Micro-Project 01 - Model systems for non-local damping

Parameter:

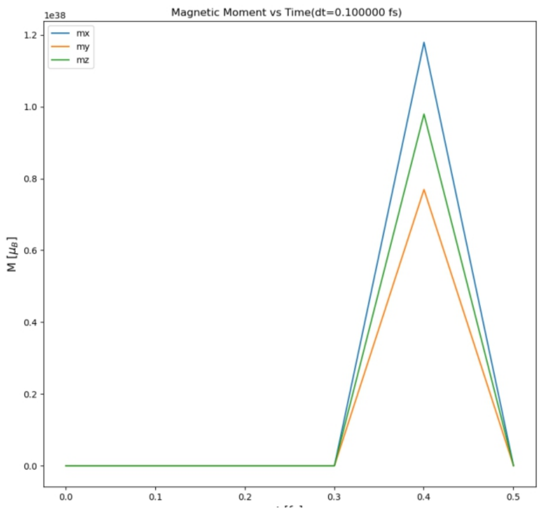
Heisenberg exchange parameter J: 1 Rydberg/μ_B^2
Magnetic moment m_i: 1 μ_B
External field B: 1 Tesla, along x axis
Time step dt: 0.0001 fs

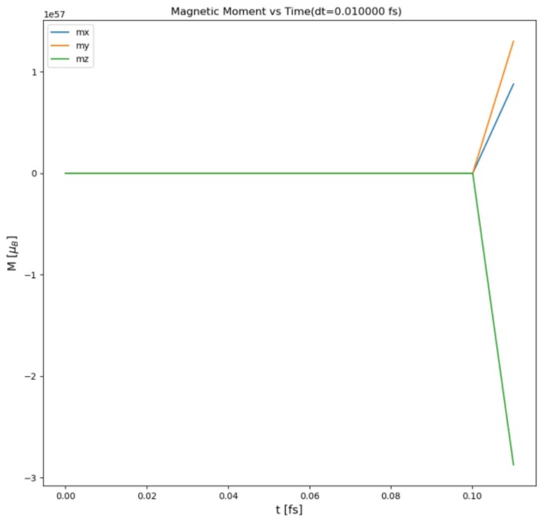
Giromagnetic Ratio ϒ : 41.39 1/(Ryd·fs)

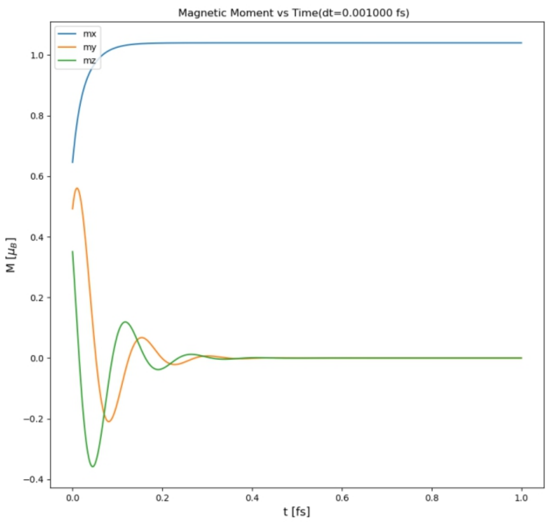
Onsite damping strength: 0.01

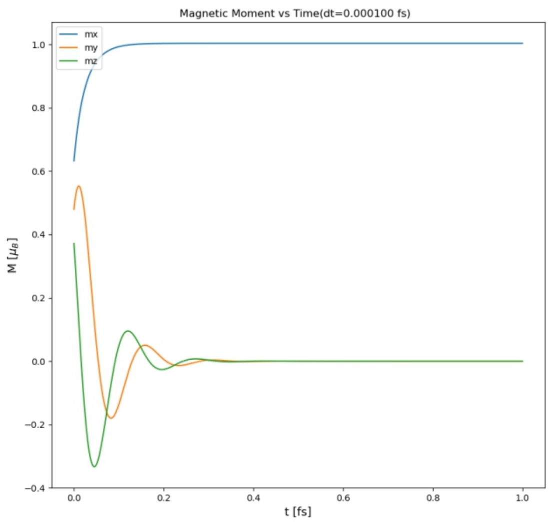
Dimer

1 Test the numerical stability by varying and observe. Use here that $\alpha_{ij}=\alpha I$, where I is unit matrix.









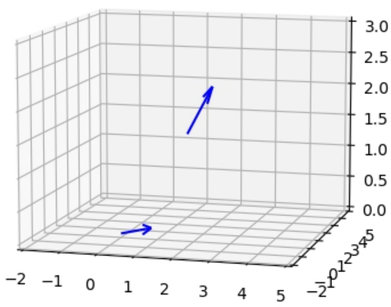
Where its damping tensor is :

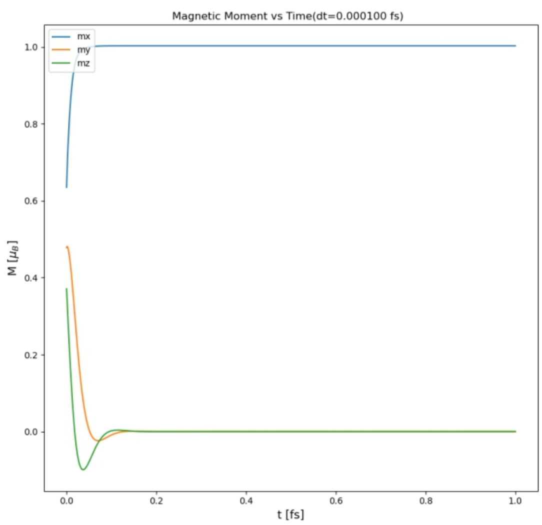
```
[[[[0.01 0.   0.  ]
   [0.   0.01 0.  ]
   [0.   0.   0.01]]

  [[0.   0.   0.  ]
   [0.   0.   0.  ]
   [0.   0.   0.  ]]]


 [[[0.   0.   0.  ]
   [0.   0.   0.  ]
   [0.   0.   0.  ]]

  [[0.01 0.   0.  ]
   [0.   0.01 0.  ]
   [0.   0.   0.01]]]]
```

2 Use a diagonal on-site damping tensor where the diagonal elements are different and observe the dynamics,where its damping tensor is:

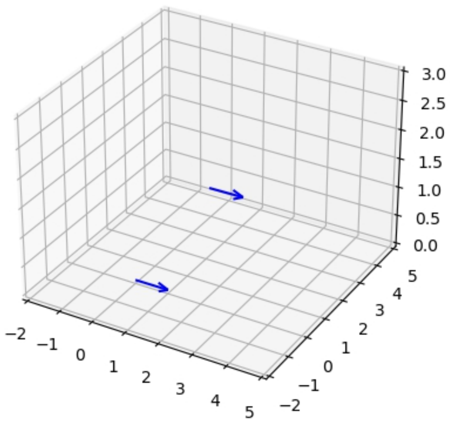
```
[[[[0.01 0.   0.  ]
   [0.   0.02 0.  ]
   [0.   0.   0.03]]

  [[0.   0.   0.  ]
   [0.   0.   0.  ]
   [0.   0.   0.  ]]]


 [[[0.   0.   0.  ]
   [0.   0.   0.  ]
   [0.   0.   0.  ]]

  [[0.01 0.   0.  ]
   [0.   0.02 0.  ]
   [0.   0.   0.03]]]]
```

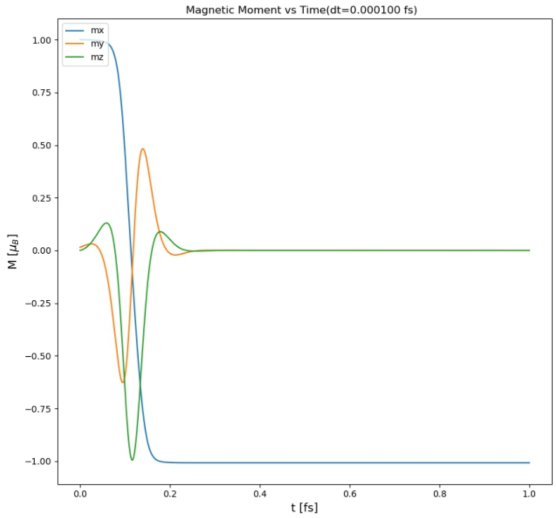
A. Start from a random configuration



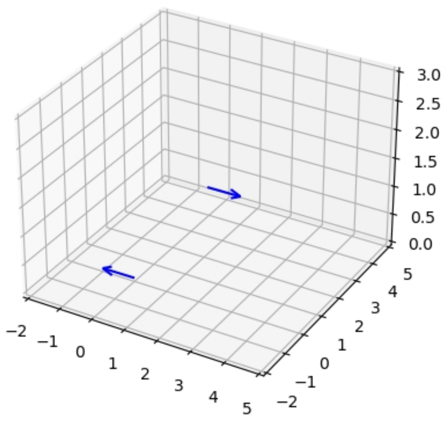


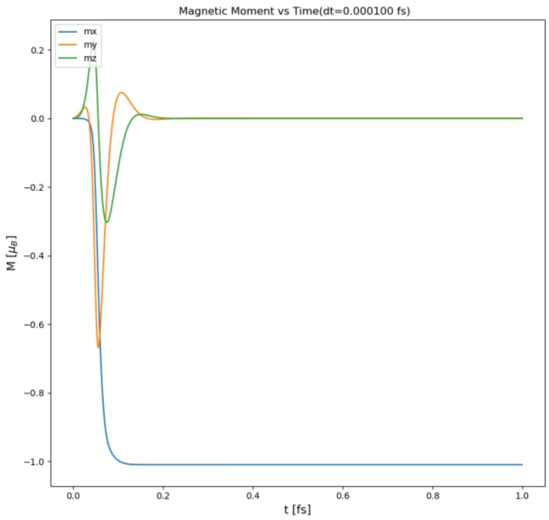
B. Start from FM configuration





C. Start from AFM configuration

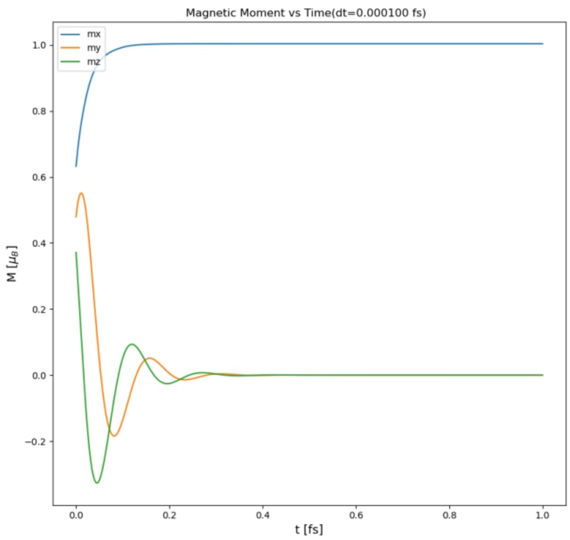




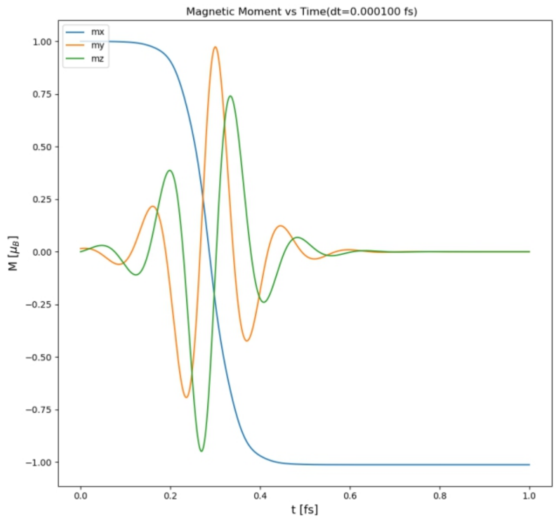
3 Use a full on-site damping tensor and observe the dynamics. Consider that the tensor need to be symmetric, where damping tensor is:

```
[[[[0.01  0.001 0.001]
   [0.001 0.01  0.001]
   [0.001 0.001 0.01 ]]

  [[0.    0.    0.   ]
   [0.    0.    0.   ]
   [0.    0.    0.   ]]]


 [[[0.    0.    0.   ]
   [0.    0.    0.   ]
   [0.    0.    0.   ]]

  [[0.01  0.001 0.001]
   [0.001 0.01  0.001]
   [0.001 0.001 0.01 ]]]]
```

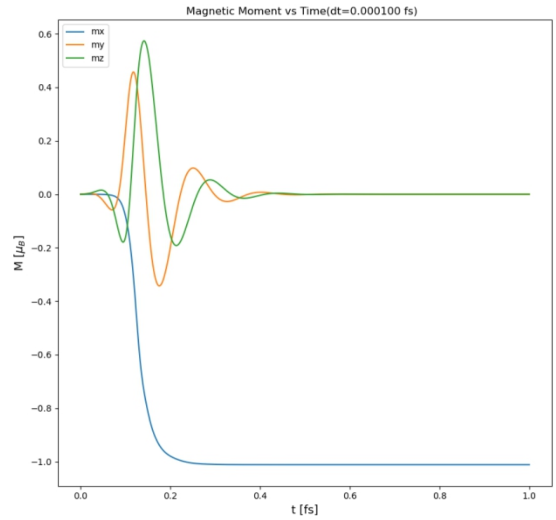
A. Start from a random configuration



B. Start from FM configuration



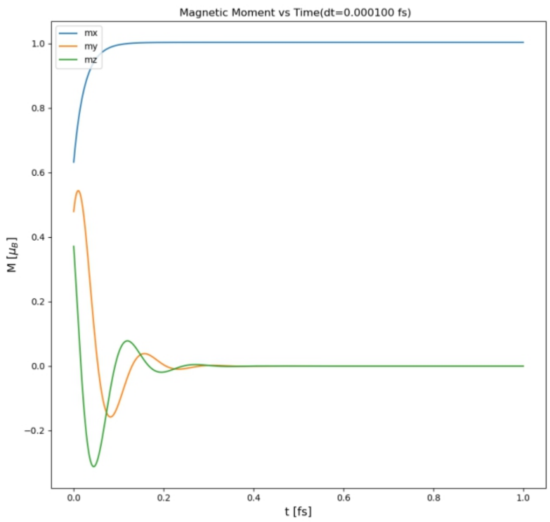
C. Start from AFM configuration



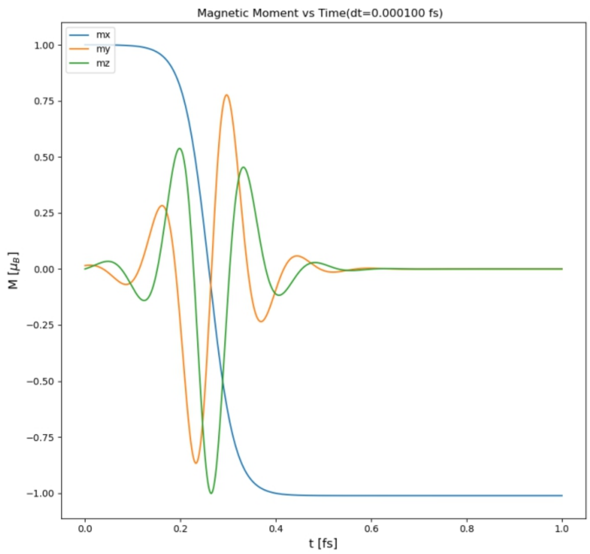
4. Use here that $\alpha_{ij}=\alpha_{ij}I$, where I is unit matrix, and observe the dynamics,where its damping tensor is:

```
[[[[0.01  0.    0.   ]
   [0.    0.01  0.   ]
   [0.    0.    0.01 ]]

  [[0.001 0.    0.   ]
   [0.    0.001 0.   ]
   [0.    0.    0.001]]]


 [[[0.001 0.    0.   ]
   [0.    0.001 0.   ]
   [0.    0.    0.001]]

  [[0.01  0.    0.   ]
   [0.    0.01  0.   ]
   [0.    0.    0.01 ]]]]
```

