
Chapter 4

Bloch simulator

The command *Utilities/Bloch module* in the main NMR-SIM menu opens a new window (Figure 4.1) with its own menu bar. You may also start the bloch simulator as stand-alone application using following option:

nmrsim -bloch

Additional parameters *-excit_profile* and *-time_evolution* may be used to start immediately the calculation of the excitation profile, or of the time evolution of the nuclear magnetization.

The stand-alone module contains only the functionality described in this chapter.

The Bloch simulator module is designed to calculate and visualize the motion of the nuclear magnetization vector during a NMR experiment. The calculation of *excitation profiles* and *waveform analysis* brings important information about the behavior of pulses or pulse sequences in a real experiment.

The motion of the magnetization vector is described by the Bloch equation

$$\dot{\bar{M}} = -\gamma(\bar{B} \times \bar{M}) \quad , \quad (4.1)$$

This is a classical equivalent of the Liouville equation (Equation 2.1) for spin 1/2.

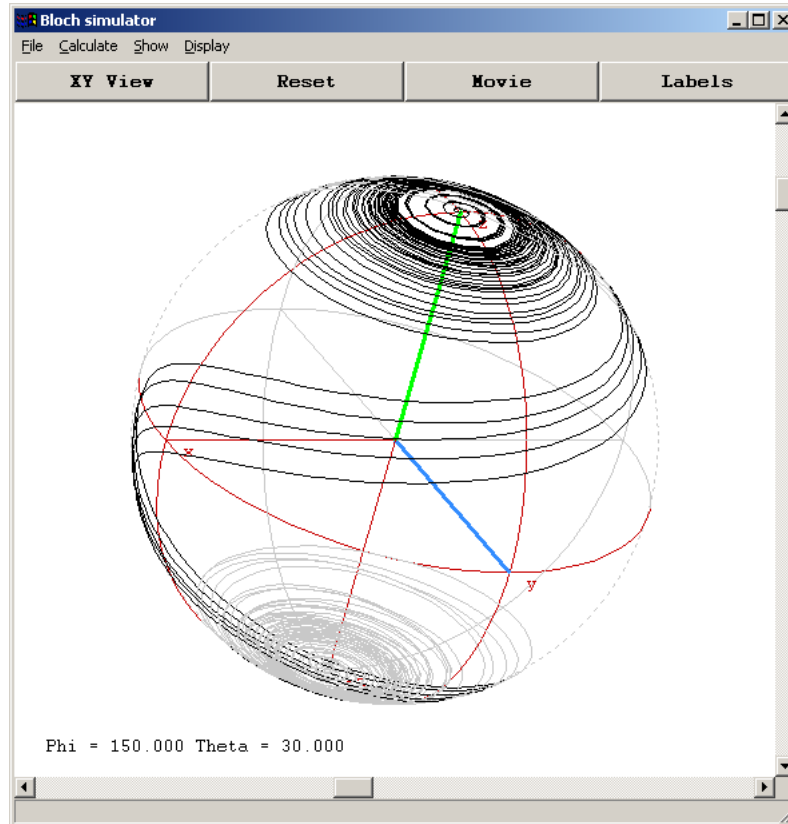


Figure 4.1

The time evolution of a nuclear magnetization vector during an adiabatic pulse, calculated for several offsets, is shown as a projection on the sphere

4.1 File

- *Select*
selects the waveform for the calculation. The waveform is immediately shown on the screen. The buttons on the top of window may be used to switch between cartesian and polar coordinates.

- **Save**
Saves the calculated information to disk. Always the displayed profile or waveform analysis will be written. This could be imported into other programs (it is a plain text file).
- **Export**
Saves the calculated data as TOPSPIN data sets. Each data set contains in the title short description of stored data.

