

tested 190817 using *SpinDynamica* 3.0.1 under *Mathematica* 11.0

Amplitude-Modulated Rf field

```
Needs["SpinDynamica`"]  
SetSpinSystem[1]  
 SetSpinSystem: the spin system has been set to  $\{\{1, \frac{1}{2}\}\}$ 
```

Amplitude-Modulated rf field simulated in the laboratory frame; no relaxation

this example shows the simulation of evolution under a time-dependent Hamiltonian. In this case a laboratory frame simulation is performed using an amplitude-modulated rf field

$\omega_0 = 2\pi 10^6$

2000000π

$\omega_{\text{nut}} = 2\pi 50 \times 10^3$

100000π

$\tau_{360} = 2\pi / \omega_{\text{nut}}$

$\frac{1}{50000}$

$\tau_{90} = \tau_{360}/4; \tau_{180} = \tau_{360}/2;$

the following syntax shows how to define a time-dependent Hamiltonian function, in this case a cosine modulated rf field

```
HamiltonianFunction = Function[t, \omega_0 opI["z"] + \omega_{\text{nut}} (2 opI["x"] Cos[\omega_0 t])]  
Function[t, \omega_0 opI[z] + \omega_{\text{nut}} (2 opI[x] Cos[\omega_0 t])]
```

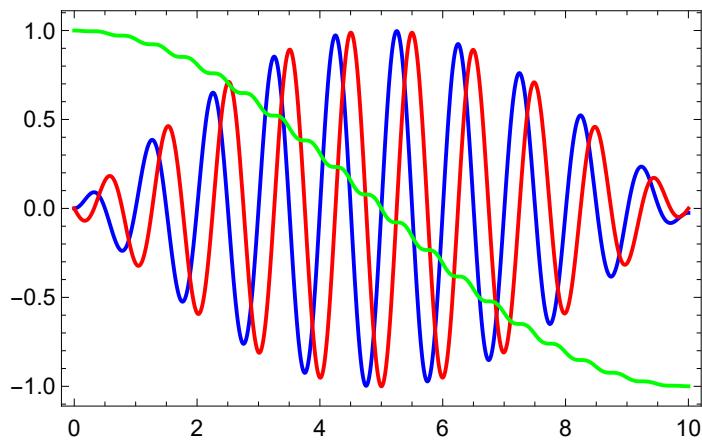
in this simple example, the time-dependent Hamiltonian is applied for the duration of a 180° pulse.
In general, any sequence of events of various types may be defined.

```
events = {{HamiltonianFunction, \tau_{180}}}  
