Python On Resonance (PyOR)

Everybody can simulate NMR

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Tutorial 2: Spin Operators for Multi spins System

In previous tutorial, you have seen how to generate spin operators for a single spin. Lets see how to generate spin operators for more than one spin.

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

In [25]:
```
pathSource = '/media/HD2/Vineeth/PostDoc_Simulations/Github/PyOR_G/Source'
```

In [26]:
```
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 [27]:
```
"""
Let me show an example of two spin system.
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]

"""
Try also
Slist1 = [1/2,1/2]
Slist1 = [1/2,1]
Slist1 = [1/2,1/2,1/2]
Slist1 = [1/2,1/2,1/2,1/2,1/2,1/2]
""";
```

In [28]:
```
"""
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 [29]:
```
"""
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)
```

Representation of Spin Operators

In PyOR you visualize a matrix (Hamitonians, Density matrix and Operators) in various forms, I hope you saw it in previous tutorials.

In [30]:
```
"""
Matrix represenatation (Sympy)
In Sx[0], 0 means the index of the first spin.
And Sx[1], 1 means the index of the second spin.
""";
Matrix(Sz[0]) # Spin operator Sz of first spin
```

Out[30]:
$$\begin{bmatrix} 0.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & -0.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.5 \end{bmatrix}$$

In [31]:
```
Matrix(Sz[1]) # Spin operator Sz of second spin
```

Out[31]:
$$\begin{bmatrix} 1.0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1.0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1.0 \end{bmatrix}$$

In [32]:
```
Matrix(Sp[0]) # Spin operator S+ of first spin
```

Out[32]:

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

In [33]:

```
Matrix(Sp[1]) # Spin operator S+ of second spin
```

Out[33]:

$$\begin{bmatrix} 0 & 1.4142135623731 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.4142135623731 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.4142135623731 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.4142135623731 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

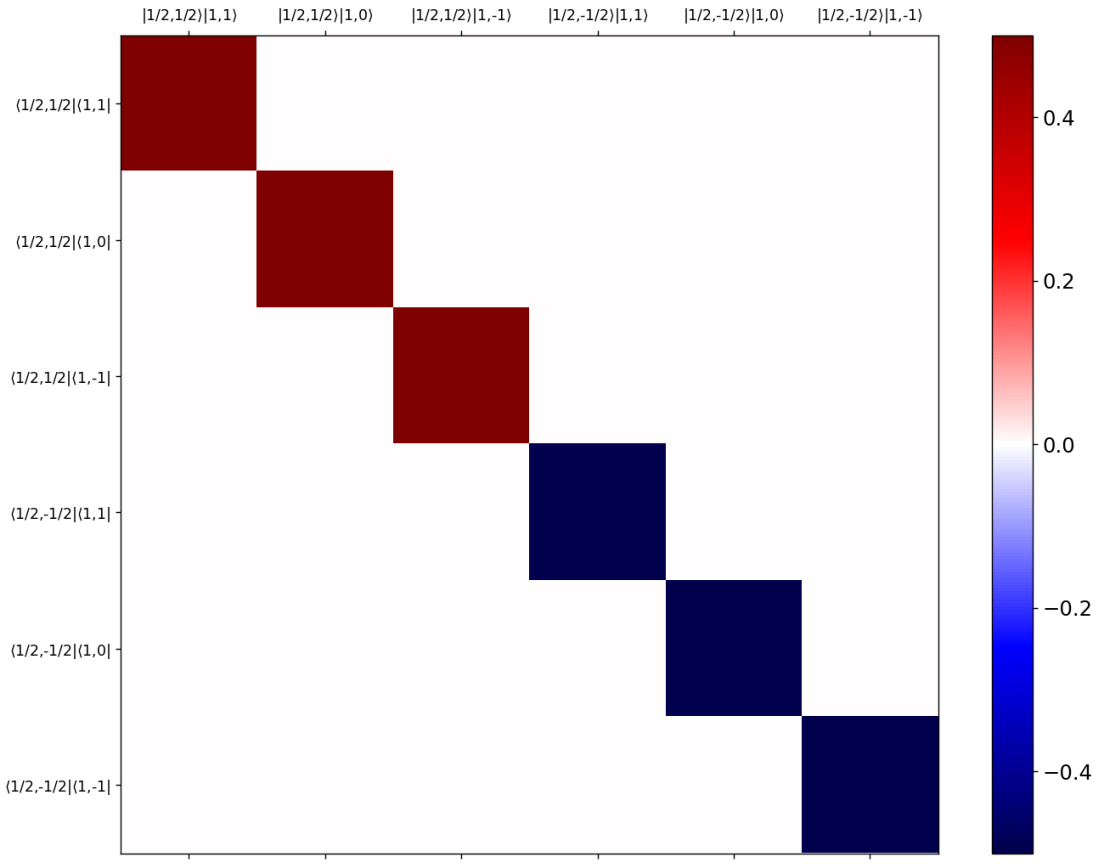
In [34]:

```
"""
I hope you understand how to call spin operators of individual spins. It is as simple.
""";
```

In [35]:

```
"""
Matrix Represenatation (matplotlib)
At the moment labelling is not possible for more than 2 spin system. In future it will be
""";

System.MatrixPlot(1,Sz[0].real)
```



Next tutorial: Zeeman and B1 Hamiltonian Part 1

In this lecture you will see how to generate Zeeman Hamiltonian (lab and rotating frame) and B1 field Hamiltonian for a single 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 [ ]: