Python On Resonance (PyOR)

Everybody can simulate NMR

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Tutorial 6: Simulation of Spin-Lock Induced Crossing (SLIC) - DeVience, et.al, PRL 111, 2013.

In this tutorial you will simulate Figure 1 (d) using Pulse sequence given in Figure 1 (c), from the paper "Preparation of Nuclear Spin Singlet States Using Spin-Lock Induced Crossing", by DeVience, et.al, Phys. Rev. Lett. 111, 173002. DOI: https://doi.org/10.1103/PhysRevLett.111.173002

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

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 = 4.7

"""
Define the chemical Shift of individual spins
Offset = [chemical Shift spin 1, chemical Shift spin 1, ..]
"""
Offset = [0,2.8] # Offset frequency in Hz
deltaV = Offset[1] - Offset[0] # Frequency difference between Spin 1 and 2
"""
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:  [-200.11400882 -200.11401162]
```

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 = 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
```

Zeeman Halitonian in Rotating Frame

In [8]:

```
off = -2*np.pi*deltaV/2
OmegaRF = [-System.gammaH1*B0 + off ,-System.gammaH1*B0 + off] # RF iradiation in the midd
Hzr = System.Zeeman_RotFrame(LarmorF, Sz, OmegaRF)
```

J Coupling Hamiltonian

In [9]:

```
"""
Define J couplings between individual spins
"""

Jlist = np.zeros((len(Slist1),len(Slist1)))
Jlist[0][1] = 17.4
Hj = System.Jcoupling(Jlist,Sx,Sy,Sz)
```

B1 Hamiltonian (Spin Lock)

In [10]:

```
Omega1 = [Jlist[0][1],Jlist[0][1]] # SLIC condition: B1 amplitude equals J coupling betwee
Omega1Phase = [0,0]
Hrf = System.Zeeman_B1(Sx,Sy,Omega1,Omega1Phase)
```

Total Hamiltonian

In [11]:

```
Hslic = Hzr + Hj + Hrf # Hamiltonina duirng Spin Lock
Hevol = Hzr + Hj # Hamiltonian during Free Evolution
```

Pulse

In [12]:

```
"""
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))
```

Relaxation Constant

In [13]:

```
'''
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([0,0])
R2 = np.asarray([0,0])
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 under first Spin Lock

In [14]:

```
dt = 50e-6
Slic_Time = 0.707/abs(deltaV)
Npoints1 = int(Slic_Time/dt)
print("Number of points in the simulation", Npoints1)

"""
option for solver, "method": "Unitary Propagator" or "ODE Solver"
"""
method = "Unitary Propagator"

start_time = time.time()
t1, rho_t1 = System.Evolution_H(rhoeq,rho,Sx,Sy,Sz,Sp,Sm,Hslic,dt,Npoints1,method,Rprocess
end_time = time.time()
timetaken = end_time - start_time
print("Total time = %s seconds " % (timetaken))
```

```
Number of points in the simulation 5050
Total time = 0.0578155517578125 seconds
```

Evolution of Density Matrix (Free Evolution)

In [15]:

```
dt = 50e-6
Evol_Time = 0.4
Npoints2 = int(Evol_Time/dt)
print("Number of points in the simulation", Npoints2)

method = "Unitary Propagator"

start_time = time.time()
t2, rho_t2 = System.Evolution_H(rhoeq,rho_t1[-1],Sx,Sy,Sz,Sp,Sm,Hevol,dt,Npoints2,method,R
end_time = time.time()
timetaken = end_time - start_time
print("Total time = %s seconds " % (timetaken))
```

```
Number of points in the simulation 8000
Total time = 0.08784270286560059 seconds
```

Evolution of Density Matrix under second Spin Lock

In [16]:

```
dt = 50e-6
Slic_Time = 0.707/abs(deltaV)
Npoints3 = int(Slic_Time/dt)
print("Number of points in the simulation", Npoints3)

method = "Unitary Propagator"
```

```
start_time = time.time()
t3, rho_t3 = System.Evolution_H(rhoeq,rho_t2[-1],Sx,Sy,Sz,Sp,Sm,Hslic,dt,Npoints3,method,F
end_time = time.time()
timetaken = end_time - start_time
print("Total time = %s seconds " % (timetaken))
```

