Using Maple, a General Mathematical Analysis Tool, for NMR Analyses: Product Operators in Maple

The product operators that we have introduced, and transformations that they undergo in the presence of scalar coupling, chemical shift offsets and rf pulses, represent an algebra that can be coded and applied using computers in the environment of symbolic problem solver applications such as Maple and Mathematica. In 1993 Peter Guntert *et al.* produced POMA (Product Operators in Mathematica) (Journal of Magnetic Resonance A 101, 103-105 (1993)) and Kanters *et al.* produced a similar treatment run under Maple (Journal of Magnetic Resonance A 101, 23-29 (1993)). These groups wrote notebooks or procedure files that define various functions such as pulses (target, spins, angle) that transform variables (product operators) according to the transformation rules we have introduced. We will learn to use one of these, Kanters' Maple package, pof (product operator functions), to analyze various 1D and 2D NMR experiments. The 'pof' procedures are part of the Maple 'share' library.

General Instructions:

1). Install Maple on your computer. In order to proceed, you need to have Maple installed on your computer. On our course website there is a tutorial for doing so.

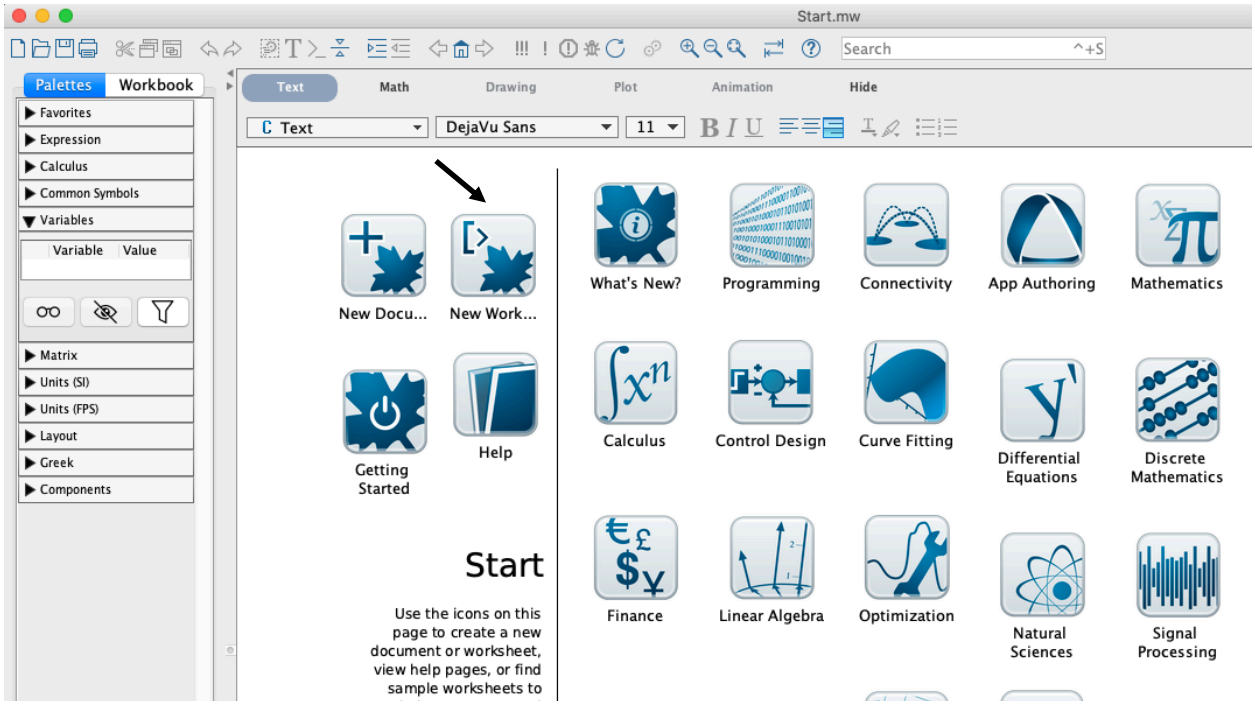
2). Install the Maple 'share' library. You can download the maple 'share' library from our course website in addition to a tutorial for installing it on your computer. So, install it now.

3). Download the data and worksheets archive from our course website ('maplelab-2-data-worksheets.tar') to the desktop of your computer. Unpack the 'tar' archive ('tar -xf') to give a folder named 'maplelab-2'. Make a directory 'maple' in your home directory (for MacOS, '/Users/username/maple', for Linux, '/home/username/maple'). Copy the 'maplelab-2' folder from your desktop into the 'maple' folder. Confirm the contents as shown below (two Maple worksheets (file extensions '.mw').

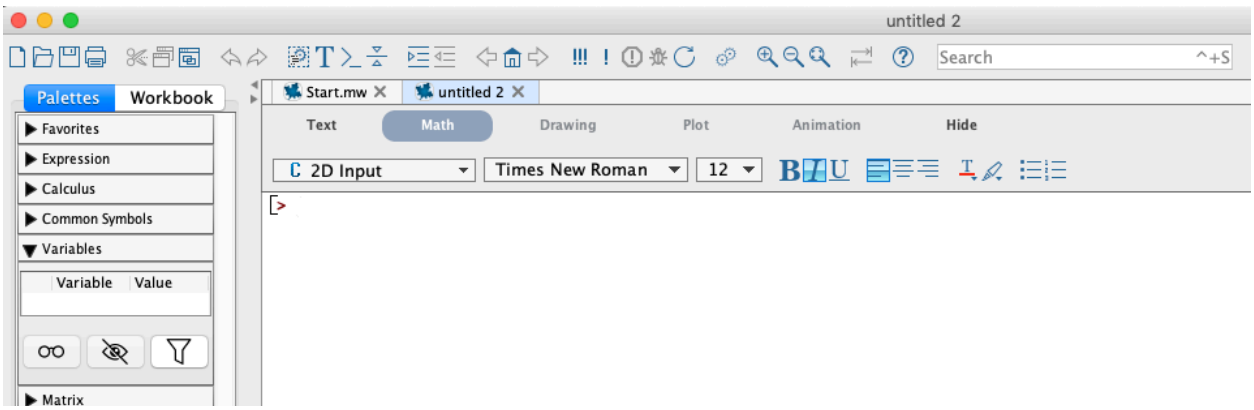
```
MacBook-Pro:~ username$ cd /Users/username/Desktop
MacBook-Pro:Desktop username$ pwd
/Users/username/Desktop
MacBook-Pro:Desktop username $ ls maplelab-2-data-worksheets.tar
maplelab-2-data-worksheets.tar
MacBook-Pro:Desktop username$ tar -xf maplelab-2-data-worksheets.tar
MacBook-Pro:Desktop username$ ls -F maplelab-2
chem-shift-refoc-1.mw*    cosy.mw*
MacBook-Pro:Desktop username$ mkdir /Users/username/maple
MacBook-Pro:Desktop username$ mv maplelab-2 /Users/username/maple
MacBook-Pro:Desktop username$ cd /Users/username/maple/maplelab-2
MacBook-Pro:maplelab-2 username$ pwd
/Users/username/maple/maplelab-2
MacBook-Pro:maplelab-2 username$ ls -F
chem-shift-refoc-1.mw*    cosy.mw*
```

Starting Maple:

For **MacOS**, double-click on the 'Maple 2018.app' (assuming you are using Maple 2018) in the folder/directory 'Maple 2018' in your 'Applications' folder. For convenience, you should probably put the icon on your Dock. For **Linux**, if you have a shortcut on your Desktop, double-click the shortcut icon. Alternatively, you may have a shortcut in your 'Applications' menu (for the 'CentOS installation, a shortcut was automatically placed in the 'Applications' menu under 'Education'. Select it to start the program. If you do not have a shortcut, enter the path to the 'xmaple' application (for the CentOS installation, the path to the 'xmaple' executable is '/opt/local/maple2018/bin/xmaple') to start the program. Notice the 'x' ('xmaple'). This starts the graphical version of the Maple interface, which is what you want. Once Maple starts, select the 'New Worksheet' option to open the program in the 'Worksheet Mode'.

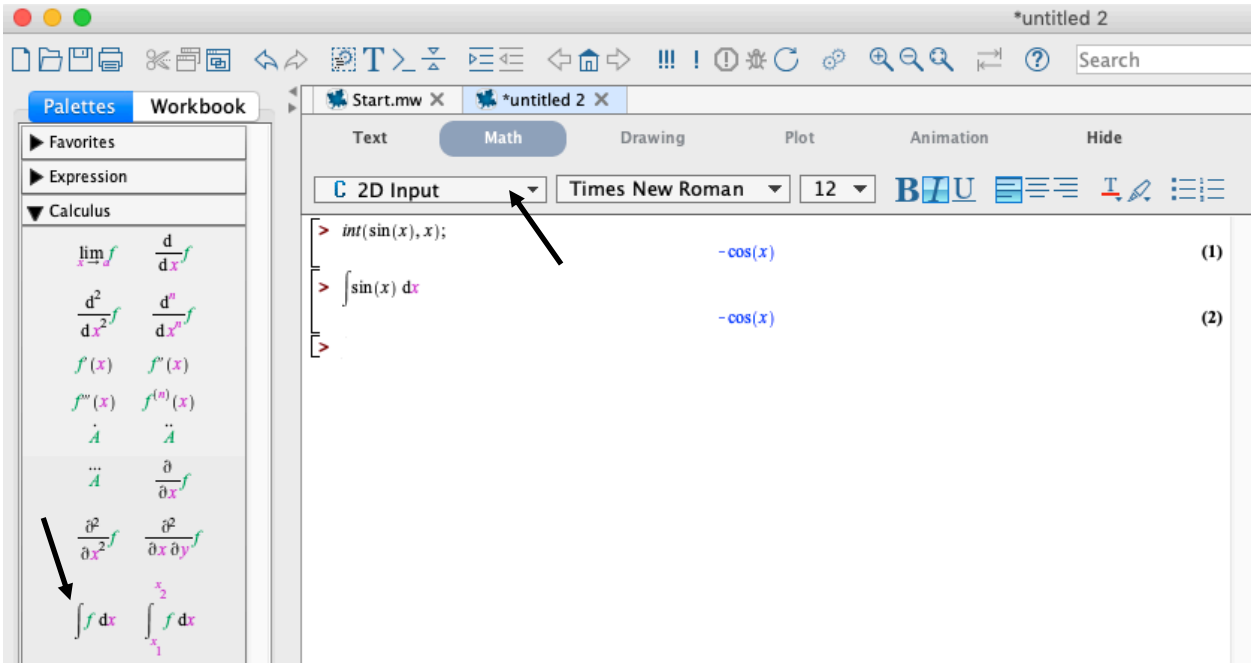


The new worksheet will open. Notice the red command prompt (>). This indicates you are in the 'Worksheet Mode'. Commands are entered at the prompt.



Using '2-D Input' ("2-D Math"):

The default Maple input style is '2D Input'. There are a number of other options (that can be selected from the drop-down menu), and we'll not attempt to describe them here, but the '2D Input' mode is a very versatile mode for mathematics. Like everything else in Maple, the '2D Input' mode allows for multiple ways to accomplish the same task. For instance, in the examples below, Maple is asked to solve an integral. In the first example, the command to integrate, 'int' is entered at the first red command prompt (>). Enclosed in the parentheses are the two variables, the integrand, 'sin(x)', and the variable of integration, 'x'. A semicolon follows the command, indicating that the output will be shown (a colon suppresses output). In the second example, an expression is selected from the 'Calculus' contextual menu on the left (with a click), and the common, familiar notation for an integral is entered automatically after the command prompt. The notation is edited manually to make 'sin(x)' the integrand. The output of the two commands is the same ('-cos(x)').



In our tutorial, we'll mostly use the first type of notation, which is the older, classical Maple notation. This notation is a bit more versatile, but has the disadvantage that the commands to accomplish various mathematical tasks must be remembered. For our tutorials, all of the commands will be entered in the worksheets, so all you have to do is execute the commands sequentially (enter <return> at the end of each line after the semicolon or colon). This is convenient for tutorials as mistakes in entering commands can make the tutorials laborious.

Also, we'll use the convention that a semicolon or colon must follow each command. As you work through the tutorials, feel free to experiment with commands. If your worksheet ceases to work properly, just reload the original and begin again.

Help:

The Maple 'Help' menu (top bar in MacOS, top of Maple window in Linux) includes the entry 'Maple Help'. Selecting this option opens a comprehensive help utility. For simple help with commands, typing '?command_name' at the red command prompt will give help on that particular command. Usually, a new window will open with an exhaustive analysis of the command and its usage. Try typing '?plot3d' at the command prompt, for instance, so you can get an idea of the usefulness of the help utilities.

Basics:

According to the book, "Maple V by Example" (Marth Abell and James Braselton, Academic Press Professional, 1994), there are five basic rules to Maple V syntax.

1) The arguments of functions are given in parentheses (…..).
2) A semicolon (;) or colon (:) must be included at the end of each command (note, the colon suppresses output, and the semicolon now is optional, although it is a good idea to include it).
3) Multiplication is represented by an asterisk (*). However, in Maple 2018 (and perhaps some previous versions) even though you type an asterisk, it unfortunately shows up as a dot (•).
4) Powers are denoted by ^ (you indicate an exponent by typing the caret sign, shift-6). However, in Maple 2018 (and perhaps some previous versions), the display that you see is an exponent (old display: 3^5, new display: 3^5).
5) If you get no response or an obviously incorrect response, most likely you entered the command incorrectly.

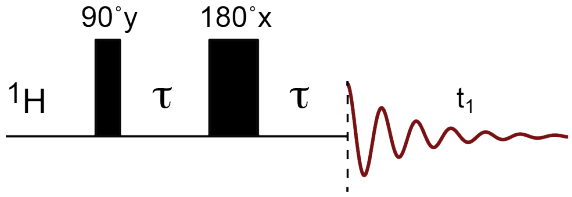
Because of #5, and to make the tutorials go smoothly, you will only need to execute commands, not enter them, to run the tutorials (see below).

Chemical Shift Refocusing (begin this tutorial):

Start Maple. From the 'File' menu, choose 'Open' and **open the file 'chem-shift-refoc-1.mw'** (for MacOS, /Users/username/maple/maplelab-2/chem-shift-refoc-1.mw', for Linux, '/home/username/maple/ maplelab-2/chem-shift-refoc-1.mw'). This file has a list of Maple commands, but no output. So, you don't have to type in all of the commands. This is so that you can see how Maple works without worrying about incorrectly typing in the commands.

All you have to do is put the cursor after the semicolon on each line and hit <return>. This will execute the command and give you the output shown below (in blue). Start at the top and execute each command in sequence from top to bottom.

In this first exercise, we'll examine the spin-echo sequence (right) and chemical shift refocusing. Following the initial 90° pulse to create transverse magnetization, the 'τ-180°-τ' sequence refocuses chemical shift evolution, magnetic field inhomogeneities, and heteronuclear scalar couplings. We'll just consider chemical shift refocusing for a single nucleus in this example.



After the 'restart' (clear memory, clear variables), the 'share' library and 'pof' procedures are loaded (both using the 'with' command). The output from loading the 'share' library indicates the library is installed. The output from loading the 'pof' procedures is an error message that can be ignored (is not fatal, the 'pof' procedures are loaded). The next command defines a 'spinsystem' (a single spin, for instance a single ^{1}H nucleus, named 'A'). The output indicates equilibrium 'z' magnetization for spin 'A'. The next command applies a 90° ('Pi/2', i.e. π/2) pulse along the 'y' axis ('ypulse') on the Iz_A magnetization ('step1') for spin 'A'. The result is transverse 'x' magnetization ('Ix_A'). The next command allows the 'A' magnetization from the previous step ('Ix_A') evolve for a time 'tau' (τ). The result is the familiar expression for precession in the transverse plane (Bloch equations). Here 'W_A' represents the frequency for spin 'A' (i.e. the chemical shift). The next command applies a 180° (π) pulse along the 'x' axis for spin 'A' on the magnetization from step 4. This has no effect on the 'x' component ('Ix_A') but converts 'y' to '-y' (-*Iy*A'). Step 5 is the final 'τ' evolution period. The result is '*Ix*A', which is the same as the magnetization present just prior to the first 't' period. So, the result of the 'τ-180°-τ' sequence is to refocus the magnetization, so there is no net chemical shift evolution.

```
> restart;
> with(share);
See ?share and ?share,contents for information about the share
library
                                  [ ]                              (1)
> with(pof);
Error, invalid input: with expects its 1st argument, pname, to be
of type {`module`, package}, but received `pof `
> step1 := spinsystem([A]);
                              step1 := Iz_A                        (2)
> step2 := ypulse(step1, {A}, Pi/2);
                              step2 := Ix_A                        (3)
> step3 := evolve(step2, {A}, tau);
                step3 := Ix_A Cos(2 π W_A τ) + Iy_A Sin(2 π W_A τ) (4)
> step4 := xpulse(step3, {A}, Pi);
                step4 := Ix_A Cos(2 π W_A τ) − Iy_A Sin(2 π W_A τ) (5)
> setp5 := evolve(step4, {A}, tau);
                              setp5 := Ix_A                        (6)
> restart;
```

The second example is the same as the first, except there are two spins ('A' and 'X') in a coupled two-spin system. The pulses are applied on both 'A' and 'X', and both 'A' and 'X' evolve together, so this could, for instance, represent a coupled homonuclear system ('A' and 'X' both ^{1}H, and coupled) or heteronuclear coupling. As shown in the output for 'step5', the result is that the magnetization is modulated by the coupling constant (*J*), but not the chemical shift (*W*). This is the basis for 1D and 2D *J*-modulated and *J*-resolved experiments.

```
> restart;
> with(share);
```

```
See ?share and ?share,contents for information about the share
library
```

$$[\,] \tag{7}$$

```
> with(pof);
```

```
Error, invalid input: with expects its 1st argument, pname, to be
of type {`module`, package}, but received `pof`
```

```
> step1 := spinsystem([A, X]);
```

$$step1 := Iz_A + Iz_X \tag{8}$$

```
> step2 := ypulse(step1, {A, X}, Pi/2);
```

$$step2 := Ix_A + Ix_X \tag{9}$$

```
> step3 := evolve(step2, {A, X}, tau);
```

$$\begin{aligned} step3 := {} & Cos(2\,\pi\,W_A\,\tau)\,Ix_A\,Cos(\pi\,J_{A,X}\,\tau) + 2\,Cos(2\,\pi\,W_A\,\tau)\,Iy_A\,Iz_X\,Sin(\pi\,J_{A,X}\,\tau) \\ & + Sin(2\,\pi\,W_A\,\tau)\,Iy_A\,Cos(\pi\,J_{A,X}\,\tau) - 2\,Sin(2\,\pi\,W_A\,\tau)\,Ix_A\,Iz_X\,Sin(\pi\,J_{A,X}\,\tau) \\ & + Cos(2\,\pi\,W_X\,\tau)\,Ix_X\,Cos(\pi\,J_{A,X}\,\tau) + 2\,Cos(2\,\pi\,W_X\,\tau)\,Iy_X\,Iz_A\,Sin(\pi\,J_{A,X}\,\tau) \\ & + Sin(2\,\pi\,W_X\,\tau)\,Iy_X\,Cos(\pi\,J_{A,X}\,\tau) - 2\,Sin(2\,\pi\,W_X\,\tau)\,Ix_X\,Iz_A\,Sin(\pi\,J_{A,X}\,\tau) \end{aligned} \tag{10}$$

```
> step4 := xpulse(step3, {A, X}, Pi);
```

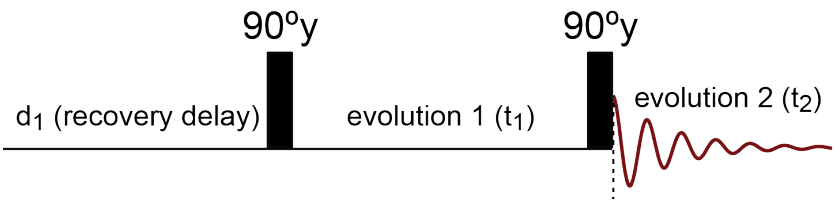
$$\begin{aligned} step4 := {} & Cos(2\,\pi\,W_A\,\tau)\,Ix_A\,Cos(\pi\,J_{A,X}\,\tau) + 2\,Cos(2\,\pi\,W_A\,\tau)\,Iy_A\,Iz_X\,Sin(\pi\,J_{A,X}\,\tau) \\ & - Sin(2\,\pi\,W_A\,\tau)\,Iy_A\,Cos(\pi\,J_{A,X}\,\tau) + 2\,Sin(2\,\pi\,W_A\,\tau)\,Ix_A\,Iz_X\,Sin(\pi\,J_{A,X}\,\tau) \\ & + Cos(2\,\pi\,W_X\,\tau)\,Ix_X\,Cos(\pi\,J_{A,X}\,\tau) + 2\,Cos(2\,\pi\,W_X\,\tau)\,Iy_X\,Iz_A\,Sin(\pi\,J_{A,X}\,\tau) \\ & - Sin(2\,\pi\,W_X\,\tau)\,Iy_X\,Cos(\pi\,J_{A,X}\,\tau) + 2\,Sin(2\,\pi\,W_X\,\tau)\,Ix_X\,Iz_A\,Sin(\pi\,J_{A,X}\,\tau) \end{aligned} \tag{11}$$

```
> step5 := evolve(step4, {A, X}, tau);
```

$$\begin{aligned} step5 := {} & Ix_A\,Cos(2\,\pi\,J_{A,X}\,\tau) + 2\,Iy_A\,Iz_X\,Sin(2\,\pi\,J_{A,X}\,\tau) + Ix_X\,Cos(2\,\pi\,J_{A,X}\,\tau) \\ & + 2\,Iy_X\,Iz_A\,Sin(2\,\pi\,J_{A,X}\,\tau) \end{aligned} \tag{12}$$

```
> restart;
```

COSY (begin this tutorial):



Start Maple. From the 'File' menu, choose 'Open' and **open the file 'cosy.mw'** (for MacOS, /Users/username/maple/maplelab-2/cosy.mw', for Linux, '/home/username/maple/ maplelab-2/cosy.mw'). This file has a list of Maple commands, but no output. So, you don't have to type in all of the commands. This is so that you can see how Maple works without worrying about incorrectly typing in the commands.

All you have to do is put the cursor after the semicolon on each line and hit <return>. This will execute the command and give you the output shown below (in blue). Start at the top and execute each command in sequence from top to bottom.

This Maple product operator tutorial describes the basic 90-t_1-90-t_2 COSY experiment. Operations (defining the spin system, pulses, evolution periods) are similar to those in the chemical shift refocusing tutorial described above. At 'step5' the 'observe' function is introduced, which generates evolution in a second time domain, t_2 (the directly observed dimension). The Fourier transformation of the data is accomplished in step6. Both dimensions are transformed, and the 'evalc' command (which returns symbolic forms of complex expressions) returns the real ('Re') values that will be used for plotting the results (the imaginary components, 'Im', are unnecessary at this point and are not used). Note that there are 32 terms offset by chemical shifts of spin 'A' and spin 'X' and by +/- J/2 in both dimensions. They describe line shapes (absorption or dispersion) in each dimension (v1 or v2). These are the autocorrelation (diagonal) peaks and cross peaks expected for the AX spin system. The 'table' commands define values for T_2 relaxation times ('T2'), chemical shifts ('Wv') and coupling constants ('Jv') to be used in subsequent plot functions. A couple of different plotting functions are illustrated. The variables in the plot functions set boundaries of the regions to be plotted and the number of points to be used. In the first instance ('nmrplot2d') you are only plotting one crosspeak (note the range of the v1 and v2 variables). You can interactively rotate the spectrum to see it more clearly. The second example ('super2d') plots the entire spectrum. These particular plotting functions are part of the share library, and as a result no Maple 'help' descriptions are available. However, the variables in the plot functions set boundaries of the region to be plotted and the number of points used. There are also extensive plotting routines available in Maple. To find some of the plotting routines open the 'Help' utility from the icon on the right side of the second menu bar (circle with question mark inside) and type 'plot' in the search window that opens.

```
> restart;
> with(share) : with(pof);
See ?share and ?share,contents for information about the share library
Error, invalid input: with expects its 1st argument, pname, to be of type
{`module`, package}, but received `pof `
```

```
> step1 := spinsystem([A, X]);
```

$$step1 := Iz_A + Iz_X \tag{1}$$

```
> step2 := ypulse(step1, {A, X}, Pi/2);
```

$$step2 := Ix_A + Ix_X \tag{2}$$

```
> step3 := evolve(step2, {A, X}, t1);
```

$$\begin{aligned} step3 := {} & Cos(2\pi W_A t1)\, Ix_A Cos(\pi J_{A,X} t1) + 2\, Cos(2\pi W_A t1)\, Iy_A Iz_X Sin(\pi J_{A,X} t1) \\ & + Sin(2\pi W_A t1)\, Iy_A Cos(\pi J_{A,X} t1) - 2\, Sin(2\pi W_A t1)\, Ix_A Iz_X Sin(\pi J_{A,X} t1) \\ & + Cos(2\pi W_X t1)\, Ix_X Cos(\pi J_{A,X} t1) + 2\, Cos(2\pi W_X t1)\, Iy_X Iz_A Sin(\pi J_{A,X} t1) \\ & + Sin(2\pi W_X t1)\, Iy_X Cos(\pi J_{A,X} t1) - 2\, Sin(2\pi W_X t1)\, Ix_X Iz_A Sin(\pi J_{A,X} t1) \end{aligned} \tag{3}$$

```
> step4 := ypulse(step3, {A, X}, Pi/2);
```

$$\begin{aligned} step4 := {} & -Cos(2\pi W_A t1)\, Iz_A Cos(\pi J_{A,X} t1) + 2\, Cos(2\pi W_A t1)\, Iy_A Ix_X Sin(\pi J_{A,X} t1) \\ & + Sin(2\pi W_A t1)\, Iy_A Cos(\pi J_{A,X} t1) + 2\, Sin(2\pi W_A t1)\, Iz_A Ix_X Sin(\pi J_{A,X} t1) \\ & - Cos(2\pi W_X t1)\, Iz_X Cos(\pi J_{A,X} t1) + 2\, Cos(2\pi W_X t1)\, Iy_X Ix_A Sin(\pi J_{A,X} t1) \\ & + Sin(2\pi W_X t1)\, Iy_X Cos(\pi J_{A,X} t1) + 2\, Sin(2\pi W_X t1)\, Iz_X Ix_A Sin(\pi J_{A,X} t1) \end{aligned} \tag{4}$$

```
> step5 := observe(step4, {A, X}, t2, 0);
```

$$\begin{aligned} step5 := {} & \frac{I\, Sin(2\pi W_A t1)\, Cos(\pi J_{A,X} t1)\, Cos(2\pi W_A t2)\, Cos(\pi J_{A,X} t2)}{2} \\ & - \frac{Sin(2\pi W_X t1)\, Sin(\pi J_{A,X} t1)\, Sin(2\pi W_A t2)\, Sin(\pi J_{A,X} t2)}{2} \\ & - \frac{Sin(2\pi W_A t1)\, Cos(\pi J_{A,X} t1)\, Sin(2\pi W_A t2)\, Cos(\pi J_{A,X} t2)}{2} \\ & + \frac{I\, Sin(2\pi W_X t1)\, Cos(\pi J_{A,X} t1)\, Cos(2\pi W_X t2)\, Cos(\pi J_{A,X} t2)}{2} \\ & + \frac{I\, Sin(2\pi W_X t1)\, Sin(\pi J_{A,X} t1)\, Cos(2\pi W_A t2)\, Sin(\pi J_{A,X} t2)}{2} \\ & - \frac{Sin(2\pi W_A t1)\, Sin(\pi J_{A,X} t1)\, Sin(2\pi W_X t2)\, Sin(\pi J_{A,X} t2)}{2} \\ & - \frac{Sin(2\pi W_X t1)\, Cos(\pi J_{A,X} t1)\, Sin(2\pi W_X t2)\, Cos(\pi J_{A,X} t2)}{2} \\ & + \frac{I\, Sin(2\pi W_A t1)\, Sin(\pi J_{A,X} t1)\, Cos(2\pi W_X t2)\, Sin(\pi J_{A,X} t2)}{2} \end{aligned} \tag{5}$$

```
> spec1 := evalc(Re(FT(FT(step5, 0, t2, v2), 0, t1, v1)));
```

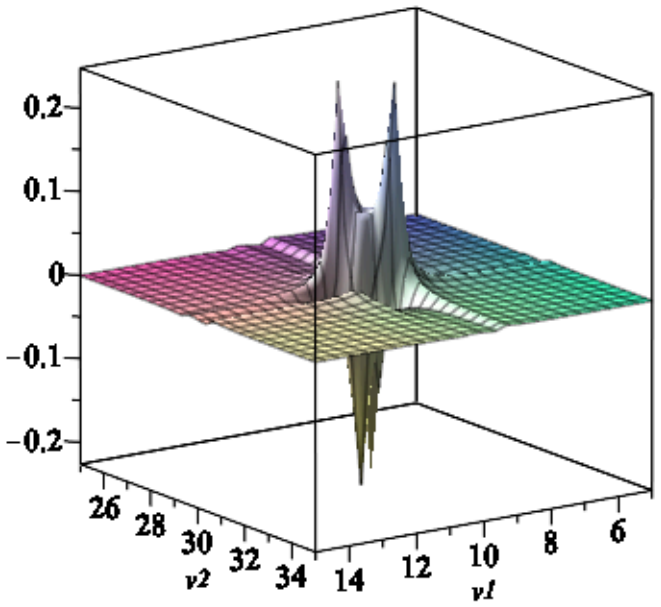
$$
\begin{aligned}
spec1 := {} & \frac{Ab\left(\frac{J_{A,X}}{2}+W_X,v2\right)Ab\left(\frac{J_{A,X}}{2}+W_X,v1\right)}{16}+\frac{Ab\left(\frac{J_{A,X}}{2}+W_X,v2\right)Ab\left(-\frac{J_{A,X}}{2}+W_X,v1\right)}{16} \\
& -\frac{Di\left(\frac{J_{A,X}}{2}+W_A,v2\right)Di\left(-\frac{J_{A,X}}{2}+W_X,v1\right)}{16}+\frac{Di\left(\frac{J_{A,X}}{2}+W_A,v2\right)Di\left(\frac{J_{A,X}}{2}+W_X,v1\right)}{16} \\
& +\frac{Ab\left(-\frac{J_{A,X}}{2}+W_A,v2\right)Ab\left(\frac{J_{A,X}}{2}+W_A,v1\right)}{16}+\frac{Ab\left(-\frac{J_{A,X}}{2}+W_A,v2\right)Ab\left(-\frac{J_{A,X}}{2}+W_A,v1\right)}{16} \\
& +\frac{Ab\left(-\frac{J_{A,X}}{2}+W_X,v2\right)Ab\left(\frac{J_{A,X}}{2}+W_X,v1\right)}{16}+\frac{Ab\left(-\frac{J_{A,X}}{2}+W_X,v2\right)Ab\left(-\frac{J_{A,X}}{2}+W_X,v1\right)}{16} \\
& -\frac{Di\left(\frac{J_{A,X}}{2}+W_A,v2\right)Di\left(\frac{J_{A,X}}{2}+W_A,v1\right)}{16}-\frac{Di\left(\frac{J_{A,X}}{2}+W_A,v2\right)Di\left(-\frac{J_{A,X}}{2}+W_A,v1\right)}{16} \\
& -\frac{Di\left(-\frac{J_{A,X}}{2}+W_A,v2\right)Di\left(\frac{J_{A,X}}{2}+W_A,v1\right)}{16}-\frac{Di\left(-\frac{J_{A,X}}{2}+W_A,v2\right)Di\left(-\frac{J_{A,X}}{2}+W_A,v1\right)}{16} \\
& +\frac{Ab\left(\frac{J_{A,X}}{2}+W_X,v2\right)Ab\left(-\frac{J_{A,X}}{2}+W_A,v1\right)}{16}-\frac{Ab\left(\frac{J_{A,X}}{2}+W_X,v2\right)Ab\left(\frac{J_{A,X}}{2}+W_A,v1\right)}{16} \\
& -\frac{Ab\left(-\frac{J_{A,X}}{2}+W_X,v2\right)Ab\left(-\frac{J_{A,X}}{2}+W_A,v1\right)}{16}+\frac{Ab\left(-\frac{J_{A,X}}{2}+W_X,v2\right)Ab\left(\frac{J_{A,X}}{2}+W_A,v1\right)}{16} \\
& +\frac{Ab\left(\frac{J_{A,X}}{2}+W_A,v2\right)Ab\left(\frac{J_{A,X}}{2}+W_A,v1\right)}{16}+\frac{Ab\left(\frac{J_{A,X}}{2}+W_A,v2\right)Ab\left(-\frac{J_{A,X}}{2}+W_A,v1\right)}{16} \\
& +\frac{Di\left(-\frac{J_{A,X}}{2}+W_A,v2\right)Di\left(-\frac{J_{A,X}}{2}+W_X,v1\right)}{16}-\frac{Di\left(-\frac{J_{A,X}}{2}+W_A,v2\right)Di\left(\frac{J_{A,X}}{2}+W_X,v1\right)}{16} \\
& -\frac{Di\left(\frac{J_{A,X}}{2}+W_X,v2\right)Di\left(-\frac{J_{A,X}}{2}+W_A,v1\right)}{16}+\frac{Di\left(\frac{J_{A,X}}{2}+W_X,v2\right)Di\left(\frac{J_{A,X}}{2}+W_A,v1\right)}{16} \\
& +\frac{Di\left(-\frac{J_{A,X}}{2}+W_X,v2\right)Di\left(-\frac{J_{A,X}}{2}+W_A,v1\right)}{16}-\frac{Di\left(-\frac{J_{A,X}}{2}+W_X,v2\right)Di\left(\frac{J_{A,X}}{2}+W_A,v1\right)}{16} \\
& -\frac{Di\left(-\frac{J_{A,X}}{2}+W_X,v2\right)Di\left(-\frac{J_{A,X}}{2}+W_X,v1\right)}{16}-\frac{Di\left(-\frac{J_{A,X}}{2}+W_X,v2\right)Di\left(\frac{J_{A,X}}{2}+W_X,v1\right)}{16} \\
& -\frac{Di\left(\frac{J_{A,X}}{2}+W_X,v2\right)Di\left(\frac{J_{A,X}}{2}+W_X,v1\right)}{16}-\frac{Di\left(\frac{J_{A,X}}{2}+W_X,v2\right)Di\left(-\frac{J_{A,X}}{2}+W_X,v1\right)}{16} \\
& -\frac{Ab\left(-\frac{J_{A,X}}{2}+W_A,v2\right)Ab\left(-\frac{J_{A,X}}{2}+W_X,v1\right)}{16}+\frac{Ab\left(-\frac{J_{A,X}}{2}+W_A,v2\right)Ab\left(\frac{J_{A,X}}{2}+W_X,v1\right)}{16} \\
& +\frac{Ab\left(\frac{J_{A,X}}{2}+W_A,v2\right)Ab\left(-\frac{J_{A,X}}{2}+W_X,v1\right)}{16}-\frac{Ab\left(\frac{J_{A,X}}{2}+W_A,v2\right)Ab\left(\frac{J_{A,X}}{2}+W_X,v1\right)}{16}
\end{aligned}
\tag{6}
$$

```
> T2 := table([A=1, X=1]) : Wv := table([A=10, X=30]) : Jv := table(symmetric, [(A, X)=1]);
```

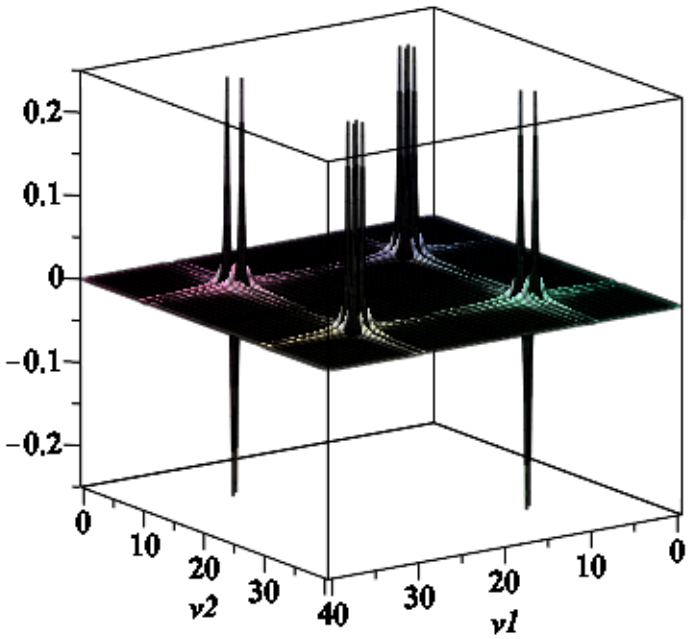
$$Jv := \text{table}(symmetric, [(A, X) = 1]) \tag{7}$$

```
> nmrplot2d(spec1, v1=5..15, v2=25..35, numpoints=5000, title="A - X spin system");
```

$$-X\ spin\ system + A$$




```
> super2d(spec1, v1, v2);
```




```
> restart :
>
```