Chapter 18. Basis set for the density matrix and the product operator formalism. Part 2. Two-spin populations

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. This software is distributed under the conditions of the BSD license and without any guarantees or warranties. Please send comments, including bug reports, to this address:

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Chapter 18 introduces the idea of using a basis set composed of operator matrices to represent the density matrix. The first section deals with a population of isolated spins, without scalar coupling, whereas the rest of the chapter deals with a population of weakly-coupled spin pairs. Because separate Maxima libraries (1spinLib.mac and 2spinLib.mac) are used for the two kinds of systems, separate workbooks are provided for the two parts of Chapter 17

The library used previously for quantum mechanical calculations for individual, weakly coupled spins also contains functions for density matrix calculations for populations of uncoupled spins. Functions with names beginning with "psi" are generally used for wavefunction calculations, whereas function names beginning with "rho" are associated with density matrix calculations.

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

2 18.2 A basis set for a population of scalar-coupled spins

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The general form of the density matrix for a population of coupled spins

```
(%i2) rhogen;
```

$$(\%o2)\quad \begin{pmatrix} avCaaConjCaa & avCaaConjCab & avCaaConjCba & avCaaConjCbb \\ avCabConjCaa & avCabConjCab & avCabConjCba & avCabConjCbb \\ avCbaConjCaa & avCbaConjCab & avCbaConjCba & avCbaConjCbb \\ avCbbConjCaa & avCbbConjCab & avCbbConjCba & avCbbConjCbb \end{pmatrix}$$

The six magnetization operator matrices

```
(%i3) Ix;
```

$$(\%o3) \quad \begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$$

```
(%i4) Iy;
```

$$(\%o4) \quad \begin{pmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{pmatrix}$$

```
(%i5) Iz;
```

$$(\%o5) \quad \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}$$

```
(%i6) Sx;
```

$$(\%o6) \quad \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \end{pmatrix}$$

```
(%i7) Sy;
```

$$(\%o7) \begin{pmatrix} 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 \end{pmatrix}$$

```
(%i8) Sz;
```

$$(\%o8) \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}$$

The nine product operator matrices

```
(%i9) IxSx;
```

$$(\%o9) \begin{pmatrix} 0 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ \frac{1}{4} & 0 & 0 & 0 \end{pmatrix}$$

```
(%i10) IxSy;
```

$$(\%o10) \begin{pmatrix} 0 & 0 & 0 & -\frac{i}{4} \\ 0 & 0 & \frac{i}{4} & 0 \\ 0 & -\frac{i}{4} & 0 & 0 \\ \frac{i}{4} & 0 & 0 & 0 \end{pmatrix}$$

```
(%i11) IxSz;
```

$$(\%o11)\quad \begin{pmatrix} 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & -\frac{1}{4} \\ \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 \end{pmatrix}$$

```
(%i12) IySx;
```

$$(\%o12)\quad \begin{pmatrix} 0 & 0 & 0 & -\frac{i}{4} \\ 0 & 0 & -\frac{i}{4} & 0 \\ 0 & \frac{i}{4} & 0 & 0 \\ \frac{i}{4} & 0 & 0 & 0 \end{pmatrix}$$

```
(%i13) IySy;
```

$$(\%o13)\quad \begin{pmatrix} 0 & 0 & 0 & -\frac{1}{4} \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ -\frac{1}{4} & 0 & 0 & 0 \end{pmatrix}$$

```
(%i14) IySz;
```

$$(\%o14)\quad \begin{pmatrix} 0 & 0 & -\frac{i}{4} & 0 \\ 0 & 0 & 0 & \frac{i}{4} \\ \frac{i}{4} & 0 & 0 & 0 \\ 0 & -\frac{i}{4} & 0 & 0 \end{pmatrix}$$

```
(%i15) IzSx;
```

$$(\%o15)\quad \begin{pmatrix} 0 & \frac{1}{4} & 0 & 0 \\ \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{4} \\ 0 & 0 & -\frac{1}{4} & 0 \end{pmatrix}$$

```
(%i16) IzSy;
```

$$(\%o16)\quad \begin{pmatrix} 0 & -\frac{i}{4} & 0 & 0 \\ \frac{i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{4} \\ 0 & 0 & -\frac{i}{4} & 0 \end{pmatrix}$$

```
(%i17) IzSz;
```

$$(\%o17)\quad \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}$$

The 4x4 identity matrix

```
(%i18) ident;
```

$$(\%o18)\quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The 2spinLib.mac file includes a function to print the representation of a density matrix as the terms in a linear combination of the magnetization operators and the product operators.
We can write an arbitrary density matrix as:

```
(%i19) rho1:cIx*Ix + cIy*Iy + cIz*Iz + cSx*Sx + cSy*Sy + cSz*Sz
       + cIxSx*IxSx + cIxSy*IxSy + cIxSz*IxSz + cIySx*IySx + cIySy*IySy + cIySz*IySz
       + cIzSx*IzSx + cIzSy*IzSy + cIzSz*IzSz;
```

$$
(\%o19)\quad \begin{pmatrix}
\frac{\mathrm{cSz}}{2}+\frac{\mathrm{cIzSz}}{4}+\frac{\mathrm{cIz}}{2} & -\frac{i\cdot \mathrm{cSy}}{2}+\frac{\mathrm{cSx}}{2}-\frac{i\cdot \mathrm{cIzSy}}{4}+\frac{\mathrm{cIzSx}}{4} & -\frac{i\cdot \mathrm{cIySz}}{4}-\frac{i\cdot \mathrm{cIy}}{2}+\frac{\mathrm{cIxSz}}{4}+\frac{\mathrm{cIx}}{2} & -\frac{\mathrm{cIySy}}{4}-\frac{i\cdot \mathrm{cIySx}}{4}-\frac{i\cdot \mathrm{cIxSy}}{4}+\frac{\mathrm{cIxSx}}{4} \\
\frac{i\cdot \mathrm{cSy}}{2}+\frac{\mathrm{cSx}}{2}+\frac{i\cdot \mathrm{cIzSy}}{4}+\frac{\mathrm{cIzSx}}{4} & -\frac{\mathrm{cSz}}{2}-\frac{\mathrm{cIzSz}}{4}+\frac{\mathrm{cIz}}{2} & \frac{\mathrm{cIySy}}{4}-\frac{i\cdot \mathrm{cIySx}}{4}+\frac{i\cdot \mathrm{cIxSy}}{4}+\frac{\mathrm{cIxSx}}{4} & \frac{i\cdot \mathrm{cIySz}}{4}-\frac{i\cdot \mathrm{cIy}}{2}-\frac{\mathrm{cIxSz}}{4}+\frac{\mathrm{cIx}}{2} \\
\frac{i\cdot \mathrm{cIySz}}{4}+\frac{i\cdot \mathrm{cIy}}{2}+\frac{\mathrm{cIxSz}}{4}+\frac{\mathrm{cIx}}{2} & \frac{\mathrm{cIySy}}{4}+\frac{i\cdot \mathrm{cIySx}}{4}-\frac{i\cdot \mathrm{cIxSy}}{4}+\frac{\mathrm{cIxSx}}{4} & \frac{\mathrm{cSz}}{2}-\frac{\mathrm{cIzSz}}{4}-\frac{\mathrm{cIz}}{2} & -\frac{i\cdot \mathrm{cSy}}{2}+\frac{\mathrm{cSx}}{2}+\frac{i\cdot \mathrm{cIzSy}}{4}-\frac{\mathrm{cIzSx}}{4} \\
-\frac{\mathrm{cIySy}}{4}+\frac{i\cdot \mathrm{cIySx}}{4}+\frac{i\cdot \mathrm{cIxSy}}{4}+\frac{\mathrm{cIxSx}}{4} & -\frac{i\cdot \mathrm{cIySz}}{4}+\frac{i\cdot \mathrm{cIy}}{2}-\frac{\mathrm{cIxSz}}{4}+\frac{\mathrm{cIx}}{2} & \frac{i\cdot \mathrm{cSy}}{2}+\frac{\mathrm{cSx}}{2}-\frac{i\cdot \mathrm{cIzSy}}{4}-\frac{\mathrm{cIzSx}}{4} & -\frac{\mathrm{cSz}}{2}+\frac{\mathrm{cIzSz}}{4}-\frac{\mathrm{cIz}}{2}
\end{pmatrix}
$$

```
(%i20) opBasisRep(rho1);
```

$$Ix:\ \mathrm{cIx}\,Iy:\ \mathrm{cIy}\,Iz:\ \mathrm{cIz}\,Sx:\ \mathrm{cSx}\,Sy:\ \mathrm{cSy}\,Sz:\ \mathrm{cSz}\,IxSx:\ \mathrm{cIxSx}\,IxSy:\ \mathrm{cIxSy}\,IxSz:\ \mathrm{cIxSz}\,IySx:\ \mathrm{cIySx}\,IySy:\ \mathrm{cIySy}\,IySz:\ \mathrm{cIySz}\,IzSx:\ \mathrm{cIzSx}\,IzSy:\ \mathrm{cIzSy}\,IzSz:\ \mathrm{cIzSz}$$

(%o20)

The opBasisRep function outputs all of the non-zero coefficients on individual lines.

The product of two operators for the same spin

```
(%i21) Ix.Iy;
```

$$
(\%o21)\quad \begin{pmatrix}
\frac{i}{4} & 0 & 0 & 0 \\
0 & \frac{i}{4} & 0 & 0 \\
0 & 0 & -\frac{i}{4} & 0 \\
0 & 0 & 0 & -\frac{i}{4}
\end{pmatrix}
$$

This product is related to Iz

```
(%i22) Iz;
```

$$
(\%o22)\quad \begin{pmatrix}
\frac{1}{2} & 0 & 0 & 0 \\
0 & \frac{1}{2} & 0 & 0 \\
0 & 0 & -\frac{1}{2} & 0 \\
0 & 0 & 0 & -\frac{1}{2}
\end{pmatrix}
$$

Taking products clockwise along the circle represented in Fig. 18.2

```
(%i23) opBasisRep(Ix.Iy);
```

$$Iz:\ \frac{i}{2}$$

(%o23)

```
(%i24) opBasisRep(Iy.Iz);
```

$$Ix:\ \frac{i}{2}$$

(%o24)

```
(%i25) opBasisRep(Iz.Ix);
```

$$Iy: \frac{i}{2}$$

(%o25)

Taking products counter-clockwise along the circle represented in Fig. 18.2

```
(%i26) opBasisRep(Ix.Iz);
```

$$Iy: -\frac{i}{2}$$

(%o26)

```
(%i27) opBasisRep(Iz.Iy);
```

$$Ix: -\frac{i}{2}$$

(%o27)

```
(%i28) opBasisRep(Iy.Ix);
```

$$Iz: -\frac{i}{2}$$

(%o28)

The equivalent relationships for the S magnetization operators

```
(%i29) opBasisRep(Sx.Sy);
```

$$Sz: \frac{i}{2}$$

(%o29)

```
(%i30) opBasisRep(Sy.Sz);
```

$$Sx: \frac{i}{2}$$

(%o30)

```
(%i31) opBasisRep(Sz.Sx);
```

$$Sy: \frac{i}{2}$$

(%o31)

The average magnetization components for a density matrix represented by the linear combination of the magnetization operators and product operators.

```
(%i32) mattrace(Iz.rho1);
```

$$(\%o32) \quad \frac{\frac{cIz}{2}+\frac{cIzSz}{4}+\frac{cSz}{2}}{2}-\frac{-\frac{cIz}{2}-\frac{cIzSz}{4}+\frac{cSz}{2}}{2}-\frac{-\frac{cIz}{2}+\frac{cIzSz}{4}-\frac{cSz}{2}}{2}+\frac{\frac{cIz}{2}-\frac{cIzSz}{4}-\frac{cSz}{2}}{2}$$

```
(%i33) ratsimp(%);
```

(%o33) cIz

Looking only at the Iz component

```
(%i34) Iz.(cIz*Iz);
```

$$(\%o34)\quad \begin{pmatrix} \frac{cIz}{4} & 0 & 0 & 0 \\ 0 & \frac{cIz}{4} & 0 & 0 \\ 0 & 0 & \frac{cIz}{4} & 0 \\ 0 & 0 & 0 & \frac{cIz}{4} \end{pmatrix}$$

```
(%i35) mattrace(%);
```

$$(\%o35)\quad cIz$$

All of the magnetization components of the arbitrary linear combination

```
(%i36) allMagRho(rho1);
```

$$< Ix >= cIx < Iy >= cIy < Iz >= cIz < Sx >= cSx < Sy >= cSy < Sz >= cSz$$

(%o36)

Each magnetization component is simply the coefficient of the corresponding operator matrix.

The correlations calculated using the product operators.

```
(%i37) IxSy.(cIxSy*IxSy);
```

$$(\%o37)\quad \begin{pmatrix} \frac{cIxSy}{16} & 0 & 0 & 0 \\ 0 & \frac{cIxSy}{16} & 0 & 0 \\ 0 & 0 & \frac{cIxSy}{16} & 0 \\ 0 & 0 & 0 & \frac{cIxSy}{16} \end{pmatrix}$$

```
(%i38) mattrace(%);
```

$$(\%o38)\quad \frac{cIxSy}{4}$$

The 2spinLib.mac file contains a function to calculate all of the correlations from the density matrix

```
(%i39) allCorrRho(rho1);
```

$$< IxSx >= \frac{cIxSx}{4} < IxSy >= \frac{cIxSy}{4} < IxSz >= \frac{cIxSz}{4} < IySx >= \frac{cIySx}{4} < IySy >= \frac{cIySy}{4} < IySz >= \frac{cIySz}{4} < IzSx >= \frac{cIzSx}{4} < IzSy >= \frac{cIzSy}{4} < IzSz >= \frac{cIzSz}{4}$$

(%o39)

The correlation products are the coefficients of the product operator matrices divided by 4.

2.1 18.2.2 Representation of the equilibrium density matrix

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```
(%i40) rhoEq;
```

$$(\%o40)\quad \begin{pmatrix} \frac{deltaPS}{4}+\frac{deltaPI}{4} & 0 & 0 & 0 \\ 0 & \frac{deltaPI}{4}-\frac{deltaPS}{4} & 0 & 0 \\ 0 & 0 & \frac{deltaPS}{4}-\frac{deltaPI}{4} & 0 \\ 0 & 0 & 0 & -\frac{deltaPS}{4}-\frac{deltaPI}{4} \end{pmatrix}$$

```
(%i41) opBasisRep(rhoEq);
```

$$Iz:\ \frac{deltaPI}{2}Sz:\ \frac{deltaPS}{2}$$

(%o41)

2.2 18.2.3 Pulses

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Pulse of angle a along the x'-axis

```
(%i42) rhoPulseX(Ix,a)$
(%i43) opBasisRep(%);
```

$$Ix:\ 1$$

(%o43)

```
(%i44) opBasisRep(rhoPulseX(Iy,a));
```

$$Iy:\ \cos(a)Iz:\ \sin(a)$$

(%o44)

```
(%i45) opBasisRep(rhoPulseX(Iz,a));
```

$$Iy:\ -\sin(a)Iz:\ \cos(a)$$

(%o45)

Pulse of angle a along the y'-axis

```
(%i46) opBasisRep(rhoPulseY(Ix,a));
```

$$Ix:\ \cos(a)Iz:\ -\sin(a)$$

(%o46)

```
(%i47) opBasisRep(rhoPulseY(Iy,a));
```

$$Iy:\ 1$$

(%o47)

```
(%i48) opBasisRep(rhoPulseY(Iz,a));
```

$$Ix:\ \sin(a)Iz:\ \cos(a)$$

(%o48)

Fig. 18.7

pi/2 y pulse to I spin of density matrix represented by IzSz

(%i49) rhoPi2YI(IzSz);

$$(\%o49) \quad \begin{pmatrix} 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & -\frac{1}{4} \\ \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 \end{pmatrix}$$

(%i50) opBasisRep(rhoPi2YI(IzSz));

$IxSz\colon\ 1$

(%o50)

Fig. 18.8

2.3 18.2.4 Time evolution in the absence of scalar coupling

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The 2spinLib.mac file includes functions to calculate separately the change in density matrix with time due to chemical shift and scalar coupling. These functions are rhoTimeC(rho,t) and rhoTimeS(rho,t) where the arguments are the starting density matrix (rho) and the time of evolution (t).

Starting with density matrices equal to Ix, Iy and Iz

(%i51) rhoTimeC(Ix,t);

$$(\%o51) \quad \begin{pmatrix} 0 & 0 & \frac{e^{i\cdot\pi\cdot t\cdot(\mathrm{nuS}-\mathrm{nuI})-i\cdot\pi\cdot t\cdot(\mathrm{nuI}+\mathrm{nuS})}}{2} & 0 \\ 0 & 0 & 0 & \frac{e^{i\cdot\pi\cdot t\cdot(-\mathrm{nuS}-\mathrm{nuI})-i\cdot\pi\cdot t\cdot(\mathrm{nuI}-\mathrm{nuS})}}{2} \\ \frac{e^{i\cdot\pi\cdot t\cdot(\mathrm{nuS}+\mathrm{nuI})-i\cdot\pi\cdot t\cdot(\mathrm{nuS}-\mathrm{nuI})}}{2} & 0 & 0 & 0 \\ 0 & \frac{e^{i\cdot\pi\cdot t\cdot(\mathrm{nuI}-\mathrm{nuS})-i\cdot\pi\cdot t\cdot(-\mathrm{nuI}-\mathrm{nuS})}}{2} & 0 & 0 \end{pmatrix}$$

(%i52) opBasisRep(%);

$Ix\colon\ \cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}) Iy\colon\ \sin(2\cdot\pi\cdot t\cdot \mathrm{nuI})$

(%o52)

(%i53) opBasisRep(rhoTimeC(Iy,t));

$Ix\colon\ -\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}) Iy\colon\ \cos(2\cdot\pi\cdot t\cdot \mathrm{nuI})$

(%o53)

(%i54) opBasisRep(rhoTimeC(Iz,t));

$Iz\colon\ 1$

(%o54)

Fig. 18.9

Evolution of a density matrix component representing the product IxSz

```
(%i55) opBasisRep(rhoTimeC(IxSz,t));
```

$$IxSz:\ \cos(2\cdot\pi\cdot t\cdot \mathrm{nuI})IySz:\ \sin(2\cdot\pi\cdot t\cdot \mathrm{nuI})$$

(%o55)

Fig. 18.10

Evolution of a density matrix component representing the product IxSx

```
(%i56) opBasisRep(rhoTimeC(IxSx,t));
```

$$IxSx:\ \frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})+\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})}{2}IxSy:\ \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})+\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})}{2}IySx:\ \sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}$$

(%o56)

The individual terms can be converted to the forms shown in the text by applying the trigexpand function, which converts trig functions of sums of angles into products of trig functions.

For the IxSx component

```
(%i57) (cos(2*%pi*t*nuS+2*%pi*t*nuI)+cos(2*%pi*t*nuS-2*%pi*t*nuI))/2;
```

$$\text{(%o57)}\quad \frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})+\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})}{2}$$

```
(%i58) trigexpand(%);
```

$$\text{(%o58)}\quad \cos(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS})$$

For the IxSy component

```
(%i59) (sin(2*%pi*t*nuS+2*%pi*t*nuI)+sin(2*%pi*t*nuS-2*%pi*t*nuI))/2;
```

$$\text{(%o59)}\quad \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})+\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})}{2}$$

```
(%i60) trigexpand(%);
```

$$\text{(%o60)}\quad \cos(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS})$$

For the IySx component

```
(%i61) sin(2*%pi*t*nuS+2*%pi*t*nuI)/2-sin(2*%pi*t*nuS-2*%pi*t*nuI)/2;
```

$$\text{(%o61)}\quad \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})}{2}-\frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})}{2}$$

```
(%i62) trigexpand(%);
```

$$\text{(%o62)}\quad \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS})+\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS})}{2}-\frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS})-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS})}{2}$$

```
(%i63) ratsimp(%);
```

$$\text{(%o63)}\quad \sin(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS})$$

For the IySy component

```
(%i64) -cos(2*%pi*t*nuS+2*%pi*t*nuI)/2+cos(2*%pi*t*nuS-2*%pi*t*nuI)/2;
```

$$\text{(%o64)}\quad \frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})}{2}-\frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})}{2}$$

```
(%i65) ratsimp(%);
```

$$(\%o65) \quad -\frac{\cos(2\cdot\pi\cdot t\cdot nuS+2\cdot\pi\cdot t\cdot nuI)-\cos(2\cdot\pi\cdot t\cdot nuS-2\cdot\pi\cdot t\cdot nuI)}{2}$$

```
(%i66) trigexpand(%);
```

$$(\%o66) \quad \sin(2\cdot\pi\cdot t\cdot nuI)\cdot\sin(2\cdot\pi\cdot t\cdot nuS)$$

Setting nuS to zero

```
(%i67) opBasisRep(subst(nuS=0,rhoTimeC(IxSx,t)));
```

$$IxSx:\ \cos(2\cdot\pi\cdot t\cdot nuI) IySx:\ \sin(2\cdot\pi\cdot t\cdot nuI)$$

$$(\%o67)$$

Fig. 18.11

2.4 18.2.5 Evolution under the influence of scalar coupling

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Here, we can use the rhoTimeS function to calculate the effect of scalar coupling without chemical shift evolution.

Applied to the individual I-magnetization components, showing the conversion of magnetization components into correlations

```
(%i68) opBasisRep(rhoTimeS(Ix,t));
```

$$Ix:\ \cos(\pi\cdot t\cdot J) IySz:\ 2\cdot\sin(\pi\cdot t\cdot J)$$

$$(\%o68)$$

```
(%i69) opBasisRep(rhoTimeS(Iy,t));
```

$$Iy:\ \cos(\pi\cdot t\cdot J) IxSz:\ -2\cdot\sin(\pi\cdot t\cdot J)$$

$$(\%o69)$$

```
(%i70) opBasisRep(rhoTimeS(Iz,t));
```

$$Iz:\ 1$$

$$(\%o70)$$

Fig. 18.12

Evolution of IxSz and IySz, with the conversion to magnetization components.