```
Number of points in the simulation 5050
Total time = 0.05803656578063965 seconds
```

Expectation value

In [17]:

```
"""
Zeeman Basis
""";
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 [18]:

```
"""
Singlet Triplet Basis
""";
B_ST = System.STBasis(B_Z)
```

Basis: T_-, T_0,T_+,S_0

In [19]:

```
"""
Expectation Value of different Operators
""";

det1 = -np.matmul(B_ST[3],System.Adjoint(B_ST[3])) # |S0><S0|
det2 = -np.matmul(B_ST[1],System.Adjoint(B_ST[1])) # |T0><T0|
det3 = 0.5*(Sz[0] - Sz[1]) # I1z - I2z
det4 = 0.5*(Sx[0] + Sx[1]) # I1x + I2x
det5 = 0.5*(Sy[0] - Sy[1]) # I1y - I2y
```

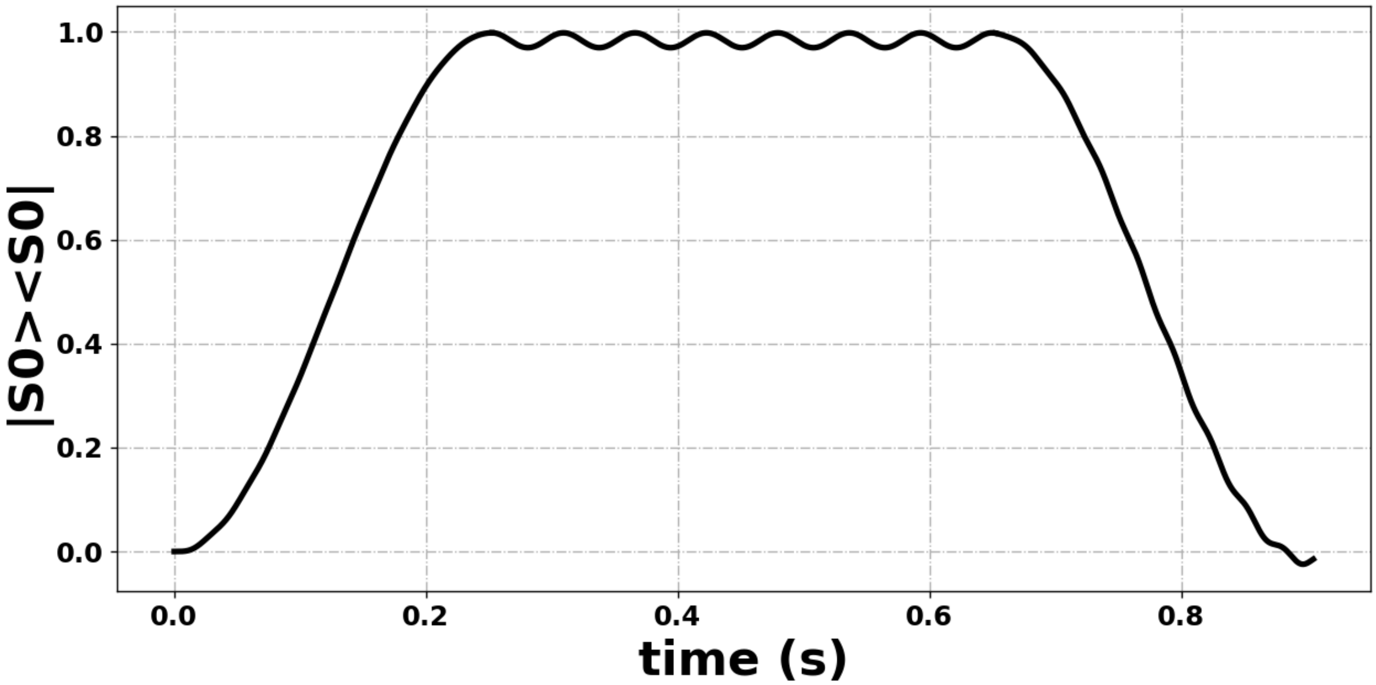
In [20]:

```
t1, det1_a = System.Expectation_H(rho_t1,det1,dt,Npoints1) # First Spin Lock
t2, det1_b = System.Expectation_H(rho_t2,det1,dt,Npoints2) # Free Evolution
t3, det1_c = System.Expectation_H(rho_t3,det1,dt,Npoints3) # Second Spin Lock

t1, det2_a = System.Expectation_H(rho_t1,det2,dt,Npoints1) # First Spin Lock
t2, det2_b = System.Expectation_H(rho_t2,det2,dt,Npoints2) # Free Evolution
t3, det2_c = System.Expectation_H(rho_t3,det2,dt,Npoints3) # Second Spin Lock

t1, det3_a = System.Expectation_H(rho_t1,det3,dt,Npoints1) # First Spin Lock
t2, det3_b = System.Expectation_H(rho_t2,det3,dt,Npoints2) # Free Evolution
t3, det3_c = System.Expectation_H(rho_t3,det3,dt,Npoints3) # Second Spin Lock

t1, det4_a = System.Expectation_H(rho_t1,det4,dt,Npoints1) # First Spin Lock
t2, det4_b = System.Expectation_H(rho_t2,det4,dt,Npoints2) # Free Evolution
t3, det4_c = System.Expectation_H(rho_t3,det4,dt,Npoints3) # Second Spin Lock

t1, det5_a = System.Expectation_H(rho_t1,det5,dt,Npoints1) # First Spin Lock
t2, det5_b = System.Expectation_H(rho_t2,det5,dt,Npoints2) # Free Evolution
t3, det5_c = System.Expectation_H(rho_t3,det5,dt,Npoints3) # Second Spin Lock
```

