Maxima workbook for Principles of NMR Spectroscopy Chapter 16: Heteronuclear NMR techniques

1 Introduction

This wxMaxima workbook is an electronic supplement to to the book Principles of NMR Spectroscopy: An Illustrated Guide, David P. Goldenberg, University Science Books, (c) 2016.
This and related files are available for download through links at: http://uscibooks.com/goldenberg.htm
wxMaxima is a graphical user interface to the computer algebra system (CAS) Maxima. General information about Maxima and wxMaxima, along with free versions of the programs, can be found at: http://maxima.sourceforge.net/ and http://andrejv.github.io/wxmaxima/
Before attempting to use this workbook, users are strongly encouraged to read and experiment with the introductory workbook, gettingStarted.wxmx, and the workbooks for the earlier chapters.

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This chapter describes NMR experiments based on dipolar coupling between different nuclei types, such as 1H and 13C, or 1H and 15N.
The worksheet uses the definitions found in 2spinLib.mac. These definitions, where appropriate, assume the weak- coupling limit.

```
(%i1) load("2spinLib.mac")$
```

Removing the $ symbol at the end of the command below and executing the command will output a list of all of the functions defined by the 2spinLib.mac library, and the packages it loads.

```
(%i2) functions$
```

2 16.1 Heteronuclear coupling and decoupling

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Decoupling after a selective pi/2 y,S pulse.
Consider a Ialpha alpha> and Ibeta alpha> starting states for a coupled spin pair, I-S.

```
(%i3) k_aa;
```

(%o3) $\begin{pmatrix}1\\0\\0\\0\end{pmatrix}$

```
(%i4) k_ba;
```

(%o4) $\begin{pmatrix}0\\0\\1\\0\end{pmatrix}$

After an initial pi/2 y,S pulse:

```
(%i5) k_aa1:psiPi2YS(k_aa);
```

(%o5) $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \\ 0 \end{pmatrix}$

```
(%i6) allMagPsi(k_aa1);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= \frac{1}{2}$
$< Sx >= \frac{1}{2}$
$< Sy >= 0$
$< Sz >= 0$

(%o6)

```
(%i7) k_ba1:psiPi2YS(k_ba);
```

(%o7) $\begin{pmatrix} 0 \\ 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$

```
(%i8) allMagPsi(k_ba1);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= -\frac{1}{2}$
$< Sx >= \frac{1}{2}$
$< Sy >= 0$
$< Sz >= 0$

(%o8)

Precession for a period tau1

```
(%i9) k_aa2:psiTime(k_aa1,tau1)$
(%i10) allMagPsi(k_aa2);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= \frac{1}{2}$
$< Sx >= \frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J)}{2}$
$< Sy >= \frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J)}{2}$
$< Sz >= 0$

(%o10)

```
(%i11) k_ba2:psiTime(k_ba1,tau1)$
(%i12) allMagPsi(k_ba2);
```

$$< Ix >= 0$$
$$< Iy >= 0$$
$$< Iz >= -\frac{1}{2}$$
$$< Sx >= \frac{\cos\left(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J\right)}{2}$$
$$< Sy >= \frac{\sin\left(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J\right)}{2}$$
$$< Sz >= 0$$

(%o12)

Fig. 16.4

pi x,I refocussing pulse:

```
(%i13) k_aa3:psiPiXI(k_aa2)$
(%i14) allMagPsi(k_aa3);
```

$$< Ix >= 0$$
$$< Iy >= 0$$
$$< Iz >= -\frac{1}{2}$$
$$< Sx >= \frac{\cos\left(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J\right)}{2}$$
$$< Sy >= \frac{\sin\left(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J\right)}{2}$$
$$< Sz >= 0$$

(%o14)

```
(%i15) k_ba3:psiPiXI(k_ba2)$
(%i16) allMagPsi(k_ba3);
```

$$< Ix >= 0$$
$$< Iy >= 0$$
$$< Iz >= \frac{1}{2}$$
$$< Sx >= \frac{\cos\left(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J\right)}{2}$$
$$< Sy >= \frac{\sin\left(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J\right)}{2}$$
$$< Sz >= 0$$

(%o16)

Evolution for period tau2

```
(%i17) k_aa4:psiTime(k_aa3,tau2)$
(%i18) allMagPsi(k_aa4);
```

$$< Ix >= 0$$
$$< Iy >= 0$$
$$< Iz >= -\frac{1}{2}$$
$$< Sx >= \frac{\cos\left(\left(2 \cdot \pi \cdot tau1 + 2 \cdot \pi \cdot tau2\right) \cdot nuS + \left(\pi \cdot tau1 - \pi \cdot tau2\right) \cdot J\right)}{2}$$
$$< Sy >= \frac{\sin\left(\left(2 \cdot \pi \cdot tau1 + 2 \cdot \pi \cdot tau2\right) \cdot nuS + \left(\pi \cdot tau1 - \pi \cdot tau2\right) \cdot J\right)}{2}$$
$$< Sz >= 0$$

(%o18)

```
(%i19) k_ba4:psiTime(k_ba3,tau2)$
(%i20) allMagPsi(k_ba4);
```

$< Ix >= 0$

$< Iy >= 0$

$< Iz >= \frac{1}{2}$

$< Sx >= \frac{\cos\left((2\cdot\pi\cdot tau1+2\cdot\pi\cdot tau2)\cdot nuS+(\pi\cdot tau2-\pi\cdot tau1)\cdot J\right)}{2}$

$< Sy >= \frac{\sin\left((2\cdot\pi\cdot tau1+2\cdot\pi\cdot tau2)\cdot nuS+(\pi\cdot tau2-\pi\cdot tau1)\cdot J\right)}{2}$

$< Sz >= 0$

(%o20)

Now, calculate magnetization components, with the condition tau2=tau1

```
(%i21) allMagPsi(subst(tau2=tau1,k_aa4));
```

$< Ix >= 0$

$< Iy >= 0$

$< Iz >= -\frac{1}{2}$

$< Sx >= \frac{\cos(4\cdot\pi\cdot tau1\cdot nuS)}{2}$

$< Sy >= \frac{\sin(4\cdot\pi\cdot tau1\cdot nuS)}{2}$

$< Sz >= 0$

(%o21)

```
(%i22) allMagPsi(subst(tau2=tau1,k_ba4));
```

$< Ix >= 0$

$< Iy >= 0$

$< Iz >= \frac{1}{2}$

$< Sx >= \frac{\cos(4\cdot\pi\cdot tau1\cdot nuS)}{2}$

$< Sy >= \frac{\sin(4\cdot\pi\cdot tau1\cdot nuS)}{2}$

$< Sz >= 0$

(%o22)

Fig. 16.5

The two populations give rise to the same average frequency.

Decoupling applied to a single population. with a superposition state giving rise to two frequencies.
A non-selective pi/2 y pulse applied to k_aa

```
(%i23) k_aa5:psiPi2Y(k_aa);
```

(%o23) $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$

```
(%i24) allMagPsi(k_aa5);
```

$< Ix >= \frac{1}{2}$

$< Iy >= 0$

$< Iz >= 0$

$< Sx >= \frac{1}{2}$

$< Sy >= 0$

$< Sz >= 0$

(%o24)

First time-evolution period, tau1

```
(%i25) k_aa6:psiTime(k_aa5,tau1)$
(%i26) allMagPsi(k_aa6);
```

$$< Ix >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)+\cos(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)}{4}$$

$$< Iy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)+\sin(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)}{4}$$

$< Iz >= 0$

$$< Sx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)+\cos(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)}{4}$$

$$< Sy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)+\sin(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)}{4}$$

$< Sz >= 0$

(%o26)

Fig. 16.6

pi x,I refocussing pulse:

```
(%i27) k_aa7:psiPiXI(k_aa6)$
(%i28) allMagPsi(k_aa7);
```

$$< Ix >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)+\cos(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)}{4}$$

$$< Iy >= -\frac{\sin(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)+\sin(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)}{4}$$

$< Iz >= 0$

$$< Sx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)+\cos(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)}{4}$$

$$< Sy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)+\sin(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)}{4}$$

$< Sz >= 0$

(%o28)

Fig. 16.7

Second evolution period, tau2

```
(%i29) k_aa8:psiTime(k_aa7,tau2)$
(%i30) allMagPsi(k_aa8);
```

$$< Ix >= \frac{\cos\left((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuI+(\pi\cdot tau1-\pi\cdot tau2)\cdot J\right)+\cos\left((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuI+(\pi\cdot tau2-\pi\cdot tau1)\cdot J\right)}{4}$$

$$< Iy >= \frac{\sin\left((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuI+(\pi\cdot tau1-\pi\cdot tau2)\cdot J\right)+\sin\left((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuI+(\pi\cdot tau2-\pi\cdot tau1)\cdot J\right)}{4}$$

$$< Iz >= 0$$

$$< Sx >= \frac{\cos\left((2\cdot\pi\cdot tau1+2\cdot\pi\cdot tau2)\cdot nuS+(\pi\cdot tau1-\pi\cdot tau2)\cdot J\right)+\cos\left((2\cdot\pi\cdot tau1+2\cdot\pi\cdot tau2)\cdot nuS+(\pi\cdot tau2-\pi\cdot tau1)\cdot J\right)}{4}$$

$$< Sy >= \frac{\sin\left((2\cdot\pi\cdot tau1+2\cdot\pi\cdot tau2)\cdot nuS+(\pi\cdot tau1-\pi\cdot tau2)\cdot J\right)+\sin\left((2\cdot\pi\cdot tau1+2\cdot\pi\cdot tau2)\cdot nuS+(\pi\cdot tau2-\pi\cdot tau1)\cdot J\right)}{4}$$

$$< Sz >= 0$$

(%o30)

Simplifying the results for Iy and Sy

```
(%i31) meanPsi(Iy,k_aa8);
```

(%o31) $$\frac{\sin\left((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuI+(\pi\cdot tau1-\pi\cdot tau2)\cdot J\right)+\sin\left((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuI+(\pi\cdot tau2-\pi\cdot tau1)\cdot J\right)}{4}$$

```
(%i32) expand(%);
```

(%o32) $$\frac{\sin\left(2\cdot\pi\cdot tau2\cdot nuI-2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau2\cdot J-\pi\cdot tau1\cdot J\right)}{4}+\frac{\sin\left(2\cdot\pi\cdot tau2\cdot nuI-2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau2\cdot J+\pi\cdot\right.}{4}$$

```
(%i33) meanPsi(Sy,k_aa8);
```

(%o33) $$\frac{\sin\left((2\cdot\pi\cdot tau1+2\cdot\pi\cdot tau2)\cdot nuS+(\pi\cdot tau1-\pi\cdot tau2)\cdot J\right)+\sin\left((2\cdot\pi\cdot tau1+2\cdot\pi\cdot tau2)\cdot nuS+(\pi\cdot tau2-\pi\cdot tau1)\cdot J\right)}{4}$$

```
(%i34) expand(%);
```

(%o34) $$\frac{\sin\left(2\cdot\pi\cdot tau2\cdot nuS+2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau2\cdot J-\pi\cdot tau1\cdot J\right)}{4}+\frac{\sin\left(2\cdot\pi\cdot tau2\cdot nuS+2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau2\cdot J+\pi\right.}{4}$$

If tau2 is set to equal tau1

```
(%i35) allMagPsi(subst(tau2=tau1, k_aa8));
```

$$< Ix >= \frac{1}{2}$$

$$< Iy >= 0$$

$$< Iz >= 0$$

$$< Sx >= \frac{\cos(4\cdot\pi\cdot tau1\cdot nuS)}{2}$$

$$< Sy >= \frac{\sin(4\cdot\pi\cdot tau1\cdot nuS)}{2}$$

$$< Sz >= 0$$

(%o35)

The I-signal is refocussed to the x'I axis, and the S-signal reflects the average precession frequency of its two components.

Following the correlations during the refocusing of magnetization beginning as Sx.

After the initial non-selective pi/2 y-pulse

```
(%i36) k_aa5;
```

(%o36) $$\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$$

(%i37) allMagPsi(k_aa5);

$< Ix >= \frac{1}{2}$

$< Iy >= 0$

$< Iz >= 0$

$< Sx >= \frac{1}{2}$

$< Sy >= 0$

$< Sz >= 0$

(%o37)

(%i38) allCorrPsi(k_aa5);

$< IxSx >= \frac{1}{4}$

$< IxSy >= 0$

$< IxSz >= 0$

$< IySx >= 0$

$< IySy >= 0$

$< IySz >= 0$

$< IzSx >= 0$

$< IzSy >= 0$

$< IzSz >= 0$

(%o38)

Time evolution during tau1 period

(%i39) k_aa6;

$$(\%o39) \quad \begin{pmatrix} \frac{e^{-i\cdot\pi\cdot tau1\cdot\left(\frac{J}{2}+nuI+nuS\right)}}{2} \\ \frac{e^{-i\cdot\pi\cdot tau1\cdot\left(-\frac{J}{2}+nuI-nuS\right)}}{2} \\ \frac{e^{-i\cdot\pi\cdot tau1\cdot\left(-\frac{J}{2}-nuI+nuS\right)}}{2} \\ \frac{e^{-i\cdot\pi\cdot tau1\cdot\left(\frac{J}{2}-nuI-nuS\right)}}{2} \end{pmatrix}$$

(%i40) allMagPsi(k_aa6);

$$< Ix >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)+\cos(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)}{4}$$

$$< Iy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)+\sin(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)}{4}$$

$< Iz >= 0$

$$< Sx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)+\cos(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)}{4}$$

$$< Sy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)+\sin(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)}{4}$$

$< Sz >= 0$

(%o40)

(%i41) allCorrPsi(k_aa6);

$$< IxSx >= \frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuS - 2 \cdot \pi \cdot tau1 \cdot nuI) + \cos(2 \cdot \pi \cdot tau1 \cdot nuS + 2 \cdot \pi \cdot tau1 \cdot nuI)}{8}$$

$$< IxSy >= \frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuS - 2 \cdot \pi \cdot tau1 \cdot nuI) + \sin(2 \cdot \pi \cdot tau1 \cdot nuS + 2 \cdot \pi \cdot tau1 \cdot nuI)}{8}$$

$$< IxSz >= \frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuI + \pi \cdot tau1 \cdot J) - \cos(2 \cdot \pi \cdot tau1 \cdot nuI - \pi \cdot tau1 \cdot J)}{8}$$

$$< IySx >= \frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuS + 2 \cdot \pi \cdot tau1 \cdot nuI) - \sin(2 \cdot \pi \cdot tau1 \cdot nuS - 2 \cdot \pi \cdot tau1 \cdot nuI)}{8}$$

$$< IySy >= -\frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuS + 2 \cdot \pi \cdot tau1 \cdot nuI) - \cos(2 \cdot \pi \cdot tau1 \cdot nuS - 2 \cdot \pi \cdot tau1 \cdot nuI)}{8}$$

$$< IySz >= \frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuI + \pi \cdot tau1 \cdot J) - \sin(2 \cdot \pi \cdot tau1 \cdot nuI - \pi \cdot tau1 \cdot J)}{8}$$

$$< IzSx >= \frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J) - \cos(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J)}{8}$$

$$< IzSy >= \frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J) - \sin(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J)}{8}$$

$$< IzSz >= 0$$

(%o41)

Fig. 16.8 The initial Sx-magnetization evolves into a mixture of Sy-magnetization and SxIz and SyIz correlations.

The pi-xI pulse

```
(%i42) k_aa7;
```

(%o42) $$\begin{pmatrix} -\frac{i \cdot e^{-i \cdot \pi \cdot tau1 \cdot \left(-\frac{J}{2} - nuI + nuS\right)}}{2} \\ -\frac{i \cdot e^{-i \cdot \pi \cdot tau1 \cdot \left(\frac{J}{2} - nuI - nuS\right)}}{2} \\ -\frac{i \cdot e^{-i \cdot \pi \cdot tau1 \cdot \left(\frac{J}{2} + nuI + nuS\right)}}{2} \\ -\frac{i \cdot e^{-i \cdot \pi \cdot tau1 \cdot \left(-\frac{J}{2} + nuI - nuS\right)}}{2} \end{pmatrix}$$

```
(%i43) allMagPsi(k_aa7);
```

$$< Ix >= \frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuI - \pi \cdot tau1 \cdot J) + \cos(2 \cdot \pi \cdot tau1 \cdot nuI + \pi \cdot tau1 \cdot J)}{4}$$

$$< Iy >= -\frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuI - \pi \cdot tau1 \cdot J) + \sin(2 \cdot \pi \cdot tau1 \cdot nuI + \pi \cdot tau1 \cdot J)}{4}$$

$$< Iz >= 0$$

$$< Sx >= \frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J) + \cos(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J)}{4}$$

$$< Sy >= \frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J) + \sin(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J)}{4}$$

$$< Sz >= 0$$

(%o43)

```
(%i44) allCorrPsi(k_aa7);
```

$$< IxSx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuS - 2\cdot\pi\cdot tau1\cdot nuI) + \cos(2\cdot\pi\cdot tau1\cdot nuS + 2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IxSy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuS - 2\cdot\pi\cdot tau1\cdot nuI) + \sin(2\cdot\pi\cdot tau1\cdot nuS + 2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IxSz >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuI + \pi\cdot tau1\cdot J) - \cos(2\cdot\pi\cdot tau1\cdot nuI - \pi\cdot tau1\cdot J)}{8}$$

$$< IySx >= -\frac{\sin(2\cdot\pi\cdot tau1\cdot nuS + 2\cdot\pi\cdot tau1\cdot nuI) - \sin(2\cdot\pi\cdot tau1\cdot nuS - 2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IySy >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuS + 2\cdot\pi\cdot tau1\cdot nuI) - \cos(2\cdot\pi\cdot tau1\cdot nuS - 2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IySz >= -\frac{\sin(2\cdot\pi\cdot tau1\cdot nuI + \pi\cdot tau1\cdot J) - \sin(2\cdot\pi\cdot tau1\cdot nuI - \pi\cdot tau1\cdot J)}{8}$$

$$< IzSx >= -\frac{\cos(2\cdot\pi\cdot tau1\cdot nuS + \pi\cdot tau1\cdot J) - \cos(2\cdot\pi\cdot tau1\cdot nuS - \pi\cdot tau1\cdot J)}{8}$$

$$< IzSy >= -\frac{\sin(2\cdot\pi\cdot tau1\cdot nuS + \pi\cdot tau1\cdot J) - \sin(2\cdot\pi\cdot tau1\cdot nuS - \pi\cdot tau1\cdot J)}{8}$$

$$< IzSz >= 0$$

(%o44)

Fig. 16.9 The signs of the IzSx and IzSy correlations are reversed by the pulse. This also interchanges the precession frequencies associated with these terms.

The second evolution period, tau2

```
(%i45) k_aa8;
```

(%o45)
$$\begin{pmatrix} -\frac{i\cdot e^{-i\cdot\pi\cdot tau1\cdot\left(-\frac{J}{2}-nuI+nuS\right)-i\cdot\pi\cdot tau2\cdot\left(\frac{J}{2}+nuI+nuS\right)}}{2} \\ -\frac{i\cdot e^{-i\cdot\pi\cdot tau1\cdot\left(\frac{J}{2}-nuI-nuS\right)-i\cdot\pi\cdot tau2\cdot\left(-\frac{J}{2}+nuI-nuS\right)}}{2} \\ -\frac{i\cdot e^{-i\cdot\pi\cdot tau2\cdot\left(-\frac{J}{2}-nuI+nuS\right)-i\cdot\pi\cdot tau1\cdot\left(\frac{J}{2}+nuI+nuS\right)}}{2} \\ -\frac{i\cdot e^{-i\cdot\pi\cdot tau2\cdot\left(\frac{J}{2}-nuI-nuS\right)-i\cdot\pi\cdot tau1\cdot\left(-\frac{J}{2}+nuI-nuS\right)}}{2} \end{pmatrix}$$

With tau2=tau1

```
(%i46) allMagPsi(subst(tau2=tau1,k_aa8));
```

$$< Ix >= \frac{1}{2}$$

$$< Iy >= 0$$

$$< Iz >= 0$$

$$< Sx >= \frac{\cos(4\cdot\pi\cdot tau1\cdot nuS)}{2}$$

$$< Sy >= \frac{\sin(4\cdot\pi\cdot tau1\cdot nuS)}{2}$$

$$< Sz >= 0$$

(%o46)

```
(%i47) allCorrPsi(subst(tau2=tau1,k_aa8));
```

$< IxSx >= \dfrac{\cos(4 \cdot \pi \cdot tau1 \cdot nuS)}{4}$

$< IxSy >= \dfrac{\sin(4 \cdot \pi \cdot tau1 \cdot nuS)}{4}$

$< IxSz >= 0$
$< IySx >= 0$
$< IySy >= 0$
$< IySz >= 0$
$< IzSx >= 0$
$< IzSy >= 0$
$< IzSz >= 0$

(%o47)

Figs. 16.10, 16.11, 16.12, 16.13

3 16.2 Suppressing chemical-shift differences while detecting scalar coupling

Starting again with k_aa and k_ba and applying a selective pi/2 YS pulse

```
(%i48) k_aa10:psiPi2YS(k_aa)$
(%i49) allMagPsi(k_aa10);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= \dfrac{1}{2}$
$< Sx >= \dfrac{1}{2}$
$< Sy >= 0$
$< Sz >= 0$

(%o49)

```
(%i50) k_ba10:psiPi2YS(k_ba)$
(%i51) allMagPsi(k_ba10);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= -\dfrac{1}{2}$
$< Sx >= \dfrac{1}{2}$
$< Sy >= 0$
$< Sz >= 0$

(%o51)

The first evolution period, tau1

```
(%i52) k_aa11:psiTime(k_aa10,tau1)$
(%i53) allMagPsi(k_aa11);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= \frac{1}{2}$
$< Sx >= \frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J)}{2}$
$< Sy >= \frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J)}{2}$
$< Sz >= 0$
(%o53)

```
(%i54) k_ba11:psiTime(k_ba10,tau1)$
(%i55) allMagPsi(k_ba11);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= -\frac{1}{2}$
$< Sx >= \frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J)}{2}$
$< Sy >= \frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J)}{2}$
$< Sz >= 0$
(%o55)

Fig. 16.14

Non-selective pi x pulse

```
(%i56) k_aa12:psiPiX(k_aa11)$
(%i57) allMagPsi(k_aa12);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= -\frac{1}{2}$
$< Sx >= \frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J)}{2}$
$< Sy >= -\frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuS + \pi \cdot tau1 \cdot J)}{2}$
$< Sz >= 0$
(%o57)

```
(%i58) k_ba12:psiPiX(k_ba11)$
(%i59) allMagPsi(k_ba12);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= \frac{1}{2}$
$< Sx >= \frac{\cos(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J)}{2}$
$< Sy >= -\frac{\sin(2 \cdot \pi \cdot tau1 \cdot nuS - \pi \cdot tau1 \cdot J)}{2}$
$< Sz >= 0$
(%o59)

Fig. 16.15

Second evolution period, tau2

```
(%i60) k_aa13:psiTime(k_aa12,tau2)$
(%i61) allMagPsi(k_aa13);
```

$$< Ix >= 0$$
$$< Iy >= 0$$
$$< Iz >= -\frac{1}{2}$$
$$< Sx >= \frac{\cos\left((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuS+(-\pi\cdot tau1-\pi\cdot tau2)\cdot J\right)}{2}$$
$$< Sy >= \frac{\sin\left((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuS+(-\pi\cdot tau1-\pi\cdot tau2)\cdot J\right)}{2}$$
$$< Sz >= 0$$

(%o61)

```
(%i62) k_ba13:psiTime(k_ba12,tau2)$
(%i63) allMagPsi(k_ba13);
```

$$< Ix >= 0$$
$$< Iy >= 0$$
$$< Iz >= \frac{1}{2}$$
$$< Sx >= \frac{\cos\left((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuS+(\pi\cdot tau1+\pi\cdot tau2)\cdot J\right)}{2}$$
$$< Sy >= \frac{\sin\left((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuS+(\pi\cdot tau1+\pi\cdot tau2)\cdot J\right)}{2}$$
$$< Sz >= 0$$

(%o63)

If tau2 is made equal to tau1

```
(%i64) allMagPsi(subst(tau2=tau1,k_aa13));
```

$$< Ix >= 0$$
$$< Iy >= 0$$
$$< Iz >= -\frac{1}{2}$$
$$< Sx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot J)}{2}$$
$$< Sy >= -\frac{\sin(2\cdot\pi\cdot tau1\cdot J)}{2}$$
$$< Sz >= 0$$

(%o64)

```
(%i65) allMagPsi(subst(tau2=tau1,k_ba13));
```

$$< Ix >= 0$$
$$< Iy >= 0$$
$$< Iz >= \frac{1}{2}$$
$$< Sx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot J)}{2}$$
$$< Sy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot J)}{2}$$
$$< Sz >= 0$$

(%o65)

Fig. 16.15

The final positions depend only on the coupling constant, J.

The same pulse-sequence applied to a single population in a superposition state giving rise to two frequencies.
A non-selective pi/2 y pulse applied to k_aa

```
(%i66) k_aa15:psiPi2Y(k_aa);
```

(%o66) $$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

```
(%i67) allMagPsi(k_aa15);
```

$< Ix >= \frac{1}{2}$
$< Iy >= 0$
$< Iz >= 0$
$< Sx >= \frac{1}{2}$
$< Sy >= 0$
$< Sz >= 0$
(%o67)

First evolution period, tau1

```
(%i68) k_aa16:psiTime(k_aa15,tau1)$
(%i69) allMagPsi(k_aa16);
```

$$< Ix >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)+\cos(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)}{4}$$
$$< Iy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)+\sin(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)}{4}$$
$< Iz >= 0$
$$< Sx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)+\cos(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)}{4}$$
$$< Sy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)+\sin(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)}{4}$$
$< Sz >= 0$
(%o69)

Fig. 16.16

```
(%i70) allCorrPsi(k_aa16);
```

$$< IxSx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuS-2\cdot\pi\cdot tau1\cdot nuI)+\cos(2\cdot\pi\cdot tau1\cdot nuS+2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IxSy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuS-2\cdot\pi\cdot tau1\cdot nuI)+\sin(2\cdot\pi\cdot tau1\cdot nuS+2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IxSz >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)-\cos(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)}{8}$$

$$< IySx >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuS+2\cdot\pi\cdot tau1\cdot nuI)-\sin(2\cdot\pi\cdot tau1\cdot nuS-2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IySy >= -\frac{\cos(2\cdot\pi\cdot tau1\cdot nuS+2\cdot\pi\cdot tau1\cdot nuI)-\cos(2\cdot\pi\cdot tau1\cdot nuS-2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IySz >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)-\sin(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)}{8}$$

$$< IzSx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)-\cos(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)}{8}$$

$$< IzSy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)-\sin(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)}{8}$$

$$< IzSz >= 0$$

(%o70)

Fig. 16.17

Non-selective pi x pulse

```
(%i71) k_aa17:psiPiX(k_aa16)$
(%i72) allMagPsi(k_aa17);
```

$$< Ix >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)+\cos(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)}{4}$$

$$< Iy >= -\frac{\sin(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)+\sin(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)}{4}$$

$$< Iz >= 0$$

$$< Sx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)+\cos(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)}{4}$$

$$< Sy >= -\frac{\sin(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)+\sin(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)}{4}$$

$$< Sz >= 0$$

(%o72)

Fig. 16.16

```
(%i73) allCorrPsi(k_aa17);
```

$$< IxSx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot nuS-2\cdot\pi\cdot tau1\cdot nuI)+\cos(2\cdot\pi\cdot tau1\cdot nuS+2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IxSy >= -\frac{\sin(2\cdot\pi\cdot tau1\cdot nuS-2\cdot\pi\cdot tau1\cdot nuI)+\sin(2\cdot\pi\cdot tau1\cdot nuS+2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IxSz >= -\frac{\cos(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)-\cos(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)}{8}$$

$$< IySx >= -\frac{\sin(2\cdot\pi\cdot tau1\cdot nuS+2\cdot\pi\cdot tau1\cdot nuI)-\sin(2\cdot\pi\cdot tau1\cdot nuS-2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IySy >= -\frac{\cos(2\cdot\pi\cdot tau1\cdot nuS+2\cdot\pi\cdot tau1\cdot nuI)-\cos(2\cdot\pi\cdot tau1\cdot nuS-2\cdot\pi\cdot tau1\cdot nuI)}{8}$$

$$< IySz >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuI+\pi\cdot tau1\cdot J)-\sin(2\cdot\pi\cdot tau1\cdot nuI-\pi\cdot tau1\cdot J)}{8}$$

$$< IzSx >= -\frac{\cos(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)-\cos(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)}{8}$$

$$< IzSy >= \frac{\sin(2\cdot\pi\cdot tau1\cdot nuS+\pi\cdot tau1\cdot J)-\sin(2\cdot\pi\cdot tau1\cdot nuS-\pi\cdot tau1\cdot J)}{8}$$

$$< IzSz >= 0$$

(%o73)

Fig. 16.18

second evolution period, tau2

```
(%i74) k_aa18:psiTime(k_aa17, tau2)$
(%i75) allMagPsi(k_aa18);
```

$$< Ix >= \frac{\cos((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuI+(-\pi\cdot tau1-\pi\cdot tau2)\cdot J)+\cos((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuI+(\pi\cdot tau1+\pi\cdot tau2)\cdot J)}{4}$$

$$< Iy >= \frac{\sin((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuI+(-\pi\cdot tau1-\pi\cdot tau2)\cdot J)+\sin((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuI+(\pi\cdot tau1+\pi\cdot tau2)\cdot J)}{4}$$

$$< Iz >= 0$$

$$< Sx >= \frac{\cos((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuS+(-\pi\cdot tau1-\pi\cdot tau2)\cdot J)+\cos((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuS+(\pi\cdot tau1+\pi\cdot tau2)\cdot J}{4}$$

$$< Sy >= \frac{\sin((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuS+(-\pi\cdot tau1-\pi\cdot tau2)\cdot J)+\sin((2\cdot\pi\cdot tau2-2\cdot\pi\cdot tau1)\cdot nuS+(\pi\cdot tau1+\pi\cdot tau2)\cdot J)}{4}$$

$$< Sz >= 0$$

(%o75)

If tau2=tau1

```
(%i76) allMagPsi(subst(tau2=tau1,k_aa18));
```

$$< Ix >= \frac{\cos(2\cdot\pi\cdot tau1\cdot J)}{2}$$

$$< Iy >= 0$$

$$< Iz >= 0$$

$$< Sx >= \frac{\cos(2\cdot\pi\cdot tau1\cdot J)}{2}$$

$$< Sy >= 0$$

$$< Sz >= 0$$

(%o76)

The correlations present in this case are

```
(%i77) allCorrPsi(subst(tau2=tau1,k_aa18));
```

$< IxSx >= \frac{1}{4}$

$< IxSy >= 0$

$< IxSz >= 0$

$< IySx >= 0$

$< IySy >= 0$

$< IySz >= \frac{\sin(2 \cdot \pi \cdot tau1 \cdot J)}{4}$

$< IzSx >= 0$

$< IzSy >= \frac{\sin(2 \cdot \pi \cdot tau1 \cdot J)}{4}$

$< IzSz >= 0$

(%o77)

Fig. 16.19

if tau1 and tau2 are both set to 1/(4J)

```
(%i78) allMagPsi(subst([tau1=1/(4*J),tau2=1/(4*J)],k_aa18));
```

$< Ix >= 0$

$< Iy >= 0$

$< Iz >= 0$

$< Sx >= 0$

$< Sy >= 0$

$< Sz >= 0$

(%o78)

```
(%i79) allCorrPsi(subst([tau1=1/(4*J),tau2=1/(4*J)],k_aa18));
```

$< IxSx >= \frac{1}{4}$

$< IxSy >= 0$

$< IxSz >= 0$

$< IySx >= 0$

$< IySy >= 0$

$< IySz >= \frac{1}{4}$

$< IzSx >= 0$

$< IzSy >= \frac{1}{4}$

$< IzSz >= 0$

(%o79)

Fig. 16.20

4 16.3 Polarization transfer and the INEPT experiment

The experiments described in this section don't really require a quantum mechanical treatment, because they can be described using just the magnetization components from the four starting states, as detailed in the text.

5 16.4 Reverse INEPT

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This pulse sequence does require a quantum mechanical description. Starting states A and B: A: S-magnetization along x'-axis, I-magnetization along Iz. B: S-magnetization along y'-axis, I-magnetization along Iz.

Both can be generated from k_aa

```
(%i80) k_riA:psiPi2YS(k_aa)$
(%i81) allMagPsi(k_riA)$
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= \frac{1}{2}$
$< Sx >= \frac{1}{2}$
$< Sy >= 0$
$< Sz >= 0$

```
(%i82) k_riB:psiPulseXS(k_aa,-%pi/2)$
(%i83) allMagPsi(k_riB);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= \frac{1}{2}$
$< Sx >= 0$
$< Sy >= \frac{1}{2}$
$< Sz >= 0$
(%o83)

After initial non-selective pi/2 y pulse

```
(%i84) k_riA1:psiPi2Y(k_riA)$
(%i85) allMagPsi(k_riA1);
```

$< Ix >= \frac{1}{2}$
$< Iy >= 0$
$< Iz >= 0$
$< Sx >= 0$
$< Sy >= 0$
$< Sz >= -\frac{1}{2}$
(%o85)

```
(%i86) k_riB1:psiPi2Y(k_riB)$
(%i87) allMagPsi(k_riB1);
```

$< Ix >= \frac{1}{2}$
$< Iy >= 0$
$< Iz >= 0$
$< Sx >= 0$
$< Sy >= \frac{1}{2}$
$< Sz >= 0$
(%o87)

Fig. 16.31

first half of evolution period

```
(%i88) k_riA2:psiTime(k_riA1, 1/(4*J))$
(%i89) allMagPsi(k_riA2);
```

$$< Ix >= \frac{\cos\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)}{2}$$
$$< Iy >= \frac{\sin\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)}{2}$$
$$< Iz >= 0$$
$$< Sx >= 0$$
$$< Sy >= 0$$
$$< Sz >= -\frac{1}{2}$$

(%o89)

```
(%i90) k_riB2:psiTime(k_riB1, 1/(4*J))$
(%i91) allMagPsi(k_riB2);
```

$$< Ix >= \frac{\cos\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)+\cos\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)}{4}$$
$$< Iy >= \frac{\sin\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)+\sin\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)}{4}$$
$$< Iz >= 0$$
$$< Sx >= -\frac{\sin\left(\frac{2\cdot\pi\cdot nuS-\pi\cdot J}{4\cdot J}\right)+\sin\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)}{4}$$
$$< Sy >= \frac{\cos\left(\frac{2\cdot\pi\cdot nuS-\pi\cdot J}{4\cdot J}\right)+\cos\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)}{4}$$
$$< Sz >= 0$$

(%o91)

Fig. 16.32

The I-spin of the state that began with the S-magnetization along the x'-axis (A) precess with a single frequency, whereas the I-spin of the state that began with the S-magnetization along the y'-axis precesses with two frequencies.

The refocusing pulse

```
(%i92) k_riA3:psiPiX(k_riA2)$
(%i93) allMagPsi(k_riA3);
```

$$< Ix >= \frac{\cos\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)}{2}$$
$$< Iy >= -\frac{\sin\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)}{2}$$
$$< Iz >= 0$$
$$< Sx >= 0$$
$$< Sy >= 0$$
$$< Sz >= \frac{1}{2}$$

(%o93)

```
(%i94) k_riB3:psiPiX(k_riB2)$
(%i95) allMagPsi(k_riB3);
```

$$< Ix >= \frac{\cos\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)+\cos\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)}{4}$$

$$< Iy >= -\frac{\sin\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)+\sin\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)}{4}$$

$$< Iz >= 0$$

$$< Sx >= -\frac{\sin\left(\frac{2\cdot\pi\cdot nuS-\pi\cdot J}{4\cdot J}\right)+\sin\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)}{4}$$

$$< Sy >= -\frac{\cos\left(\frac{2\cdot\pi\cdot nuS-\pi\cdot J}{4\cdot J}\right)+\cos\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)}{4}$$

$$< Sz >= 0$$

(%o95)

Fig. 16.32

2nd half of the evolution period

```
(%i96) k_riA4:psiTime(k_riA3,1/(4*J))$
(%i97) allMagPsi(k_riA4);
```

$$< Ix >= 0$$
$$< Iy >= \frac{1}{2}$$
$$< Iz >= 0$$
$$< Sx >= 0$$
$$< Sy >= 0$$
$$< Sz >= \frac{1}{2}$$

(%o97)

```
(%i98) k_riB4:psiTime(k_riB3,1/(4*J))$
(%i99) allMagPsi(k_riB4);
```

$$< Ix >= 0$$
$$< Iy >= 0$$
$$< Iz >= 0$$
$$< Sx >= 0$$
$$< Sy >= 0$$
$$< Sz >= 0$$

(%o99)

Fig. 16.32

Time evolution during the data-acquisition period

```
(%i100) allMagPsi(psiTime(k_riA4,t));
```

$$< Ix >= -\frac{\sin(2\cdot\pi\cdot t\cdot nuI+\pi\cdot t\cdot J)}{2}$$
$$< Iy >= \frac{\cos(2\cdot\pi\cdot t\cdot nuI+\pi\cdot t\cdot J)}{2}$$
$$< Iz >= 0$$
$$< Sx >= 0$$
$$< Sy >= 0$$
$$< Sz >= \frac{1}{2}$$

(%o100)

```
(%i101) allMagPsi(psiTime(k_riB4,t));
```

$$< Ix >= -\frac{\sin(2\cdot\pi\cdot t\cdot nuI+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J)}{4}$$
$$< Iy >= \frac{\cos(2\cdot\pi\cdot t\cdot nuI+\pi\cdot t\cdot J)-\cos(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J)}{4}$$
$$< Iz >= 0$$
$$< Sx >= \frac{\cos(2\cdot\pi\cdot t\cdot nuS+\pi\cdot t\cdot J)-\cos(2\cdot\pi\cdot t\cdot nuS-\pi\cdot t\cdot J)}{4}$$
$$< Sy >= \frac{\sin(2\cdot\pi\cdot t\cdot nuS+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot nuS-\pi\cdot t\cdot J)}{4}$$
$$< Sz >= 0$$
(%o101)

For the state that began with the S-magnetization along the x'-axis (A): a single frequency component
For the state that began with the S-magnetization along the y'-axis (B): two anti-phase components

General example

Create starting state with Iz and S-magnetization in the x-y plane at angle a from the x-axis Do this by starting with Iaa> and applying an x,S pulse of angle -a, followed by a pi/2 Sy pulse.

```
(%i102) k_riC0:psiPi2YS(psiPulseXS(k_aa,-a))$
(%i103) allMagPsi(k_riC0);
```

$$< Ix >= 0$$
$$< Iy >= 0$$
$$< Iz >= \frac{1}{2}$$
$$< Sx >= \frac{\cos(a)}{2}$$
$$< Sy >= \frac{\sin(a)}{2}$$
$$< Sz >= 0$$
(%o103)

First pulse of reverse inept: non-selective pi/2 Y

```
(%i104) k_riC1:psiPi2Y(k_riC0)$
(%i105) allMagPsi(k_riC1);
```

$$< Ix >= \frac{1}{2}$$
$$< Iy >= 0$$
$$< Iz >= 0$$
$$< Sx >= 0$$
$$< Sy >= \frac{\sin(a)}{2}$$
$$< Sz >= -\frac{\cos(a)}{2}$$
(%o105)

First delay period

```
(%i106) k_riC2:psiTime(k_riC1,1/(4*J))$
(%i107) allMagPsi(k_riC2);
```

$$< Ix >= -\frac{-2\cdot\cos\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)-2\cdot\cos\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)-\cos\left(\frac{(-4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)+\cos\left(\frac{(\pi-4\cdot a)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)-\cos\left(\frac{(4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)+\cos\left(\frac{(4\cdot a+\pi)\cdot J \ldots}{4\cdot J \ldots}\right.}{8}$$

$$< Iy >= -\frac{-2\cdot\sin\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)-2\cdot\sin\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)-\sin\left(\frac{(-4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)+\sin\left(\frac{(\pi-4\cdot a)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)-\sin\left(\frac{(4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)+\sin\left(\frac{(4\cdot a+\pi)\cdot J+2 \ldots}{4\cdot J}\right.}{8}$$

$$< Iz >= 0$$

$$< Sx >= \frac{-\cos\left(\frac{(-4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)-\cos\left(\frac{(\pi-4\cdot a)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)+\cos\left(\frac{(4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)+\cos\left(\frac{(4\cdot a+\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)}{8}$$

$$< Sy >= \frac{-\sin\left(\frac{(-4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)-\sin\left(\frac{(\pi-4\cdot a)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)+\sin\left(\frac{(4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)+\sin\left(\frac{(4\cdot a+\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)}{8}$$

$$< Sz >= -\frac{\cos(a)}{2}$$

(%o107)

That's all pretty complicated, but we go ahead with the refocusing pulse

```
(%i108) k_riC3:psiPiX(k_riC2)$
(%i109) allMagPsi(k_riC3);
```

$$< Ix >= -\frac{-2\cdot\cos\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)-2\cdot\cos\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)-\cos\left(\frac{(-4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)+\cos\left(\frac{(\pi-4\cdot a)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)-\cos\left(\frac{(4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)+\cos\left(\frac{(4\cdot a+\pi)\cdot J \ldots}{4\cdot J \ldots}\right.}{8}$$

$$< Iy >= \frac{-2\cdot\sin\left(\frac{2\cdot\pi\cdot nuI-\pi\cdot J}{4\cdot J}\right)-2\cdot\sin\left(\frac{\pi\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)-\sin\left(\frac{(-4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)+\sin\left(\frac{(\pi-4\cdot a)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)-\sin\left(\frac{(4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuI}{4\cdot J}\right)+\sin\left(\frac{(4\cdot a+\pi)\cdot J+2\cdot\pi\cdot n \ldots}{4\cdot J}\right.}{8}$$

$$< Iz >= 0$$

$$< Sx >= \frac{-\cos\left(\frac{(-4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)-\cos\left(\frac{(\pi-4\cdot a)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)+\cos\left(\frac{(4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)+\cos\left(\frac{(4\cdot a+\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)}{8}$$

$$< Sy >= -\frac{-\sin\left(\frac{(-4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)-\sin\left(\frac{(\pi-4\cdot a)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)+\sin\left(\frac{(4\cdot a-\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)+\sin\left(\frac{(4\cdot a+\pi)\cdot J+2\cdot\pi\cdot nuS}{4\cdot J}\right)}{8}$$

$$< Sz >= \frac{\cos(a)}{2}$$

(%o109)

second delay

```
(%i110) k_riC4:psiTime(k_riC3,1/(4*J))$
(%i111) allMagPsi(k_riC4);
```

$$< Ix >= 0$$

$$< Iy >= \frac{\cos(a)}{2}$$

$$< Iz >= 0$$

$$< Sx >= 0$$

$$< Sy >= 0$$

$$< Sz >= \frac{\cos(a)}{2}$$

(%o111)

This corresponds to the state illustrated with vector diagrams in the rightmost drawing of Fig. 13.4, where both the I- and S-magnetization components are represented by two vectors. The net I-magnetization is represents the difference between two vectors pointing in opposite directions along the y' axis and is determined by the initial angle a between the S-magnetization and the x'-axis.

time evolution following reverse inept

```
(%i112) allMagPsi(psiTime(k_riC4,t));
```

$$< Ix >= -\frac{-2\cdot\sin(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J)+\sin(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J-a)+\sin(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J+a)+2\cdot\sin(2\cdot\pi\cdot t\cdot nuI+\pi}{8}$$

$$< Iy >= \frac{-2\cdot\cos(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J)+\cos(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J-a)+\cos(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J+a)+2\cdot\cos(2\cdot\pi\cdot t\cdot nuI+\pi}{8}$$

$$< Iz >= 0$$

$$< Sx >= \frac{\sin(2\cdot\pi\cdot t\cdot nuS-\pi\cdot t\cdot J-a)-\sin(2\cdot\pi\cdot t\cdot nuS-\pi\cdot t\cdot J+a)-\sin(2\cdot\pi\cdot t\cdot nuS+\pi\cdot t\cdot J-a)+\sin(2\cdot\pi\cdot t\cdot nuS+\pi\cdot t\cdot}{8}$$

$$< Sy >= -\frac{\cos(2\cdot\pi\cdot t\cdot nuS-\pi\cdot t\cdot J-a)-\cos(2\cdot\pi\cdot t\cdot nuS-\pi\cdot t\cdot J+a)-\cos(2\cdot\pi\cdot t\cdot nuS+\pi\cdot t\cdot J-a)+\cos(2\cdot\pi\cdot t\cdot nuS+\pi}{8}$$

$$< Sz >= \frac{\cos(a)}{2}$$

(%o112)

Look specifically at the Iy component

```
(%i113) Iy_t:meanPsi(Iy,psiTime(k_riC4,t));
```

(%o113) $$\frac{-2\cdot\cos(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J)+\cos(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J-a)+\cos(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J+a)+2\cdot\cos(2\cdot\pi\cdot t\cdot nuI+}{8}$$

The trick to making this look like the version in the text is to separate out the initial angle a from the terms arising from precession. trig expand converts all of the sums in the arguments of the trig functions into products of trig functions.

```
(%i114) trigexpand(Iy_t);
```

(%o114) $$\frac{4\cdot\cos(a)\cdot\cos(\pi\cdot t\cdot J)\cdot\cos(2\cdot\pi\cdot t\cdot nuI)+2\cdot(\cos(\pi\cdot t\cdot J)\cdot\cos(2\cdot\pi\cdot t\cdot nuI)-\sin(\pi\cdot t\cdot J)\cdot\sin(2\cdot\pi\cdot t\cdot nuI))-2\cdot(\cos}{8}$$

```
(%i115) ratsimp(%);
```

(%o115) $$-\frac{\sin(\pi\cdot t\cdot J)\cdot\sin(2\cdot\pi\cdot t\cdot nuI)-\cos(a)\cdot\cos(\pi\cdot t\cdot J)\cdot\cos(2\cdot\pi\cdot t\cdot nuI)}{2}$$

Now, substitute an arbitrary symbol for the cos(a) term, so that it is not affected by the next manipulations.

```
(%i116) subst(zz,cos(a),%);
```

(%o116) $$-\frac{\sin(\pi\cdot t\cdot J)\cdot\sin(2\cdot\pi\cdot t\cdot nuI)-zz\cdot\cos(\pi\cdot t\cdot J)\cdot\cos(2\cdot\pi\cdot t\cdot nuI)}{2}$$

Use trigreduce to convert products back into sums of arguments

```
(%i117) trigreduce(%);
```

(%o117) $$\frac{(zz-1)\cdot\cos(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J)+(zz+1)\cdot\cos(2\cdot\pi\cdot t\cdot nuI+\pi\cdot t\cdot J)}{4}$$

substitute back cos(a)

```
(%i118) subst(cos(a),zz,%);
```

(%o118) $$\frac{(\cos(a)-1)\cdot\cos(2\cdot\pi\cdot t\cdot nuI-\pi\cdot t\cdot J)+(\cos(a)+1)\cdot\cos(2\cdot\pi\cdot t\cdot nuI+\pi\cdot t\cdot J)}{4}$$

This is the form presented in the text, with nuI1=nuI+J/2 and nuI2=nuI-J/2

6 16.5 The heteronuclear single-quantum coherence (HSQC) experiment

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Following the population that begins in the k_aa state, as in the text, the INEPT sequence is equivalent to a pi/2 y,S pulse

```
(%i119) k_hsqc1:psiPi2YS(k_aa)$
(%i120) allMagPsi(k_hsqc1);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= \frac{1}{2}$
$< Sx >= \frac{1}{2}$
$< Sy >= 0$
$< Sz >= 0$

(%o120)

First half of the S-evolution period

```
(%i121) k_hsqc2:psiTime(k_hsqc1,t1/2)$
(%i122) allMagPsi(k_hsqc2);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= \frac{1}{2}$
$< Sx >= \frac{\cos\left(\frac{\pi \cdot t1 \cdot J+2 \cdot \pi \cdot t1 \cdot nuS}{2}\right)}{2}$
$< Sy >= \frac{\sin\left(\frac{\pi \cdot t1 \cdot J+2 \cdot \pi \cdot t1 \cdot nuS}{2}\right)}{2}$
$< Sz >= 0$

(%o122)

I refocussing pulse

```
(%i123) k_hsqc3:psiPiXI(k_hsqc2)$
(%i124) allMagPsi(k_hsqc3);
```

$< Ix >= 0$
$< Iy >= 0$
$< Iz >= -\frac{1}{2}$
$< Sx >= \frac{\cos\left(\frac{\pi \cdot t1 \cdot J+2 \cdot \pi \cdot t1 \cdot nuS}{2}\right)}{2}$
$< Sy >= \frac{\sin\left(\frac{\pi \cdot t1 \cdot J+2 \cdot \pi \cdot t1 \cdot nuS}{2}\right)}{2}$
$< Sz >= 0$

(%o124)

2nd half of the S-evolution period

```
(%i125) k_hsqc4:psiTime(k_hsqc3,t1/2)$
(%i126) allMagPsi(k_hsqc4);
```

$< Ix >= \; 0$

$< Iy >= \; 0$

$< Iz >= \; -\frac{1}{2}$

$< Sx >= \; \frac{\cos\left(2 \cdot \pi \cdot t1 \cdot nuS\right)}{2}$

$< Sy >= \; \frac{\sin\left(2 \cdot \pi \cdot t1 \cdot nuS\right)}{2}$

$< Sz >= \; 0$

(%o126)

Fig. 16.36

This corresponds to the starting point for the reverse INEPT sequence described in the previous section, with the initial displacement angle from the x'-axis, a, equal to 2*pi*t1*nuS
The reverse INEPT sequence then converts the Sx component into an Iy component, and the Sy sine term into an Sz cosine term.

7 16.6 The heteronuclear multiple-quantum coherence (HMQC) spectrum

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Starting with k_aa, apply pi/2 y,I pulse

```
(%i127) k_hmqc1:psiPi2YI(k_aa)$
(%i128) allMagPsi(k_hmqc1);
```

$< Ix >= \; \frac{1}{2}$

$< Iy >= \; 0$

$< Iz >= \; 0$

$< Sx >= \; 0$

$< Sy >= \; 0$

$< Sz >= \; \frac{1}{2}$

(%o128)

I-evolution period for1/(2J)

```
(%i129) k_hmqc2:psiTime(k_hmqc1,1/(2*J))$
(%i130) allMagPsi(k_hmqc2);
```

$< Ix >= \; -\frac{\sin\left(\frac{\pi \cdot nuI}{J}\right)}{2}$

$< Iy >= \; \frac{\cos\left(\frac{\pi \cdot nuI}{J}\right)}{2}$

$< Iz >= \; 0$

$< Sx >= \; 0$

$< Sy >= \; 0$

$< Sz >= \; \frac{1}{2}$

(%o130)

pi/2 y,S pulse

```
(%i131) k_hmqc3:psiPi2YS(k_hmqc2)$
(%i132) allMagPsi(k_hmqc3);
```

$< Ix >= -\frac{\sin\left(\frac{\pi \cdot nuI}{J}\right)}{2}$

$< Iy >= \frac{\cos\left(\frac{\pi \cdot nuI}{J}\right)}{2}$

$< Iz >= 0$

$< Sx >= \frac{1}{2}$

$< Sy >= 0$

$< Sz >= 0$

(%o132)

Fig. 16.39

First half of S-evolution period

```
(%i133) k_hmqc4:psiTime(k_hmqc3,t1/2)$
(%i134) allMagPsi(k_hmqc4);
```

$< Ix >= -\frac{\sin\left(\frac{(2 \cdot \pi \cdot t1 \cdot J+2 \cdot \pi) \cdot nuI-\pi \cdot t1 \cdot J^2}{2 \cdot J}\right)+\sin\left(\frac{\pi \cdot t1 \cdot J^2+(2 \cdot \pi \cdot t1 \cdot J+2 \cdot \pi) \cdot nuI}{2 \cdot J}\right)}{4}$

$< Iy >= \frac{\cos\left(\frac{(2 \cdot \pi \cdot t1 \cdot J+2 \cdot \pi) \cdot nuI-\pi \cdot t1 \cdot J^2}{2 \cdot J}\right)+\cos\left(\frac{\pi \cdot t1 \cdot J^2+(2 \cdot \pi \cdot t1 \cdot J+2 \cdot \pi) \cdot nuI}{2 \cdot J}\right)}{4}$

$< Iz >= 0$

$< Sx >= \frac{\cos\left(\frac{2 \cdot \pi \cdot t1 \cdot nuS-\pi \cdot t1 \cdot J}{2}\right)+\cos\left(\frac{\pi \cdot t1 \cdot J+2 \cdot \pi \cdot t1 \cdot nuS}{2}\right)}{4}$

$< Sy >= \frac{\sin\left(\frac{2 \cdot \pi \cdot t1 \cdot nuS-\pi \cdot t1 \cdot J}{2}\right)+\sin\left(\frac{\pi \cdot t1 \cdot J+2 \cdot \pi \cdot t1 \cdot nuS}{2}\right)}{4}$

$< Sz >= 0$

(%o134)

pi I-pulse

```
(%i135) k_hmqc5:psiPiXI(k_hmqc4)$
(%i136) allMagPsi(k_hmqc5);
```

$< Ix >= -\frac{\sin\left(\frac{(2 \cdot \pi \cdot t1 \cdot J+2 \cdot \pi) \cdot nuI-\pi \cdot t1 \cdot J^2}{2 \cdot J}\right)+\sin\left(\frac{\pi \cdot t1 \cdot J^2+(2 \cdot \pi \cdot t1 \cdot J+2 \cdot \pi) \cdot nuI}{2 \cdot J}\right)}{4}$

$< Iy >= -\frac{\cos\left(\frac{(2 \cdot \pi \cdot t1 \cdot J+2 \cdot \pi) \cdot nuI-\pi \cdot t1 \cdot J^2}{2 \cdot J}\right)+\cos\left(\frac{\pi \cdot t1 \cdot J^2+(2 \cdot \pi \cdot t1 \cdot J+2 \cdot \pi) \cdot nuI}{2 \cdot J}\right)}{4}$

$< Iz >= 0$

$< Sx >= \frac{\cos\left(\frac{2 \cdot \pi \cdot t1 \cdot nuS-\pi \cdot t1 \cdot J}{2}\right)+\cos\left(\frac{\pi \cdot t1 \cdot J+2 \cdot \pi \cdot t1 \cdot nuS}{2}\right)}{4}$

$< Sy >= \frac{\sin\left(\frac{2 \cdot \pi \cdot t1 \cdot nuS-\pi \cdot t1 \cdot J}{2}\right)+\sin\left(\frac{\pi \cdot t1 \cdot J+2 \cdot \pi \cdot t1 \cdot nuS}{2}\right)}{4}$

$< Sz >= 0$

(%o136)

Second half of S-evolution period

```
(%i137) k_hmqc6:psiTime(k_hmqc5,t1/2)$
(%i138) allMagPsi(k_hmqc6);
```

$$< Ix >= -\frac{\sin\left(\frac{\pi \cdot nuI}{J}\right)}{2}$$

$$< Iy >= -\frac{\cos\left(\frac{\pi \cdot nuI}{J}\right)}{2}$$

$$< Iz >= 0$$

$$< Sx >= \frac{\cos(2 \cdot \pi \cdot t1 \cdot nuS)}{2}$$

$$< Sy >= \frac{\sin(2 \cdot \pi \cdot t1 \cdot nuS)}{2}$$

$$< Sz >= 0$$

(%o138)

Fig. 16.40

pi/2 y,S pulse

```
(%i139) k_hmqc7:psiPi2YS(k_hmqc6)$
(%i140) allMagPsi(k_hmqc7);
```

$$< Ix >= -\frac{\sin\left(\frac{\pi \cdot nuI}{J}\right)}{2}$$

$$< Iy >= -\frac{\cos\left(\frac{\pi \cdot nuI}{J}\right)}{2}$$

$$< Iz >= 0$$

$$< Sx >= 0$$

$$< Sy >= \frac{\sin(2 \cdot \pi \cdot t1 \cdot nuS)}{2}$$

$$< Sz >= -\frac{\cos(2 \cdot \pi \cdot t1 \cdot nuS)}{2}$$

(%o140)

Final evolution period, t=1/(2J)

```
(%i141) k_hmqc8:psiTime(k_hmqc7,1/(2*J))$
(%i142) allMagPsi(k_hmqc8);
```

$$< Ix >= -\frac{\cos(2 \cdot \pi \cdot t1 \cdot nuS)}{2}$$

$$< Iy >= 0$$

$$< Iz >= 0$$

$$< Sx >= 0$$

$$< Sy >= 0$$

$$< Sz >= -\frac{\cos(2 \cdot \pi \cdot t1 \cdot nuS)}{2}$$

(%o142)

Fig. 16.41 The net Ix magnetization is modulated by t1 and nuS.

Data acquisition period

```
(%i143) allMagPsi(psiTime(k_hmqc8,t2));
```

$$< Ix >= -\frac{2\cdot\cos(2\cdot\pi\cdot t2\cdot nuI-\pi\cdot t2\cdot J)-2\cdot\cos(2\cdot\pi\cdot t2\cdot nuI+\pi\cdot t2\cdot J)+\cos(2\cdot\pi\cdot t1\cdot nuS-2\cdot\pi\cdot t2\cdot nuI-\pi\cdot t2\cdot J)+\cos(2}{}$$

$$< Iy >= -\frac{2\cdot\sin(2\cdot\pi\cdot t2\cdot nuI-\pi\cdot t2\cdot J)-2\cdot\sin(2\cdot\pi\cdot t2\cdot nuI+\pi\cdot t2\cdot J)-\sin(2\cdot\pi\cdot t1\cdot nuS-2\cdot\pi\cdot t2\cdot nuI-\pi\cdot t2\cdot J)-\sin(2\cdot}{}$$

$$< Iz >= 0$$

$$< Sx >= -\frac{\sin\left(\frac{((2\cdot\pi\cdot t2-2\cdot\pi\cdot t1)\cdot J+\pi)\cdot nuS-\pi\cdot t2\cdot J^2}{J}\right)-\sin\left(\frac{\pi\cdot t2\cdot J^2+((2\cdot\pi\cdot t2-2\cdot\pi\cdot t1)\cdot J+\pi)\cdot nuS}{J}\right)-\sin\left(\frac{((2\cdot\pi\cdot t1+2\cdot\pi\cdot t2)\cdot J+\pi)\cdot nuS-\pi\cdot t2\cdot J^2}{J}\right)+\sin\left(\frac{\pi\cdot t2\cdot J^2+((2\cdot\pi\cdot t1+2\cdot\pi\cdot t2)\cdot J}{J}\right.}{8}$$

$$< Sy >= \frac{\cos\left(\frac{((2\cdot\pi\cdot t2-2\cdot\pi\cdot t1)\cdot J+\pi)\cdot nuS-\pi\cdot t2\cdot J^2}{J}\right)-\cos\left(\frac{\pi\cdot t2\cdot J^2+((2\cdot\pi\cdot t2-2\cdot\pi\cdot t1)\cdot J+\pi)\cdot nuS}{J}\right)-\cos\left(\frac{((2\cdot\pi\cdot t1+2\cdot\pi\cdot t2)\cdot J+\pi)\cdot nuS-\pi\cdot t2\cdot J^2}{J}\right)+\cos\left(\frac{\pi\cdot t2\cdot J^2+((2\cdot\pi\cdot t1+2\cdot\pi\cdot t2)\cdot J}{J}\right.}{8}$$

$$< Sz >= -\frac{\cos(2\cdot\pi\cdot t1\cdot nuS)}{2}$$

(%o143)

Using the same approach as before for the reverse INEPT result to simplify the result.

```
(%i144) Iy_hmqct2:-(cos(2*%pi*t1*nuS+2*%pi*t2*nuI+%pi*t2*J)+cos(2*%pi*t1*nuS+2*%pi*t2*nuI-%pi*t2*J)+cos(2*%pi*t1*nuS-2*
        cos(2*%pi*t1*nuS-2*%pi*t2*nuI-%pi*t2*J)-2*cos(2*%pi*t2*nuI+%pi*t2*J)+2*cos(2*%pi*t2*nuI-%pi*t2*J))/(8);
```

(%o144) $$\frac{-2\cdot\cos(2\cdot\pi\cdot t2\cdot nuI-\pi\cdot t2\cdot J)+2\cdot\cos(2\cdot\pi\cdot t2\cdot nuI+\pi\cdot t2\cdot J)-\cos(2\cdot\pi\cdot t1\cdot nuS-2\cdot\pi\cdot t2\cdot nuI-\pi\cdot t2\cdot J)-\cos(}{}$$

```
(%i145) trigexpand(Iy_hmqct2);
```

(%o145) $$\frac{2\cdot(\cos(\pi\cdot t2\cdot J)\cdot\cos(2\cdot\pi\cdot t2\cdot nuI)-\sin(\pi\cdot t2\cdot J)\cdot\sin(2\cdot\pi\cdot t2\cdot nuI))-2\cdot(\cos(\pi\cdot t2\cdot J)\cdot\cos(2\cdot\pi\cdot t2\cdot nuI)+\sin(\pi\cdot}{8}$$

```
(%i146) ratsimp(%);
```

(%o146) $$-\frac{\sin(\pi\cdot t2\cdot J)\cdot\sin(2\cdot\pi\cdot t2\cdot nuI)+\cos(\pi\cdot t2\cdot J)\cdot\cos(2\cdot\pi\cdot t2\cdot nuI)\cdot\cos(2\cdot\pi\cdot t1\cdot nuS)}{2}$$

```
(%i147) subst(zz,cos(2*%pi*t1*nuS),%);
```

(%o147) $$-\frac{zz\cdot\cos(\pi\cdot t2\cdot J)\cdot\cos(2\cdot\pi\cdot t2\cdot nuI)+\sin(\pi\cdot t2\cdot J)\cdot\sin(2\cdot\pi\cdot t2\cdot nuI)}{2}$$

```
(%i148) trigreduce(%);
```

(%o148) $$\frac{(-zz-1)\cdot\cos(2\cdot\pi\cdot t2\cdot nuI-\pi\cdot t2\cdot J)+(1-zz)\cdot\cos(2\cdot\pi\cdot t2\cdot nuI+\pi\cdot t2\cdot J)}{4}$$

```
(%i149) subst(cos(2*%pi*t1*nuS),zz,%);
```

(%o149) $$\frac{\cos(2\cdot\pi\cdot t2\cdot nuI-\pi\cdot t2\cdot J)\cdot(-\cos(2\cdot\pi\cdot t1\cdot nuS)-1)+\cos(2\cdot\pi\cdot t2\cdot nuI+\pi\cdot t2\cdot J)\cdot(1-\cos(2\cdot\pi\cdot t1\cdot nuS))}{4}$$

We have two I-frequency components with amplitudes of opposite signs and modulated by t1*nuS. With decoupling, these are combined into one frequency component with an amplitude determined by t1*nuS
