ST[3] # Singlet state
```

Out[27]:
```
array([[ 0.        ],
       [ 0.70710678],
       [-0.70710678],
       [ 0.        ]])
```

Next tutorial: Initial Density Matrix

In this lecture you will see how to generate initial density matrix for spin ensemble at thermal equlibrium

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 [ ]:
```

```