Plotting

In [21]:

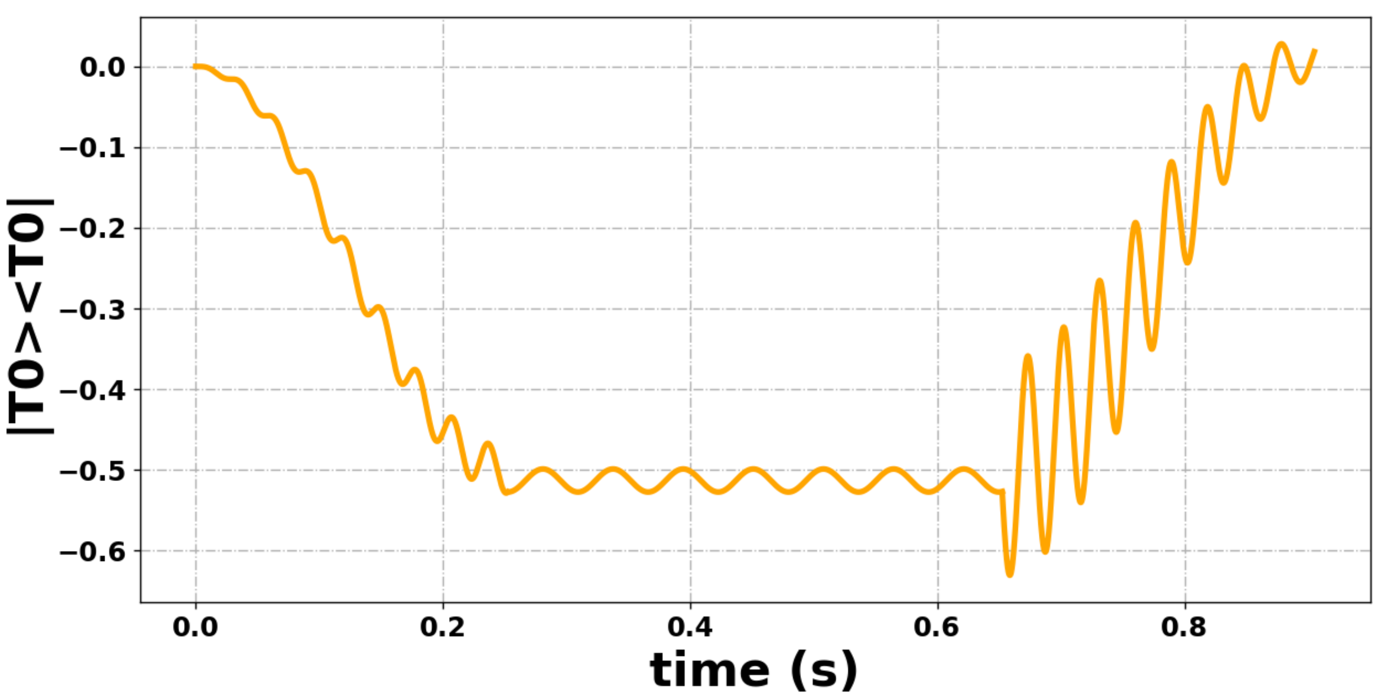
```
System.PlottingMulti(1,[t1,t1[-1]+t2,t1[-1]+t2[-1]+t3],[det1_a,det1_b,det1_c],"time (s)",'
```




```
/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)
/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)
/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 [22]:

```
System.PlottingMulti(2,[t1,t1[-1]+t2,t1[-1]+t2[-1]+t3],[det2_a,det2_b,det2_c],"time (s)",'
```

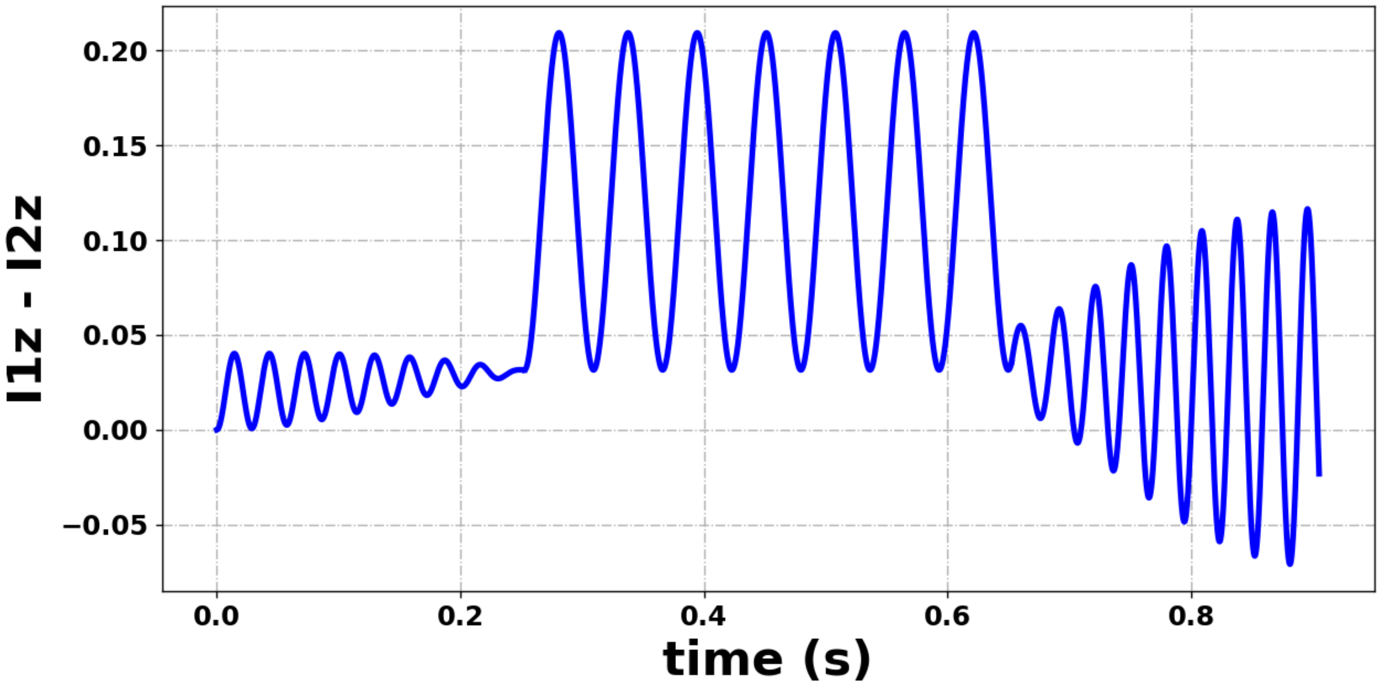