```
(%i71) opBasisRep(rhoTimeS(IxSz,t));
```

$$Iy:\ \frac{\sin(\pi\cdot t\cdot J)}{2} IxSz:\ \cos(\pi\cdot t\cdot J)$$

$$(\%o71)$$

```
(%i72) opBasisRep(rhoTimeS(IySz,t));
```

$$Ix:\ -\frac{\sin(\pi\cdot t\cdot J)}{2} IySz:\ \cos(\pi\cdot t\cdot J)$$

$$(\%o72)$$

Fig. 18.13

Evolution of the other correlations

```
(%i73) opBasisRep(rhoTimeS(IzSz,t));
```

$IzSz:\ 1$

(%o73)

```
(%i74) opBasisRep(rhoTimeS(IxSx,t));
```

$IxSx:\ 1$

(%o74)

```
(%i75) opBasisRep(rhoTimeS(IxSy,t));
```

$IxSy:\ 1$

(%o75)

```
(%i76) opBasisRep(rhoTimeS(IySx,t));
```

$IySx:\ 1$

(%o76)

```
(%i77) opBasisRep(rhoTimeS(IySy,t));
```

$IySy:\ 1$

(%o77)

None of these correlations is affected by scalar coupling, but they will evolve with chemical shift differences.

3 18.3 Some examples

3.1 18.3.1 Refocusing pulses

3.1.1 A decoupling pulse sequence

Evolution of Sx during the first time period starting with chemical-shift evolution, followed by scalar-coupling evolution

```
(%i78) rho_dc1:rhoTimeC(Sx,tau/2)$
(%i79) opBasisRep(%);
```

$$Sx:\ \cos(\pi\cdot\tau\cdot \mathrm{nuS}) Sy:\ \sin(\pi\cdot\tau\cdot \mathrm{nuS})$$

(%o79)

```
(%i80) rho_dc2:rhoTimeS(rho_dc1,tau/2)$
(%i81) opBasisRep(%);
```

$$Sx:\ \frac{\cos\left(\frac{2\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot \mathrm{nuS}}{2}\right)}{2} Sy:\ \frac{\sin\left(\frac{2\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\sin\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot \mathrm{nuS}}{2}\right)}{2} IzSx:\ \cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot \mathrm{nuS}}{2}\right)-\cos\left(\frac{2\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)$$

(%o81)

Fig. 18.14

These are in a different form than shown in the text, but they can be shown to be equivalent.

The pi x-pulse to the I spins

```
(%i82) rho_dc3:rhoPiXI(rho_dc2);
```

$$(\%o82)\quad \begin{pmatrix} 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 & 0 \\ \frac{e^{i\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot J}{2}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} \\ 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}+i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 \end{pmatrix}$$

```
(%i83) opBasisRep(rho_dc3);
```

$$Sx:\ \frac{\cos\left(\frac{2\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot \mathrm{nuS}}{2}\right)}{2} Sy:\ \frac{\sin\left(\frac{2\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\sin\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot \mathrm{nuS}}{2}\right)}{2} IzSx:\ \cos\left(\frac{2\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)-\cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot \mathrm{nuS}}{2}\right)$$

(%o83)

Fig. 18.15

This changes the signs of the IzSx and IzSy components.

Scalar-coupling evolution during the second delay period

```
(%i84) rho_dc4:rhoTimeS(rho_dc3,tau/2);
```

$$(\%o84)\quad \begin{pmatrix} 0 & \frac{e^{-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 & 0 \\ \frac{e^{i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} \\ 0 & 0 & \frac{e^{i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 \end{pmatrix}$$

```
(%i85) opBasisRep(rho_dc4);
```

$$Sx:\ \cos(\pi\cdot\tau\cdot \mathrm{nuS}) Sy:\ \sin(\pi\cdot\tau\cdot \mathrm{nuS})$$

(%o85)

Chemical-shift evolution during the second delay period

```
(%i86) rho_dc5:rhoTimeC(rho_dc4,tau/2);
```

$$(\%o86)\quad \begin{pmatrix} 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 \\ \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} \\ 0 & 0 & \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} & 0 \end{pmatrix}$$

```
(%i87) opBasisRep(rho_dc5);
```

$$Sx:\ \cos(2\cdot\pi\cdot\tau\cdot\mathrm{nuS})Sy:\ \sin(2\cdot\pi\cdot\tau\cdot\mathrm{nuS})$$

(%o87)

Fig. 18.16

In summary, the selective refocusing pulse suppresses the effect of scalar coupling, so that the S-spins evolve with a single apparent frequency.

3.1.2 A decoupling pulse applied to IzSy

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In this example a decoupling pulse is applied to the I component of IzSy
We can define new functions to incorporate multiple steps in a pulse sequence

```
(%i88) decoupleI(rho,tau):=block([rho1,rho2],
          rho1:rhoTime(rho,tau/2),
          rho2:rhoPiXI(rho1),
          rhoTime(rho2,tau/2));
```

$$(\%o88)\quad \mathrm{decoupleI}(\rho,\tau):=\mathrm{block}\left([\mathrm{rho1},\mathrm{rho2}],\mathrm{rho1}:\mathrm{rhoTime}\left(\rho,\frac{\tau}{2}\right),\mathrm{rho2}:\mathrm{rhoPiXI}(\mathrm{rho1}),\mathrm{rhoTime}\left(\mathrm{rho2},\frac{\tau}{2}\right)\right)$$

The block function is used to define a function with multiple lines. The optional first argument is a list of local variables. If defined, these variable can be used within the function without perturbing variables with the same name outside of the function.

Testing the decouple function with Sx

```
(%i89) decoupleI(Sx,tau);
```

$$(\%o89)\quad \begin{pmatrix} 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}+\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{2} & 0 & \cdots \\ \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}+\cdots} \\ 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{2} & \cdots \end{pmatrix}$$

```
(%i90) opBasisRep(%);
```

$$Sx:\ \cos(2\cdot\pi\cdot\tau\cdot \mathrm{nuS}) Sy:\ \sin(2\cdot\pi\cdot\tau\cdot\mathrm{nuS})$$

(%o90)

Now, apply the function to IzSy

```
(%i91) decoupleI(IzSy,tau);
```

$$(\%o91)\quad \begin{pmatrix} 0 & \frac{i\cdot e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}+\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{4} & 0 & \cdots \\ -\frac{i\cdot e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{4} & 0 & 0 & \cdots \\ 0 & 0 & 0 & -i\cdot e^{\cdots} \\ 0 & 0 & \frac{i\cdot e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{4} & \cdots \end{pmatrix}$$

```
(%i92) opBasisRep(%);
```

$$IzSx:\ \sin(2\cdot\pi\cdot\tau\cdot\mathrm{nuS}) IzSy:\ -\cos(2\cdot\pi\cdot\tau\cdot\mathrm{nuS})$$

(%o92)

Fig. 18.17

3.1.3 A refocusing pulse applied to transverse components

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In this example the refocusing pulse is applied to the S-spin during the evolution beginning with Sx

First the chemical-shift evolution

```
(%i93) rho_dcS1:rhoTimeC(Sx,tau/2);
```

$$(\%o93)\quad \begin{pmatrix} 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 \\ \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} \\ 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}}}{2} & 0 \end{pmatrix}$$

```
(%i94) opBasisRep(rho_dcS1);
```

$$Sx:\ \cos(\pi\cdot\tau\cdot\mathrm{nuS})Sy:\ \sin(\pi\cdot\tau\cdot\mathrm{nuS})$$

(%o94)

Then the scalar-coupling evolution

```
(%i95) rho_dcS2:rhoTimeS(rho_dcS1,tau/2);
```

$$(\%o95)\quad \begin{pmatrix} 0 & \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 \\ \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}+\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} \\ 0 & 0 & \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} & 0 \end{pmatrix}$$

```
(%i96) opBasisRep(%);
```

$$Sx:\ \frac{\cos\left(\frac{2\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot\mathrm{nuS}}{2}\right)}{2}Sy:\ \frac{\sin\left(\frac{2\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\sin\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot\mathrm{nuS}}{2}\right)}{2}IzSx:\ \cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot\mathrm{nuS}}{2}\right)-\cos\left(\frac{2\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)$$

(%o96)

pi x-pulse to the S-spins

```
(%i97) rho_dcS3:rhoPiXS(rho_dcS2);
```

$$(\%o97) \begin{pmatrix} 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}+i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 & 0 \\ \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{i\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot J}{2}}}{2} \\ 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 \end{pmatrix}$$

```
(%i98) opBasisRep(%);
```

$$Sx:\ \frac{\cos\left(\frac{2\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot \mathrm{nuS}}{2}\right)}{2} Sy:\ -\frac{\sin\left(\frac{2\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\sin\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot \mathrm{nuS}}{2}\right)}{2} IzSx:\ \cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot \mathrm{nuS}}{2}\right)-\cos\left(\frac{2\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right.$$

(%o98)

Scalar-coupling evolution during the second half of the period

```
(%i99) rho_dcS4:rhoTimeS(rho_dcS3,tau/2);
```

$$(\%o99) \begin{pmatrix} 0 & \frac{e^{i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 & 0 \\ \frac{e^{-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} \\ 0 & 0 & \frac{e^{-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 \end{pmatrix}$$

```
(%i100) opBasisRep(%);
```

$$Sx:\ \cos(\pi\cdot\tau\cdot \mathrm{nuS}) Sy:\ -\sin(\pi\cdot\tau\cdot \mathrm{nuS})$$

(%o100)

Chemical-shift evolution during the second half of the period

```
(%i101) rho_dcS5:rhoTimeC(rho_dcS4,tau/2);
```

$$(\%o101)\quad \begin{pmatrix} 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 \\ \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} \\ 0 & 0 & \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} & 0 \end{pmatrix}$$

```
(%i102) opBasisRep(%);
```

$$Sx:\ 1$$

(%o102)

Fig. 18.18

A function for decoupling with the pi pulse applied to the S-spins

```
(%i103) decoupleS(rho,tau):=block([rho1,rho2],
          rho1:rhoTime(rho,tau/2),
          rho2:rhoPiXS(rho1),
          rhoTime(rho2,tau/2));
```

$$(\%o103)\quad \mathrm{decoupleS}(\rho,\tau):=\mathrm{block}\left([\mathrm{rho1},\mathrm{rho2}],\ \mathrm{rho1}:\mathrm{rhoTime}\left(\rho,\frac{\tau}{2}\right),\ \mathrm{rho2}:\mathrm{rhoPiXS}(\mathrm{rho1}),\ \mathrm{rhoTime}\left(\mathrm{rho2},\frac{\tau}{2}\right)\right)$$

Testing the function with Sx

```
(%i104) decoupleS(Sx,tau);
```

$$(\%o104)\quad \begin{pmatrix} 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}+\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{2} & 0 & \cdots \\ \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}+\cdots} \\ 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{2} & \cdots \end{pmatrix}$$

```
(%i105) opBasisRep(%);
```

$$Sx:\ 1$$

(%o105)

Applying the same sequence to Sy