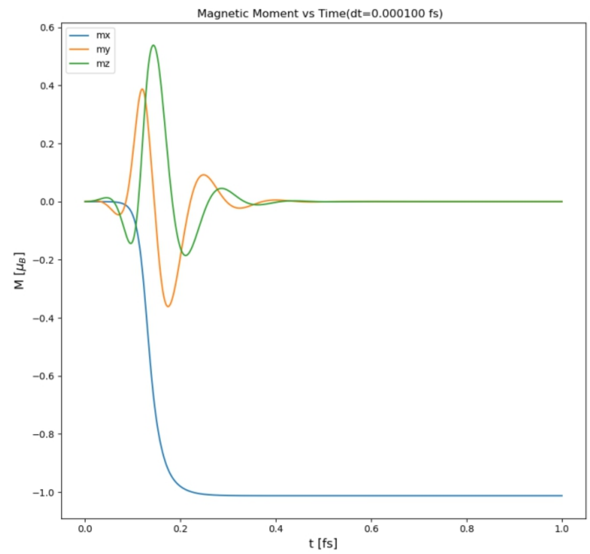
A. Start from a random configuration



B. Start from FM configuration



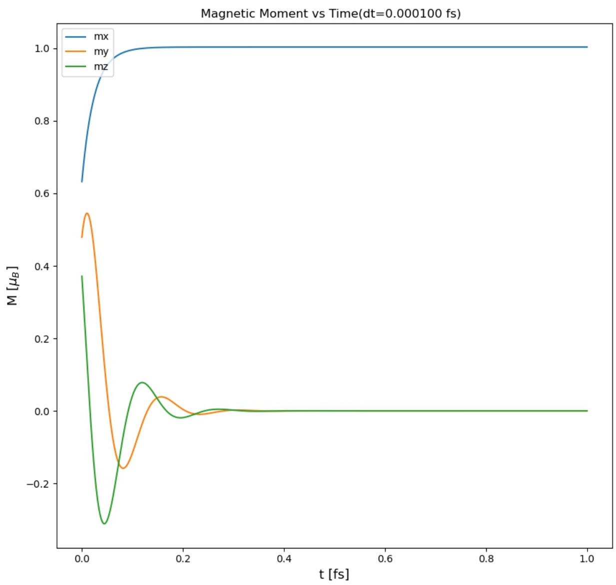
C. Start from AFM configuration



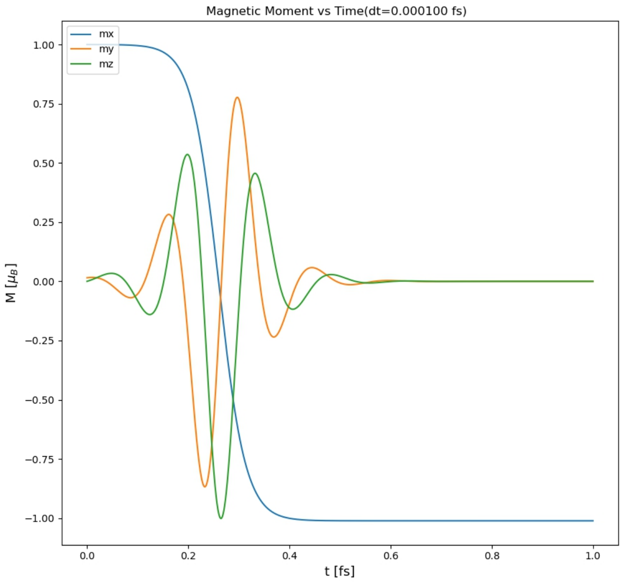
5. Use a full non-local damping tensor and observe the dynamics, where its damping tensor is:

```
[[[[0.01   0.     0.    ]
   [0.     0.01   0.    ]
   [0.     0.     0.01  ]]

  [[0.001  0.0001 0.0001]
   [0.0001 0.001  0.0001]
   [0.0001 0.0001 0.001 ]]]


 [[[0.001  0.0001 0.0001]
   [0.0001 0.001  0.0001]
   [0.0001 0.0001 0.001 ]]

  [[0.01   0.     0.    ]
   [0.     0.01   0.    ]
   [0.     0.     0.01  ]]]]
```

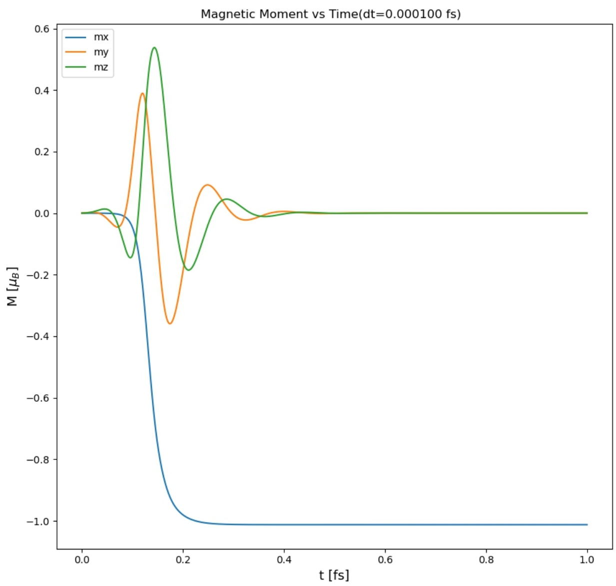
A. Start from a random configuration



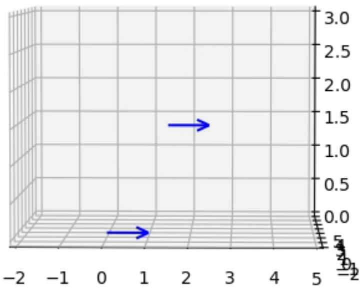
B. Start from FM configuration



C. Start from AFM configuration

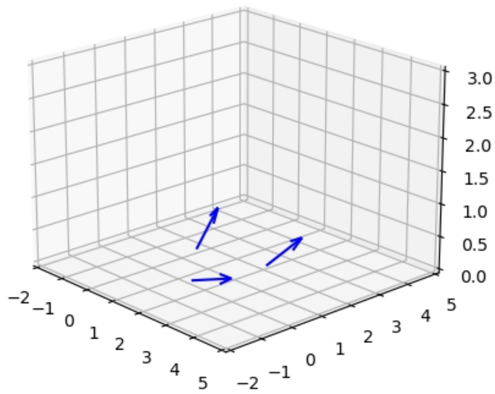


The end configuration of dimer in the dynamics:

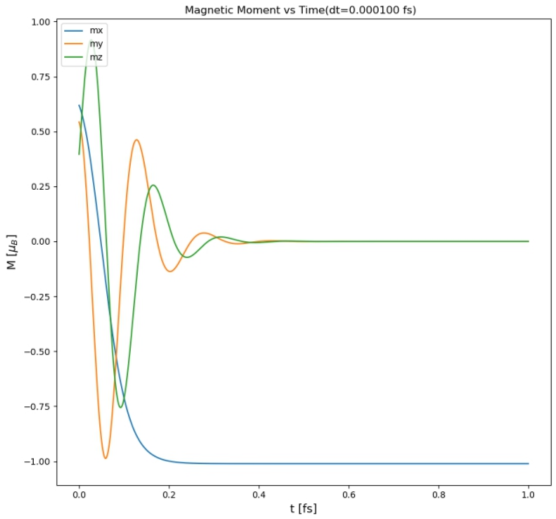


Trimer

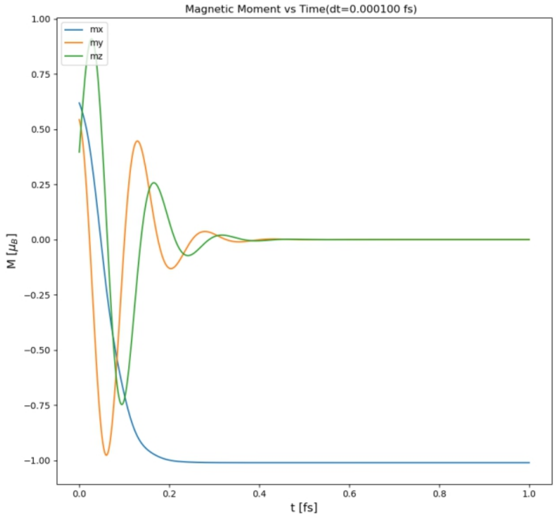
A. Start from a random configuration



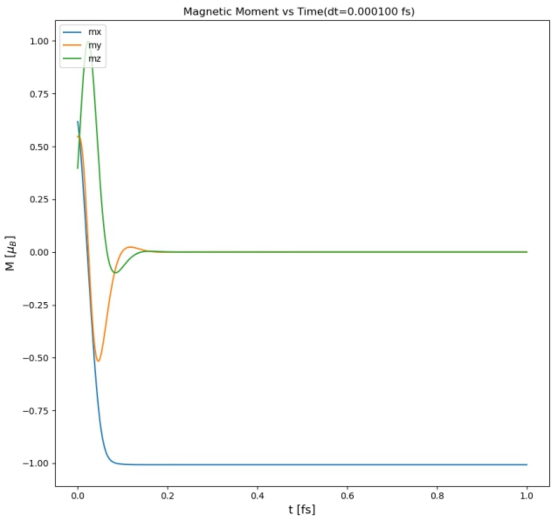
Diagonal_onsite_damping



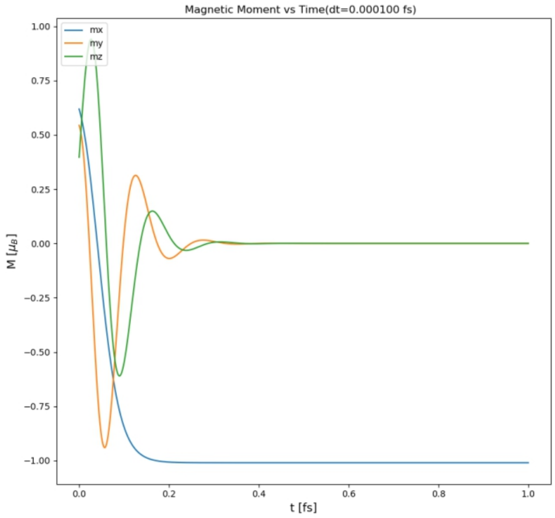
Full_onsite_damping



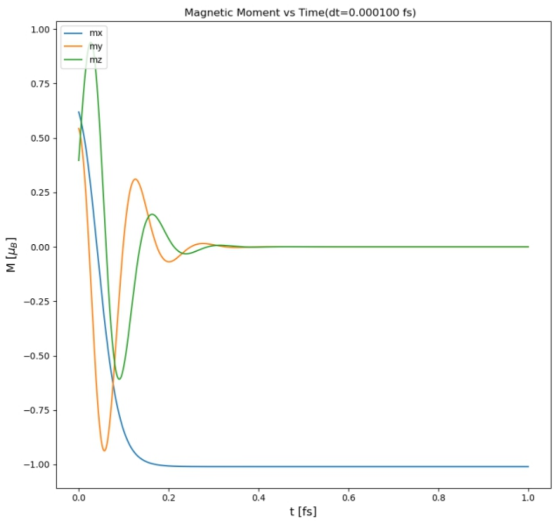
Different_diagonal_element_onsite_damping



Diagonal_nonlocal_damping

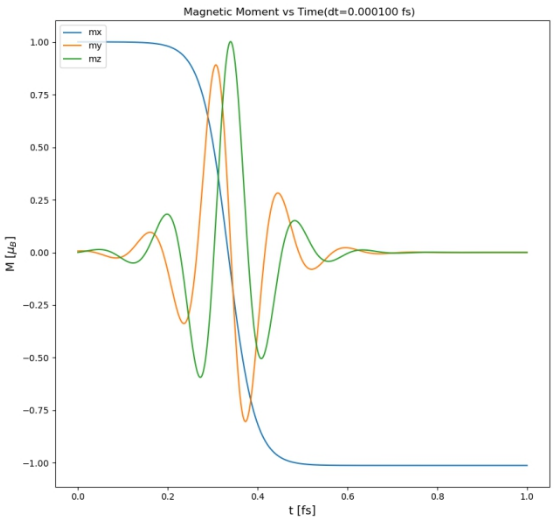


Full_nonlocal_damping

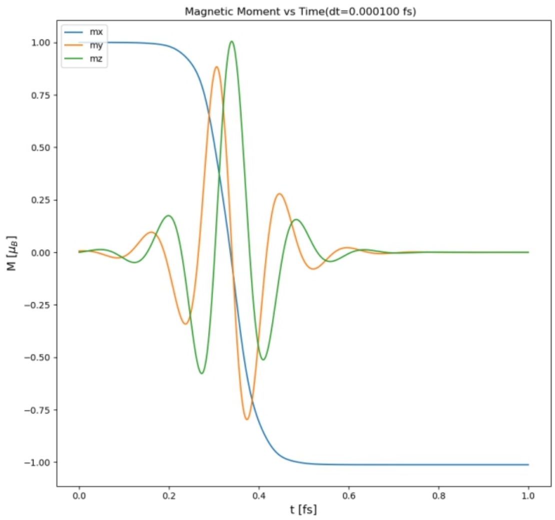


B. Start from FM configuration

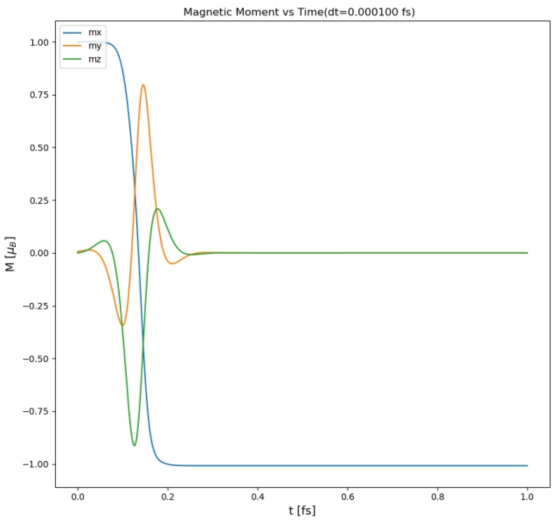
Diagonal_onsite_damping



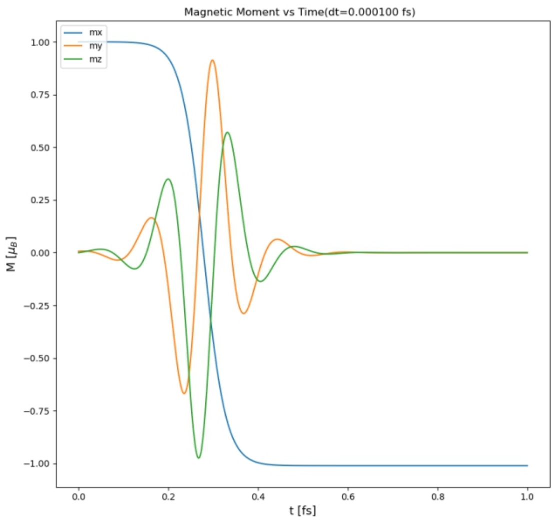
Full_onsite_damping



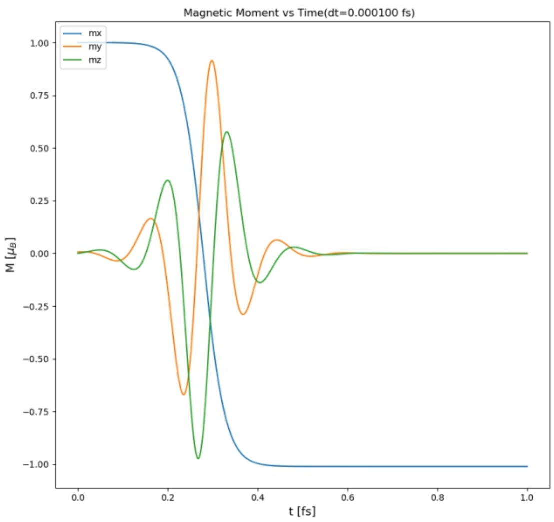
Different_diagonal_element_onsite_damping



Diagonal_nonlocal_damping



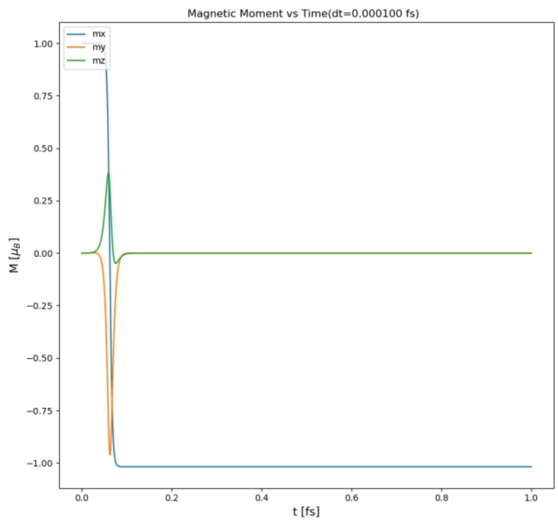
Full_nonlocal_damping



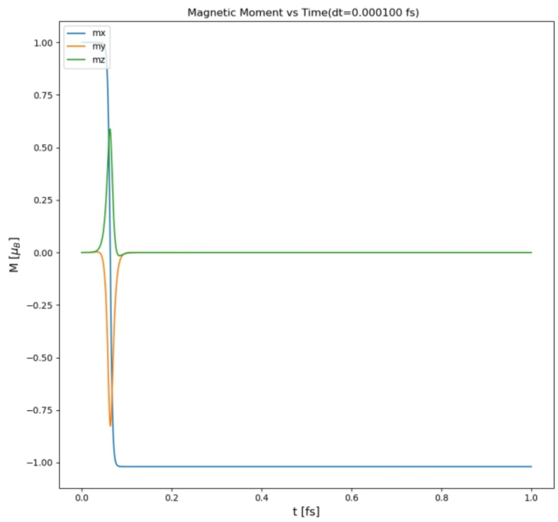
Other results of dimer

A.Onsite damping strength now is 0.1, start from FM configuration.

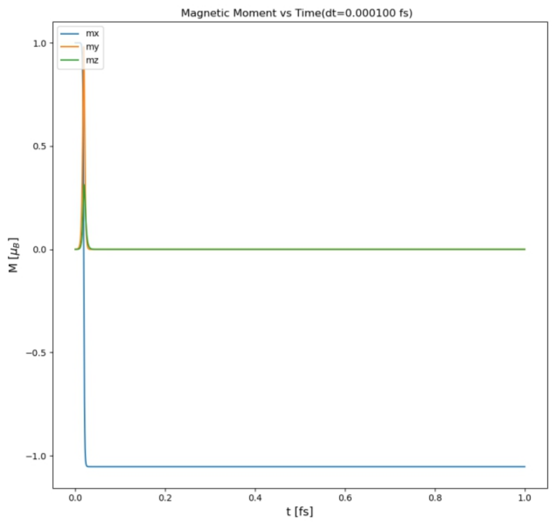
Diagonal_onsite_damping



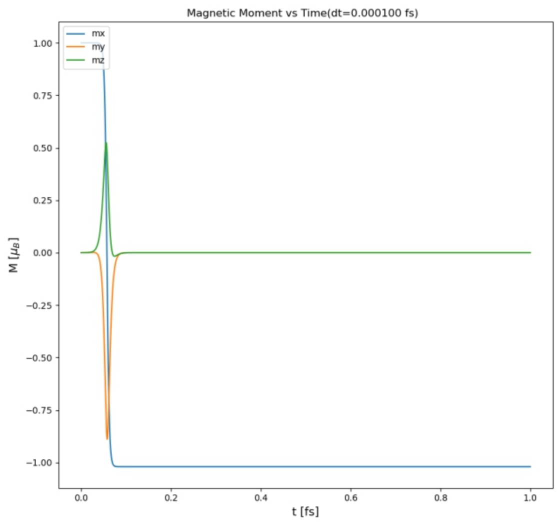
Full_onsite_damping



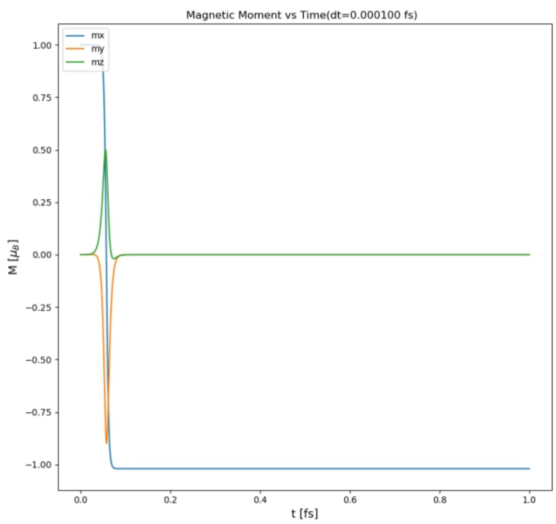
Different_diagonal_element_onsite_damping



Diagonal_nonlocal_damping

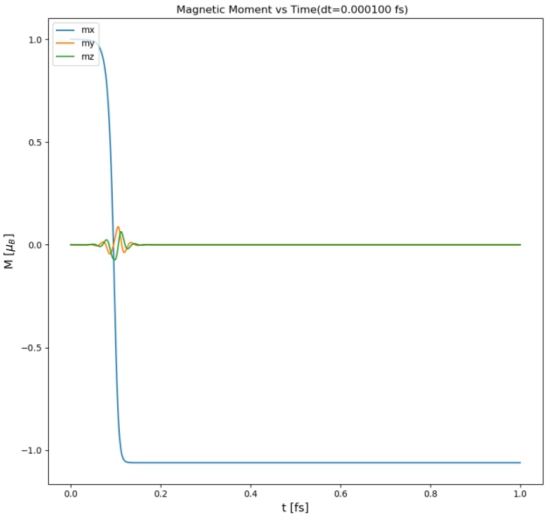


Full_nonlocal_damping

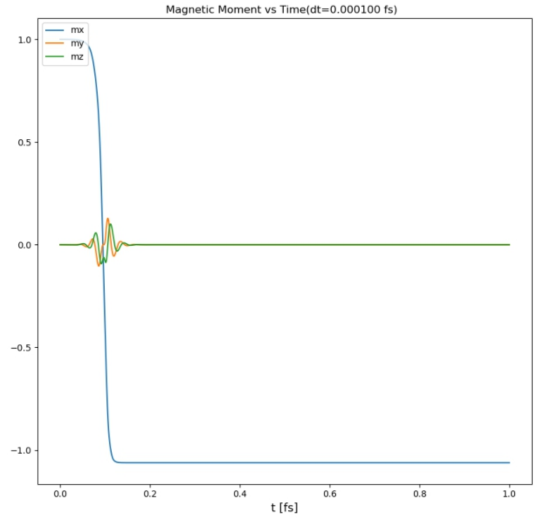


B External field now is 5 Tesla, start from FM configuration.

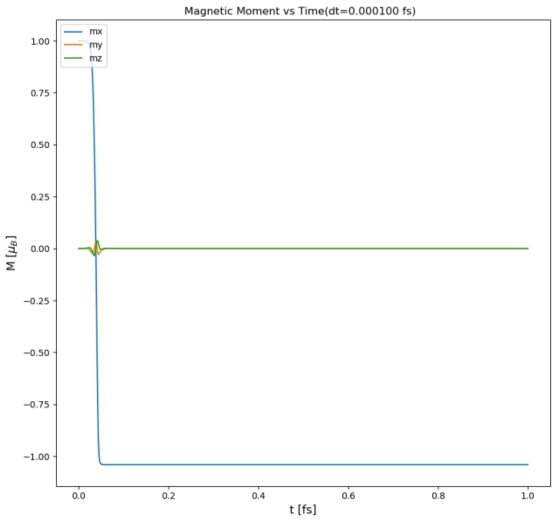
Diagonal_onsite_damping



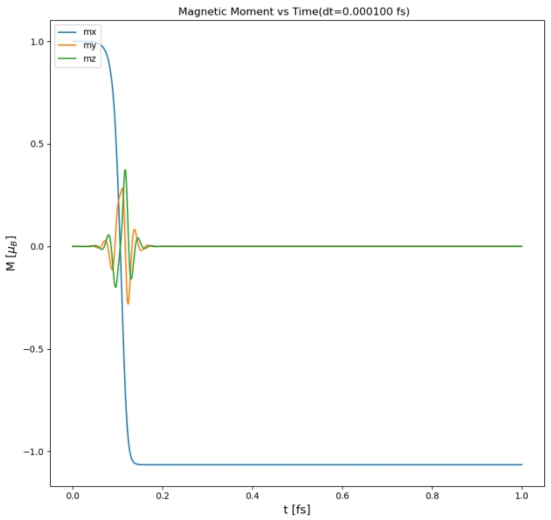
Full_onsite_damping



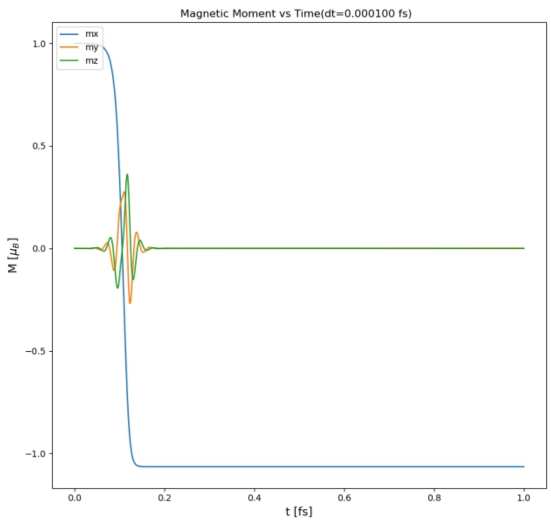
Different_diagonal_element_onsite_damping



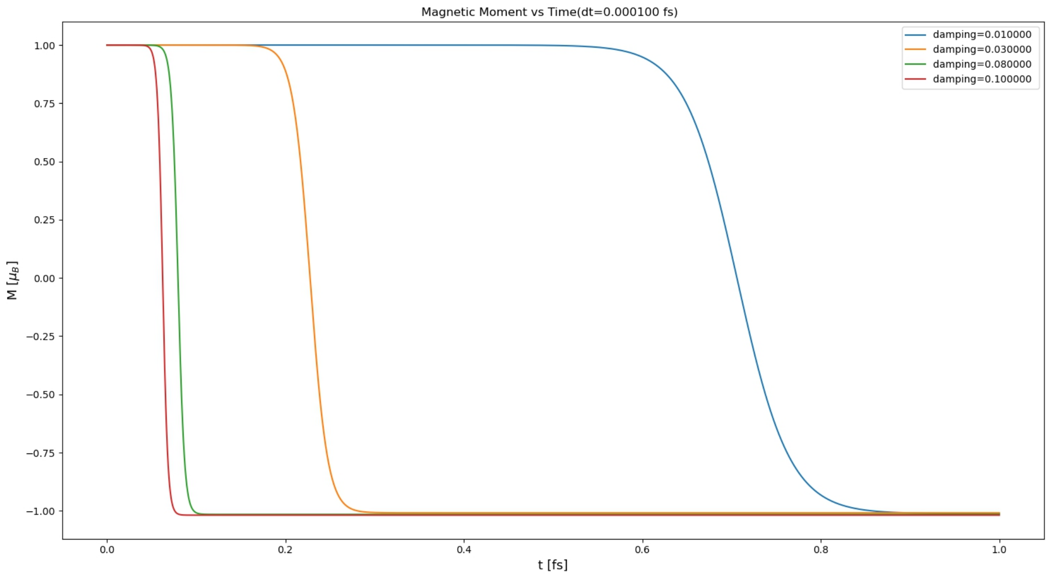
Diagonal_nonlocal_damping



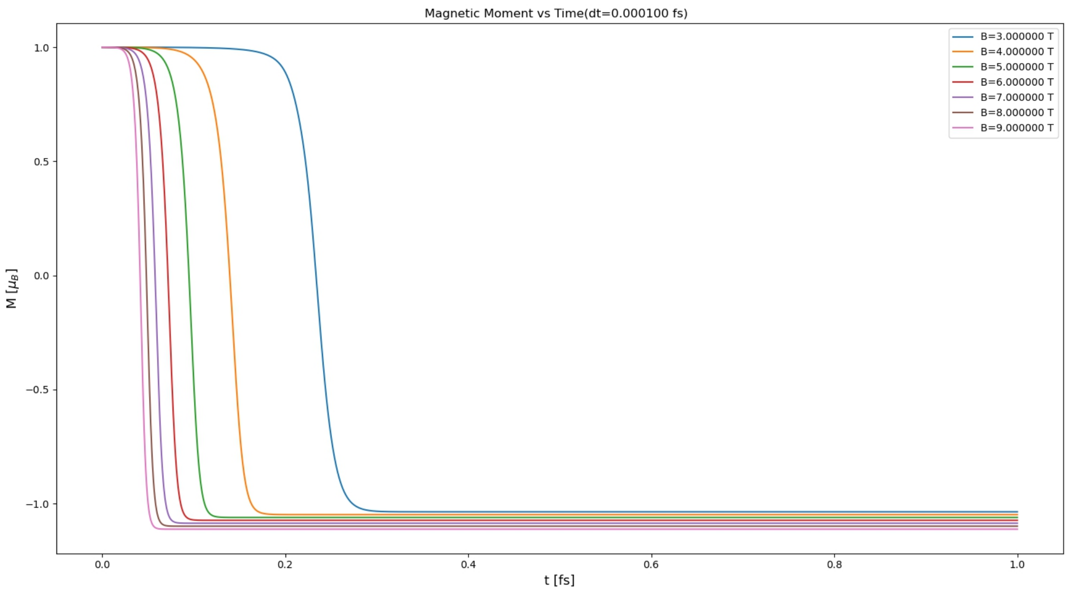
Full_nonlocal_damping



C


Magnetic Moment vs Time(dt=0.000100 fs)
damping=0.010000
damping=0.030000
damping=0.080000
damping=0.100000
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
M [μ_B]
0.0
0.2
0.4
0.6
0.8
1.0
t [fs]

D


Magnetic Moment vs Time(dt=0.000100 fs)
B=3.000000 T
B=4.000000 T
B=5.000000 T
B=6.000000 T
B=7.000000 T
B=8.000000 T
B=9.000000 T
1.0
0.5
0.0
−0.5
−1.0
M [μ_B]
0.0
0.2
0.4
0.6
0.8
1.0
t [fs]

F
Comparing the system with and without non-local damping effect