Tutorial: Product Operator Basis (Zeeman and PMZ) in Liouvillie Space

PyOR Version: Jeener (release date not decided)

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

Import necessery packages and define source code of PyOR

In [1]:
```
from IPython.display import display, HTML
display(HTML("<style>.container { width:100% !important; }</style>"))
import sys
sys.path.append('/media/HD2/Vineeth/PostDoc_Simulations/Github/PyOR_V1/Source')

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 [2]:
```
Slist1 = [1/2,1/2]
hbarEQ1 = True

System = PyOR.Numerical_MR(Slist1,hbarEQ1)
Sx,Sy,Sz = System.SpinOperator()
Sp,Sm = System.PMoperators(Sx,Sy)
```

Generating Product Operator Basis: PMZ Basis (Hilbert Space)

In [3]:
```
# Product Operators Basis
sort = 'negative to positive'
Index = False
Normal = True
Basis_PMZ, coh_PMZ, dic_PMZ = System.ProductOperators_SpinHalf_PMZ(sort,Index,Normal)
OpB_H = System.String_to_Matrix(dic_PMZ, Basis_PMZ)
```

```
['Im1Im2', 'Im2', 'Im1', 'Im1Iz2', 'Iz1Im2', '', 'Iz2', 'Im1Ip2', 'Iz1', 'Iz1Iz2', 'Ip1Im
2', 'Ip2', 'Iz1Ip2', 'Ip1', 'Ip1Iz2', 'Ip1Ip2']
```

In [4]:
```
Matrix(OpB_H["Im1Im2"])
```

Out[4]:

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

Generating Zeeman Hamiltonian (Lab and Rotating Frame)

In [5]:
```
# Gyromagnetic Ratio
Gamma = [System.gammaH1,System.gammaH1]

# B0 Field in Tesla, Static Magnetic field (B0) along Z
B0 = 1.0

# Offset Frequency in Hz
Offset = [10.0,20.0]

# generate Larmor Frequencies
LarmorF = System.LarmorFrequency(Gamma,B0,Offset)

# Rotating Frame Frequency
OmegaRF = [-System.gammaH1*B0,-System.gammaH1*B0]

# Lab Frame Hamiltonian
Hz_lab = System.Zeeman(LarmorF,Sz)

# Rotating Frame Hamiltonian
Hz = System.Zeeman_RotFrame(LarmorF,Sz,OmegaRF)
```

```
Larmor Frequency in MHz:  [-42.57745869 -42.57746869]
```

Hamiltonian in Hilbert Space

In [6]:
```
Matrix(Hz/(2.0*np.pi))
```

Out[6]:
$$\begin{bmatrix} -15.0000000000126 & 0 & 0 & 0 \\ 0 & 5.00000000158526 & 0 & 0 \\ 0 & 0 & -5.00000000158526 & 0 \\ 0 & 0 & 0 & 15.0000000000126 \end{bmatrix}$$

Zeeman Basis State

In [7]:
```
Basis_Zeeman_state = System.ZBasis_H(Hz_lab)
```

In [8]:
```
Basis_Zeeman_state
```

Out[8]:
```
[array([[1.],
        [0.],
        [0.],
        [0.]]),
 array([[0.],
        [1.],
        [0.],
        [0.]]),
 array([[0.],
        [0.],
```

```
       [1.],
       [0.]]),
 array([[0.],
       [0.],
       [0.],
       [1.]])]
```

Singlet Triplet Basis State

In [9]:
```
Basis_ST_state = System.STBasis(Hz_lab)
```

Basis: T_-, T_0,T_+,S_0

In [10]:
```
Basis_ST_state
```

Out[10]:
```
[array([[1.],
       [0.],
       [0.],
       [0.]]),
 array([[0.        ],
       [0.70710678],
       [0.70710678],
       [0.        ]]),
 array([[0.],
       [0.],
       [0.],
       [1.]]),
 array([[ 0.        ],
       [ 0.70710678],
       [-0.70710678],
       [ 0.        ]])]
```

Transformation Between Zeeman state and Singlelet state

In [11]:
```
U_Z_ST = System.Transform_StateBasis(Basis_Zeeman_state,Basis_ST_state)
Matrix(U_Z_ST)
```

Out[11]:
$$\begin{bmatrix} 1.0 & 0 & 0 & 0 \\ 0 & 0.707106781186547 & 0 & 0.707106781186547 \\ 0 & 0.707106781186547 & 0 & -0.707106781186547 \\ 0 & 0 & 1.0 & 0 \end{bmatrix}$$

In [12]:
```
Matrix(System.State_BasisChange(Basis_Zeeman_state[3],U_Z_ST))
```

Out[12]:
$$\begin{bmatrix} 0 \\ 0.707106781186547 \\ -0.707106781186547 \\ 0 \end{bmatrix}$$

J Coupling Hamiltonian

In [13]:
```
Jlist = np.zeros((len(Slist1),len(Slist1)))
Jlist[0][1] = 1
```