 $\left\{ \left\{ \text{Function}[t, \omega_0 \text{opI}[z] + \omega_{\text{nut}} (2 \text{opI}[x] \text{Cos}[\omega_0 t])], \frac{1}{100000} \right\} \right\}$   
  
 $\{I_x^{traj}, I_y^{traj}, I_z^{traj}\} =$   
 $\text{Trajectory}[\text{opI}["z"] \rightarrow \{\text{opI}["x"], \text{opI}["y"], \text{opI}["z"]\}, \text{events}]$   
 $\{\text{TrajectoryFunction}[\{\{0, 10. \times 10^{-6}\}\}, \text{<>}],$   
 $\text{TrajectoryFunction}[\{\{0, 10. \times 10^{-6}\}\}, \text{<>}], \text{TrajectoryFunction}[\{\{0, 10. \times 10^{-6}\}\}, \text{<>}\}]\}$   
  
 $\text{EventDuration}[\text{events}]$   
 $\frac{1}{100000}$ 
```

```

Plot[
 Evaluate[Through[{Ixtraj, Iytraj, Iztraj}[t $\mu$ s  $\times$  10 $^{-6}$ ]]],
 {t $\mu$ s, 0, EventDuration[events]  $\times$  10 $^6$  },
 Frame  $\rightarrow$  True,
 PlotStyle  $\rightarrow$  {{Thick, Blue}, {Thick, Red}, {Thick, Green}},
 LabelStyle  $\rightarrow$  Directive[Medium, FontFamily  $\rightarrow$  "Helvetica"]
]

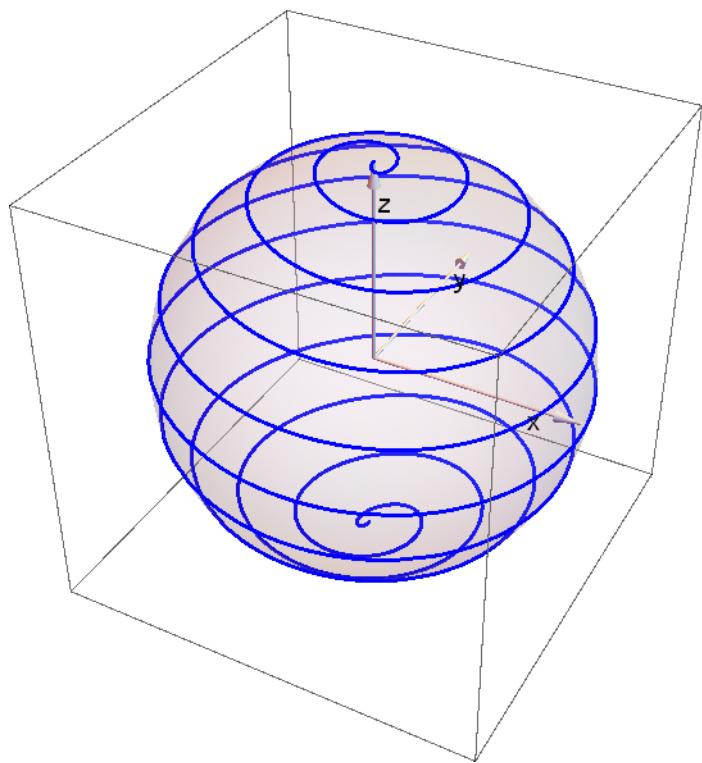
```



```

Show[
 Graphics3D@{Opacity[0.2], Sphere[{0, 0, 0}, 1]},
 ParametricPlot3D[
 Through[{Ixtraj, Iytraj, Iztraj}[t]], {t, 0, EventDuration[events]} ],
 Boxed  $\rightarrow$  True, Axes  $\rightarrow$  None, PlotStyle  $\rightarrow$  {{Thick, Blue}}
],
 Axes3D[]
]

```



Amplitude-Modulated rf field simulated in the laboratory frame; with relaxation

in this case a strong relaxation superoperator is included in the BackgroundGenerator. Evolution over 5 complete nutations is simulated.

```
w0 = 2 π 10^6;
ωnut = 2 π 50 × 10^3;
τ360 = 2 π / ωnut;
τ90 = τ360 / 4; τ180 = τ360 / 2;

HamiltonianFunction = Function[t, w0 opI["z"] + ωnut × (2 opI["x"] Cos[w0 t])]
Function[t, w0 opI[z] + ωnut (2 opI[x] Cos[w0 t])]
```

the relaxation superoperator defined below corresponds to fluctuating random fields along the z-axis.

```
relaxationstrength = 10^5;

RelaxationSuperoperator =
- relaxationstrength DoubleCommutationSuperoperator[opT[1, {1, 0}], opT[1, {1, 0}]]
- 100 000 DoubleCommutationSuperoperator[I1z, I1z]

events = {{HamiltonianFunction, 5 τ360} }

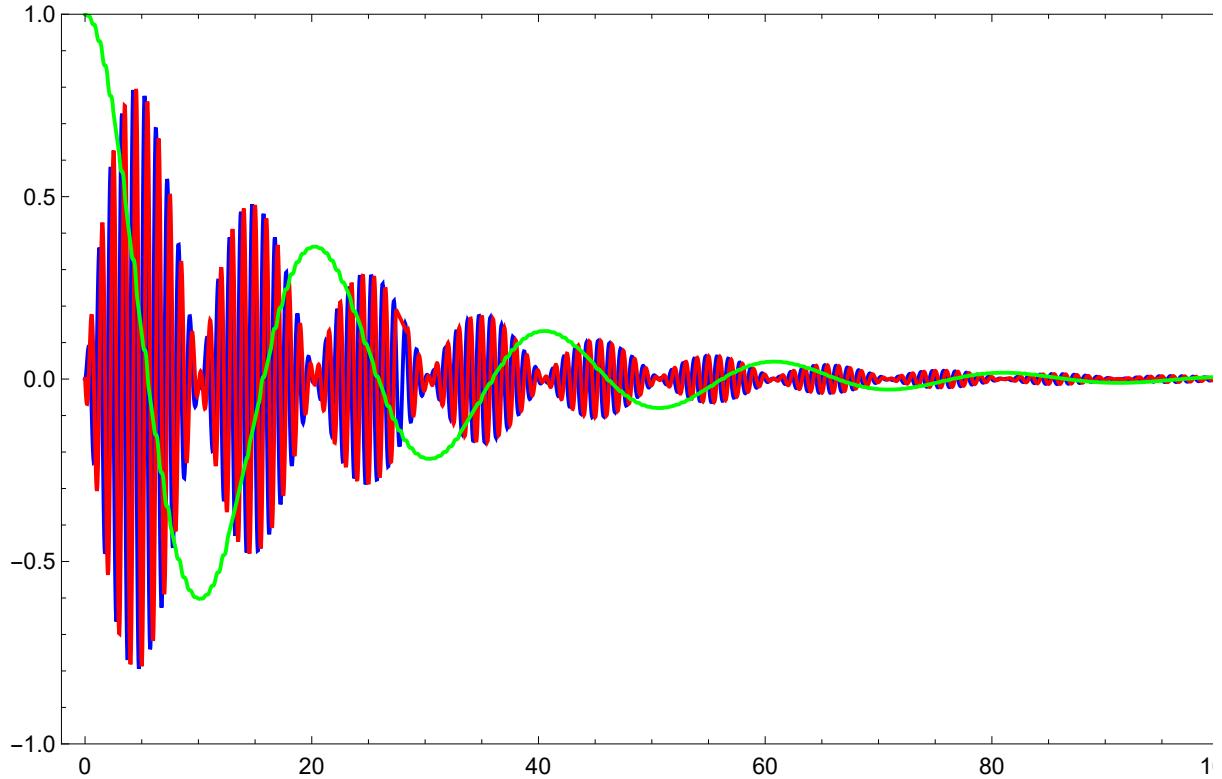
{{Function[t, w0 opI[z] + ωnut (2 opI[x] Cos[w0 t])], 1/10 000} }

traj = Trajectory[
opI["z"] -> opI["z"],
events,
BackgroundGenerator -> RelaxationSuperoperator
]
TrajectoryFunction[{{0, 100. × 10^-6}} , <>]

Trajectory[
opI["z"] -> {opI["x"], opI["y"], opI["z"]},
events,
BackgroundGenerator -> RelaxationSuperoperator
]
{TrajectoryFunction[{{0, 100. × 10^-6}} , <>],
 TrajectoryFunction[{{0, 100. × 10^-6}} , <>],
 TrajectoryFunction[{{0, 100. × 10^-6}} , <>]}

{Ixtraj, Iytraj, Iztraj} =
Trajectory[
opI["z"] -> {opI["x"], opI["y"], opI["z"]},
events,
BackgroundGenerator -> RelaxationSuperoperator
]
{TrajectoryFunction[{{0, 100. × 10^-6}} , <>],
 TrajectoryFunction[{{0, 100. × 10^-6}} , <>],
 TrajectoryFunction[{{0, 100. × 10^-6}} , <>]}
```

```
Plot[Evaluate[Through[{Ixtraj, Iytraj, Iztraj}[t $\mu$ s  $\times$  10 $^{-6}$ ])),  
{t $\mu$ s, 0, EventDuration[events]  $\times$  10 $^6$ }, Frame  $\rightarrow$  True,  
PlotStyle  $\rightarrow$  {{Thick, Blue}, {Thick, Red}, {Thick, Green}},  
PlotRange  $\rightarrow$  {-1, 1}, LabelStyle  $\rightarrow$  Directive[Medium, FontFamily  $\rightarrow$  "Helvetica"]]
```



```
Show[  
  Graphics3D@{Opacity[0.2], Sphere[{0, 0, 0}, 1]},  
  ParametricPlot3D[  
    Through[{Ixtraj, Iytraj, Iztraj}[t]], {t, 0, EventDuration[events]}],  
  Boxed → True, Axes → None, PlotStyle → {{Thick, Blue}}]  
,  
Axes3D[]  
]
```