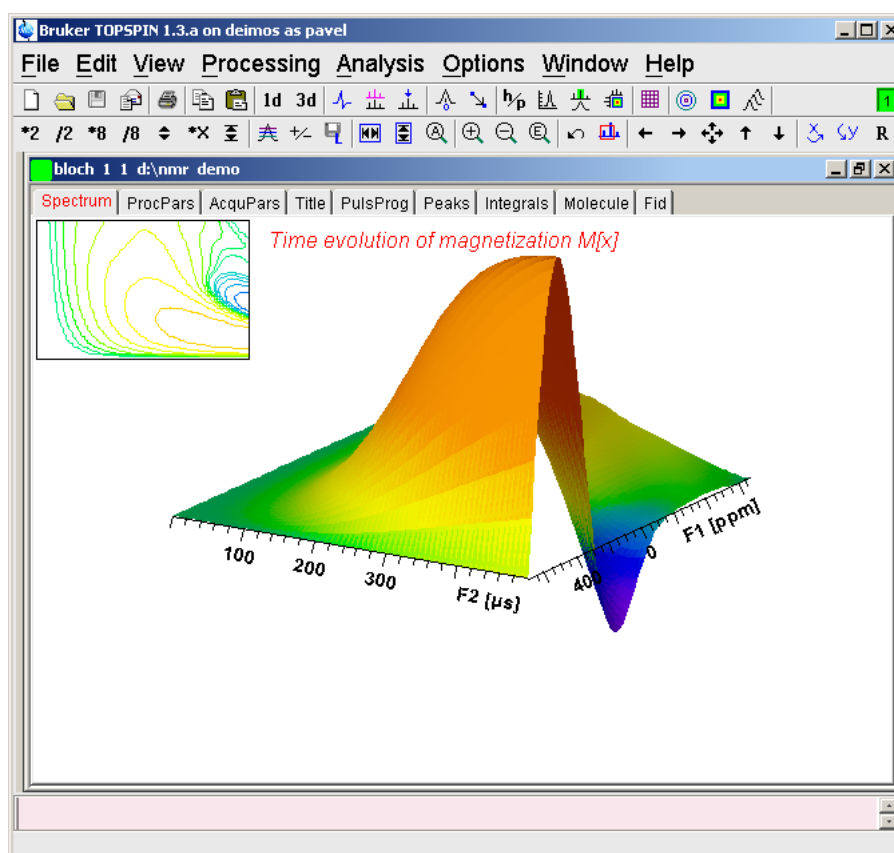


Figure 4.2 Exported time evolution of the magnetization shown in TOPSPIN

- **Print**
Prints the current picture. The UNIX version supports only output to disk file in PostScript format. The MS-WINDOWS versions support all MS-WINDOWS printers, including color ones.
- **Copy to Clipboard**
Copies the picture into MS-WINDOWS clipboard.
- **Close**
Closes the Bloch module window and pops up the NMR-SIM main window.

Windows

4.2 Calculate

The calculations are started from the pull down menu *Calculate*. It is also possi-

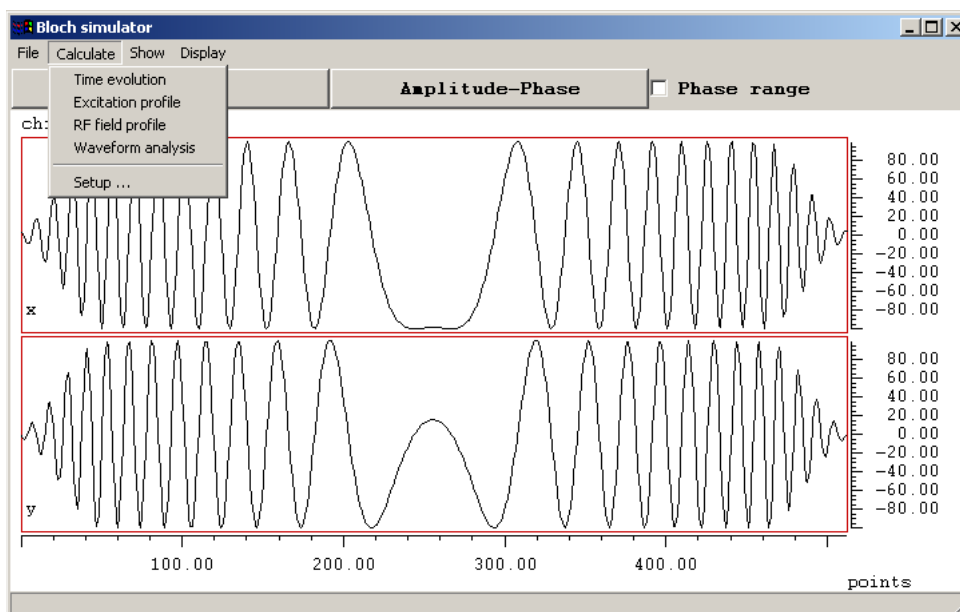


Figure 4.3 *Calculate* pull-down menu

ble, to start the calculation from the command line. The arguments *-excit_profile* and *-time_evolution* combined with the *-bloch* argument will start the calculation immediately.

Example:

```
nrmrsim -config chirp.cfg -bloch -time_evolution
```

starts the bloch module, loads all settings from the configuration file *chirp.cfg* and calculates the time evolution of the magnetization.

4.3 Time evolution

Command *Time evolution* calculates the motion of the magnetization vector during the pulse for several radio frequency offsets and shows it on the sphere (Figure 4.1).

The command opens dialog box (Figure 4.4), which defines following experiment parameters:

Parameter	Value	Unit	Description
SPNAM0	chirp2.shp		filename for sp0
Mx (0)	0		initial magnetization
My (0)	0		initial magnetization
Mz (0)	1		initial magnetization
P 0	9600	us	fixed pulse
SP 0	1000	Hz	power for shaped pulses
N	1		number of calculated offsets
Start	0	Hz	first RF offset
Step	100	Hz	offset increment

Enter a FLOAT value between -1.0 and 1.0

OK Cancel

Figure 4.4 Parameters for the calculation of the time evolution of the magnetization

- ***MX(0),MY(0),MZ(0)***
The initial value of the magnetization vector. The values are later so normalized, that the ***vector length is 1***.

Example:

(0,10,0) is equivalent to ***(0,1,0)***,

(1,1,1) is equivalent to $(1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$

The value ***(0,0,0)*** is identical to the equilibrium value ***(0,0,1)***.

- ***SPNAM0***
Waveform name.

A list of all pulses, delays and variables that occur in the pulse program:

- ***SP 0***
The radio frequency field intensity for the shaped pulse.
- ***TSlice***
This parameter defines the maximal time step between two samples. It is necessary to set it only to sample the evolution during rectangular pulses. The value 0 means, that this parameter is ignored and the magnetization is sampled only at the end of each interval in the shaped pulse.
- ***N***
Number of slices (offset values) which will be calculated. One slice represents the simulated experiment for one radio frequency offset.
- ***Start***
The first value of radio frequency offset used for the calculation.
- ***Step***
The radio frequency offset increment between two slices.

The result of the calculation may be shown either using spherical coordinates (Figure 4.5) or in cartesian coordinate system (Figure 4.6). Use the buttons on the top of the Bloch simulator window to select the type of coordinates and the visible magnetization component. The scroll-bars on the bottom and on the side of the window may be used to adjust the angle of view. The button ***Reset*** will restore default angle of view. The button ***Labels*** toggles the display of time labels. Each labels shows the time elapsed form the start of the pulse.