```
Hj = System.Jcoupling(Jlist,Sx,Sy,Sz)
Matrix(Hj)
```

Out[13]:

$$\begin{bmatrix} 1.5707963267949 & 0 & 0 & 0 \\ 0 & -1.5707963267949 & 3.14159265358979 & 0 \\ 0 & 3.14159265358979 & -1.5707963267949 & 0 \\ 0 & 0 & 0 & 1.5707963267949 \end{bmatrix}$$

Transformation of J Coupling Hamiltonian from Zeeman to Singlet Triplet

In [14]:

```
Hj_ST = System.Operator_BasisChange(Hj,U_Z_ST)
Matrix(System.Matrix_Round(System.Matrix_Tol(Hj_ST/(2.0*np.pi),1.0e-5),2))
```

Out[14]:

$$\begin{bmatrix} 0.25 & 0 & 0 & 0 \\ 0 & 0.25 & 0 & 0 \\ 0 & 0 & 0.25 & 0 \\ 0 & 0 & 0 & -0.75 \end{bmatrix}$$

Basis Kets

In [15]:

```
Kets = System.Basis_Ket()
Kets
```

Out[15]:

```
['|1/2,1/2>|1/2,1/2>',
 '|1/2,1/2>|1/2,-1/2>',
 '|1/2,-1/2>|1/2,1/2>',
 '|1/2,-1/2>|1/2,-1/2>']
```

Basis Bras

In [16]:

```
Bras = System.Basis_Bra()
Bras
```

Out[16]:

```
['<1/2,1/2|<1/2,1/2|',
 '<1/2,1/2|<1/2,-1/2|',
 '<1/2,-1/2|<1/2,1/2|',
 '<1/2,-1/2|<1/2,-1/2|']
```

Product Operator Basis: Zeeman (Hilbert Space)

In [17]:

```
Basis_Zeeman, dic_Zeeman = System.ProductOperators_Zeeman(Hz_lab)
```

In [18]:

```
Matrix(Basis_Zeeman[0])
```

Out[18]:

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

In [19]:
```
# Dictionary
dic_Zeeman
```

Out[19]:
```
['|1/2,1/2>|1/2,1/2><1/2,1/2|<1/2,1/2|',
 '|1/2,1/2>|1/2,1/2><1/2,1/2|<1/2,-1/2|',
 '|1/2,1/2>|1/2,1/2><1/2,-1/2|<1/2,1/2|',
 '|1/2,1/2>|1/2,1/2><1/2,-1/2|<1/2,-1/2|',
 '|1/2,1/2>|1/2,-1/2><1/2,1/2|<1/2,1/2|',
 '|1/2,1/2>|1/2,-1/2><1/2,1/2|<1/2,-1/2|',
 '|1/2,1/2>|1/2,-1/2><1/2,-1/2|<1/2,1/2|',
 '|1/2,1/2>|1/2,-1/2><1/2,-1/2|<1/2,-1/2|',
 '|1/2,-1/2>|1/2,1/2><1/2,1/2|<1/2,1/2|',
 '|1/2,-1/2>|1/2,1/2><1/2,1/2|<1/2,-1/2|',
 '|1/2,-1/2>|1/2,1/2><1/2,-1/2|<1/2,1/2|',
 '|1/2,-1/2>|1/2,1/2><1/2,-1/2|<1/2,-1/2|',
 '|1/2,-1/2>|1/2,-1/2><1/2,1/2|<1/2,1/2|',
 '|1/2,-1/2>|1/2,-1/2><1/2,1/2|<1/2,-1/2|',
 '|1/2,-1/2>|1/2,-1/2><1/2,-1/2|<1/2,1/2|',
 '|1/2,-1/2>|1/2,-1/2><1/2,-1/2|<1/2,-1/2|']
```

Hamiltonian in Liouvillie Space (Zeeman basis)

In [20]:
```
Hz_L = System.CommutationSuperoperator(Hz)
Matrix(System.Matrix_Round(Hz_L/(2.0*np.pi),2))
```

Out[20]:

$$\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -20.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -10.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -30.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 20.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 10.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -10.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10.0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -10.0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -20.0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 30.0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10.0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 20. \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

Product Operator Basis: Zeeman Liouvillie

In [21]:
```
Basis_Zeeman_L = System.ProductOperators_ConvertToLiouville(Basis_Zeeman)
```

In [22]:
```
Matrix(Basis_Zeeman_L[0])
```

Out[22]:

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

Product Operator Basis: PMZ Liouvillie

In [23]:
```
Basis_PMZ_L = System.ProductOperators_ConvertToLiouville(Basis_PMZ)
```

In [24]:
```
Matrix(Basis_PMZ_L[0])
```

Out[24]:
$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1.0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Eigen Frequencies: Hilbert

In [25]:
```
System.EigFreq_ProductOperator_H(Hz,OpB_H["Im1Im2"])
```

Out[25]:
```
30.000000000025157
```

Eigen Frequencies: Liouvillie

In [26]:
```
for i in range(System.Ldim):
    print("Eigen frequency of " + dic_PMZ[i] + "(" + str(coh_PMZ[i]) + ") :", System.EigFr
```

