# Maxima workbook for Principles of NMR Spectroscopy Chapter 14: NMR spectroscopy of a weakly-coupled spin pair

## 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 Chapters 11-13

Please send comments, including bug reports, to this address:
David P. Goldenberg
Department of Biology
University of Utah
257 South 1400 East
Salt Lake City, UT 84112-0840
goldenberg@biology.utah.edu

This chapter covers the effects of pulses and evolution periods on a weakly coupled spin pair.
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 14.1 Time evolution of wavefunction

Page 393.

Under the weak-coupling limit, the eigenfunctions of the Hamilton are the eigenfunctions of the Iz and Sz operators

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

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

```
(%i4) k_ab;
```

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

```
(%i5) k_bb;
```

$$(\%o5) \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

```
(%i6) k_bb;
```

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

The general form of the wavefunction is given, in the column vector form representing the ket, as

```
(%i7) k_psi;
```

$$(\%o7) \quad \begin{pmatrix} \mathrm{caa} \\ \mathrm{cab} \\ \mathrm{cba} \\ \mathrm{cbb} \end{pmatrix}$$

caa, cab, cba and cbb are the complex coefficients of the eigenfunctions of the z-operator, k_aa, k_ab, k_ba and k_bb The bra for the general form of the wavefunction is given in row vector form as:

```
(%i8) b_psi;
```

$$(\%o8) \quad \begin{pmatrix} \overline{\mathrm{caa}} & \overline{\mathrm{cab}} & \overline{\mathrm{cba}} & \overline{\mathrm{cbb}} \end{pmatrix}$$

In the vector representation, the time evolution of the wavefunction is expressed as a matrix, defined here as a function of t, nuI,nuS and J

```
(%i9) Uh(t,nuI,nuS,J);
```

$$(\%o9) \quad \begin{pmatrix} e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)} & 0 & 0 & 0 \\ 0 & e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)} & 0 & 0 \\ 0 & 0 & e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)} & 0 \\ 0 & 0 & 0 & e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)} \end{pmatrix}$$

Starting with k_psi, the wavefunction at time, t, is calculated as the product of Uh and k_psi:

```
(%i10) Uh(t,nuI,nuS,J).k_psi;
```

$$(\%o10) \quad \begin{pmatrix} \mathrm{caa}\cdot e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)} \\ \mathrm{cab}\cdot e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)} \\ \mathrm{cba}\cdot e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)} \\ \mathrm{cbb}\cdot e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)} \end{pmatrix}$$

This expression is incorporated into the function psiTime, which requires two arguments, the starting ket and the final time value, t.

```
(%i11) psiTime(k_psi,t);
```

$$(\%o11)\quad \begin{pmatrix} caa\cdot e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+nuI+nuS\right)} \\ cab\cdot e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}+nuI-nuS\right)} \\ cba\cdot e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}-nuI+nuS\right)} \\ cbb\cdot e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}-nuI-nuS\right)} \end{pmatrix}$$

# 3 14.2 Pulses

Pulses are represented as matrix multiplications. There are four matrices, for rotations of the I- and S-spins about the x'- and y'- axes.

```
(%i12) RIx(a);
```

$$(\%o12)\quad \begin{pmatrix} \cos\left(\frac{a}{2}\right) & 0 & -i\cdot\sin\left(\frac{a}{2}\right) & 0 \\ 0 & \cos\left(\frac{a}{2}\right) & 0 & -i\cdot\sin\left(\frac{a}{2}\right) \\ -i\cdot\sin\left(\frac{a}{2}\right) & 0 & \cos\left(\frac{a}{2}\right) & 0 \\ 0 & -i\cdot\sin\left(\frac{a}{2}\right) & 0 & \cos\left(\frac{a}{2}\right) \end{pmatrix}$$

```
(%i13) RIy(a);
```

$$(\%o13)\quad \begin{pmatrix} \cos\left(\frac{a}{2}\right) & 0 & -\sin\left(\frac{a}{2}\right) & 0 \\ 0 & \cos\left(\frac{a}{2}\right) & 0 & -\sin\left(\frac{a}{2}\right) \\ \sin\left(\frac{a}{2}\right) & 0 & \cos\left(\frac{a}{2}\right) & 0 \\ 0 & \sin\left(\frac{a}{2}\right) & 0 & \cos\left(\frac{a}{2}\right) \end{pmatrix}$$

```
(%i14) RSx(a);
```

$$(\%o14)\quad \begin{pmatrix} \cos\left(\frac{a}{2}\right) & -i\cdot\sin\left(\frac{a}{2}\right) & 0 & 0 \\ -i\cdot\sin\left(\frac{a}{2}\right) & \cos\left(\frac{a}{2}\right) & 0 & 0 \\ 0 & 0 & \cos\left(\frac{a}{2}\right) & -i\cdot\sin\left(\frac{a}{2}\right) \\ 0 & 0 & -i\cdot\sin\left(\frac{a}{2}\right) & \cos\left(\frac{a}{2}\right) \end{pmatrix}$$

```
(%i15) RSy(a);
```

$$(\%o15)\quad \begin{pmatrix} \cos\left(\frac{a}{2}\right) & -\sin\left(\frac{a}{2}\right) & 0 & 0 \\ \sin\left(\frac{a}{2}\right) & \cos\left(\frac{a}{2}\right) & 0 & 0 \\ 0 & 0 & \cos\left(\frac{a}{2}\right) & -\sin\left(\frac{a}{2}\right) \\ 0 & 0 & \sin\left(\frac{a}{2}\right) & \cos\left(\frac{a}{2}\right) \end{pmatrix}$$

For the rotation if the I-spin about the y'-axis, the multiplication is

```
(%i16) RIy(a).k_psi;
```

$$(\%o16)\quad \begin{pmatrix} \cos\left(\frac{a}{2}\right)\cdot \mathrm{caa}-\sin\left(\frac{a}{2}\right)\cdot \mathrm{cba} \\ \cos\left(\frac{a}{2}\right)\cdot \mathrm{cab}-\sin\left(\frac{a}{2}\right)\cdot \mathrm{cbb} \\ \cos\left(\frac{a}{2}\right)\cdot \mathrm{cba}+\sin\left(\frac{a}{2}\right)\cdot \mathrm{caa} \\ \cos\left(\frac{a}{2}\right)\cdot \mathrm{cbb}+\sin\left(\frac{a}{2}\right)\cdot \mathrm{cab} \end{pmatrix}$$

The two-spin library incorporates this multiplication into a function

```
(%i17) psiPulseYI(k_psi,a);
```

$$(\%o17)\quad \begin{pmatrix} \cos\left(\frac{a}{2}\right)\cdot \mathrm{caa}-\sin\left(\frac{a}{2}\right)\cdot \mathrm{cba} \\ \cos\left(\frac{a}{2}\right)\cdot \mathrm{cab}-\sin\left(\frac{a}{2}\right)\cdot \mathrm{cbb} \\ \cos\left(\frac{a}{2}\right)\cdot \mathrm{cba}+\sin\left(\frac{a}{2}\right)\cdot \mathrm{caa} \\ \cos\left(\frac{a}{2}\right)\cdot \mathrm{cbb}+\sin\left(\frac{a}{2}\right)\cdot \mathrm{cab} \end{pmatrix}$$

There are also specific functions for pi/2- and pi-pulses

```
(%i18) psiPi2Y(k_psi);
```

$$(\%o18)\quad \begin{pmatrix} \frac{\frac{caa}{\sqrt{2}}-\frac{cab}{\sqrt{2}}}{\sqrt{2}}-\frac{\frac{cba}{\sqrt{2}}-\frac{cbb}{\sqrt{2}}}{\sqrt{2}} \\ \frac{\frac{caa}{\sqrt{2}}+\frac{cab}{\sqrt{2}}}{\sqrt{2}}-\frac{\frac{cba}{\sqrt{2}}+\frac{cbb}{\sqrt{2}}}{\sqrt{2}} \\ \frac{\frac{cba}{\sqrt{2}}-\frac{cbb}{\sqrt{2}}}{\sqrt{2}}+\frac{\frac{caa}{\sqrt{2}}-\frac{cab}{\sqrt{2}}}{\sqrt{2}} \\ \frac{\frac{cba}{\sqrt{2}}+\frac{cbb}{\sqrt{2}}}{\sqrt{2}}+\frac{\frac{caa}{\sqrt{2}}+\frac{cab}{\sqrt{2}}}{\sqrt{2}} \end{pmatrix}$$

```
(%i19) factor(%);
```

$$(\%o19)\quad \begin{pmatrix} \frac{caa-cab-cba+cbb}{2} \\ -\frac{-caa-cab+cba+cbb}{2} \\ -\frac{-caa+cab-cba+cbb}{2} \\ \frac{caa+cab+cba+cbb}{2} \end{pmatrix}$$

```
(%i20) psiPiY(k_psi);
```

$$(\%o20)\quad \begin{pmatrix} cbb \\ -cba \\ -cab \\ caa \end{pmatrix}$$

The 2spinLib.mac library contains corresponding functions for I-pulses along the x'-axis, and S-pulses along the x'- and y'-axes.

Pulse examples

Starting with the k_aa state. The average magnetization components can all be calculated using the allMagPsi command.

```
(%i21) allMagPsi(k_aa);
```

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

(%o21)

Applying a pi/2-pulse along the y'-axis to the I-spin:

```
(%i22) psiPi2YI(k_aa);
```

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

```
(%i23) allMagPsi(%);
```

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

(%o23)

Fig. 14.2.

Applying a pi/2 pulse along the y'-axis to the S-spin, after a pi/2 y-pulse to the I spin

```
(%i24) psiPi2YS(psiPi2YI(k_aa));
```

$$(\%o24)\quad \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

```
(%i25) allMagPsi(%);
```

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

(%o25)

Fig. 14.3

Applying a pi/2-pulse along the y '-axis to the I-spin of the result of the previous S-pulse

Another function in the library can be used to calculate a non-specific pi/2 y-pulse.

```
(%i26) psiPi2Y(k_aa);
```

$$(\%o26)\quad \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

A pi/2 x,I-pulse

```
(%i27) psiPi2XI(k_aa);
```

$$(\%o27) \quad \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ -\frac{i}{\sqrt{2}} \\ 0 \end{pmatrix}$$

```
(%i28) allMagPsi(psiPi2XI(k_aa));
```

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

(%o28)

Fig. 14.4

# 4 14.3 Time evolution following a selective pulse

Page 397

Apply a pi/2 y,I pulse to k_aa and call the result k_aa1

```
(%i29) k_aa1:psiPi2YI(k_aa);
```

$$(\%o29) \quad \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

The time evolution of the wavefunction is then given by:

```
(%i30) psiTime(k_aa1,t);
```

$$(\%o30) \quad \begin{pmatrix} \frac{e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}}{\sqrt{2}} \\ 0 \\ \frac{e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}}{\sqrt{2}} \\ 0 \end{pmatrix}$$

The time evolution of the magnetization components

```
(%i31) allMagPsi(psiTime(k_aa1,t));
```

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

(%o31)

Fig. 14.5

The same manipulations, starting with k_ab

```
(%i32) k_ab1:psiPi2YI(k_ab);
```

$$(\%o32) \quad \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
(%i33) allMagPsi(k_ab1);
```

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

(%o33)

Fig. 14.6

```
(%i34) allMagPsi(psiTime(k_ab1,t));
```

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

(%o34)

The same manipulations, starting with k_ba

```
(%i35) k_ba1:psiPi2YI(k_ba);
```

$$(\%o35) \quad \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

```
(%i36) allMagPsi(k_ba1);
```

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

(%o36)

Fig. 14.7

```
(%i37) allMagPsi(psiTime(k_ba1,t));
```

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

(%o37)

The same manipulations starting with k_bb

```
(%i38) k_bb1:psiPi2YI(k_bb);
```

$$(\%o38)\quad \begin{pmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
(%i39) allMagPsi(k_bb1);
```

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

(%o39)

Fig. 14.8

```
(%i40) allMagPsi(psiTime(k_bb1,t));
```

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

(%o40)

# *5 14.4 Time evolution following a pi/2 pulse to both spins*

Page 400

We will call the wavefunctions generated by a non-selective pi/2 y-pulse k_aa2, k_ab2, k_ba2, k_bb2

```
(%i41) k_aa2:psiPi2Y(k_aa);
```

$$(\%o41)\quad \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

```
(%i42) allMagPsi(k_aa2);
```

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

(%o42)

```
(%i43) psiTime(k_aa2,t);
```

$$(\%o43) \quad \begin{pmatrix} \frac{e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}}{2} \\ \frac{e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}}{2} \\ \frac{e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}}{2} \\ \frac{e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}}{2} \end{pmatrix}$$

```
(%i44) allMagPsi(psiTime(k_aa2,t));
```

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

(%o44)

Figs. 14.9 and 14.10

# 6 14.5 Some more exotic examples

To generate a wavefunction with the I-magnetization aligned with the x'-axis and the S-magnetization half-way between the z- and x'axis, we apply two pulses to a starting k_aa state
First is a pi/4 y,S pulse

```
(%i45) k_aa3:psiPulseYS(k_aa,%p/4);
```

$$(\%o45) \quad \begin{pmatrix} \cos\left(\frac{\%p}{8}\right) \\ \sin\left(\frac{\%p}{8}\right) \\ 0 \\ 0 \end{pmatrix}$$

Then a pi/2 y,I pulse

```
(%i46) k_aa4:psiPi2YI(k_aa3);
```

$$(\%o46) \quad \begin{pmatrix} \frac{\cos\left(\frac{\%p}{8}\right)}{\sqrt{2}} \\ \frac{\sin\left(\frac{\%p}{8}\right)}{\sqrt{2}} \\ \frac{\cos\left(\frac{\%p}{8}\right)}{\sqrt{2}} \\ \frac{\sin\left(\frac{\%p}{8}\right)}{\sqrt{2}} \end{pmatrix}$$

```
(%i47) allMagPsi(k_aa4);
```

$$< Ix >= \frac{1}{2} < Iy >= 0 < Iz >= 0 < Sx >= \frac{\sin\left(\frac{\%p}{4}\right)}{2} < Sy >= 0 < Sz >= \frac{\cos\left(\frac{\%p}{4}\right)}{2} \quad (\%o47)$$

Fig. 14.11

The evolution of the resulting wavefunction

```
(%i48) psiTime(k_aa4,t);
```

$$(\%o48) \quad \begin{pmatrix} \frac{\cos\left(\frac{\%p}{8}\right) \cdot e^{-i \cdot \pi \cdot t \cdot \left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}}{\sqrt{2}} \\ \frac{\sin\left(\frac{\%p}{8}\right) \cdot e^{-i \cdot \pi \cdot t \cdot \left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}}{\sqrt{2}} \\ \frac{\cos\left(\frac{\%p}{8}\right) \cdot e^{-i \cdot \pi \cdot t \cdot \left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}}{\sqrt{2}} \\ \frac{\sin\left(\frac{\%p}{8}\right) \cdot e^{-i \cdot \pi \cdot t \cdot \left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}}{\sqrt{2}} \end{pmatrix}$$

```
(%i49) allMagPsi(psiTime(k_aa4,t));
```

$$< Ix >= \frac{2 \cdot \cos(2 \cdot \pi \cdot t \cdot \mathrm{nuI} - \pi \cdot t \cdot J) + 2 \cdot \cos(2 \cdot \pi \cdot t \cdot \mathrm{nuI} + \pi \cdot t \cdot J) - \cos\left(\frac{-\%p - 4 \cdot \pi \cdot t \cdot J + 8 \cdot \pi \cdot t \cdot \mathrm{nuI}}{4}\right) - \cos\left(\frac{\%p - 4 \cdot \pi \cdot t \cdot J + 8 \cdot \pi \cdot t \cdot \mathrm{nuI}}{4}\right) + \cos\left(\frac{-\%p + 4 \cdot \pi \cdot t \cdot J + 8 \cdot \pi \cdot t \cdot \mathrm{nuI}}{4}\right) + \mathrm{co}}{8} \quad (\%o49)$$

Figs. 14.12 and 14.13

This can be reconciled with the result shown in the text by showing that cos(pi/8)^2 = (sqrt(2)+1)/(2*sqrt(2)) and that sin(pi/8)^2 = (sqrt(2)-1)/(2*sqrt(2))

```
(%i50) cos(%pi/8)^2;
```

$$(\%o50) \quad \cos\left(\frac{\pi}{8}\right)^2$$

```
(%i51) trigrat(%);
```

$$(\%o51) \quad \frac{2+\sqrt{2}}{4}$$

```
(%i52) sin(%pi/8)^2;
```

$$(\%o52) \quad \sin\left(\frac{\pi}{8}\right)^2$$

```
(%i53) trigrat(%);
```

$$(\%o53)\quad -\frac{\sqrt{2}-2}{4}$$

The more general case:
Rotation of the S-spin by a rad from the z-axis, followed by rotation of the I-spin to the x'-axis

```
(%i54) k_aa5:psiPi2YI(psiPulseYS(k_aa,a));
```

$$(\%o54)\quad \begin{pmatrix} \frac{\cos\left(\frac{a}{2}\right)}{\sqrt{2}} \\ \frac{\sin\left(\frac{a}{2}\right)}{\sqrt{2}} \\ \frac{\cos\left(\frac{a}{2}\right)}{\sqrt{2}} \\ \frac{\sin\left(\frac{a}{2}\right)}{\sqrt{2}} \end{pmatrix}$$

```
(%i55) allMagPsi(k_aa5);
```

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

(%o55)

Time evolution of wavefunction

```
(%i56) psiTime(k_aa5,t);
```

$$(\%o56)\quad \begin{pmatrix} \frac{\cos\left(\frac{a}{2}\right)\cdot e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}}{\sqrt{2}} \\ \frac{\sin\left(\frac{a}{2}\right)\cdot e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}}{\sqrt{2}} \\ \frac{\cos\left(\frac{a}{2}\right)\cdot e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}}{\sqrt{2}} \\ \frac{\sin\left(\frac{a}{2}\right)\cdot e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}}{\sqrt{2}} \end{pmatrix}$$

Time evolution of <Ix>

```
(%i57) meanPsi(Ix,psiTime(k_aa5,t));
```

$$(\%o57)\quad \frac{2\cdot\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J)-\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J-a)-\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J+a)+2\cdot\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J)+\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J-a)}{8}$$

In this case, the simplification rules within the meanPsi function lead to an "over simplification", combining the term related to the initial rotation angle, a, with the time evolution terms. To obtain the result shown in the text, we first do the calculation explicitly, without any simplification:

```
(%i58) k_aa5t:psiTime(k_aa5,t);
```

$$(\%o58)\quad \begin{pmatrix} \frac{\cos\left(\frac{a}{2}\right)\cdot e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}}{\sqrt{2}} \\ \frac{\sin\left(\frac{a}{2}\right)\cdot e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}+\mathrm{nuI}-\mathrm{nuS}\right)}}{\sqrt{2}} \\ \frac{\cos\left(\frac{a}{2}\right)\cdot e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}}{\sqrt{2}} \\ \frac{\sin\left(\frac{a}{2}\right)\cdot e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{nuS}\right)}}{\sqrt{2}} \end{pmatrix}$$

```
(%i59) bra(k_aa5t).Ix.k_aa5t;
```

$$(\%o59)\quad \frac{\cos\left(\frac{a}{2}\right)^2\cdot e^{i\cdot\pi\cdot t\cdot\left(\mathrm{nuS}+\mathrm{nuI}+\frac{J}{2}\right)-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}}{4}+\frac{\cos\left(\frac{a}{2}\right)^2\cdot e^{i\cdot\pi\cdot t\cdot\left(\mathrm{nuS}-\mathrm{nuI}-\frac{J}{2}\right)-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}}{4}+\frac{\sin\left(\frac{a}{2}\right)^2\cdot e^{i\cdot\pi\cdot t\cdot\left(-\mathrm{nuS}+\mathrm{nuI}-\frac{J}{2}\right)-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}-\mathrm{nuI}-\mathrm{n}\right.}}{4}$$

The complex exponential terms can then be converted to trigonometric forms, using the Maxima demoivre function, which is based on the formula of Abraham de Moivre: (cos x + i  sin x)^n = cos (nx) + i sin (nx), where x is a real number and n is an integer.

```
(%i60) demoivre(%);
```

$$(\%o60)\quad \frac{\cos\left(\frac{a}{2}\right)^2\cdot\left(\cos\left(\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)-\pi\cdot t\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)\right)+i\cdot\sin\left(\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)-\pi\cdot t\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)\right)\right)}{4}+\frac{\cos\left(\frac{a}{2}\right)^2\cdot\left(\cos\left(\pi\cdot t\cdot\left(\frac{J}{2}\right.\right.\right.}{}$$

Algebraic simplification gives:

```
(%i61) ratsimp(%);
```

$$(\%o61)\quad \frac{\sin\left(\frac{a}{2}\right)^2\cdot\cos(2\cdot\pi\cdot t\cdot\mathrm{nuI}-\pi\cdot t\cdot J)+\cos\left(\frac{a}{2}\right)^2\cdot\cos(2\cdot\pi\cdot t\cdot\mathrm{nuI}+\pi\cdot t\cdot J)}{2}$$

This result can then be converted to the version shown in the text with these trigonometric identities:

```
(%i62) cos(a/2)^2;
```

$$(\%o62)\quad \cos\left(\frac{a}{2}\right)^2$$

```
(%i63) trigreduce(%);
```

$$(\%o63)\quad \frac{1+\cos(a)}{2}$$

```
(%i64) sin(a/2)^2;
```

$$(\%o64)\quad \sin\left(\frac{a}{2}\right)^2$$

```
(%i65) trigreduce(%);
```

(%o65) $\frac{1-\cos(a)}{2}$

# 7 14.6 Effects of pulses and evolution on spin-spin correlations

Page 406

Individual correlations are calculated by applying the operators formed as products of the appropriate magnetization operators. For instance, the correlation between the z-magnetization of the I and S spins is calculated from the IzSz product operator

```
(%i66) Iz.Sz;
```

$$(\%o66)\quad \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}$$

This operator is also defined explicitly in the 2spinLib.mac library

```
(%i67) IzSz;
```

$$(\%o67)\quad \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}$$

To calculate the Iz-Sz correlation for the Ialpha alpha> wavefunction

```
(%i68) b_aa.IzSz.k_aa;
```

$$(\%o68)\quad \frac{1}{4}$$

The 2spinLib.mac library includes a function to calculate all nine of the possible correlations from a wavefunction

```
(%i69) allCorrPsi(k_aa);
```

$$< IxSx >= 0 < IxSy >= 0 < IxSz >= 0 < IySx >= 0 < IySy >= 0 < IySz >= 0 < IzSx >= 0 < IzSy >= 0 < IzSz >= \frac{1}{4}$$

(%o69)

Applying a pi/2 y,I pulse to Ialpha alpha>

```
(%i70) psiPi2YI(k_aa);
```

$$(\%o70)\quad \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

All of the magnetization components for the resulting wavefunction

```
(%i71) allMagPsi(psiPi2YI(k_aa));
```

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

(%o71)

All of the correlations for the resulting wavefunction

```
(%i72) allCorrPsi(psiPi2YI(k_aa));
```

$$< IxSx >= 0 < IxSy >= 0 < IxSz >= \frac{1}{4} < IySx >= 0 < IySy >= 0 < IySz >= 0 < IzSx >= 0 < IzSy >= 0 < IzSz >= 0$$

(%o72)

## 7.1 14.6.1 Correlation vector diagrams

The wavefunction Ipsi1>, from Chapter 13

```
(%i73) k_psi1:(k_ab+k_ba)/sqrt(2);
```

$$(\%o73)\quad \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

The average magnetization components when measured for k_psi1

```
(%i74) allMagPsi(k_psi1);
```

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

(%o74)

The correlations for k_psi1

```
(%i75) allCorrPsi(k_psi1);
```

$$< IxSx >= \frac{1}{4} < IxSy >= 0 < IxSz >= 0 < IySx >= 0 < IySy >= \frac{1}{4} < IySz >= 0 < IzSx >= 0 < IzSy >= 0 < IzSz >= -\frac{1}{4}$$

(%o75)

Fig. 14.16

Applying a pi/2 y,I pulse to k_psi1

```
(%i76) allMagPsi(psiPi2YI(k_psi1));
```

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

(%o76)

There are still no observable magnetization components.

The correlations after the pulse

```
(%i77) allCorrPsi(psiPi2YI(k_psi1));
```

$$< IxSx >= \ 0 < IxSy >= \ 0 < IxSz >= \ -\frac{1}{4} < IySx >= \ 0 < IySy >= \ \frac{1}{4} < IySz >= \ 0 < IzSx >= \ -\frac{1}{4} < IzSy >= \ 0 < IzSz >= \ 0$$

(%o77)

Fig. 14.17

The IxSx correlation is converted to a negative IzSx correlation The IySy correlation is unaffected The IzSz correlation is converted to a negative IxSz correlation

## 7.2 14.6.2 Time evolution of correlations

Start with the state generated by applying a pi/2 y,I pulse to k_aa. The resulting wavefunction was previously defined as k_aa1

```
(%i78) k_aa1;
```

$$(\%o78) \quad \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

```
(%i79) allMagPsi(k_aa1);
```

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

(%o79)

The wavefunction after allowing the previous wavefunction to evolve for time, t:

```
(%i80) k_aa1t:psiTime(k_aa1,t);
```

$$(\%o80) \quad \begin{pmatrix} \frac{e^{-i\cdot\pi\cdot t\cdot\left(\frac{J}{2}+\mathrm{nuI}+\mathrm{nuS}\right)}}{\sqrt{2}} \\ 0 \\ \frac{e^{-i\cdot\pi\cdot t\cdot\left(-\frac{J}{2}-\mathrm{nuI}+\mathrm{nuS}\right)}}{\sqrt{2}} \\ 0 \end{pmatrix}$$

The average magnetization components after time, t:

```
(%i81) allMagPsi(k_aa1t);
```

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

(%o81)

The average correlations after time, t:

```
(%i82) allCorrPsi(k_aa1t);
```

$$< IxSx >= \; 0 < IxSy >= \; 0 < IxSz >= \; \frac{\cos(2 \cdot \pi \cdot t \cdot \mathrm{nuI} + \pi \cdot t \cdot J)}{4} < IySx >= \; 0 < IySy >= \; 0 < IySz >= \; \frac{\sin(2 \cdot \pi \cdot t \cdot \mathrm{nuI} + \pi \cdot t \cdot J)}{4} < IzSx >= \; 0 < IzSy >= \; 0 < IzSz >= \; 0$$

(%o82)

Fig. 14.18

Evolution of correlations after a non-selective pi/2 y pulse. The wavefunction immediately after the pulse was defined as k_aa2

```
(%i83) k_aa2;
```

$$(\%o83) \quad \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

Magnetization components after the pulse

```
(%i84) allMagPsi(k_aa2);
```

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

(%o84)

Correlations after the pulse

```
(%i85) allCorrPsi(k_aa2);
```

$$< IxSx >= \; \frac{1}{4} < IxSy >= \; 0 < IxSz >= \; 0 < IySx >= \; 0 < IySy >= \; 0 < IySz >= \; 0 < IzSx >= \; 0 < IzSy >= \; 0 < IzSz >= \; 0$$

(%o85)

The time-dependent wavefunction after the pulse

```
(%i86) k_aa2t:psiTime(k_aa2,t);
```

$$(\%o86) \quad \begin{pmatrix} \frac{e^{-i \cdot \pi \cdot t \cdot \left(\frac{J}{2} + \mathrm{nuI} + \mathrm{nuS}\right)}}{2} \\ \frac{e^{-i \cdot \pi \cdot t \cdot \left(-\frac{J}{2} + \mathrm{nuI} - \mathrm{nuS}\right)}}{2} \\ \frac{e^{-i \cdot \pi \cdot t \cdot \left(-\frac{J}{2} - \mathrm{nuI} + \mathrm{nuS}\right)}}{2} \\ \frac{e^{-i \cdot \pi \cdot t \cdot \left(\frac{J}{2} - \mathrm{nuI} - \mathrm{nuS}\right)}}{2} \end{pmatrix}$$

Set nuI and nuS to zero, corresponding to matching the rotating frame frequencies. The time-dependent wavefunction under this assumption will be called k_aa2tNu0

```
(%i87) k_aa2tNu0:subst([nuI=0,nuS=0],k_aa2t);
```

$$(\%o87)\quad \begin{pmatrix} \frac{e^{-\frac{i\cdot\pi\cdot t\cdot J}{2}}}{2} \\ \frac{e^{\frac{i\cdot\pi\cdot t\cdot J}{2}}}{2} \\ \frac{e^{\frac{i\cdot\pi\cdot t\cdot J}{2}}}{2} \\ \frac{e^{-\frac{i\cdot\pi\cdot t\cdot J}{2}}}{2} \end{pmatrix}$$

```
(%i88) allMagPsi(k_aa2tNu0);
```

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

(%o88)

Fig. 14.19

```
(%i89) allCorrPsi(k_aa2tNu0);
```

$$< IxSx >= \frac{1}{4} < IxSy >= 0 < IxSz >= 0 < IySx >= 0 < IySy >= 0 < IySz >= \frac{\sin(\pi\cdot t\cdot J)}{4} < IzSx >= 0 < IzSy >= \frac{\sin(\pi\cdot t\cdot J)}{4} < IzSz >= 0$$

(%o89)

Fig. 14.20

Without constraining nuI=0 and nuS=0

```
(%i90) allMagPsi(k_aa2t);
```

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

(%o90)

```
(%i91) allCorrPsi(k_aa2t);
```

$$< IxSx >= \frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})+\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})}{8} < IxSy >= \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})+\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})}{8} < IxSz >= \frac{c}{}$$

(%o91)

These are in a different trigonometric form than shown in the text, but can be converted using the trigexpand command. IxSx

```
(%i92) meanPsi(IxSx,k_aa2t);
```

$$(\%o92)\quad \frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})+\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})}{8}$$

```
(%i93) trigexpand(%);
```

$$(\%o93)\quad \frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS})}{4}$$

IxSy

```
(%i94) meanPsi(IxSy,k_aa2t);
```

$$\frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})+\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})}{8} \tag{\%o94}$$

```
(%i95) trigexpand(%);
```

$$\frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS})}{4} \tag{\%o95}$$

IySx

```
(%i96) meanPsi(IySx,k_aa2t);
```

$$\frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})}{8} \tag{\%o96}$$

```
(%i97) trigexpand(%);
```

$$\frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS})}{4} \tag{\%o97}$$

IySy

```
(%i98) meanPsi(IySy,k_aa2t);
```

$$-\frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}+2\cdot\pi\cdot t\cdot \mathrm{nuI})-\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS}-2\cdot\pi\cdot t\cdot \mathrm{nuI})}{8} \tag{\%o98}$$

```
(%i99) trigexpand(%);
```

$$\frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI})\cdot\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS})}{4} \tag{\%o99}$$

IySz

```
(%i100) meanPsi(IySz,k_aa2t);
```

$$\frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J)}{8} \tag{\%o100}$$

```
(%i101) trigexpand(%);
```

$$\frac{\sin(\pi\cdot t\cdot J)\cdot\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI})}{4} \tag{\%o101}$$

IzSy

```
(%i102) meanPsi(IzSy,k_aa2t);
```

$$\frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-\pi\cdot t\cdot J)}{8} \tag{\%o102}$$

```
(%i103) trigexpand(%);
```

$$\frac{\sin(\pi\cdot t\cdot J)\cdot\cos(2\cdot\pi\cdot t\cdot \mathrm{nuS})}{4} \tag{\%o103}$$

## 7.3 14.6.3 Multiple quantum coherence and some nomenclature

Page 412

The form of the average correlations shown in Eq. 14.41 are the ones directly produced by the allCorrPsi command.

```
(%i104) allCorrPsi(k_aa2t);
```

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

(%o104)

# 8 14.7 Some demonstration experiments

Page 414

## 8.1 14.7.1 Experiment 1

Start with a selective pi/2 y-pulse to the I spin, starting from the k_aa state.

```
(%i105) k_exp1aa:psiPi2YS(k_aa);
```

$$(\%o105)\quad \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \\ 0 \end{pmatrix}$$

```
(%i106) allMagPsi(k_exp1aa);
```

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

(%o106)

Time evolution of the magnetization components immediately after the pulse, with nuI and nuS set to zero in the rotating frame

```
(%i107) allMagPsi(psiTime(k_exp1aa,t));
```

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

(%o107)

Introducing a delay of tau=1/(2J)

```
(%i108) k_exp1aa2:subst([nuI=0,nuS=0],psiTime(k_exp1aa,1/(2*J)));
```

$$(\%o108)\quad \begin{pmatrix} \frac{\frac{1}{\sqrt{2}} - \frac{i}{\sqrt{2}}}{\sqrt{2}} \\ \frac{\frac{1}{\sqrt{2}} + \frac{i}{\sqrt{2}}}{\sqrt{2}} \\ 0 \\ 0 \end{pmatrix}$$

Magnetization after the delay

```
(%i109) allMagPsi(k_exp1aa2);
```

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

(%o109)

Time evolution of magnetization after the delay

```
(%i110) allMagPsi(psiTime(k_exp1aa2,t));
```

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

(%o110)

Note the phase difference between this result and the one without the tau=1/(2J) delay.

From the initial k_ba state

```
(%i111) k_exp1ba:psiPi2YS(k_ba);
```

$$(\%o111) \begin{pmatrix} 0 \\ 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
(%i112) allMagPsi(k_exp1ba);
```

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

(%o112)

Time evolution of magnetization components immediately after the pulse to k_ba

```
(%i113) allMagPsi(psiTime(k_exp1ba,t));
```

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

(%o113)

Introducing a delay of tau=1/(2J)

```
(%i114) k_exp1ba2:subst([nuI=0,nuS=0],psiTime(k_exp1ba,1/(2*J)));
```

$$(\%o114) \begin{pmatrix} 0 \\ 0 \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{\sqrt{2}} \\ \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{\sqrt{2}} \end{pmatrix}$$

magnetization components after the delay

```
(%i115) allMagPsi(k_exp1ba2);
```

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

(%o115)

Time evolution of magnetization components after the delay

```
(%i116) allMagPsi(psiTime(k_exp1ba2,t));
```

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

(%o116)

These components represent the second S-frequency and are opposite in sign from those that are generated from the k_aa state.

## 8.2 14.7.2 Experiment 2

Page 415

With the delay time, tau, set to zero, this experiment represents a non-selective pi/2 y-pulse, followed by data acquisition. When applied to the k_aa state, the results are:

```
(%i117) k_exp2aa:psiPi2Y(k_aa);
```

$$(\%o117)\quad \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

The time evolution of magnetization after the pulse

```
(%i118) allMagPsi(psiTime(k_exp2aa,t));
```

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

(%o118)

As discussed earlier in the chapter, this represents evolution with two frequencies, separated by J. The other three starting eigenstates will also each give rise to two frequencies, but with different signs of the amplitudes.

With tau=1/(2J), the experiment consists of a pi/2 y,S pulse, the delay period, a pi/2 y,I pulse, and then the data acquisition period. For analyzing the effects on each of the four starting eigenstates, it is useful to define a function to carryout all of the manipulations of a given starting state. The function can be defined by nesting the functions for each of the individual steps. The values of nuI and nuS are set to zero in the rotating frame.

```
(%i119) psiExp2(k):=psiPi2YI(subst([nuI=0,nuS=0],psiTime(psiPi2YS(k),1/(2*J))));
```

$$(\%o119)\quad \mathrm{psiExp2}(k):=\mathrm{psiPi2YI}\left(\mathrm{subst}\left([\mathrm{nuI}=0,\mathrm{nuS}=0],\mathrm{psiTime}\left(\mathrm{psiPi2YS}(k),\frac{1}{2\cdot J}\right)\right)\right)$$

Starting with k_aa

```
(%i120) k_exp2aa2:psiExp2(k_aa);
```

$$(\%o120)\quad \begin{pmatrix} \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2} \end{pmatrix}$$

```
(%i121) allMagPsi(k_exp2aa2);
```

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

(%o121)

Fig. 14.23

```
(%i122) allMagPsi(psiTime(k_exp2aa2,t));
```

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

(%o122)

Starting with k_ab

```
(%i123) k_exp2ab2:psiExp2(k_ab);
```

$$(\%o123)\quad \begin{pmatrix} -\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2} \\ -\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2} \end{pmatrix}$$

```
(%i124) allMagPsi(k_exp2ab2);
```

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

(%o124)

Fig. 14.24

```
(%i125) allMagPsi(psiTime(k_exp2ab2,t));
```

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

(%o125)

Starting with k_ba

```
(%i126) k_exp2ba2:psiExp2(k_ba);
```

$$(\%o126)\quad \begin{pmatrix} -\frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2} \\ -\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2} \end{pmatrix}$$

```
(%i127) allMagPsi(k_exp2ba2);
```

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

(%o127)

Fig. 14.24

```
(%i128) allMagPsi(psiTime(k_exp2ba2,t));
```

$$< Ix >= -\frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J)+\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J)}{4} < Iy >= -\frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J)+\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J)}{4} < Iz >= 0 < Sx >= \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nu}}{}$$

(%o128)

Starting from k_bb

```
(%i129) k_exp2bb2:psiExp2(k_bb);
```

$$(\%o129) \quad \begin{pmatrix} \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2} \\ -\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2} \\ -\frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2} \end{pmatrix}$$

```
(%i130) allMagPsi(k_exp2bb2);
```

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

(%o130)

Fig. 14.24

```
(%i131) allMagPsi(psiTime(k_exp2bb2,t));
```

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

(%o131)

The relative populations starting in the k_aa, k_ab, k_ba and k_bb states are given in terms of the DeltaI and DeltaS equilibrium population differences as:

```
(%i132) faa:(1+ deltaPI+deltaPS)/4;
```

$$(\%o132) \quad \frac{1+\mathrm{deltaPI}+\mathrm{deltaPS}}{4}$$

```
(%i133) fab:(1+deltaPI-deltaPS)/4;
```

$$(\%o133) \quad \frac{1+\mathrm{deltaPI}-\mathrm{deltaPS}}{4}$$

```
(%i134) fba:(1-deltaPI+deltaPS)/4;
```

$$(\%o134) \quad \frac{1-\mathrm{deltaPI}+\mathrm{deltaPS}}{4}$$

```
(%i135) fbb:(1-deltaPI-deltaPS)/4;
```

$$(\%o135) \quad \frac{1-\mathrm{deltaPI}-\mathrm{deltaPS}}{4}$$

Check to make sure that the sum of the fractional populations is 1

```
(%i136) faa+fab+fba+fbb;
```

$$(\%o136) \quad \frac{1+\mathrm{deltaPI}+\mathrm{deltaPS}}{4}+\frac{1-\mathrm{deltaPI}+\mathrm{deltaPS}}{4}+\frac{1+\mathrm{deltaPI}-\mathrm{deltaPS}}{4}+\frac{1-\mathrm{deltaPI}-\mathrm{deltaPS}}{4}$$

```
(%i137) ratsimp(%);
```

$$(\%o137) \quad 1$$

From the earlier calculations, the initial Sy magnetization components from the wavefunctions that begin in the four eigenstates are:
from k_aa: 1/2 from k_ab: -1/2 from k_ba: -1/2 from k_bb: 1/2
The net Sy magnetization after the second pulse is then:

```
(%i138) faa*(1/2)+fab*(-1/2) + fba*(-1/2) +fbb*(1/2);
```

$$(\%o138)\quad \frac{1+\mathrm{deltaPI}+\mathrm{deltaPS}}{8}-\frac{1-\mathrm{deltaPI}+\mathrm{deltaPS}}{8}-\frac{1+\mathrm{deltaPI}-\mathrm{deltaPS}}{8}+\frac{1-\mathrm{deltaPI}-\mathrm{deltaPS}}{8}$$

```
(%i139) ratsimp(%);
```

$$(\%o139)\quad 0$$

## 8.3 14.7.3 Experiment 3

Page 418

Starting with k_aa, with the delay time, tau, equal to 0. This corresponds to a nonselective pi/2 y pulse, followed immediately by a selective pulse to the I spin.

```
(%i140) k_exp3aa:psiPi2YI(psiPi2Y(k_aa));
```

$$(\%o140)\quad \begin{pmatrix} 0 \\ 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
(%i141) allMagPsi(k_exp3aa);
```

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

(%o141)

Time evolution of magnetization immediately after the pulses.

```
(%i142) allMagPsi(psiTime(k_exp3aa,t));
```

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

(%o142)

Fig. 14.25

The other frequency will be produced by the excess of k_ba over k_bb at equilibrium.

The effects on the population starting from k_aa, with the delay time set to tau=1/(2J).
After the initial pulse and the delay period:

```
(%i143) k_exp3aa2:subst([nuI=0,nuS=0],psiTime(psiPi2Y(k_aa),1/(2*J)));
```

$$(\%o143)\quad \begin{pmatrix} \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2} \\ \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2} \end{pmatrix}$$

```
(%i144) allMagPsi(k_exp3aa2);
```

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

(%o144)

There are no observable magnetization components at this point, but there are correlations:

```
(%i145) allCorrPsi(k_exp3aa2);
```

$$< IxSx >= \ \frac{1}{4} < IxSy >= \ 0 < IxSz >= \ 0 < IySx >= \ 0 < IySy >= \ 0 < IySz >= \ \frac{1}{4} < IzSx >= \ 0 < IzSy >= \ \frac{1}{4} < IzSz >= \ 0$$

(%o145)

Figs. 14.26 and 14.28

The second pulse, pi/2 y applied only to the I-spin

```
(%i146) k_exp3aa3:psiPi2YI(k_exp3aa2);
```

$$(\%o146)\quad \begin{pmatrix} \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}-\frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}-\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}+\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}+\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \end{pmatrix}$$

```
(%i147) allMagPsi(k_exp3aa3);
```

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

(%o147)

There are still no magnetization components, but the correlations have been altered:

```
(%i148) allCorrPsi(k_exp3aa3);
```

$$< IxSx >= 0 < IxSy >= \frac{1}{4} < IxSz >= 0 < IySx >= 0 < IySy >= 0 < IySz >= \frac{1}{4} < IzSx >= -\frac{1}{4} < IzSy >= 0 < IzSz >= 0$$

(%o148)

Figs. 14.27 and 14.29

The time evolution after the second pulse

```
(%i149) allMagPsi(psiTime(k_exp3aa3,t));
```

$$< Ix >= -\frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J)}{4} < Iy >= \frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J)-\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J)}{4} < Iz >= 0 < Sx >= -\cos(2\cdot\pi\cdot t\cdot \mathrm{nu}$$

(%o149)

To handle the other three starting states, it is convenient, again to define a function. This time, we will include in the definition a variable for the time delay, so that the results with or without the results can be calculated easily.

```
(%i150) psiExp3(k,tau):=psiPi2YI(subst([nuI=0,nuS=0],psiTime(psiPi2Y(k),tau)));
```

(%o150) $\mathrm{psiExp3}(k,\tau):=\mathrm{psiPi2YI}(\mathrm{subst}([\mathrm{nuI}=0,\mathrm{nuS}=0],\mathrm{psiTime}(\mathrm{psiPi2Y}(k),\tau)))$

Check this by recalculating the results for k_aa, with tau=0 and tau=1/(2J)

```
(%i151) psiExp3(k_aa,0);
```

$$(\%o151)\quad \begin{pmatrix} 0 \\ 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
(%i152) allMagPsi(%);
```

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

(%o152)

```
(%i153) psiExp3(k_aa,1/(2*J));
```

$$(\%o153) \quad \begin{pmatrix} \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}-\frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}-\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}+\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}+\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \end{pmatrix}$$

```
(%i154) allMagPsi(%);
```

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

(%o154)

```
(%i155) allCorrPsi(psiExp3(k_aa,1/(2*J)));
```

$$< IxSx >= \ 0 < IxSy >= \ \frac{1}{4} < IxSz >= \ 0 < IySx >= \ 0 < IySy >= \ 0 < IySz >= \ \frac{1}{4} < IzSx >= \ -\frac{1}{4} < IzSy >= \ 0 < IzSz >= \ 0$$

(%o155)

```
(%i156) allMagPsi(psiTime(psiExp3(k_aa,1/(2*J)),t));
```

$$< Ix >= \ -\frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J)}{4} < Iy >= \ \frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J)-\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J)}{4} < Iz >= \ 0 < Sx >= \ -\frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nu}}{}$$

(%o156)

Starting with k_ab

```
(%i157) psiExp3(k_ab,1/(2*J));
```

$$(\%o157)\quad \begin{pmatrix} \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} - \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} - \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ -\frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} - \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} + \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \end{pmatrix}$$

```
(%i158) allMagPsi(psiTime(%,t));
```

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

(%o158)

Starting with k_ba

```
(%i159) psiExp3(k_ba,1/(2*J));
```

$$(\%o159)\quad \begin{pmatrix} -\frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} - \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ -\frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} - \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} - \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} - \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \end{pmatrix}$$

```
(%i160) allMagPsi(psiTime(%,t));
```

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

(%o160)

Starting with k_bb

```
(%i161) psiExp3(k_bb,1/(2*J));
```

$$(\%o161)\quad \begin{pmatrix} \frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}+\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ -\frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}-\frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}-\frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \\ \frac{\frac{1}{\sqrt{2}}-\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}}-\frac{\frac{1}{\sqrt{2}}+\frac{i}{\sqrt{2}}}{2^{\frac{3}{2}}} \end{pmatrix}$$

```
(%i162) allMagPsi(psiTime(%,t));
```

$$< Ix >= \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J)}{4} < Iy >= -\frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}+\pi\cdot t\cdot J)-\cos(2\cdot\pi\cdot t\cdot \mathrm{nuI}-\pi\cdot t\cdot J)}{4} < Iz >= 0 < Sx >= -\frac{\cos(2\cdot\pi\cdot t\cdot \mathrm{nu}}{}$$

(%o162)

To add up contributions from all four starting states, assign the expressions for the time-dependent Sy components to some variables

```
(%i163) Sy_aa:-(sin(2*%pi*t*nuS+%pi*t*J)-sin(2*%pi*t*nuS-%pi*t*J))/4;
```

$$(\%o163)\quad \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+\pi\cdot t\cdot J)}{4}$$

```
(%i164) Sy_ab:(sin(2*%pi*t*nuS+%pi*t*J)-sin(2*%pi*t*nuS-%pi*t*J))/4;
```

$$(\%o164)\quad \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-\pi\cdot t\cdot J)}{4}$$

```
(%i165) Sy_ba:(sin(2*%pi*t*nuS+%pi*t*J)-sin(2*%pi*t*nuS-%pi*t*J))/4;
```

$$(\%o165)\quad \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-\pi\cdot t\cdot J)}{4}$$

```
(%i166) Sy_bb:-(sin(2*%pi*t*nuS+%pi*t*J)-sin(2*%pi*t*nuS-%pi*t*J))/4;
```

$$(\%o166)\quad \frac{\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+\pi\cdot t\cdot J)}{4}$$

These components are weighted by the fractions of the populations corresponding to each initial state

```
(%i167) faa*Sy_aa + fab*Sy_ab + fba*Sy_ba + fbb*Sy_bb;
```

$$(\%o167)\quad \frac{(1-\mathrm{deltaPI}+\mathrm{deltaPS})\cdot(\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-\pi\cdot t\cdot J))}{16}+\frac{(1+\mathrm{deltaPI}-\mathrm{deltaPS})\cdot(\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}+\pi\cdot t\cdot J)-\sin(2\cdot\pi\cdot t\cdot \mathrm{nuS}-\pi\cdot}{16}$$

```
(%i168) ratsimp(%);
```

$$(\%o168)\quad 0$$

The net magnetization components cancel out.

---

Created with wxMaxima.