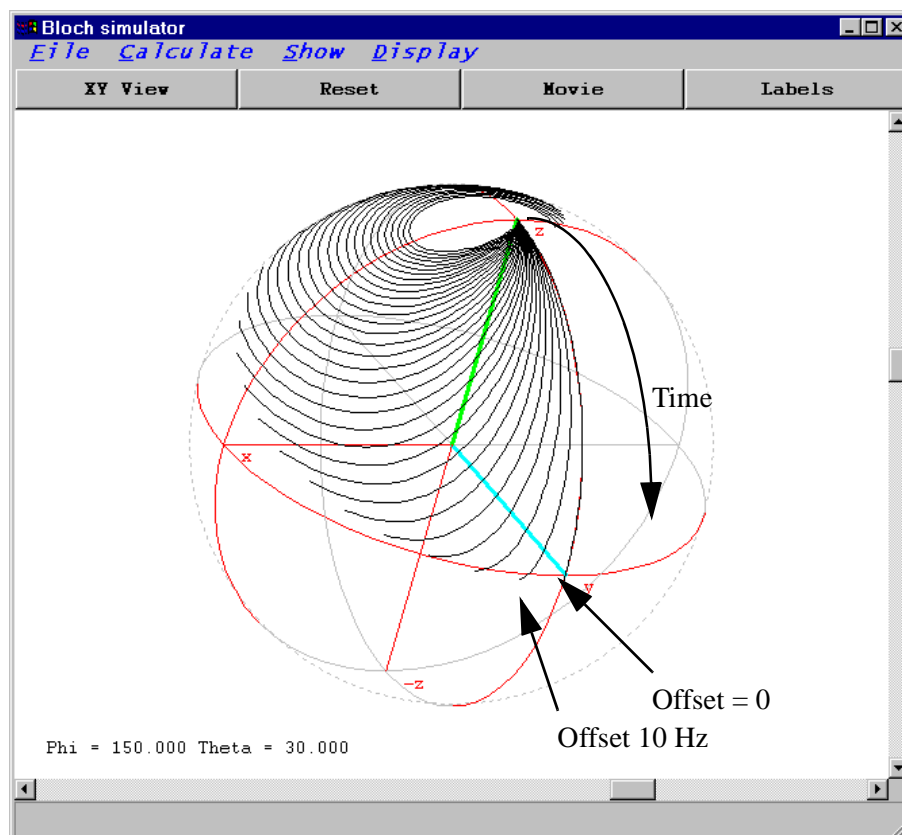


Figure 4.5 The time evolution of the magnetization vector shown as a projection on the sphere.

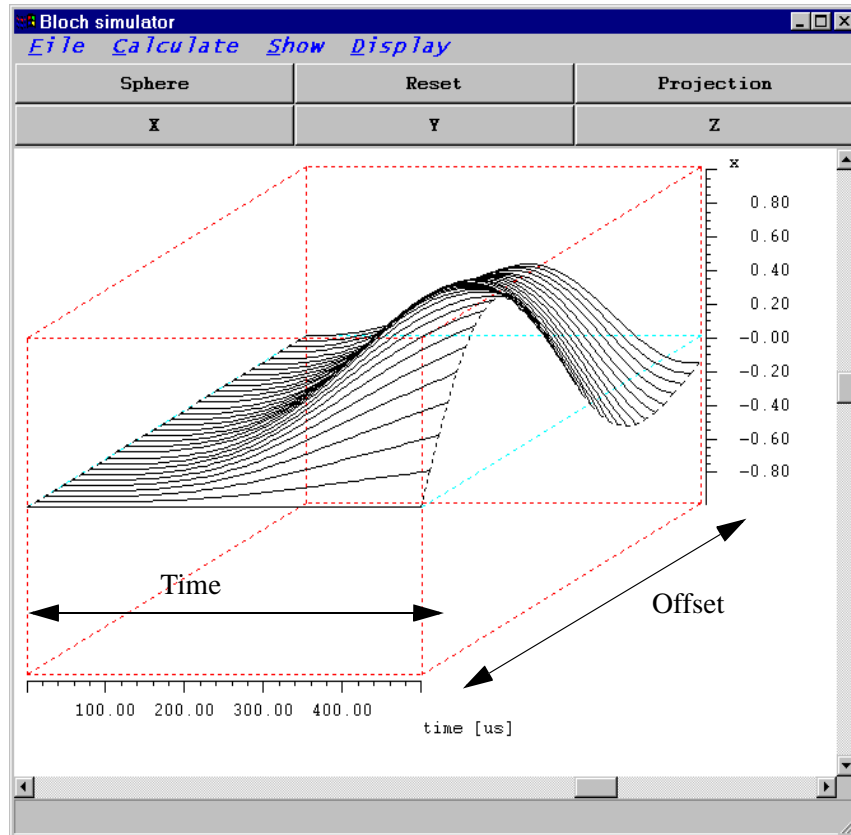


Figure 4.6 The time evolution of the M_x magnetization component shown as a surface.

4.3.1 Excitation profile

The command *Excitation profile* calculates the excitation profile of a shaped pulse.

Parameter	Value	Unit	Description
SPNAME0	gauss.shp		filename for sp0
Mx (0)	0		initial magnetization
My (0)	0		initial magnetization
Mz (0)	0		initial magnetization
P 0	500	us	fixed pulse
SP 0	1000	Hz	power for shaped pulses
N	400		number of calculated points
Start	-4000	Hz	first RF offset
Step	20	Hz	offset increment

Figure 4.7 Parameters for the excitation profile calculation

The parameters are the same as for the time sequence. The window layout changes and the calculated excitation profile is shown (Figure 4.8). The buttons on the top of the window allow you to select the visible component. You may select either one magnetization component, the fourier transformation of the waveform¹, or combination of them. The button *Phase range* toggles the phase display between <0..360> and full phase range.

The buttons on the bottom may be used to scale the graph. On the bottom of the window is shown the position of the mouse cursor in the coordinates used for the axis.

1. The fourier transformation of the waveform is in the first approximation (small flip angles) very near to the excitation profile of the pulse.

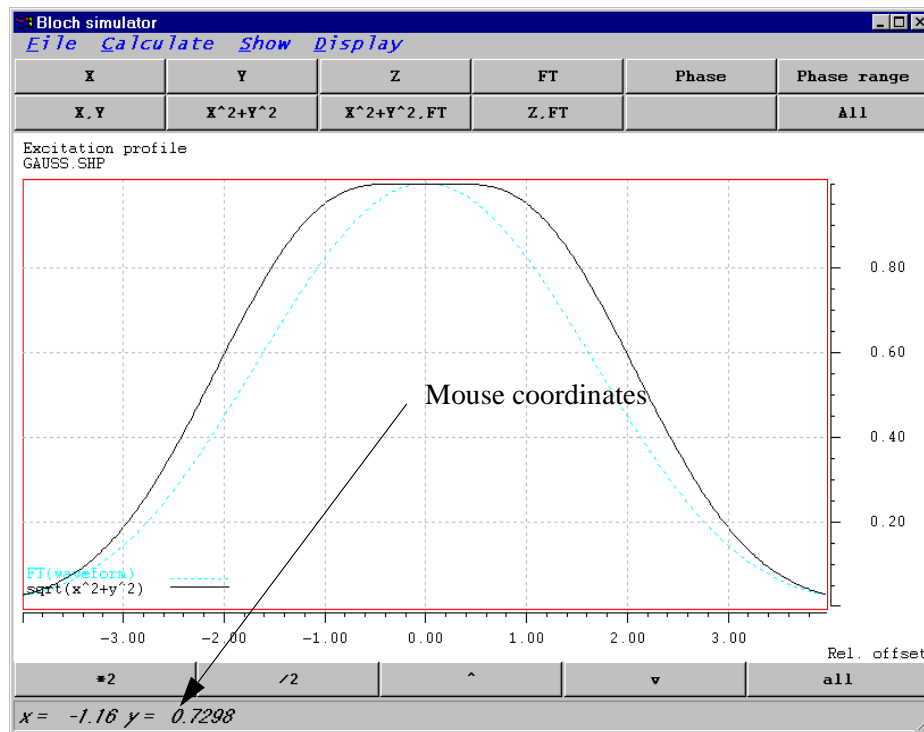
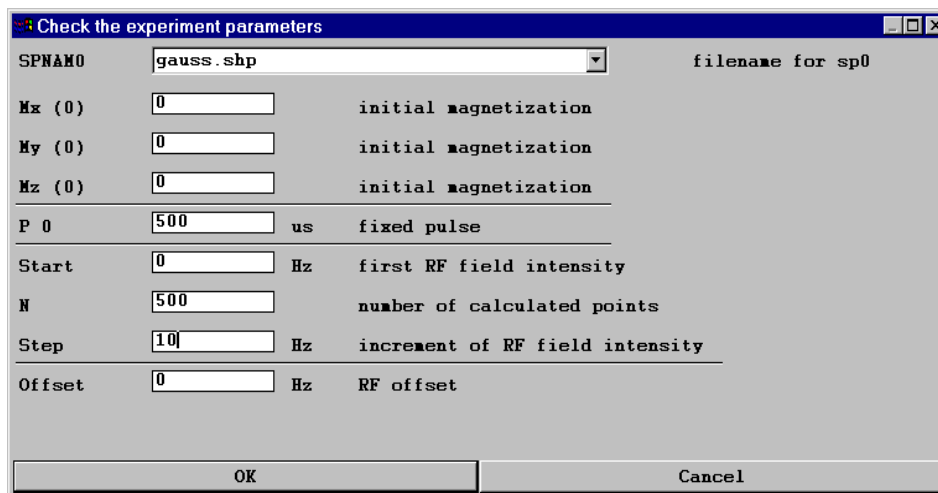


Figure 4.8

The excitation profile of the gaussian 90 degree pulse. The x axis uses as a unit the relative offset - the ratio of the radio frequency field and offset. Such a presentation is independent on the absolute value of radio frequency fields. The bottom status line shows the coordinate of the mouse cursor in this graph.

4.3.2 RF field profile

The RF field profile command calculates the dependency of the magnetization on the RF field intensity. You define the pulse length, the RF offset, the starting value of used radio frequency field, number of calculated points and the step (Figure 4.9)



Parameter	Value	Unit	Description
SPNAME	gauss.shp		filename for sp0
Mx (0)	0		initial magnetization
My (0)	0		initial magnetization
Mz (0)	0		initial magnetization
P 0	500	us	fixed pulse
Start	0	Hz	first RF field intensity
N	500		number of calculated points
Step	10	Hz	increment of RF field intensity
Offset	0	Hz	RF offset

Figure 4.9

Parameters used for the calculation of radio frequency profiles

Calculated profile (Figure 4.10) is shown as a dependency of magnetization components on the RF field intensity. The displayed component may be selected using the buttons on the top of the window. The cursor position is shown on the bottom status line.

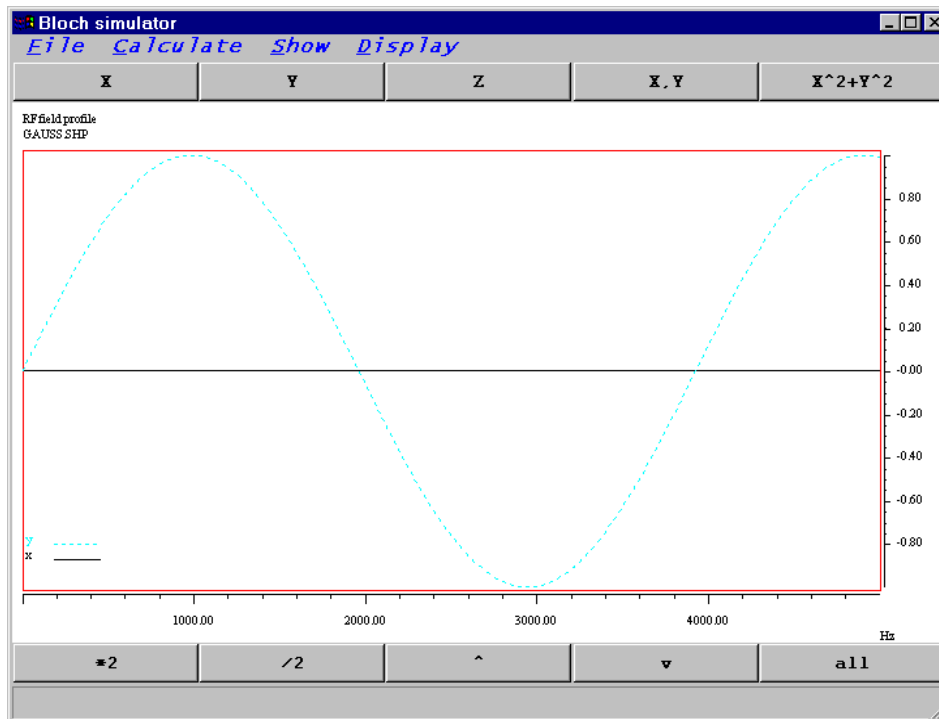


Figure 4.10

Calculated radio frequency profile. The length of the 90 degree pulse is 1000 ms.

4.3.3 Waveform analysis

The command “Calculate/Waveform analysis” is used to analyze features of adia-

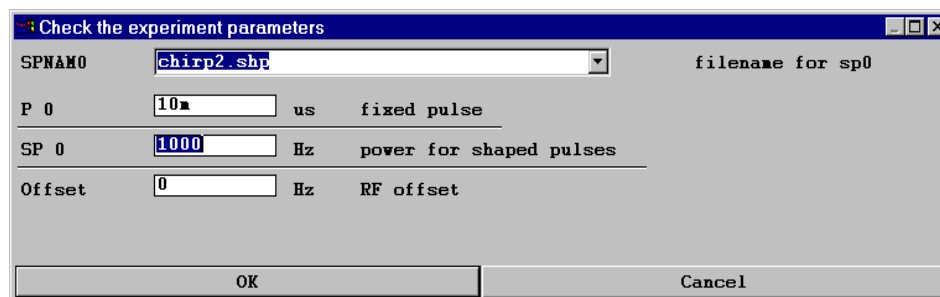


Figure 4.11 Parameters used for the waveform analysis

batic pulses. The program requires the pulse length, the rf intensity and the offset of the examined pulse and calculates following output:

- Θ_M and Θ_{B1eff} are the angles between the magnetization or $B1_{eff}$ vectors and the xy plane .

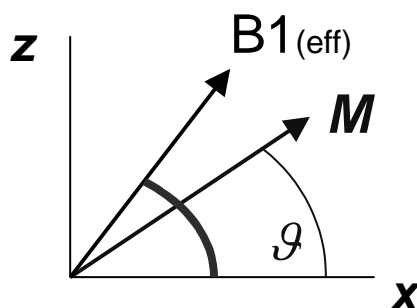


Figure 4.12

The definition of adiabatic condition requires, that the magnetization vector M follows the trajectory of the effective radio frequency field vector $B1_{eff}$.

- Quality factor
- Frequency sweep.

Following pictures show the same pulse analyzed under two experimental conditions - on resonance and off resonance. The on resonance picture shows very good adiabatic condition, the off resonance case shows rising misalignment between the magnetization and rf field vectors - the adiabatic condition is not valid anymore.

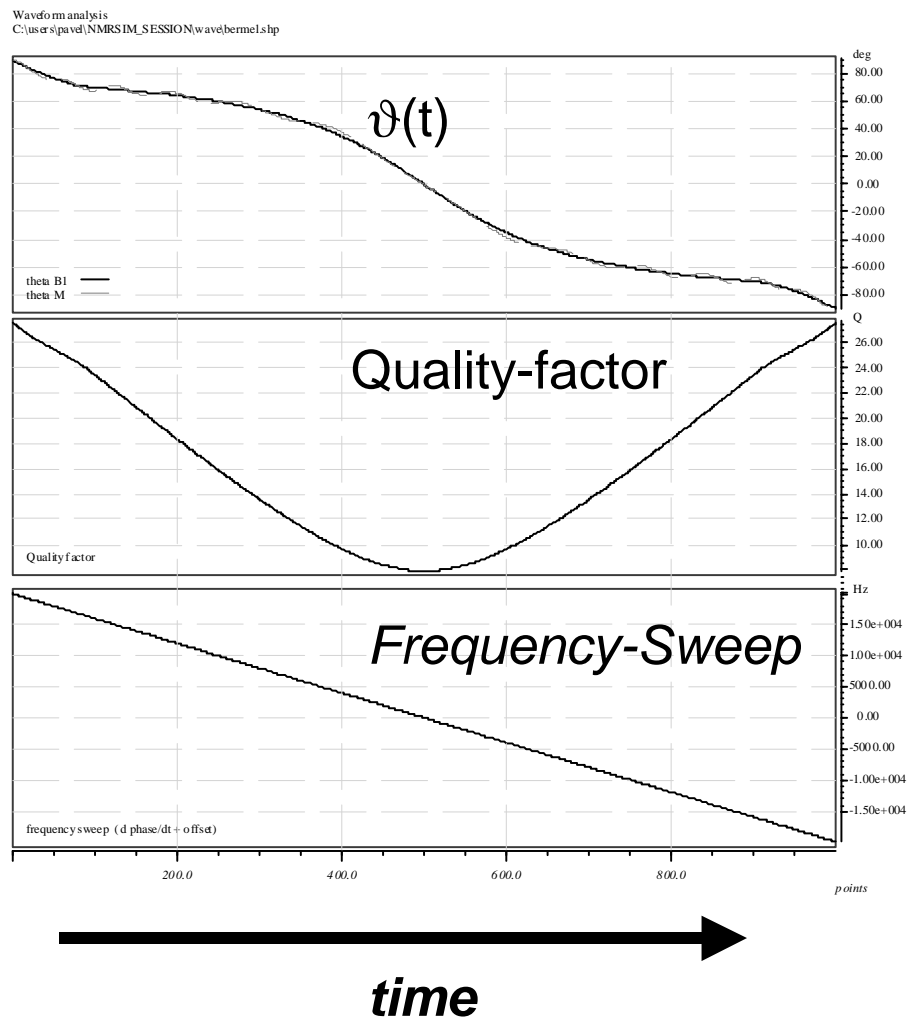


Figure 4.13 On resonance

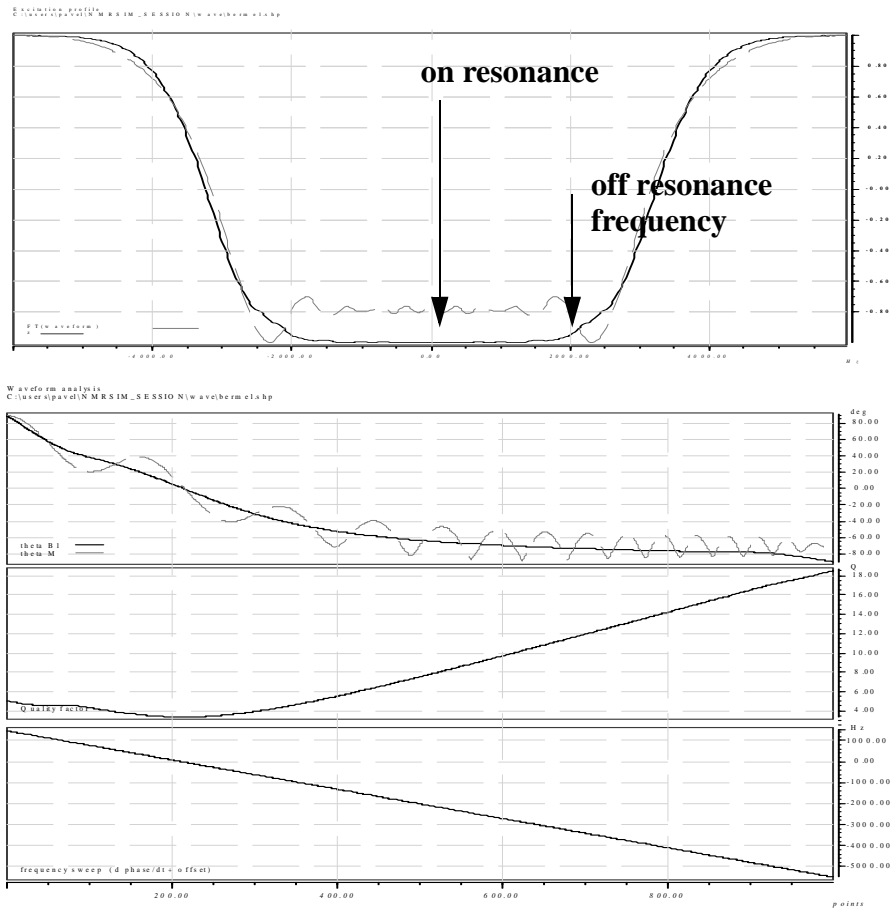


Figure 4.14

4.3.4 Calculation setup

Command *Setup* opens a dialog box which allows you to select the calculation mode and the names of input files.

NMR-SIM supports two calculation modes:

1. *Shaped Pulse*

The shaped pulses are used for the calculation in this mode.

2. *Pulse sequence fragment*

You can calculate the excitation profile or time evolution of the magnetization through any pulse sequence. You must write your own pulse program to do this.

Follow this scheme:

```
ze
1 sample ; starts sampling
; the pulse sequence fragment begins here
; you can use any pulse, loop or delay command
  p1 ph1
.....
.....
; finish the sampling
  sample
;
; increment the hamiltonian variables
; and start the next run
  ihc
  lo to 1 times l2
exit
;
; specify phases
;
```

```
ph1 = 0
ph2 = 2
```

The command *sample* is used to record the magnetization value. It replaces the command *go=* used in normal pulse programs.

4.4 Show

This command selects the information shown on the display.

- **Time evolution**
Shows the calculated time evolution projected on the sphere. The position of the viewpoint can be changed using the slider on the sides of the drawing area. You can also set the position directly from the *Options* dialog box. The position is defined using the two *Euler angles* ψ and θ . The button *Reset* brings the sphere back to the standard position.
- **Excitation profile**
- **RF profile**
- **Analysis**
- **Waveform**
Show the selected waveform (*SPNAM0*). You may toggle the display between polar and Cartesian (x,y) coordinates (Figure 4.15)..

4.5 Options

This command opens a dialog box, which defines the current position of the viewpoint on the sphere, the step for the sphere rotation and controls the display of hidden lines for the sphere (by default are the hidden lines dashed and dark).

The switch *Background* selects the background color for all graphics in the bloch module. Other windows (pulse program display,...) are not affected.

The units for the frequency axis may also be set here. There are two possibilities:

- **Hz**
The x axis of the excitation profile shows the rf offset in *absolute* units - Hz.

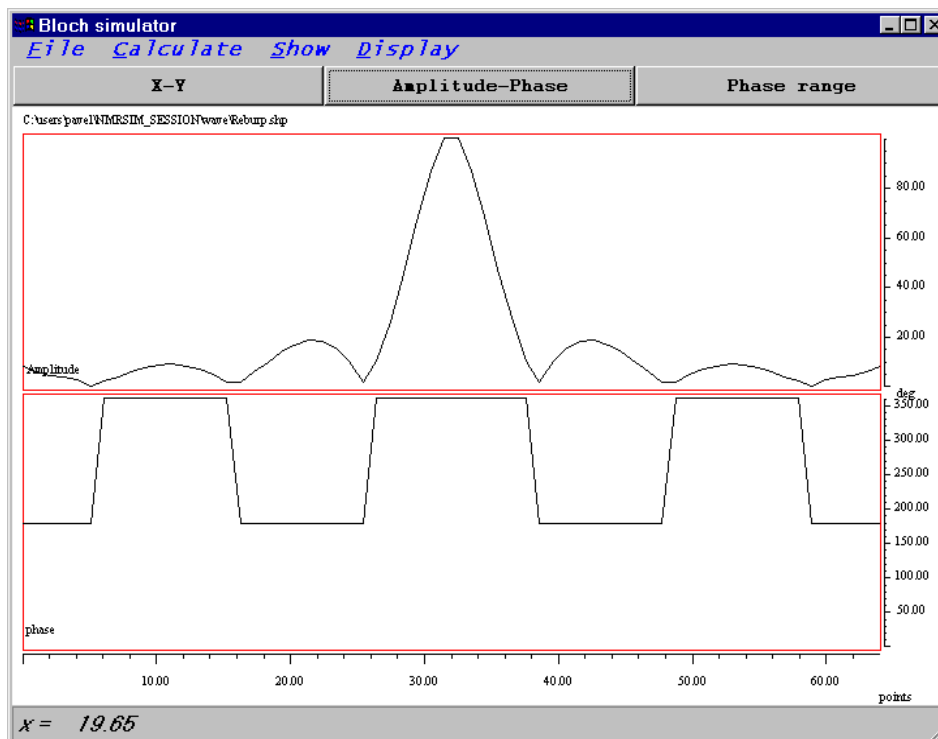


Figure 4.15 Shaped pulse display in NMR-SIM

- **Offset/H1**
The x axis shows the rf offset *relative* to the radio frequency field strength used during the shaped pulse.

4.6 Examples

There are two predefined configuration files which may be used to start your own work with this part of program: *bloch.cfg* and *chirp.cfg*.

Load the configuration saved in the *bloch.cfg* (use the main menu command *File/*

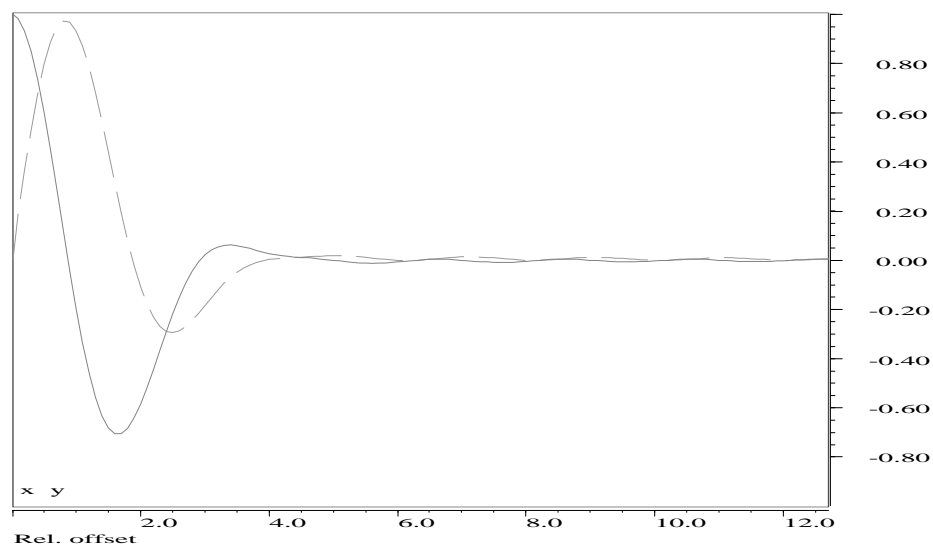


Figure 4.16 The excitation profile of shaped gauss pulse. The M_x and M_y components are shown. The x axis is in relative offset units ω/B_1

Experiment setup/Load from file).

Command *Calculate/Time evolution* shows the trajectories of the magnetization for a gaussian 90 degree pulse. It is not necessary to change any parameters.

The result of command *Calculate/Excitation profile* is on the Figure 4.16. The picture was copied into the MS-WINDOWS clipboard (*File/Copy to clipboard*) and pasted in this document.

The next example shows the behavior of the magnetization vector during composite inverse pulse.

Load the configuration file *bloch.cfg* and change the calculation mode (in *Calculate/Setup*) to *Sequence fragment*.

The command *Calculate/Time evolution* opens a dialog box. The meaning of all parameters is the same as in the previous case. Change the value of the *TSlice* parameter to 10 μ s. The preview of the analyzed pulse program *inverse.seq* is

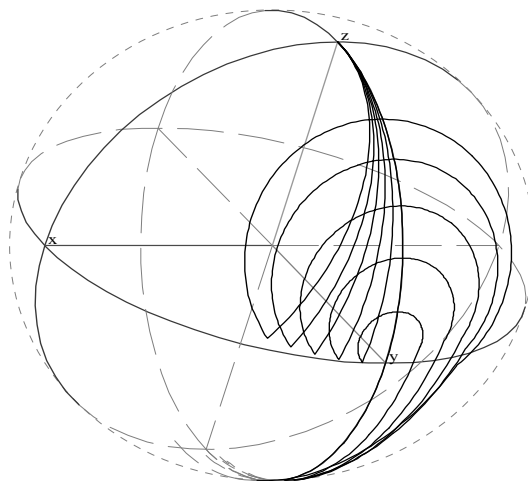


Figure 4.17 The time evolution of magnetization during composite $90_x 240_y 90_x$ pulse.

shown additionally:

```

;NMR-SIM example sequence - 1 3 1 inversion pulse
;avance-version
;
ze
1 sample
p1
p2 ph2
p1
sample
ihc
lo to 1 times 11
exit

```

ph2 = 1

You may use this pulse program fragment as an example for your further development. It is possible to use the command ***Edit/Pulse program*** in the main window to modify it.

The Figure 4.17 shows the result, the self refocusing feature of this pulse is apparent.

The file *chirp.cfg* contains the setup for the phase modulated inverse chirp pulse. The result of the time evolution calculation is on the Figure 4.1.

4.7 Waveform analysis using the TOPSPIN shape tool

Standard tool for the definition of waveforms is the TOPSPIN *Shapetool*. Start it using *stdisp* command on the TOPSPIN command line. You may generate a lot of different waveforms. The Shapetool command ***Analyze/Simulate*** opens the Bloch simulator window and shows the excitation profile of your pulse (Figure 4.18). Each ***Analyze/Simulate*** command opens a new Bloch simulator window.

You may now use all Bloch module functionality to investigate the features of your pulse.

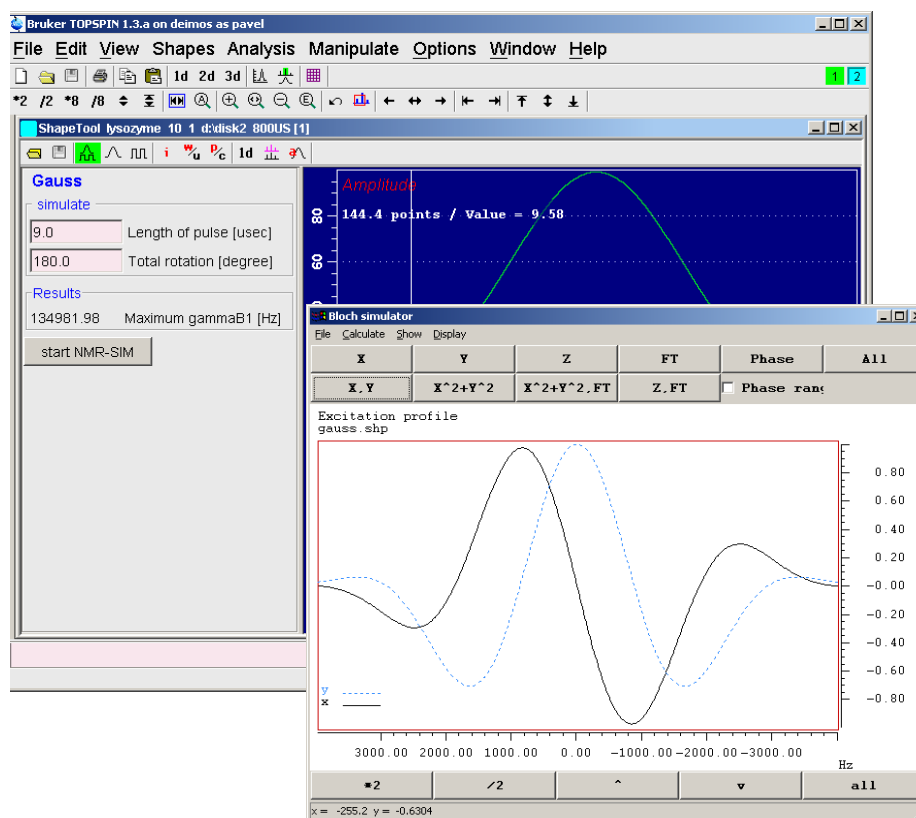


Figure 4.18 TOPSPIN Shape tool and Bloch simulator windows