```
Eigen frequency of Im1 Im2 (-2) : 30.000000000025157
Eigen frequency of Id1 Im2 (-1) : 20.00000000159783
Eigen frequency of Im1 Id2 (-1) : 9.999999998427322
Eigen frequency of Im1 Iz2 (-1) : 9.999999656141906
Eigen frequency of Iz1 Im2 (-1) : 19.999999317026997
Eigen frequency of Id1 Id2 (0) : 0.0
Eigen frequency of Id1 Iz2 (0) : 0.0
Eigen frequency of Im1 Ip2 (0) : -10.000000003170511
Eigen frequency of Iz1 Id2 (0) : 0.0
Eigen frequency of Iz1 Iz2 (0) : 0.0
Eigen frequency of Ip1 Im2 (0) : 10.000000003170511
Eigen frequency of Id1 Ip2 (1) : -20.00000000159783
Eigen frequency of Iz1 Ip2 (1) : -19.999999317026997
Eigen frequency of Ip1 Id2 (1) : -9.999999998427322
Eigen frequency of Ip1 Iz2 (1) : -9.999999656141906
Eigen frequency of Ip1 Ip2 (2) : -30.000000000025157
```

Basis Transformation Matrix: From Zeeman to PMZ Basis (Liouvillie Space)

In [27]:
```
U_Z_PMZ = System.Transform_StateBasis(Basis_Zeeman_L,Basis_PMZ_L)
```

In [28]:
```
Matrix(U_Z_PMZ)
```

Out[28]:

$$\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0.5 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.707106781186547 & 0 & 0 & 0.70710676908493 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.5 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.707106781186547 & 0.70710676908493 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.5 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1.0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.707106781186547 & -0.70710676908493 & 0 & 0 \\
0 & 0.707106781186547 & 0 & 0 & -0.70710676908493 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.5
\end{bmatrix}$$

In [29]:
```
Matrix(System.State_BasisChange(Basis_Zeeman_L[0],U_Z_PMZ))
```

Out[29]:

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

Liouvillie Bracket

In [30]:
```
System.Liouville_Bracket(Basis_Zeeman_L[0],Hz_L/(2.0*np.pi),Basis_Zeeman_L[0])
```

Out[30]:
```
0.0
```

In [31]:
```
System.Liouville_Bracket(Basis_PMZ_L[0],Hz_L/(2.0*np.pi),Basis_PMZ_L[0])
```

Out[31]:
```
30.000000000025157
```

Hamiltonian in Liouvillie Space (PMZ basis)

In [32]:
```
Hz_L_PMZ = System.Operator_BasisChange(Hz_L,U_Z_PMZ)
```

In [33]:
```
Matrix(System.Matrix_Round(System.Matrix_Tol(Hz_L_PMZ/(2.0*np.pi),1.0e-5),2))
```

Out[33]:

$$\begin{bmatrix}
30.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 20.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 10.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 10.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 20.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -10.0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10.0 & 0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -20.0 & 0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -20.0 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -10.0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -10.0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -
\end{bmatrix}$$

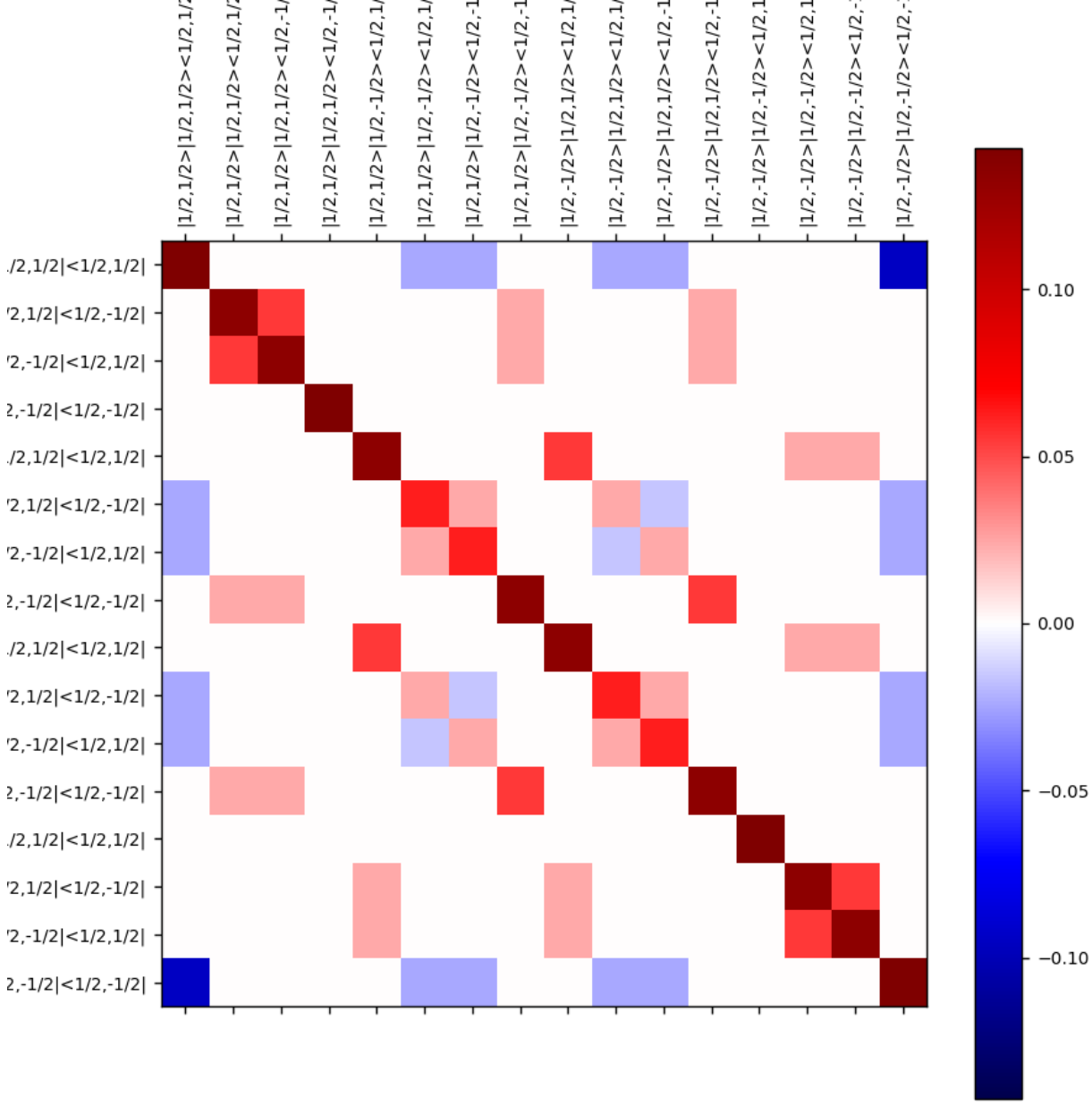
Dipolar Homonuclear Relaxation

In [34]:

```
R = None
Rprocess = "Auto-correlated Dipolar Homonuclear"
tau = 10.0e-12
bIS = [20.0e3]
System.Relaxation_Parameters(LarmorF, OmegaRF, tau, bIS)
R_L = System.Relaxation_L(Rprocess,R,Sx,Sy,Sz,Sp,Sm)
```

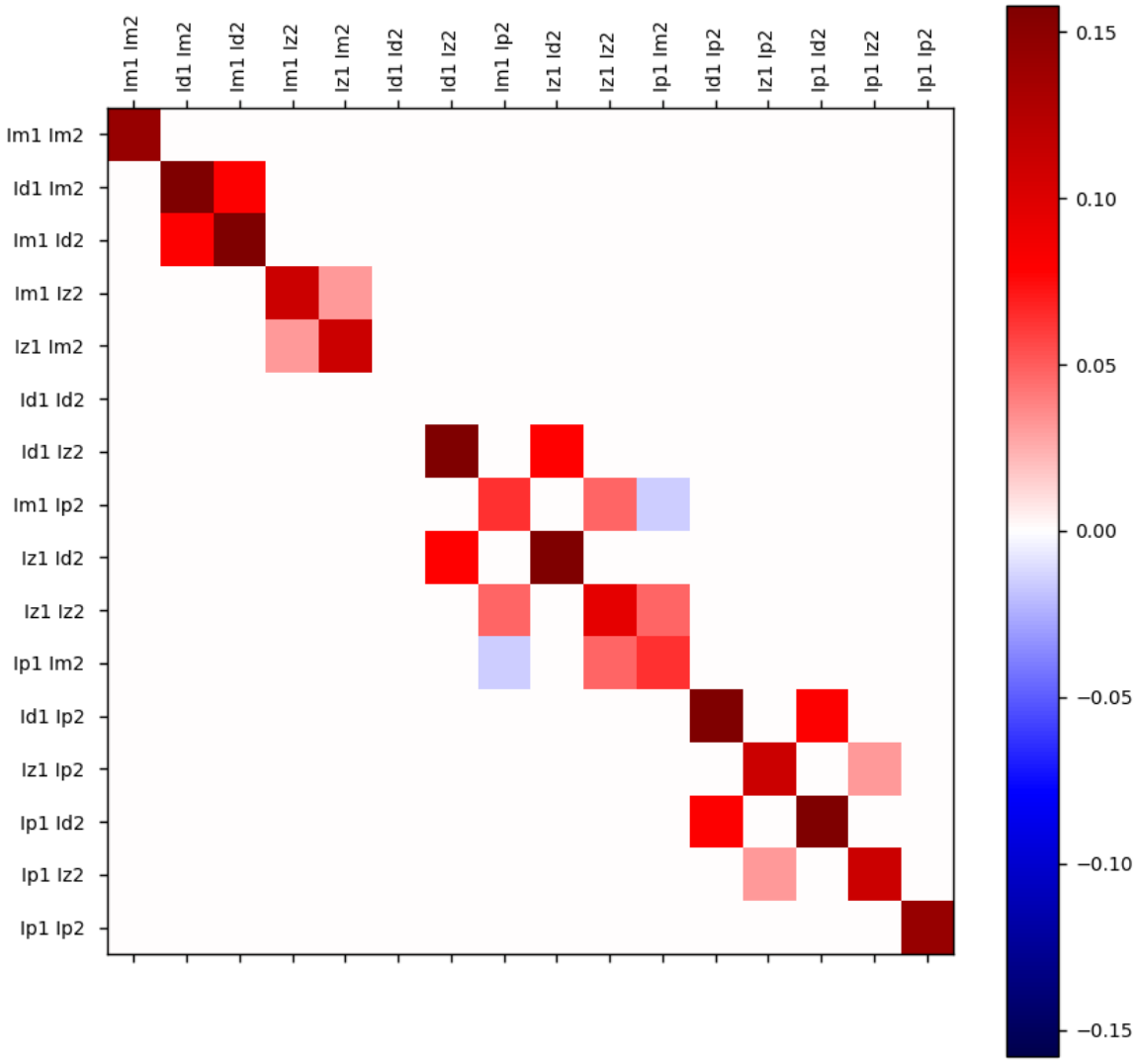
In [35]:

```
System.MatrixPlot(1,R_L.real,dic_Zeeman,dic_Zeeman)
```



In [36]:

```
System.MatrixPlot(2,System.Operator_BasisChange(R_L.real,U_Z_PMZ).real,dic_PMZ,dic_PMZ)
```



Any suggestion? write to me

vineethfrancis.physics@gmail.com