```
/opt/anaconda3/lib/python3.9/site-packages/numpy/core/_asarray.py:102: ComplexWarning: Cas
ting complex values to real discards the imaginary part
  return array(a, dtype, copy=False, order=order)
```

```
/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)
/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 [23]:

```
# There is a small difference between this result from the paper
System.PlottingMulti(3,[t1,t1[-1]+t2,t1[-1]+t2[-1]+t3],[det3_a,det3_b,det3_c],"time (s)",'
```




```
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ting complex values to real discards the imaginary part
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/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)
/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.
```
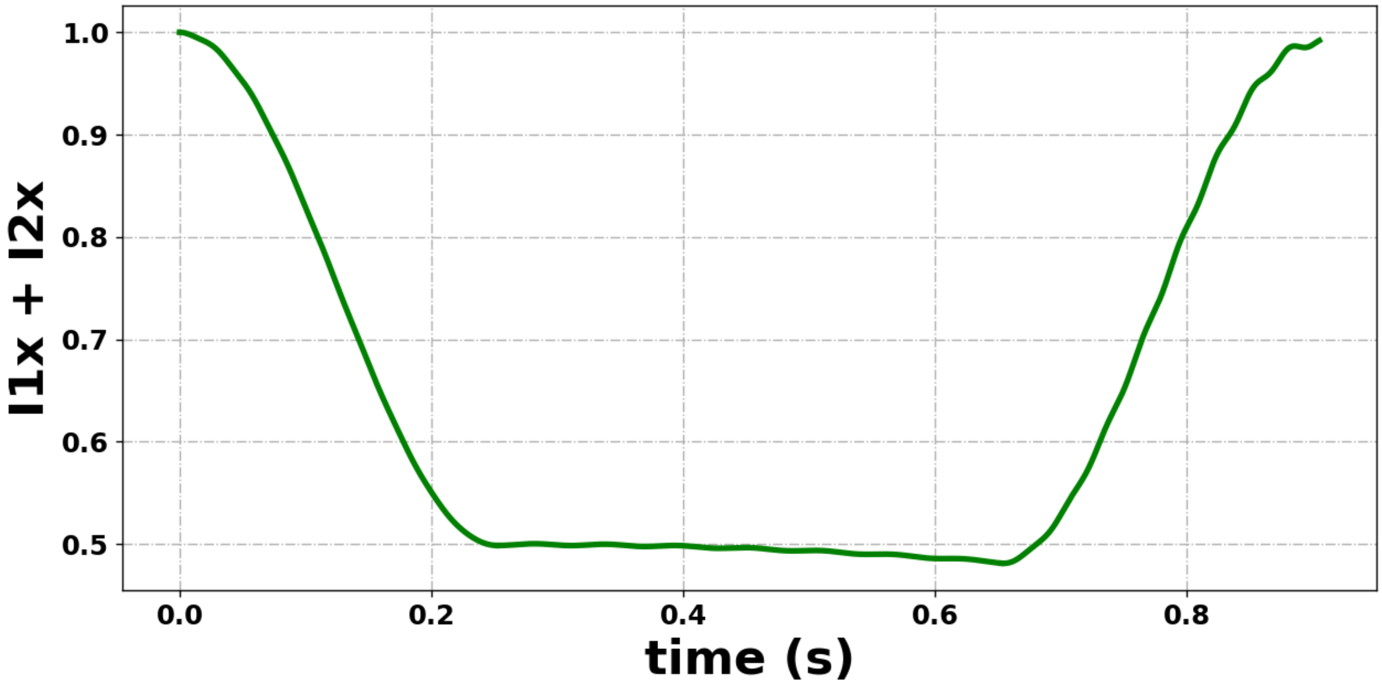