```
(%i106) decoupleS(Sy,tau);
```

$$(\%o106)\quad \left(\begin{matrix} 0 & \dfrac{i\cdot e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}+\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{2} & 0 & \\ -\dfrac{i\cdot e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{2} & 0 & 0 & \\ 0 & 0 & 0 & i\cdot \\ 0 & 0 & -\dfrac{i\cdot e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{2} & \end{matrix}\right.$$

```
(%i107) opBasisRep(%);
```

$$Sy:\ -1$$

(%o107)

3.1.4 A non-selective refocusing pulse

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Starting with Sx

```
(%i108) rho_ns1:rhoTimeC(Sx,tau/2);
```

$$(\%o108)\quad \begin{pmatrix} 0 & \dfrac{e^{\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 \\ \dfrac{e^{\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \dfrac{e^{\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} \\ 0 & 0 & \dfrac{e^{\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}}}{2} & 0 \end{pmatrix}$$

```
(%i109) opBasisRep(%);
```

$$Sx:\ \cos(\pi\cdot\tau\cdot\mathrm{nuS})Sy:\ \sin(\pi\cdot\tau\cdot\mathrm{nuS})$$

(%o109)

```
(%i110) rho_ns2:rhoTimeS(rho_ns1,tau/2);
```

$$(\%o110)\quad \begin{pmatrix} 0 & \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 \\ \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}+\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} \\ 0 & 0 & \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}-\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} & 0 \end{pmatrix}$$

```
(%i111) opBasisRep(%);
```

$$Sx:\ \frac{\cos\left(\frac{2\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot\mathrm{nuS}}{2}\right)}{2}\ Sy:\ \frac{\sin\left(\frac{2\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\sin\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot\mathrm{nuS}}{2}\right)}{2}\ IzSx:\ \cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot\mathrm{nuS}}{2}\right)-\cos\left(\frac{2\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)$$

(%o111)

refocusing pulse to both spins

```
(%i112) rho_ns3:rhoPiX(rho_ns2);
```

$$(\%o112)\quad \begin{pmatrix} 0 & \frac{e^{i\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot J}{2}}}{2} & 0 & 0 \\ \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{\frac{i\cdot\pi\cdot\tau\cdot J}{2}+i\cdot\pi\cdot\tau\cdot\mathrm{nuS}}}{2} \\ 0 & 0 & \frac{e^{-\frac{i\cdot\pi\cdot\tau\cdot J}{2}-i\cdot\pi\cdot\tau\cdot\mathrm{nuS}}}{2} & 0 \end{pmatrix}$$

```
(%i113) opBasisRep(%);
```

$$Sx:\ \frac{\cos\left(\frac{2\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot\mathrm{nuS}}{2}\right)}{2}\ Sy:\ -\frac{\sin\left(\frac{2\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)+\sin\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot\mathrm{nuS}}{2}\right)}{2}\ IzSx:\ \cos\left(\frac{2\cdot\pi\cdot\tau\cdot\mathrm{nuS}-\pi\cdot\tau\cdot J}{2}\right)-\cos\left(\frac{\pi\cdot\tau\cdot J+2\cdot\pi\cdot\tau\cdot\mathrm{nuS}}{2}\right.$$

(%o113)

Second half of the evolution period

```
(%i114) rho_ns4:rhoTimeS(rho_ns3,tau/2);
```

(%o114)
$$\begin{pmatrix} 0 & \frac{e^{i\cdot\pi\cdot\tau\cdot \mathrm{nuS}-i\cdot\pi\cdot\tau\cdot J}}{2} & 0 & 0 \\ \frac{e^{i\cdot\pi\cdot\tau\cdot J-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{i\cdot\pi\cdot\tau\cdot J+i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} \\ 0 & 0 & \frac{e^{-i\cdot\pi\cdot\tau\cdot J-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}}}{2} & 0 \end{pmatrix}$$

(%i115) opBasisRep(%);

$$Sx:\ \frac{\cos(\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J)+\cos(\pi\cdot\tau\cdot \mathrm{nuS}+\pi\cdot\tau\cdot J)}{2} Sy:\ -\frac{\sin(\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J)+\sin(\pi\cdot\tau\cdot \mathrm{nuS}+\pi\cdot\tau\cdot J)}{2} IzSx:\ \cos(\pi\cdot\tau\cdot \mathrm{nuS}-\pi\cdot\tau\cdot J)-\cos(\pi\cdot\tau\cdot \mathrm{nuS}+\pi\cdot\tau\cdot J)$$

(%o115)

(%i116) rho_ns5:rhoTimeC(rho_ns4,tau/2);

(%o116)
$$\begin{pmatrix} 0 & \frac{e^{-i\cdot\pi\cdot\tau\cdot J+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}+i\cdot\pi\cdot\tau\cdot \mathrm{nuS}-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 \\ \frac{e^{i\cdot\pi\cdot\tau\cdot J-\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}-\mathrm{nuS})}{2}-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuI}+\mathrm{nuS})}{2}}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{e^{i\cdot\pi\cdot\tau\cdot J+\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}+i\cdot\pi\cdot\tau\cdot \mathrm{nuS}-}}{2} \\ 0 & 0 & \frac{e^{-i\cdot\pi\cdot\tau\cdot J-\frac{i\cdot\pi\cdot\tau\cdot(-\mathrm{nuI}-\mathrm{nuS})}{2}-i\cdot\pi\cdot\tau\cdot \mathrm{nuS}+\frac{i\cdot\pi\cdot\tau\cdot(\mathrm{nuS}-\mathrm{nuI})}{2}}}{2} & 0 \end{pmatrix}$$

(%i117) opBasisRep(%);

$$Sx:\ \cos(\pi\cdot\tau\cdot J) IzSy:\ 2\cdot\sin(\pi\cdot\tau\cdot J)$$

(%o117)

Fig. 18.19

Only the effect of scalar coupling is observed.

Setting tau to 1/(2*J)

(%i118) opBasisRep(subst(tau=1/(2*J),rho_ns5));

$$IzSy:\ 2$$

(%o118)

Sx is completely converted to IzSy

3.2 18.3.2 INEPT

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(%i119) rhoEq;

$$(\%o119) \begin{pmatrix} \frac{deltaPS}{4}+\frac{deltaPI}{4} & 0 & 0 & 0 \\ 0 & \frac{deltaPI}{4}-\frac{deltaPS}{4} & 0 & 0 \\ 0 & 0 & \frac{deltaPS}{4}-\frac{deltaPI}{4} & 0 \\ 0 & 0 & 0 & -\frac{deltaPS}{4}-\frac{deltaPI}{4} \end{pmatrix}$$

```
(%i120) opBasisRep(rhoEq);
```

$$Iz:\ \frac{deltaPI}{2} Sz:\ \frac{deltaPS}{2}$$

(%o120)

Starting with the Iz component

```
(%i121) rho_ineptI1:rhoPi2YI((deltaPI/2)*Iz);
```

$$(\%o121) \begin{pmatrix} 0 & 0 & \frac{deltaPI}{4} & 0 \\ 0 & 0 & 0 & \frac{deltaPI}{4} \\ \frac{deltaPI}{4} & 0 & 0 & 0 \\ 0 & \frac{deltaPI}{4} & 0 & 0 \end{pmatrix}$$

```
(%i122) opBasisRep(%);
```

$$Ix:\ \frac{deltaPI}{2}$$

(%o122)

Here we will calculate the chemical-shift and scalar-coupling evolution in a single step, using the rhoTime function.

```
(%i123) rho_ineptI2:rhoTime(rho_ineptI1,1/(4*J));
```

$$(\%o123) \begin{pmatrix} 0 & 0 & \frac{deltaPI\cdot e^{\frac{i\cdot\pi\cdot\left(-\frac{J}{2}-nuI+nuS\right)}{4\cdot J}-\frac{i\cdot\pi\cdot\left(\frac{J}{2}+nuI+nuS\right)}{4\cdot J}}}{4} & 0 \\ 0 & 0 & 0 & \frac{deltaPI\cdot e^{\frac{i\cdot\pi\cdot\left(\frac{J}{2}-nuI-nuS\right)}{4\cdot J}-\frac{i\cdot\pi\cdot\left(-\frac{J}{2}+nuI-nuS\right)}{4\cdot J}}}{4} \\ \frac{deltaPI\cdot e^{\frac{i\cdot\pi\cdot\left(\frac{J}{2}+nuI+nuS\right)}{4\cdot J}-\frac{i\cdot\pi\cdot\left(-\frac{J}{2}-nuI+nuS\right)}{4\cdot J}}}{4} & 0 & 0 & 0 \\ 0 & \frac{deltaPI\cdot e^{\frac{i\cdot\pi\cdot\left(-\frac{J}{2}+nuI-nuS\right)}{4\cdot J}-\frac{i\cdot\pi\cdot\left(\frac{J}{2}-nuI-nuS\right)}{4\cdot J}}}{4} & 0 & 0 \end{pmatrix}$$

```
(%i124) opBasisRep(%);
```

$$Ix: \frac{\mathrm{deltaPI}\cdot\cos\left(\frac{\pi\cdot \mathrm{nuI}}{2\cdot J}\right)}{2^{\frac{3}{2}}} Iy: \frac{\mathrm{deltaPI}\cdot\sin\left(\frac{\pi\cdot \mathrm{nuI}}{2\cdot J}\right)}{2^{\frac{3}{2}}} IxSz: -\frac{\mathrm{deltaPI}\cdot\sin\left(\frac{\pi\cdot \mathrm{nuI}}{2\cdot J}\right)}{\sqrt{2}} IySz: \frac{\mathrm{deltaPI}\cdot\cos\left(\frac{\pi\cdot \mathrm{nuI}}{2\cdot J}\right)}{\sqrt{2}} \quad (\%o124)$$

The non-selective refocusing pulse

```
(%i125) rho_ineptI3:rhoPiX(rho_ineptI2);
```

$$(\%o125) \begin{pmatrix} 0 & 0 & \frac{\mathrm{deltaPI}\cdot e^{\frac{i\cdot\pi\cdot \mathrm{nuI}}{2\cdot J}}}{2^{\frac{3}{2}}\cdot i+2^{\frac{3}{2}}} & 0 \\ 0 & 0 & 0 & \frac{\left(\sqrt{2}+\sqrt{2}\cdot i\right)\cdot\mathrm{deltaPI}\cdot e^{\frac{i\cdot\pi\cdot \mathrm{nuI}}{2\cdot J}}}{8} \\ \frac{\left(\sqrt{2}+\sqrt{2}\cdot i\right)\cdot\mathrm{deltaPI}\cdot e^{-\frac{i\cdot\pi\cdot \mathrm{nuI}}{2\cdot J}}}{8} & 0 & 0 & 0 \\ 0 & \frac{\mathrm{deltaPI}\cdot e^{-\frac{i\cdot\pi\cdot \mathrm{nuI}}{2\cdot J}}}{2^{\frac{3}{2}}\cdot i+2^{\frac{3}{2}}} & 0 & 0 \end{pmatrix}$$

```
(%i126) opBasisRep(%);
```

$$Ix: \frac{\mathrm{deltaPI}\cdot\cos\left(\frac{\pi\cdot \mathrm{nuI}}{2\cdot J}\right)}{2^{\frac{3}{2}}} Iy: -\frac{\mathrm{deltaPI}\cdot\sin\left(\frac{\pi\cdot \mathrm{nuI}}{2\cdot J}\right)}{2^{\frac{3}{2}}} IxSz: \frac{\mathrm{deltaPI}\cdot\sin\left(\frac{\pi\cdot \mathrm{nuI}}{2\cdot J}\right)}{\sqrt{2}} IySz: \frac{\mathrm{deltaPI}\cdot\cos\left(\frac{\pi\cdot \mathrm{nuI}}{2\cdot J}\right)}{\sqrt{2}} \quad (\%o126)$$

The second half of the evolution period

```
(%i127) rho_ineptI4:rhoTime(rho_ineptI3,1/(4*J));
```

$$(\%o127) \begin{pmatrix} 0 & 0 & \frac{\left(\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}\right)\cdot\mathrm{deltaPI}}{2^{\frac{3}{2}}\cdot i+2^{\frac{3}{2}}} & 0 \\ 0 & 0 & 0 & \frac{\left(\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}\right)\cdot\left(\sqrt{2}+\sqrt{2}\cdot i\right)\cdot\mathrm{deltaPI}}{8} \\ \frac{\left(\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}\right)\cdot\left(\sqrt{2}+\sqrt{2}\cdot i\right)\cdot\mathrm{deltaPI}}{8} & 0 & 0 & 0 \\ 0 & \frac{\left(\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}\right)\cdot\mathrm{deltaPI}}{2^{\frac{3}{2}}\cdot i+2^{\frac{3}{2}}} & 0 & 0 \end{pmatrix}$$

```
(%i128) opBasisRep(%);
```

$$IySz: \text{deltaPI}$$

(%o128)

Fig. 18.21

Starting with the initial Sz component, nothing happens until the pi x-pulse

```
(%i129) rho_ineptS1:rhoPiX((deltaS/2)*Sz);
```

$$(\%o129)\quad \begin{pmatrix} -\frac{\text{deltaS}}{4} & 0 & 0 & 0 \\ 0 & \frac{\text{deltaS}}{4} & 0 & 0 \\ 0 & 0 & -\frac{\text{deltaS}}{4} & 0 \\ 0 & 0 & 0 & \frac{\text{deltaS}}{4} \end{pmatrix}$$

```
(%i130) opBasisRep(%);
```

$$Sz: -\frac{\text{deltaS}}{2}$$

(%o130)

Then the pi/2 y-pulse to the S-spin

```
(%i131) rho_ineptS2:rhoPi2YS(rho_ineptS1);
```

$$(\%o131)\quad \begin{pmatrix} 0 & -\frac{\text{deltaS}}{4} & 0 & 0 \\ -\frac{\text{deltaS}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\text{deltaS}}{4} \\ 0 & 0 & -\frac{\text{deltaS}}{4} & 0 \end{pmatrix}$$

```
(%i132) opBasisRep(%);
```

$$Sx: -\frac{\text{deltaS}}{2}$$

(%o132)

Fig. 18.23

We define a function for the INEPT sequence

```
(%i133) inept(rho):=block([rho1,rho2,rho3,rho4,rho5],
          rho1:rhoPi2YI(rho),
          rho2:rhoTime(rho1,1/(4*J)),
          rho3:rhoPiX(rho2),
          rho4:rhoTime(rho3,1/(4*J)),
          rho5:rhoPi2XI(rho4),
          rhoPi2YS(rho5));
```

$$(\%o133)\quad \text{inept}(\rho) := \text{block}\left([\text{rho1}, \text{rho2}, \text{rho3}, \text{rho4}, \text{rho5}], \text{rho1}: \text{rhoPi2YI}(\rho), \text{rho2}: \text{rhoTime}\left(\text{rho1}, \frac{1}{4 \cdot J}\right), \text{rho3}: \text{rhoPiX}(\text{rho2}), \text{rho4}: \text{rhoTime}\left(\text{rho3}, \frac{1}{4 \cdot J}\right), \text{rho5}: \text{rhoPi2XI}(\text{rho4}\right.$$

```
(%i134) inept(Iz);
```

$$\text{(\%o134)} \quad \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \end{pmatrix}$$

```
(%i135) opBasisRep(%);
```

$$IzSx: \ 2$$

(%o135)

```
(%i136) inept(Sz);
```

$$\text{(\%o136)} \quad \begin{pmatrix} 0 & -\frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \end{pmatrix}$$

```
(%i137) opBasisRep(%);
```

$$Sx: \ -1$$

(%o137)

Applying this to the equilibrium density matrix

```
(%i138) inept(rhoEq);
```

$$\text{(\%o138)} \quad \begin{pmatrix} 0 & -\frac{\mathrm{deltaPS}-\mathrm{deltaPI}}{4} & 0 & 0 \\ -\frac{\mathrm{deltaPS}-\mathrm{deltaPI}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\mathrm{deltaPI}+\mathrm{deltaPS}}{4} \\ 0 & 0 & -\frac{\mathrm{deltaPI}+\mathrm{deltaPS}}{4} & 0 \end{pmatrix}$$

```
(%i139) opBasisRep(%);
```

$$Sx: \ -\frac{\mathrm{deltaPS}}{2} IzSx: \ \mathrm{deltaPI}$$

(%o139)

Time evolution during the data-acquisition period

From the Sx component

```
(%i140) rhoTime(-(deltaPS/2)*Sx,t);
```

(%o140)
$$\begin{pmatrix} 0 & -\frac{\mathrm{deltaPS}\cdot e^{i\cdot\pi\cdot t\cdot\left(-\mathrm{nuS}+\mathrm{nuI}-\frac{J}{2}\right)-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}}{4} & 0 & 0 \\ -\frac{\mathrm{deltaPS}\cdot e^{i\cdot\pi\cdot t\cdot\left(\mathrm{nuS}+\mathrm{nuI}+\frac{J}{2}\right)-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\mathrm{deltaPS}\cdot e^{i\cdot\pi\cdot t\cdot\left(-\mathrm{nuS}-\mathrm{nuI}\right.}}{} \\ 0 & 0 & -\frac{\mathrm{deltaPS}\cdot e^{i\cdot\pi\cdot t\cdot\left(\mathrm{nuS}-\mathrm{nuI}-\frac{J}{2}\right)-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}}{4} & 0 \end{pmatrix}$$

```
(%i141) opBasisRep(%);
```

$$Sx:\ -\frac{\mathrm{deltaPS}\cdot(\cos(2\cdot\pi\cdot t\cdot\mathrm{nuS}-\pi\cdot t\cdot J)+\cos(2\cdot\pi\cdot t\cdot\mathrm{nuS}+\pi\cdot t\cdot J))}{4}\ Sy:\ -\frac{\mathrm{deltaPS}\cdot(\sin(2\cdot\pi\cdot t\cdot\mathrm{nuS}-\pi\cdot t\cdot J)+\sin(2\cdot\pi\cdot t\cdot\mathrm{nuS}+\pi\cdot t\cdot J))}{4}\ IzSx:\ -\frac{\mathrm{deltaPS}\cdot(\cos}{}$$

(%o141)

From the IzSx component

```
(%i142) rhoTime(deltaPI*IzSx,t);
```

(%o142)
$$\begin{pmatrix} 0 & \frac{\mathrm{deltaPI}\cdot e^{i\cdot\pi\cdot t\cdot\left(-\mathrm{nuS}+\mathrm{nuI}-\frac{J}{2}\right)-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}}{4} & 0 & 0 \\ \frac{\mathrm{deltaPI}\cdot e^{i\cdot\pi\cdot t\cdot\left(\mathrm{nuS}+\mathrm{nuI}+\frac{J}{2}\right)-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\mathrm{deltaPI}\cdot e^{i\cdot\pi\cdot t\cdot\left(-\mathrm{nuS}-\mathrm{nuI}+\frac{J}{2}\right)-}}{4} \\ 0 & 0 & -\frac{\mathrm{deltaPI}\cdot e^{i\cdot\pi\cdot t\cdot\left(\mathrm{nuS}-\mathrm{nuI}-\frac{J}{2}\right)-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}}{4} & 0 \end{pmatrix}$$

```
(%i143) opBasisRep(%);
```

$$Sx:\ \frac{\mathrm{deltaPI}\cdot(\cos(2\cdot\pi\cdot t\cdot\mathrm{nuS}+\pi\cdot t\cdot J)-\cos(2\cdot\pi\cdot t\cdot\mathrm{nuS}-\pi\cdot t\cdot J))}{4}\ Sy:\ \frac{\mathrm{deltaPI}\cdot(\sin(2\cdot\pi\cdot t\cdot\mathrm{nuS}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot\mathrm{nuS}-\pi\cdot t\cdot J))}{4}\ IzSx:\ \frac{\mathrm{deltaPI}\cdot(\cos(2\cdot\pi\cdot t\cdot}{}$$

(%o143)

Fig. 18.24

Combining the Sx components

```
(%i144) -(deltaPS*(cos(2*%pi*t*nuS-%pi*t*J)+cos(2*%pi*t*nuS+%pi*t*J)))/4+
        (deltaPI*(cos(2*%pi*t*nuS+%pi*t*J)-cos(2*%pi*t*nuS-%pi*t*J)))/4;
```

$$(\%o144)\quad \frac{\mathrm{deltaPI}\cdot(\cos(2\cdot\pi\cdot t\cdot\mathrm{nuS}+\pi\cdot t\cdot J)-\cos(2\cdot\pi\cdot t\cdot\mathrm{nuS}-\pi\cdot t\cdot J))}{4}-\frac{\mathrm{deltaPS}\cdot(\cos(2\cdot\pi\cdot t\cdot\mathrm{nuS}-\pi\cdot t\cdot J)+\cos(2\cdot\pi\cdot t\cdot\mathrm{nuS}+\pi\cdot t\cdot J))}{4}$$

```
(%i145) ratsimp(%);
```

$$(\%o145)\quad -\frac{(\mathrm{deltaPS}+\mathrm{deltaPI})\cdot\cos(2\cdot\pi\cdot t\cdot\mathrm{nuS}-\pi\cdot t\cdot J)+(\mathrm{deltaPS}-\mathrm{deltaPI})\cdot\cos(2\cdot\pi\cdot t\cdot\mathrm{nuS}+\pi\cdot t\cdot J)}{4}$$

Combining the Sy components

```
(%i146) -(deltaPS*(sin(2*%pi*t*nuS-%pi*t*J)+sin(2*%pi*t*nuS+%pi*t*J)))/4 +
        (deltaPI*(sin(2*%pi*t*nuS+%pi*t*J)-sin(2*%pi*t*nuS-%pi*t*J)))/4;
```

$$\text{(\%o146)}\quad \frac{\mathrm{deltaPI}\cdot(\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-\pi\cdot t\cdot J))}{4}-\frac{\mathrm{deltaPS}\cdot(\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-\pi\cdot t\cdot J)+\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+\pi\cdot t\cdot J))}{4}$$

```
(%i147) ratsimp(%);
```

$$\text{(\%o147)}\quad -\frac{(\mathrm{deltaPS}+\mathrm{deltaPI})\cdot\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-\pi\cdot t\cdot J)+(\mathrm{deltaPS}-\mathrm{deltaPI})\cdot\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+\pi\cdot t\cdot J)}{4}$$

The signal with frequency nuS-J/2 has amplitude of -(deltaPI+deltaPS) The signal with frequency nS+J/2 has amplitude of (deltaPI-deltaPS)

3.3 18.3.3 HSQC

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The INEPT sequence forms the first part of the HSQC experiment, so we can begin the analysis of the HSQC with the results from INEPT shown above.

```
(%i148) opBasisRep(inept(rhoEq));
```

$$Sx:\ -\frac{\mathrm{deltaPS}}{2} IzSx:\ \mathrm{deltaPI}$$

(%o148)

For the S-evolution period, we can use the function defined earlier for an I-decoupling sequence

```
(%i149) fundef(decoupleI);
```

$$\text{(\%o149)}\quad \mathrm{decoupleI}(\rho,\tau):=\mathrm{block}\left([\mathrm{rho1},\mathrm{rho2}],\mathrm{rho1}:\mathrm{rhoTime}\left(\rho,\frac{\tau}{2}\right),\mathrm{rho2}:\mathrm{rhoPiXI}(\mathrm{rho1}),\mathrm{rhoTime}\left(\mathrm{rho2},\frac{\tau}{2}\right)\right)$$

The component beginning as Sx

```
(%i150) rho_hsqcS1:decoupleI(-(deltaPS/2)*Sx,t1);
```

$$\text{(\%o150)}\quad \begin{pmatrix} 0 & -\frac{\mathrm{deltaPS}\cdot e^{\frac{i\cdot\pi\cdot \mathrm{t1}\cdot J}{2}+\frac{i\cdot\pi\cdot\mathrm{t1}\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}-i\cdot\pi\cdot\mathrm{t1}\cdot\mathrm{nuS}-\frac{i\cdot\pi\cdot\mathrm{t1}\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{4} & 0 \\ -\frac{\mathrm{deltaPS}\cdot e^{-\frac{i\cdot\pi\cdot\mathrm{t1}\cdot J}{2}-\frac{i\cdot\pi\cdot\mathrm{t1}\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}+i\cdot\pi\cdot\mathrm{t1}\cdot\mathrm{nuS}+\frac{i\cdot\pi\cdot\mathrm{t1}\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{4} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\mathrm{deltaPS}\cdot e^{\frac{i\cdot\pi\cdot\mathrm{t1}\cdot J}{2}-\frac{i\cdot\pi\cdot\mathrm{t1}\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}{2}+i\cdot\pi\cdot\mathrm{t1}}}{4} \end{pmatrix}$$

```
(%i151) opBasisRep(%);
```

$$Sx:\ -\frac{\mathrm{deltaPS}\cdot\cos(2\cdot\pi\cdot\mathrm{t1}\cdot\mathrm{nuS})}{2} Sy:\ -\frac{\mathrm{deltaPS}\cdot\sin(2\cdot\pi\cdot\mathrm{t1}\cdot\mathrm{nuS})}{2}$$

(%o151)

Fig. 18.26

The reverse INEPT sequence for this component

The non-selective pi/2 y-pulse

```
(%i152) rho_hsqcS2:rhoPi2Y(rho_hsqcS1);
```

(%o152)
$$\begin{pmatrix} \frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}\right)}{8} & \frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}-deltaPS\right)}{8} & 0 & 0 \\ -\frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}-deltaPS\right)}{8} & -\frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}\right)}{8} & 0 & 0 \\ 0 & 0 & \frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}\right)}{8} & \frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS\cdot e^{4}\right.}{8} \\ 0 & 0 & -\frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}-deltaPS\right)}{8} & -\frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS+\right.}{8} \end{pmatrix}$$

```
(%i153) opBasisRep(%);
```

$$Sy:\ -\frac{deltaPS\cdot\sin(2\cdot\pi\cdot t1\cdot nuS)}{2}\ Sz:\ \frac{deltaPS\cdot\cos(2\cdot\pi\cdot t1\cdot nuS)}{2}$$

(%o153)

Fig. 18.27

Refocused 1/(2*J) period

```
(%i154) rho_hsqcS3:rhoTime(rho_hsqcS2,1/(4*J));
```

(%o154)
$$\begin{pmatrix} \frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}\right)}{8} & \frac{\left(deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}-deltaPS\right)\cdot e^{\frac{i\cdot\pi\cdot\left(-\frac{J}{2}+nuI-nuS\right)}{4\cdot J}-2\cdot i\cdot\pi\cdot t1\cdot nuS-\frac{i\cdot\pi\cdot\left(\frac{J}{2}+nuI+nuS\right)}{4\cdot J}}}{8} & \cdots \\ -\frac{\left(deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}-deltaPS\right)\cdot e^{-\frac{i\cdot\pi\cdot\left(-\frac{J}{2}+nuI-nuS\right)}{4\cdot J}-2\cdot i\cdot\pi\cdot t1\cdot nuS+\frac{i\cdot\pi\cdot\left(\frac{J}{2}+nuI+nuS\right)}{4\cdot J}}}{8} & -\frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}\right)}{8} & \cdots \\ 0 & 0 & \cdots \\ 0 & 0 & -\frac{\left(deltaPS\cdot e^{4}\right.}{} \end{pmatrix}$$

```
(%i155) opBasisRep(%);
```

$$Sx:\ -\frac{deltaPS\cdot\left(\cos\left(\frac{(\pi+4\cdot\pi\cdot t1\cdot J)\cdot nuS}{2\cdot J}\right)-\cos\left(\frac{(4\cdot\pi\cdot t1\cdot J-\pi)\cdot nuS}{2\cdot J}\right)\right)}{2^{\frac{5}{2}}}\ Sy:\ -\frac{deltaPS\cdot\left(\sin\left(\frac{(4\cdot\pi\cdot t1\cdot J-\pi)\cdot nuS}{2\cdot J}\right)+\sin\left(\frac{(\pi+4\cdot\pi\cdot t1\cdot J)\cdot nuS}{2\cdot J}\right)\right)}{2^{\frac{5}{2}}}\ Sz:\ \frac{deltaPS\cdot\cos(2\cdot\pi\cdot t1\cdot nuS)}{2}$$

(%o155)

```
(%i156) rho_hsqcS4:rhoPiX(rho_hsqcS3);
```

(%o156)
$$\begin{pmatrix} -\frac{e^{-2\cdot i\cdot \pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot \pi\cdot t1\cdot nuS}\right)}{8} & -\frac{e^{-2\cdot i\cdot \pi\cdot t1\cdot nuS}\cdot\left(deltaPS\cdot e^{4\cdot i\cdot \pi\cdot t1\cdot nuS}-deltaPS\right)\cdot e^{\frac{i\cdot \pi\cdot nuS}{2\cdot J}}}{2^{\frac{5}{2}}\cdot i+2^{\frac{5}{2}}} & 0 \ldots \\ \frac{\left(\left(-\sqrt{2}\cdot i-\sqrt{2}\right)\cdot deltaPS+\left(\sqrt{2}\cdot i+\sqrt{2}\right)\cdot deltaPS\cdot e^{4\cdot i\cdot \pi\cdot t1\cdot nuS}\right)\cdot e^{-2\cdot i\cdot \pi\cdot t1\cdot nuS-\frac{i\cdot \pi\cdot nuS}{2\cdot J}}}{16} & \frac{e^{-2\cdot i\cdot \pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot \pi\cdot t1\cdot nuS}\right)}{8} & 0 \ldots \\ 0 & 0 & -\frac{e^{-2\cdot i\cdot \pi\cdot t1\cdot nuS}\cdot\left(deltaPS+delta\ldots\right.}{8} \\ 0 & 0 & \frac{\left(deltaPS\cdot e^{4\cdot i\cdot \pi\cdot t1\cdot nuS}-deltaPS\right)\cdot e\ldots}{2^{\frac{5}{2}}\cdot i+2^{\frac{5}{2}}} \end{pmatrix}$$

```
(%i157) opBasisRep(%);
```

$$Sx:\ -\frac{deltaPS\cdot\left(\cos\left(\frac{(\pi+4\cdot\pi\cdot t1\cdot J)\cdot nuS}{2\cdot J}\right)-\cos\left(\frac{(4\cdot\pi\cdot t1\cdot J-\pi)\cdot nuS}{2\cdot J}\right)\right)}{2^{\frac{5}{2}}} Sy:\ \frac{deltaPS\cdot\left(\sin\left(\frac{(4\cdot\pi\cdot t1\cdot J-\pi)\cdot nuS}{2\cdot J}\right)+\sin\left(\frac{(\pi+4\cdot\pi\cdot t1\cdot J)\cdot nuS}{2\cdot J}\right)\right)}{2^{\frac{5}{2}}} Sz:\ -\frac{deltaPS\cdot\cos(2\cdot\pi\cdot t1\cdot nuS)}{2}\ldots$$

(%o157)

```
(%i158) rho_hsqcS5:rhoTime(rho_hsqcS4,1/(4*J));
```

(%o158)
$$\begin{pmatrix} -\frac{e^{-2\cdot i\cdot \pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot \pi\cdot t1\cdot nuS}\right)}{8} & -\frac{\left(\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}\right)\cdot e^{-2\cdot i\cdot \pi\cdot t1\cdot nuS}\cdot\left(deltaPS\cdot e^{4\cdot i\cdot \pi\cdot t1\cdot nuS}-deltaPS\right)}{2^{\frac{5}{2}}\cdot i+2^{\frac{5}{2}}} & \ldots \\ \frac{\left(\frac{i}{\sqrt{2}}+\frac{1}{\sqrt{2}}\right)\cdot e^{-2\cdot i\cdot \pi\cdot t1\cdot nuS}\cdot\left(\left(-\sqrt{2}\cdot i-\sqrt{2}\right)\cdot deltaPS+\left(\sqrt{2}\cdot i+\sqrt{2}\right)\cdot deltaPS\cdot e^{4\cdot i\cdot \pi\cdot t1\cdot nuS}\right)}{16} & \frac{e^{-2\cdot i\cdot \pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot \pi\cdot t1\cdot nuS}\right)}{8} & \ldots \\ 0 & 0 & -\frac{e^{-2\cdot i\cdot \pi\cdot t1\cdot nuS}\cdot\left(\ldots\right.}{\ldots} \\ 0 & 0 & \left(\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}\right)\cdot e^{-2\cdot i\cdot \pi\cdot t1\cdot n\ldots} \end{pmatrix}$$

```
(%i159) opBasisRep(%);
```

$$Sz:\ -\frac{deltaPS\cdot\cos(2\cdot\pi\cdot t1\cdot nuS)}{2} IzSx:\ -deltaPS\cdot\sin(2\cdot\pi\cdot t1\cdot nuS)$$

(%o159)

Neither of these components contributes to I-magnetization during the data-acquisition period.

Back to the IzSx component present at the end of the INEPT sequence

```
(%i160) deltaPI*IzSx;
```

$$(\%o160)\quad \begin{pmatrix} 0 & \frac{\mathrm{deltaPI}}{4} & 0 & 0 \\ \frac{\mathrm{deltaPI}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\mathrm{deltaPI}}{4} \\ 0 & 0 & -\frac{\mathrm{deltaPI}}{4} & 0 \end{pmatrix}$$

The refocused S-evolution period

```
(%i161) rho_hsqcIS1:decoupleI(deltaPI*IzSx,t1);
```

$$(\%o161)\quad \begin{pmatrix} 0 & -\frac{\mathrm{deltaPI}\cdot e^{\frac{i\cdot\pi\cdot \mathrm{t1}\cdot J}{2}+\frac{i\cdot\pi\cdot \mathrm{t1}\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}-i\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS}-\frac{i\cdot\pi\cdot \mathrm{t1}\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{4} & 0 \\ -\frac{\mathrm{deltaPI}\cdot e^{-\frac{i\cdot\pi\cdot \mathrm{t1}\cdot J}{2}-\frac{i\cdot\pi\cdot \mathrm{t1}\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}{2}+i\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS}+\frac{i\cdot\pi\cdot \mathrm{t1}\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}{2}}}{4} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\mathrm{deltaPI}\cdot e^{\frac{i\cdot\pi\cdot \mathrm{t1}\cdot J}{2}-\frac{i\cdot\pi\cdot \mathrm{t1}\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}{2}+i\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS}}}{4} \end{pmatrix}$$

```
(%i162) opBasisRep(%);
```

$$IzSx:\ -\mathrm{deltaPI}\cdot\cos(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS})IzSy:\ -\mathrm{deltaPI}\cdot\sin(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS})$$

(%o162)

Fig. 18.28

The IzSx component evolves into a mixture of IzSx and IzSy, depending on the nuS and the length of the t1 period.

Define a function for the reverse INEPT sequence

```
(%i163) rinept(rho):=block([rho1,rho2,rho3],
          rho1:rhoPi2Y(rho),
          rho2:rhoTime(rho1,1/(4*J)),
        rho3:rhoPiX(rho2),
          rhoTime(rho3,1/(4*J)));
```

$$(\%o163)\quad \mathrm{rinept}(\rho):=\mathrm{block}\left([\mathrm{rho1},\mathrm{rho2},\mathrm{rho3}],\mathrm{rho1}:\mathrm{rhoPi2Y}(\rho),\mathrm{rho2}:\mathrm{rhoTime}\left(\mathrm{rho1},\frac{1}{4\cdot J}\right),\mathrm{rho3}:\mathrm{rhoPiX}(\mathrm{rho2}),\mathrm{rhoTime}\left(\mathrm{rho3},\frac{1}{4\cdot J}\right)\right)$$

Test this with the mixture Sx and Sy present at the end of the t1 evolution period, which began as Sx at the end of the INEPT segment

```
(%i164) opBasisRep(rho_hsqcS1);
```

$$Sx:\ -\frac{\mathrm{deltaPS}\cdot\cos(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS})}{2}Sy:\ -\frac{\mathrm{deltaPS}\cdot\sin(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS})}{2}$$

(%o164)

```
(%i165) rinept(rho_hsqcS1);
```

(%o165)
$$\begin{pmatrix} -\frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}\right)}{8} & -\frac{\left(\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}\right)\cdot e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}-deltaPS\right)}{2^{\frac{5}{2}}\cdot i+2^{\frac{5}{2}}} & \cdots \\ \frac{\left(\frac{i}{\sqrt{2}}+\frac{1}{\sqrt{2}}\right)\cdot e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(\left(-\sqrt{2}\cdot i-\sqrt{2}\right)\cdot deltaPS+\left(\sqrt{2}\cdot i+\sqrt{2}\right)\cdot deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}\right)}{16} & \frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(deltaPS+deltaPS\cdot e^{4\cdot i\cdot\pi\cdot t1\cdot nuS}\right)}{8} & \cdots \\ 0 & 0 & -\frac{e^{-2\cdot i\cdot\pi\cdot t1\cdot nuS}\cdot\left(\cdots\right.}{\cdots} \\ 0 & 0 & \left(\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}\right)\cdot e^{-2\cdot i\cdot\pi\cdot t1\cdot n\cdots} \end{pmatrix}$$

```
(%i166) opBasisRep(%);
```

$$Sz:\ -\frac{deltaPS\cdot\cos(2\cdot\pi\cdot t1\cdot nuS)}{2} IzSx:\ -deltaPS\cdot\sin(2\cdot\pi\cdot t1\cdot nuS)$$

(%o166)

Now apply the reverse INEPT sequence to the two components that evolve from IzSx during the t1 period

First, the -IzSy component

```
(%i167) rinept(-deltaPI*sin(2*%pi*t1*nuS)*IzSy);
```

(%o167)
$$\begin{pmatrix} 0 & 0 & \cdots \\ 0 & 0 & i\cdot deltaPI\cdot e^{\frac{i\cdot\pi\cdot nuI}{2\cdot J}-\cdots} \\ 0 & -\frac{i\cdot deltaPI\cdot e^{-\frac{i\cdot\pi\cdot nuI}{2\cdot J}+\frac{i\cdot\pi\cdot\left(-\frac{J}{2}+nuI-nuS\right)}{4\cdot J}+\frac{i\cdot\pi\cdot nuS}{2\cdot J}-\frac{i\cdot\pi\cdot\left(-\frac{J}{2}-nuI+nuS\right)}{4\cdot J}}\cdot\sin(2\cdot\pi\cdot t1\cdot nuS)}{4} & \cdots \\ \frac{i\cdot deltaPI\cdot e^{-\frac{i\cdot\pi\cdot nuI}{2\cdot J}-\frac{i\cdot\pi\cdot\left(\frac{J}{2}-nuI-nuS\right)}{4\cdot J}-\frac{i\cdot\pi\cdot nuS}{2\cdot J}+\frac{i\cdot\pi\cdot\left(\frac{J}{2}+nuI+nuS\right)}{4\cdot J}}\cdot\sin(2\cdot\pi\cdot t1\cdot nuS)}{4} & 0 & \cdots \end{pmatrix}$$

```
(%i168) opBasisRep(%);
```

$$IxSy:\ deltaPI\cdot\sin(2\cdot\pi\cdot t1\cdot nuS)$$

(%o168)

Fig. 18.30

This component does not contribute to observable magnetization during the data-acquisition period.

Then the -IzSx correlation component

```
(%i169) rinept(-deltaPI*cos(2*%pi*t1*nuS)*IzSx);
```

(%o169)
$$\begin{pmatrix} 0 & 0 & -\frac{\left(\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}\right)\cdot \mathrm{deltaPI}\cdot\cos(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS})}{2^{\frac{3}{2}}\cdot i+2^{\frac{3}{2}}} & 0 \\ 0 & 0 & 0 & \frac{\left(\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}\right)\cdot\left(\sqrt{2}+\sqrt{2}\cdot i\right)\cdot \mathrm{deltaPI}\cdot\cos(2}{8} \\ -\frac{\left(\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}\right)\cdot\left(\sqrt{2}+\sqrt{2}\cdot i\right)\cdot \mathrm{deltaPI}\cdot\cos(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS})}{8} & 0 & 0 & 0 \\ 0 & \frac{\left(\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}\right)\cdot \mathrm{deltaPI}\cdot\cos(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS})}{2^{\frac{3}{2}}\cdot i+2^{\frac{3}{2}}} & 0 & 0 \end{pmatrix}$$

```
(%i170) opBasisRep(%);
```

$$Iy: \ -\frac{\mathrm{deltaPI}\cdot\cos(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuS})}{2}$$

(%o170)

Fig. 18.32

This is the component that generates the signal in the data-acquisition period! The magnitude of this component is determined by the initial equilibrium population difference for the I-spin and the evolution of the S-spin during the t1 period.

3.4 18.3.4 Homonuclear COSY

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Starting with the Ix component present after the initial pi/2 y-pulse.

The evolution during t1

```
(%i171) rho_hhCosy1:rhoTime(Ix,t1);
```

(%o171)
$$\begin{pmatrix} 0 & 0 & \frac{e^{i\cdot\pi\cdot \mathrm{t1}\cdot\left(\mathrm{nuS}-\mathrm{nuI}-\frac{J}{2}\right)-i\cdot\pi\cdot \mathrm{t1}\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}}{2} & 0 \\ 0 & 0 & 0 & \frac{e^{i\cdot\pi\cdot \mathrm{t1}\cdot\left(-\mathrm{nuS}-\mathrm{nuI}+\frac{J}{2}\right)-i\cdot\pi\cdot \mathrm{t1}\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}}{2} \\ \frac{e^{i\cdot\pi\cdot \mathrm{t1}\cdot\left(\mathrm{nuS}+\mathrm{nuI}+\frac{J}{2}\right)-i\cdot\pi\cdot \mathrm{t1}\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}}{2} & 0 & 0 & 0 \\ 0 & \frac{e^{i\cdot\pi\cdot \mathrm{t1}\cdot\left(-\mathrm{nuS}+\mathrm{nuI}-\frac{J}{2}\right)-i\cdot\pi\cdot \mathrm{t1}\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}}{2} & 0 & 0 \end{pmatrix}$$

```
(%i172) opBasisRep(%);
```

$Ix: \dfrac{\cos(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)+\cos(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J)}{2} Iy: \dfrac{\sin(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)+\sin(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J)}{2} IxSz: \cos(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J)-\cos($

(%o172)

Fig. 18.34

The second pi/2 y-pulse

```
(%i173) rho_hhCosy2:rhoPi2Y(rho_hhCosy1);
```

\mathrm{\tt (\%o173) }\quad \begin{pmatrix}-\frac{\left(1+{{e}^{2\cdot i\cdot \pi \cdot \mathit{t1}\cdot J}}+\left({{e}^{2\cdot i\cdot \pi \cdot \mathit{t1}\cdot J}}+1\right) \c

```
(%i174) opBasisRep(%);
```

$Iy: \dfrac{\sin(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)+\sin(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J)}{2} Iz: -\dfrac{\cos(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)+\cos(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J)}{2} IySx: \sin(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J)-\sin$

(%o174)

Evolution of the Iy component during the data-acquisition period, t2

```
(%i175) rhoIyt:rhoTime(((sin(2*%pi*t1*nuI-%pi*t1*J)+sin(2*%pi*t1*nuI+%pi*t1*J))/2)*Iy,t2);
```

$$(\%o175)\quad \left(\begin{matrix} 0 & 0 \\ 0 & 0 \\ \dfrac{i\cdot(\sin(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)+\sin(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J))\cdot e^{i\cdot\pi\cdot t2\cdot\left(nuS+nuI+\frac{J}{2}\right)-i\cdot\pi\cdot t2\cdot\left(-\frac{J}{2}-nuI+nuS\right)}}{4} & 0 \\ 0 & \dfrac{i\cdot(\sin(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)+\sin(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J))\cdot e^{i\cdot\pi\cdot t2\cdot\left(-nuS+nuI-\frac{J}{2}\right)-i}}{4} \end{matrix}\right.$$

```
(%i176) opBasisRep(rhoIyt);
```

$Ix: \dfrac{-\cos((2\cdot\pi\cdot t2-2\cdot\pi\cdot t1)\cdot nuI+(-\pi\cdot t1-\pi\cdot t2)\cdot J)-\cos((2\cdot\pi\cdot t2-2\cdot\pi\cdot t1)\cdot nuI+(\pi\cdot t1-\pi\cdot t2)\cdot J)-\cos((2\cdot\pi\cdot t2-2\cdot\pi\cdot t1)\cdot nuI+(\pi\cdot t2-\pi\cdot t1)\cdot J)-\cos}{}$

(%o176)

Simplifying the Ix component

```
(%i177) meanRho(Ix,rhoIyt);
```

$$(\%o177)\quad \frac{-\cos((2\cdot\pi\cdot t2-2\cdot\pi\cdot t1)\cdot nuI+(-\pi\cdot t1-\pi\cdot t2)\cdot J)-\cos((2\cdot\pi\cdot t2-2\cdot\pi\cdot t1)\cdot nuI+(\pi\cdot t1-\pi\cdot t2)\cdot J)-\cos((2\cdot\pi\cdot t2-2\cdot\pi\cdot t1)\cdot nuI+(\pi\cdot t2-\pi\cdot t1)\cdot J}{}$$

```
(%i178) trigreduce(%);
```

$$(\%o178)\quad \frac{-\cos(2\cdot\pi\cdot t2\cdot nuI-2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t2\cdot J-\pi\cdot t1\cdot J)-\cos(2\cdot\pi\cdot t2\cdot nuI-2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t2\cdot J+\pi\cdot t1\cdot J)-\cos(2\cdot\pi\cdot t2\cdot nuI-2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t2\cdot}{}$$

```
(%i179) trigexpand(%);
```

$$(\%o179)\quad -\cos(\pi\cdot t1\cdot J)\cdot\cos(\pi\cdot t2\cdot J)\cdot\sin(2\cdot\pi\cdot t1\cdot nuI)\cdot\sin(2\cdot\pi\cdot t2\cdot nuI)$$

```
(%i180) temp:%;
```

$$(\%o180)\quad -\cos(\pi\cdot t1\cdot J)\cdot\cos(\pi\cdot t2\cdot J)\cdot\sin(2\cdot\pi\cdot t1\cdot nuI)\cdot\sin(2\cdot\pi\cdot t2\cdot nuI)$$

To separate the t1 and t2 terms, first make substitutions for the t2 terms

```
(%i181) subst([cos(%pi*t2*J)=a,sin(2*%pi*t2*nuI)=b],temp);
```

$$(\%o181)\quad -a\cdot b\cdot \cos(\pi\cdot \mathrm{t1}\cdot J)\cdot \sin(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuI})$$

```
(%i182) trigreduce(%);
```

$$(\%o182)\quad -\frac{a\cdot b\cdot \sin(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuI}+\pi\cdot \mathrm{t1}\cdot J)}{2}-\frac{a\cdot b\cdot \sin(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuI}-\pi\cdot \mathrm{t1}\cdot J)}{2}$$

```
(%i183) factor(%);
```

$$(\%o183)\quad -\frac{a\cdot b\cdot (\sin(\pi\cdot \mathrm{t1}\cdot (2\cdot \mathrm{nuI}-J))+\sin(\pi\cdot \mathrm{t1}\cdot (2\cdot \mathrm{nuI}+J)))}{2}$$

```
(%i184) temp2:%;
```

$$(\%o184)\quad -\frac{a\cdot b\cdot (\sin(\pi\cdot \mathrm{t1}\cdot (2\cdot \mathrm{nuI}-J))+\sin(\pi\cdot \mathrm{t1}\cdot (2\cdot \mathrm{nuI}+J)))}{2}$$

Define a new term to substitute back in

```
(%i185) ab:cos(%pi*t2*J)*sin(2*%pi*t2*nuI);
```

$$(\%o185)\quad \cos(\pi\cdot \mathrm{t2}\cdot J)\cdot \sin(2\cdot\pi\cdot \mathrm{t2}\cdot \mathrm{nuI})$$

```
(%i186) ab:trigreduce(ab);
```

$$(\%o186)\quad \frac{\sin(2\cdot\pi\cdot \mathrm{t2}\cdot \mathrm{nuI}+\pi\cdot \mathrm{t2}\cdot J)}{2}+\frac{\sin(2\cdot\pi\cdot \mathrm{t2}\cdot \mathrm{nuI}-\pi\cdot \mathrm{t2}\cdot J)}{2}$$

```
(%i187) subst(ab,a*b, temp2);
```

$$(\%o187)\quad -\frac{a\cdot b\cdot (\sin(\pi\cdot \mathrm{t1}\cdot (2\cdot \mathrm{nuI}-J))+\sin(\pi\cdot \mathrm{t1}\cdot (2\cdot \mathrm{nuI}+J)))}{2}$$

The subst function does not allow a substitution for a term made up of two parts, like a*b, but ratsubst does

```
(%i188) ratsubst(ab,a*b,temp2);
```

$$(\%o188)\quad -\frac{(\sin(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuI}+\pi\cdot \mathrm{t1}\cdot J)+\sin(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuI}-\pi\cdot \mathrm{t1}\cdot J))\cdot \sin(2\cdot\pi\cdot \mathrm{t2}\cdot \mathrm{nuI}-\pi\cdot \mathrm{t2}\cdot J)+(\sin(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuI}+\pi\cdot \mathrm{t1}\cdot J)+\sin(2\cdot\pi\cdot \mathrm{t1}\cdot \mathrm{nuI}-\pi\cdot \mathrm{t1}\cdot J))\cdot}{4}$$

```
(%i189) factor(%);
```

$$(\%o189)\quad -\frac{(\sin(\pi\cdot \mathrm{t1}\cdot (2\cdot \mathrm{nuI}-J))+\sin(\pi\cdot \mathrm{t1}\cdot (2\cdot \mathrm{nuI}+J)))\cdot(\sin(\pi\cdot \mathrm{t2}\cdot (2\cdot \mathrm{nuI}-J))+\sin(\pi\cdot \mathrm{t2}\cdot (2\cdot \mathrm{nuI}+J)))}{4}$$

The term for Iy can be treated in the same way. Both of these components give rise to diagonal elements, determined by only nuI

Evolution of the -IzSx component after the second pulse

```
(%i190) rhoIzSxt:rhoTime((cos(2*%pi*t1*nuI-%pi*t1*J)-cos(2*%pi*t1*nuI+%pi*t1*J))*IzSx,t2);
```

(%o190)
$$\begin{pmatrix} 0 & \frac{(\cos(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)-\cos(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J))\cdot e^{i\cdot\pi\cdot t2\cdot\left(-nuS+nuI-\frac{J}{2}\right)-i\cdot\pi}}{4} \\ \frac{(\cos(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)-\cos(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J))\cdot e^{i\cdot\pi\cdot t2\cdot\left(nuS+nuI+\frac{J}{2}\right)-i\cdot\pi\cdot t2\cdot\left(-\frac{J}{2}+nuI-nuS\right)}}{4} & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

```
(%i191) opBasisRep(%);
```

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

(%o191)

Looking at the Sx component

```
(%i192) meanRho(Sx,rhoIzSxt);
```

(%o192) $$-\frac{-\cos(2\cdot\pi\cdot t2\cdot nuS-2\cdot\pi\cdot t1\cdot nuI+(-\pi\cdot t1-\pi\cdot t2)\cdot J)+\cos(2\cdot\pi\cdot t2\cdot nuS-2\cdot\pi\cdot t1\cdot nuI+(\pi\cdot t1-\pi\cdot t2)\cdot J)+\cos(2\cdot\pi\cdot t2\cdot nuS-2\cdot\pi\cdot t1\cdot nuI+(\pi}{}$$

```
(%i193) trigreduce(%);
```

(%o193) $$-\frac{-\cos(2\cdot\pi\cdot t2\cdot nuS-2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t2\cdot J-\pi\cdot t1\cdot J)+\cos(2\cdot\pi\cdot t2\cdot nuS-2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t2\cdot J+\pi\cdot t1\cdot J)+\cos(2\cdot\pi\cdot t2\cdot nuS-2\cdot\pi\cdot t1\cdot nuI+\pi}{}$$

```
(%i194) trigexpand(%);
```

(%o194) $$-\sin(\pi\cdot t1\cdot J)\cdot\sin(\pi\cdot t2\cdot J)\cdot\sin(2\cdot\pi\cdot t1\cdot nuI)\cdot\sin(2\cdot\pi\cdot t2\cdot nuS)$$

```
(%i195) temp3:%;
```

(%o195) $$-\sin(\pi\cdot t1\cdot J)\cdot\sin(\pi\cdot t2\cdot J)\cdot\sin(2\cdot\pi\cdot t1\cdot nuI)\cdot\sin(2\cdot\pi\cdot t2\cdot nuS)$$

Substitute for the t2 terms, as above

```
(%i196) subst([sin(%pi*t2*J)=a,sin(2*%pi*t2*nuS)=b],temp3);
```

(%o196) $$-a\cdot b\cdot\sin(\pi\cdot t1\cdot J)\cdot\sin(2\cdot\pi\cdot t1\cdot nuI)$$

```
(%i197) trigreduce(%);
```

(%o197) $$\frac{a\cdot b\cdot\cos(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J)}{2}-\frac{a\cdot b\cdot\cos(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)}{2}$$

```
(%i198) temp4:%;
```

(%o198) $$\frac{a\cdot b\cdot\cos(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J)}{2}-\frac{a\cdot b\cdot\cos(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)}{2}$$

```
(%i199) ab:sin(%pi*t2*J)*sin(2*%pi*t2*nuS);
```

(%o199) $$\sin(\pi\cdot t2\cdot J)\cdot\sin(2\cdot\pi\cdot t2\cdot nuS)$$

```
(%i200) ab:trigreduce(ab);
```

(%o200) $$\frac{\cos(2\cdot\pi\cdot t2\cdot nuS-\pi\cdot t2\cdot J)}{2}-\frac{\cos(2\cdot\pi\cdot t2\cdot nuS+\pi\cdot t2\cdot J)}{2}$$

```
(%i201) ratsubst(ab,a*b,temp4);
```

$$(\%o201)\quad -\frac{\cos(2\cdot\pi\cdot t1\cdot nuI-\pi\cdot t1\cdot J)\cdot(\cos(2\cdot\pi\cdot t2\cdot nuS-\pi\cdot t2\cdot J)-\cos(2\cdot\pi\cdot t2\cdot nuS+\pi\cdot t2\cdot J))+\cos(2\cdot\pi\cdot t1\cdot nuI+\pi\cdot t1\cdot J)\cdot(\cos(2\cdot\pi\cdot t2\cdot nuS+\pi\cdot t2\cdot J)}{4}$$

```
(%i202) factor(%);
```

$$(\%o202)\quad -\frac{(\cos(\pi\cdot t1\cdot(2\cdot nuI+J))-\cos(\pi\cdot t1\cdot(2\cdot nuI-J)))\cdot(\cos(\pi\cdot t2\cdot(2\cdot nuS+J))-\cos(\pi\cdot t2\cdot(2\cdot nuS-J)))}{4}$$

This represents a cross peak, with the t1 term determined by nuI and the t2 term determined by nuS.

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