

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

propagation of magnetization down a chain of 5 spins-1/2 in the presence of a scalar coupling Hamiltonian and a repeating sequence of composite pulses

```
Needs["SpinDynamica`"]
```

```
nspin = 5;
```

```
SetSpinSystem[nspin]
```

```
SetSpinSystem: the spin system has been set to {{1, 1/2}, {2, 1/2}, {3, 1/2}, {4, 1/2}, {5, 1/2}}
```

■ define a chain of nearest neighbour J-couplings, each 20 Hz

```
HJ = Plus @@ Table[2 π 20 opI[i] . opI[i + 1], {i, 1, nspin - 1}]
```

```
40 π (I1x•I2x + I1y•I2y + I1z•I2z) + 40 π (I2x•I3x + I2y•I3y + I2z•I3z) +  
40 π (I3x•I4x + I3y•I4y + I3z•I4z) + 40 π (I4x•I5x + I4y•I5y + I4z•I5z)
```

■ define a composite pulse with a rf field giving a nutation frequency of 2 kHz.

```
ωnut = 2 π × 2 × 103;
```

```
τ360 = 2 π / ωnut; τ180 = τ360 / 2; τ90 = τ360 / 4;
```

```
CompositePulse = {{ωnut opI["x"], τ90}, {ωnut opI["y"], τ180}, {ωnut opI["x"], τ90}};
```

```
T = EventDuration[CompositePulse]
```

```
1  
-----  
2000
```

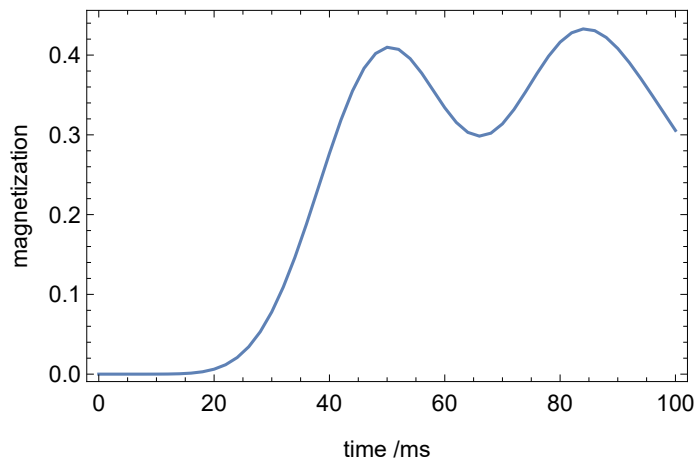
■ trajectory of I<sub>z</sub> for the last spin in the chain

use the option TableCoordinates to label with the pulse sequence duration, in units of ms

```
table =
```

```
TransformationAmplitudeTable[  
  opI[1, "z"] -> opI[nspin, "z"],  
  Repeat[CompositePulse, n],  
  {n, 0, 200, 4},  
  BackgroundGenerator -> HJ,  
  TableCoordinates -> n T × 103  
];
```

```
ListPlot[table, PlotRange -> All, Joined -> True, Frame -> True,  
  LabelStyle -> Directive[Medium, FontFamily -> "Helvetica"],  
  FrameLabel -> {"time /ms", "magnetization"}  
]
```



■ trajectory for all magnetization components at the same time

```
Iztable = Table[opI[i, "z"], {i, 1, nspin}]
```

```
{I1z, I2z, I3z, I4z, I5z}
```

```
table =
```

```
TransformationAmplitudeTable[
  opI[1, "z"] → Iztable,
  Repeat[CompositePulse, n],
  {n, 0, 200, 4},
  BackgroundGenerator → HJ,
  TableCoordinates → n T × 103
];
```

```
ListPlot[table, PlotRange → All, Joined → True, Frame → True,
  LabelStyle → Directive[Medium, FontFamily → "Helvetica"],
  FrameLabel → {"time /ms", "magnetization"},
  PlotStyle → Table[{Thick, ColorData[3, "ColorList"][[i]]}, {i, 1, nspin}]
]
```