In [24]:

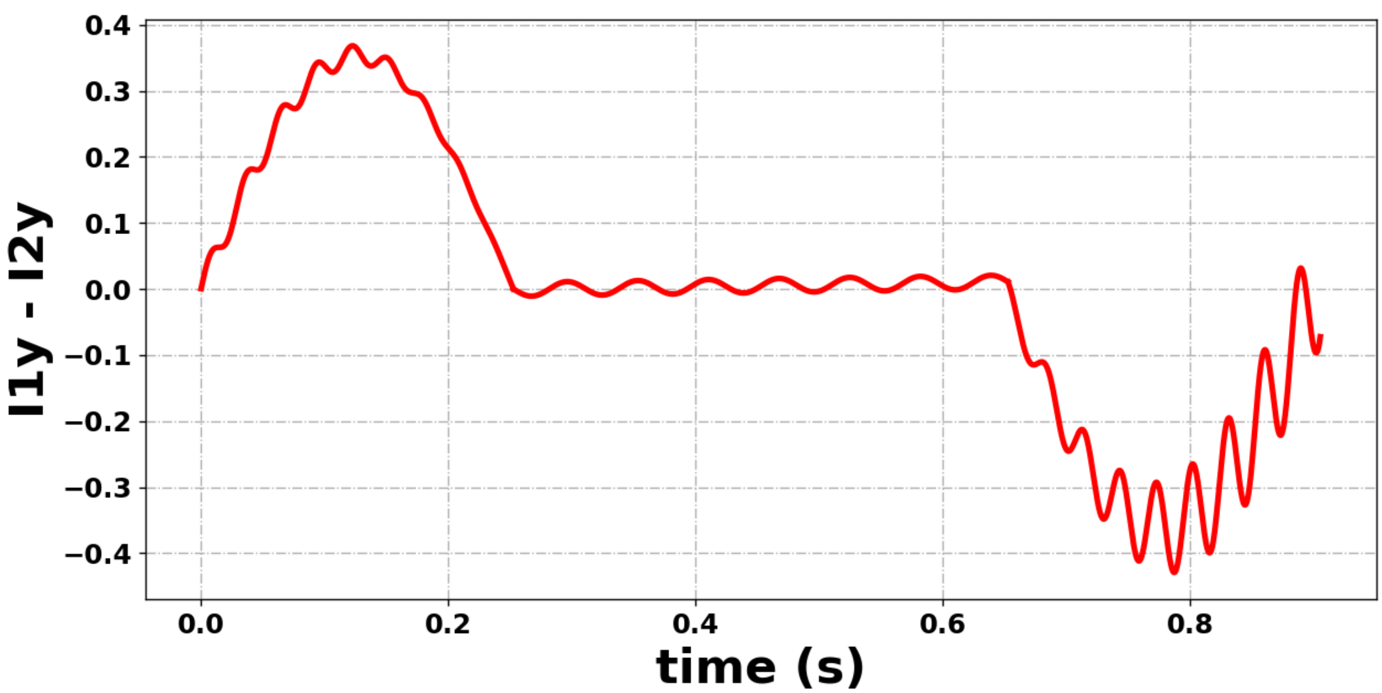
```
System.PlottingMulti(4,[t1,t1[-1]+t2,t1[-1]+t2[-1]+t3],[det4_a,det4_b,det4_c],"time (s)",'
```




```
/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)
/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)
/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 [25]:

```
System.PlottingMulti(5,[t1,t1[-1]+t2,t1[-1]+t2[-1]+t3],[det5_a,det5_b,det5_c],"time (s)",'
```




```
/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)
/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)
```

```
/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 using ODE Solver and phenomenological Relaxation

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 [ ]: