Introduction to shaped pulses

Introduction to shaped pulses

Definition:

a 'shaped pulse' is an amplitude modulated RF-pulse

Shaped pulses are not necessarily selective

- they are pulses with a customized bandwidth and behavior

Bandwidth considerations:

- selective excitation/inversion/refocussing of a narrow bandwidth
(e.g. 270^o Gaussian pulse in 1D-COSY, 1D-TOCSY)

- selective excitation / inversion / refocussing of a larger bandwidth
(e.g. G4 pulses for ^{13}C bandselective excitation in HSQC)

- wideband excitation at lowest possible power level
(e.g. CHIRP and WURST decoupling pulses)

Examples of shaped pulses

Classical

Square
Gauss
Sinc
Burp
- e-Burp1
- e-Burp2
- i-Burp1
- i-Burp2
- re-Burp
- u-Burp

Gaussian Cascades
- G4
- G3
- Q5
- Q3

Snob
- e-Snob
- i-Snob2
- r-Snob

Vega
- EVega1
- IVega

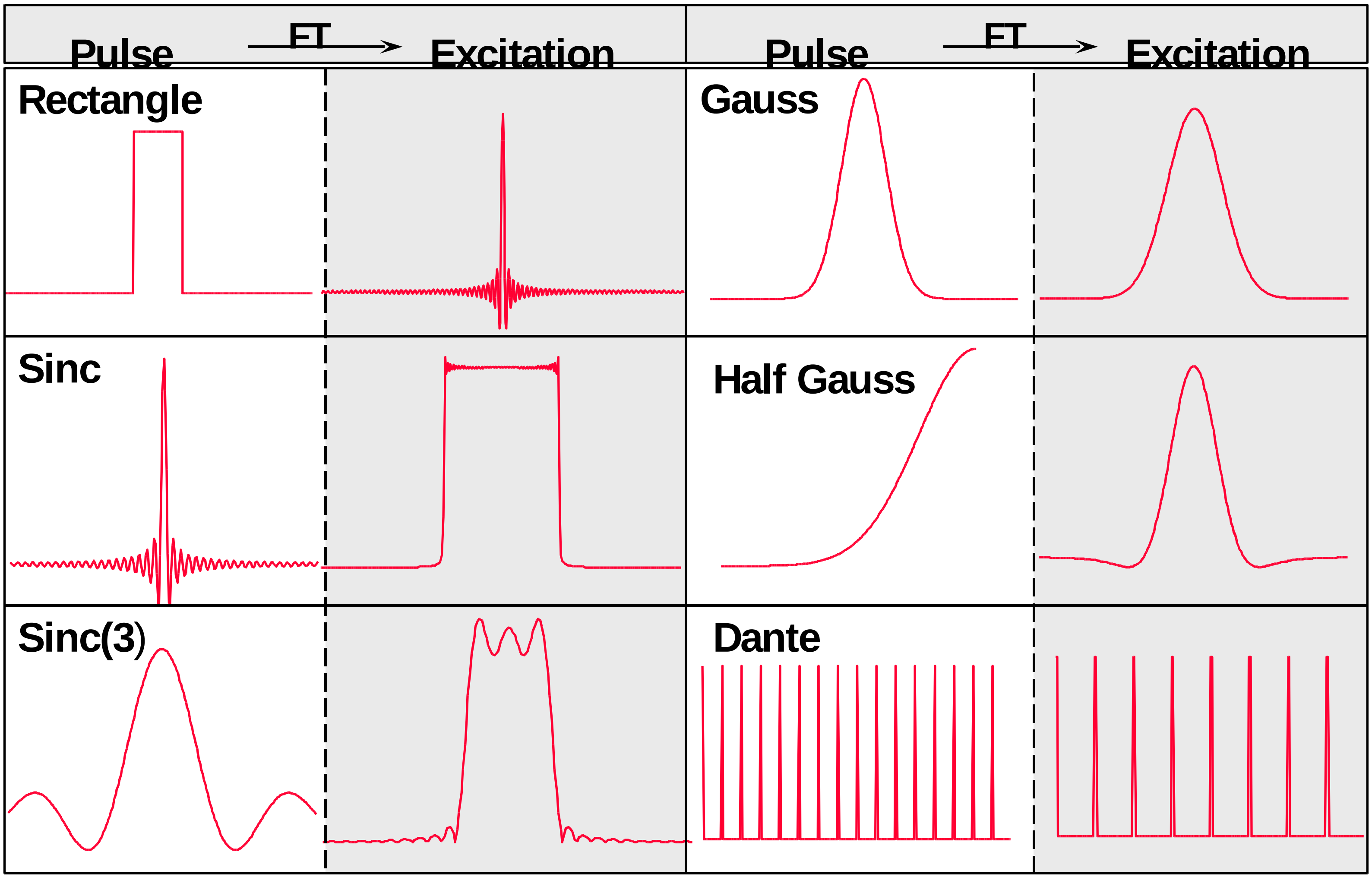
Adiabatic

Hyperbolic Secant
Sine/Cosine
- Smoothed Chirp
- Composite smoothed Chirp
- Wurst

Decoupling Swirl

e=excitation 90°
i=inversion 180°
r=refocusing 180°
u=universal 90°, 180°

Common pulse shapes and their FT

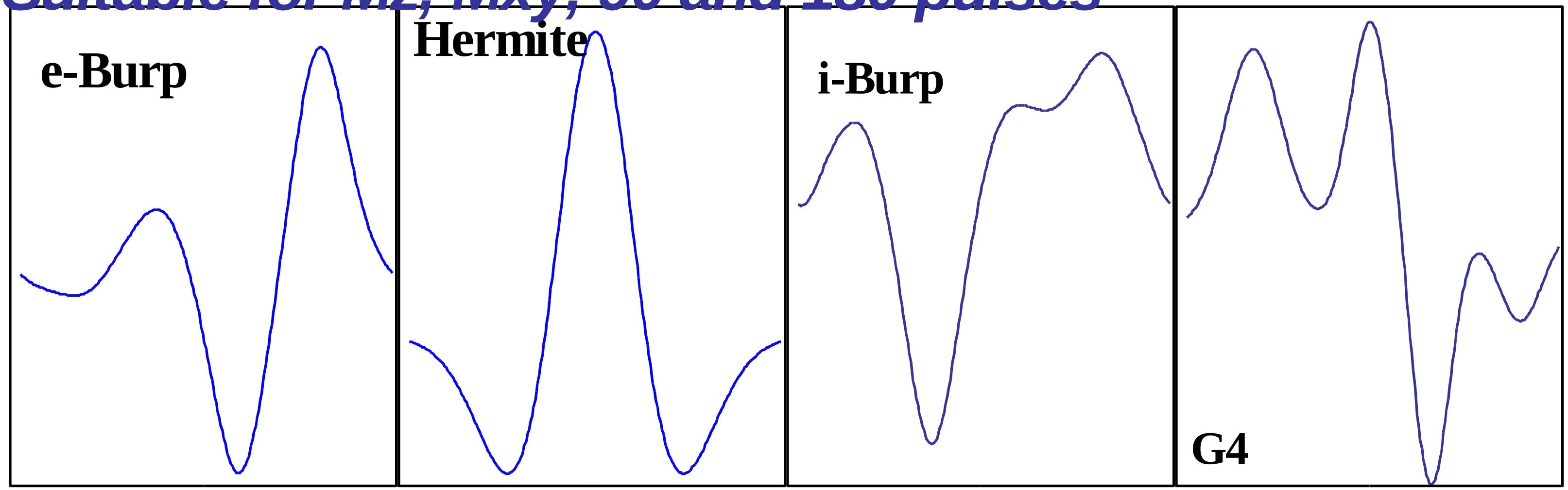


Computer optimized pulse shapes

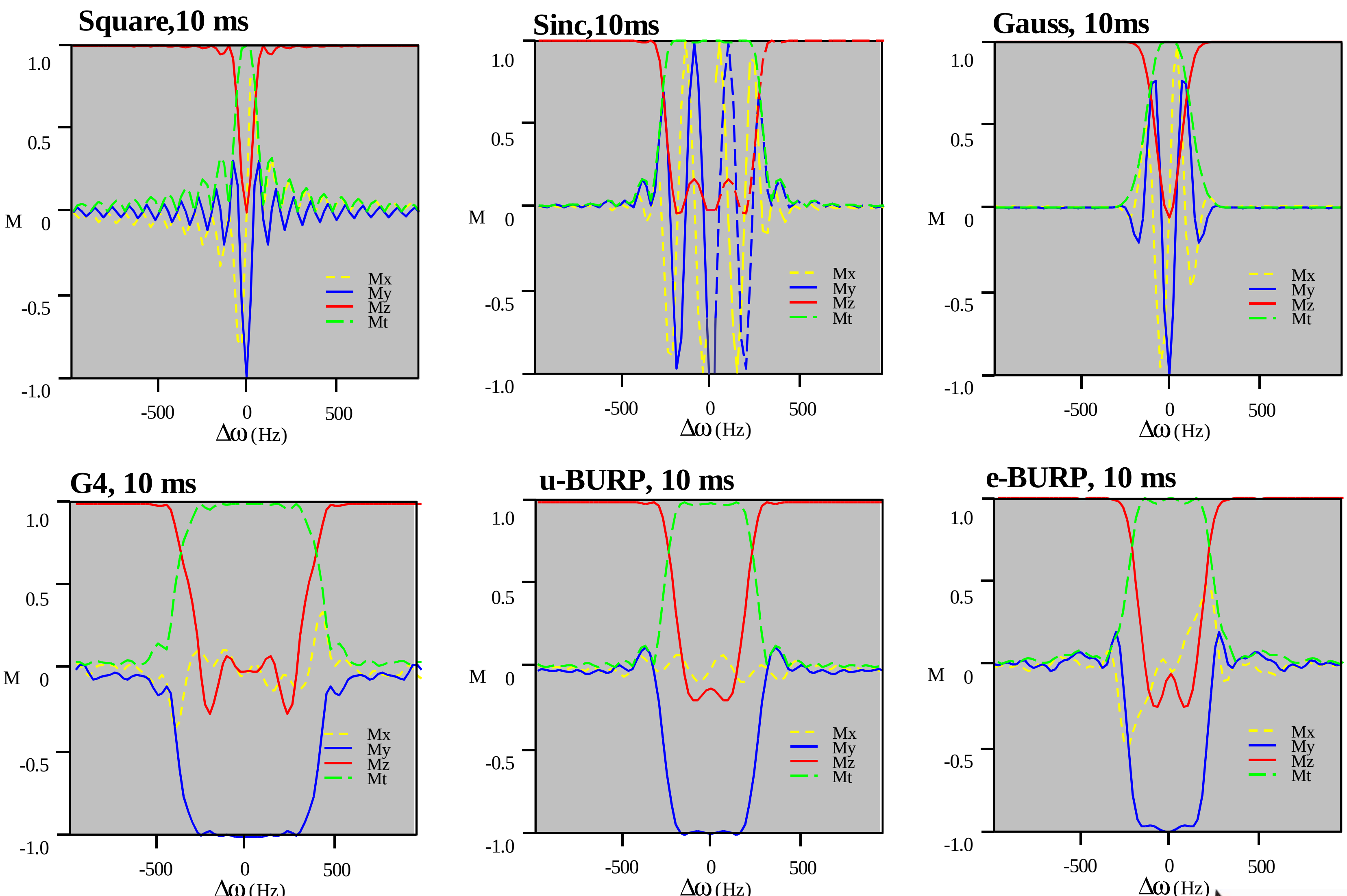
Ideal selective pulse:

- *Selects a rectangular narrow region*
- *Uniform excitation (flat top)*
- *Negligible sidebands*
- *Uniform phase response (self refocussing)*
- *Short time duration (relaxation, J-coupling)*
- *Suitable for Mz, Mxy, 90 and 180 pulses*

Some are highly specialized pulses (single application)

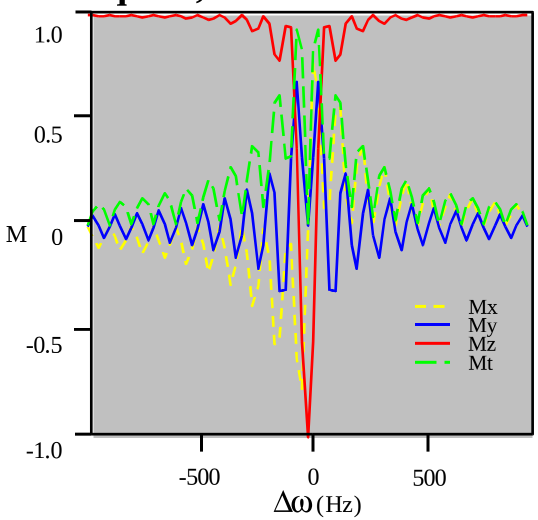


Selective 90 degree pulses

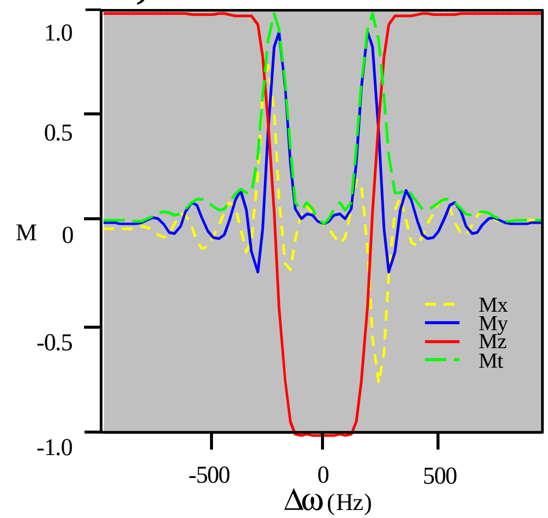


Selective 180 degree pulses

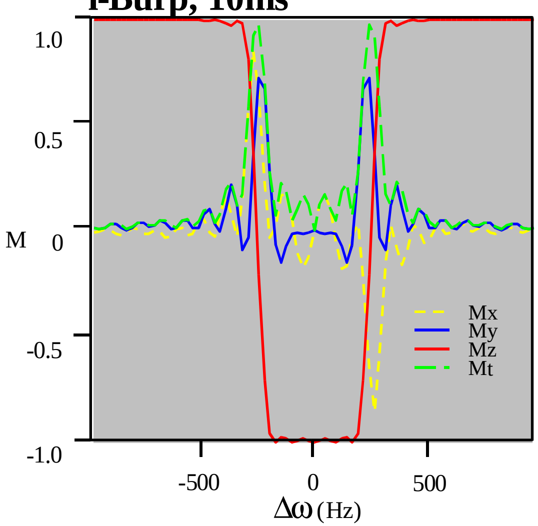
Square, 10 ms



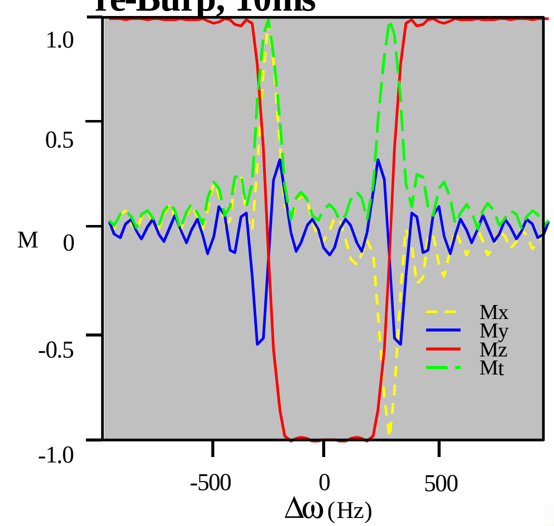
G3, 10 ms



i-Burp, 10ms



re-Burp, 10ms



How to choose
a shaped pulse

Criteria for the selection of best shaped pulse

1) Selectivity

The region of interest should be irradiated as selectively as possible

2) Length

Relaxation and J-evolution might take place during shaped pulses

3) Power

Low integral power or low peak power

4) Phase

Pulse should give pure phase within the region of interest

Selecting a shape

- according to its ´top hat' behaviour (simulated profile):

Excitation

- e-Burp2
- G4
- EVega1

↑ higher priority

Refocussing

- re-Burp
- Q3
- Hermite
- r-Snob
- Sinc (3)
- Gauss
- Hyperbolic Secant
- composite smoothed CHIRP (wideband refocussing)

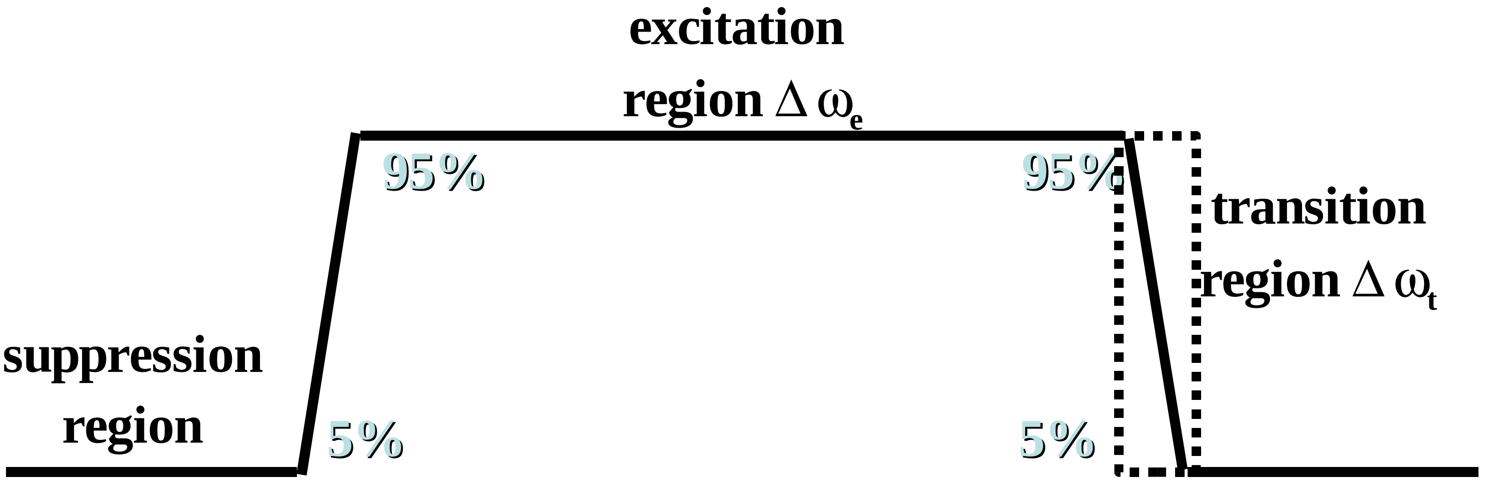
↑ higher priority

Inversion

- G3
- Hyperbolic Secant
- i-Burp2
- i-Snob3
- Hermite
- Sinc (3)
- CHIRP (wideband inversion)

↑ higher priority

The bandwidth parameter $\Delta\omega_e / \Delta\omega_t$



$\Delta\omega_e / \Delta\omega_t$ =excitation region/ transition region

width of excitation	$\Delta\omega_e$
width of transition region	$\Delta\omega_t$
bandwidth	$\Delta\omega$
pulse length	ΔT
peak amplitude	$\gamma B_1 max$

The bandwidth parameter $\Delta\omega_e / \Delta\omega_t$

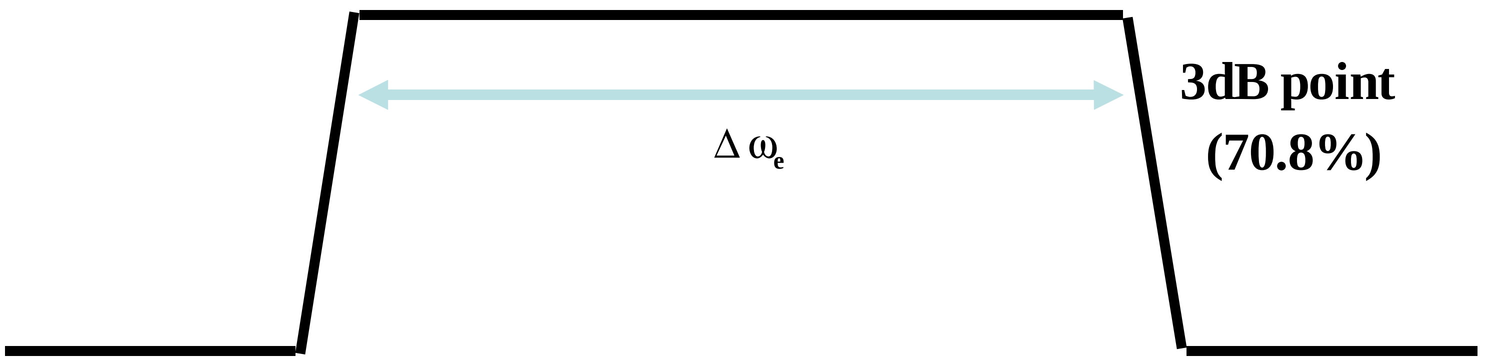
Values for refocussing:

Gauss	0.16
Square	0.38
Sinc (3)	0.41
Sinc (7)	0.92
Hermite	0.97
r-Snob	0.99
G3	1.69
Q3	2.10
re-Burp	3.33
IVega	6.88

higher priority

larger value for $\Delta\omega_e / \Delta\omega_t$ means better selectivity

The bandwidth factor Δω* ΔT



How long the pulse must be to give a certain excitation bandwidth?

width of excitation	$\Delta\omega_e$
width of transition region	$\Delta\omega_t$
bandwidth	$\Delta\omega$
pulse length	ΔT
peak amplitude	$\gamma B_1 max$

The bandwidth factor $\Delta\omega * \Delta T$

Values for refocussing:

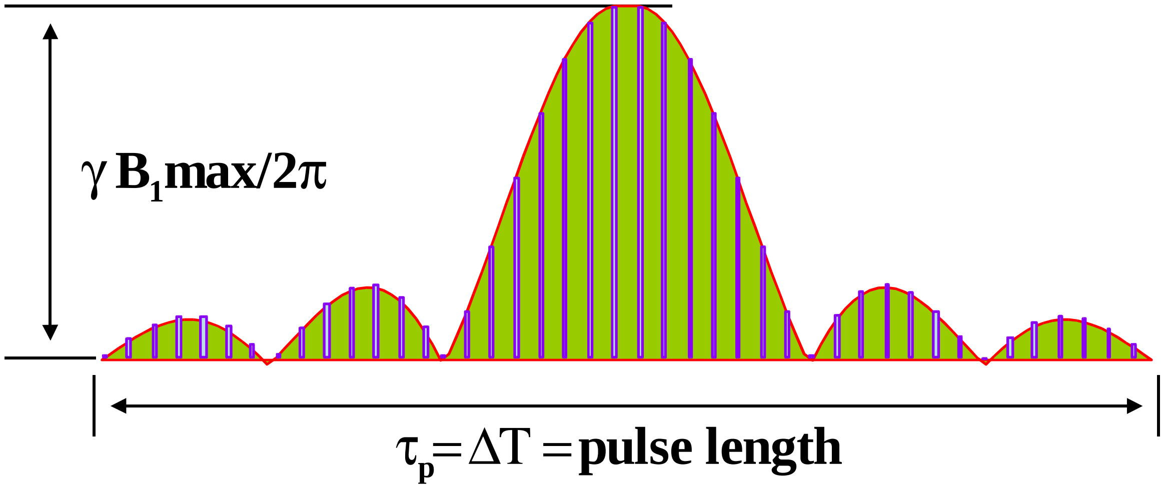
Square		0.75
Gauss		0.88
Hermite	2.24	
r-Snob		2.33
G3		3.42
Q3		3.45
Sinc (3)		4.52
re-Burp		5.81
Sinc (7)		8.66
IVega		9.25

↑ higher priority

smaller value for $\Delta\omega * \Delta T$ means <u>shorter pulse length</u> required for a certain bandwidth

Integral ratio and maximum pulse power

maximum pulse power=γB_1 max (peak amplitude)



Shaped pulse $I = (A_i) * \gamma B_1 max/2\pi * \tau_p$

Square pulse $I = \gamma B_1 max/2\pi * \tau_p$

Maximum pulse power γB_1 max

Values for refocussing 25Hz region (high selectivity, $\Delta\omega$ is constant):

Shape	$\Delta\omega_e / \Delta\omega_t$	pulse length [ms]	$\gamma B_1 max/2\pi$ [Hz]
Sinc (3)	0.41	180.8	15.6
IVega	6.88	369.6	16.6
Square	0.38	30.0	16.7
Sinc (7)	0.92	346.0	19.7
Q3	2.10	138.0	23.9
r-Snob	0.99	93.2	25.1
G3	1.69	136.8	26.2
re-Burp	3.33	232.4	26.9
Hermite	0.97	89.6	30.4
Gauss	0.16	35.2	34.5

↑ Less power

Maximum pulse power γB_1 max

Values for refocussing 25Hz region (high selectivity, $\Delta\omega$ is constant):

Shape	$\Delta\omega_e / \Delta\omega_t$	pulse length [ms]	$\gamma B_1 max/2\pi$ [Hz]
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re-Burp	3.33	232.4	26.9
Hermite	0.97	89.6	30.4
Gauss	0.16	35.2	34.5

Less power

Comparison of the best pulses

for band-selective excitation

Shape	$\Delta\omega_e / \Delta\omega_t$ selectivity	$\Delta\omega * \Delta T$ length	$\gamma B_1 max/2\pi$ [Hz] (25Hz region) power
re-Burp	3.33	5.81	26.9
Q3	2.10	3.45	23.9
Hermite	0.97	2.24	30.4
r-Snob	0.99	2.33	25.1
Sinc (3)	0.41	4.52	15.6

hoose either re-Burp or Q3 as a good refocussing pulse:

re-Burp: *advantage: more selective*
disadvantage: longer pulse length, more power

Q3 *advantage: shorter pulse, less peak power*
disadvantage: less selective

3. Introduction to adiabatic pulses

Properties of adiabatic pulses

1) Insensitive to B_1 inhomogeneity

- magnetization can be 'picked up' , excited or inverted in coil regions of reduced B_1 homogeneity

- increased signal-to-noise can be expected

2) Wide inversion bandwidth

- HSQC / DEPT experiments: solving the problem of ^{13}C pulse offset effects

- CHIRP95 and WURST decoupling: less power or wider decoupling range

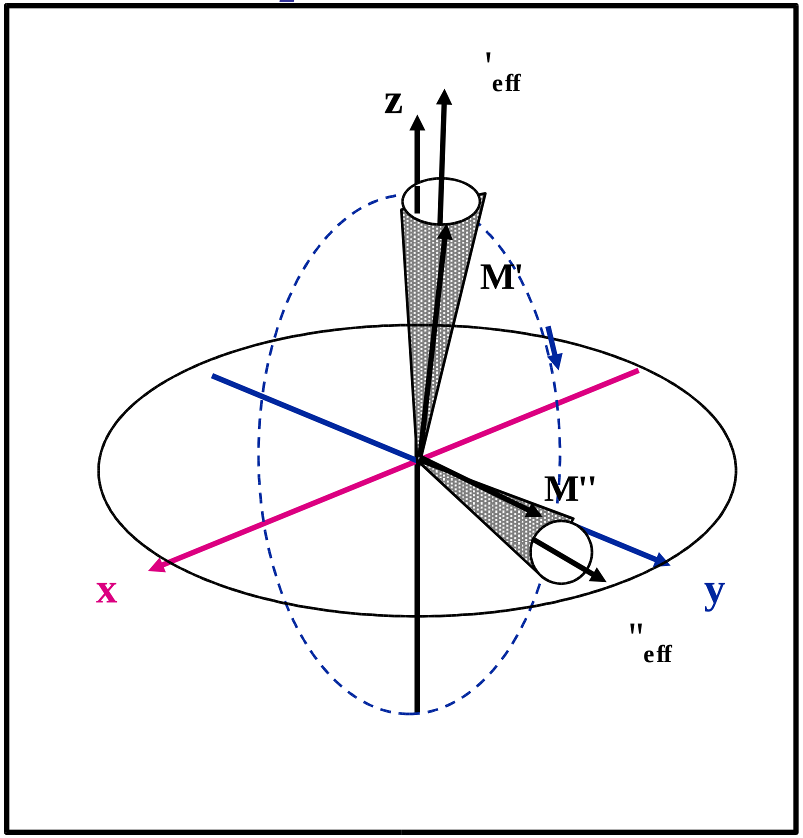
3) Insensitive to power missettings

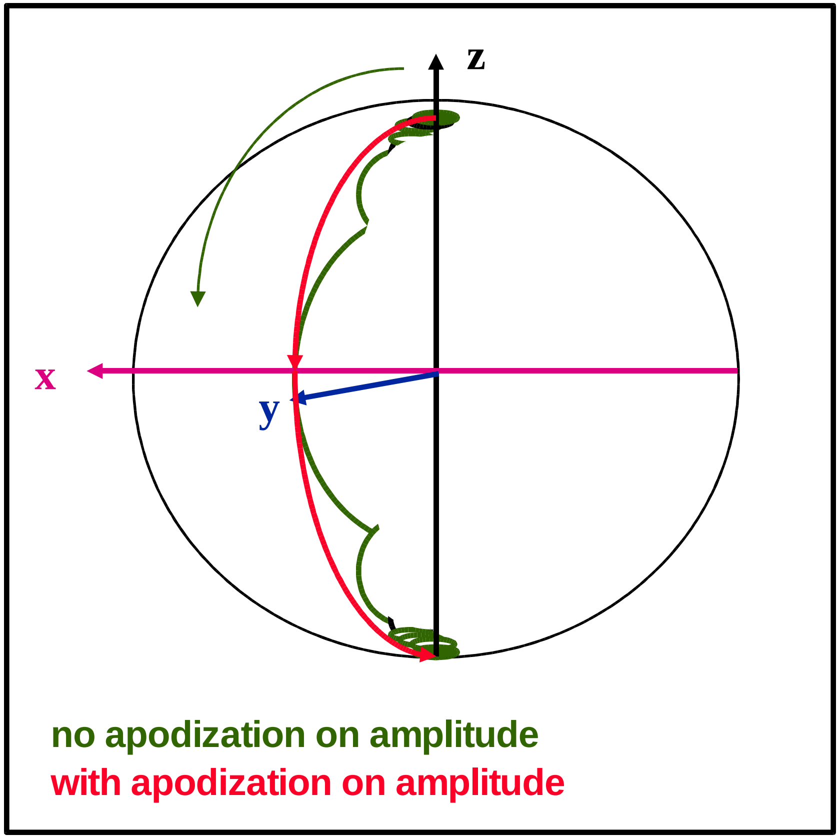
- threshold of minimum and maximum RF field where pulses are adiabatic

Note: Adiabatic 180-degree pulses discussed only

The adiabatic rotation

Schematic representation of movement of magnetization along the effective B_1 field during an adiabatic pulse





a) magnetization M during an adiabatic pulse, no apodization on amplitude

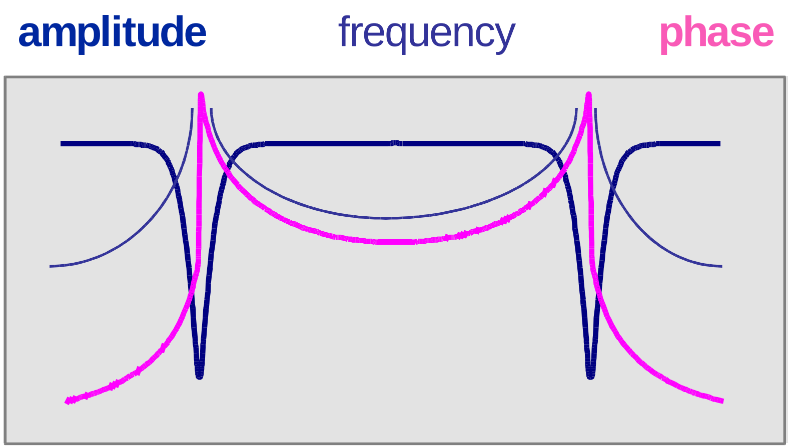
b) trajectory of M on a sphere during an adiabatic pulse

The adiabatic condition

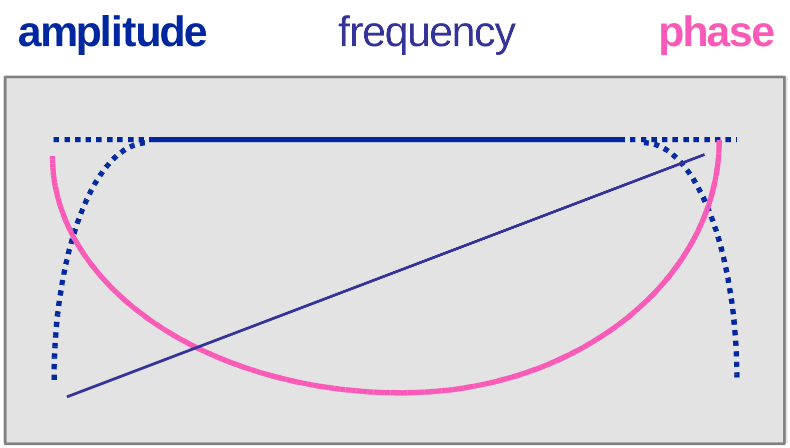
The adiabatic condition:

ω / γ **Bo << 1**

The adiabatic pulse:
- ***'rapid passage' of frequency***
- ***quasi parabolic phase change***
- ***magnetization 'spin-locked' during pulse***



BIR-4 pulse:
'apodization' of amplitude
off-resonance: fast frequency change
on-resonance: slow frequency change



CHIRP pulse:
optional 'apodization' of amplitude
constant frequency sweep
quasi-parabolic phase change
NOTE: SLP-pulses have constant phase change

BRUKER BIOSPIN

Adiabatic inversion pulses

Shape	$\Delta\omega_e / \Delta\omega_t$ selectivity	$\Delta\omega * \Delta T$ length	$\gamma B_1 max * \Delta T$ power*length
sm. CHIRP (30%)	2.81	29.16	6.18
sm. CHIRP (10%)	1.49	29.52	6.18
wurst (n=20)	2.16	28.26	6.18
power h. secant (n=8)	2.33	34.10	6.94
sincos	4.57	35.12	7.71
power wurst (n=2)	5.48	36.70	10.1

↑ higher priority

∴All these pulses are quite similar

Working with adiabatic pulses

Which shape?

CHIRP and WURST are the most common adiabatic pulses

What are the typical parameters?

for inversion: smoothed CHIRP

0.5ms, 20% smoothing, 60-80kHz sweep

for refocussing: composite smoothed CHIRP

2ms, 20% smoothing, 60-80kHz sweep

CHIRP-decoupling: smoothed CHIRP

1.5ms, 20% smoothing, 18-40kHz sweep

use decoupling program p5m4sp180

Working with adiabatic pulses

Should all 180° pulses in HSQC be substituted by adiabatic pulses?

organic molecules: CHIRP's for refocussing and inversion
^{13}C labeled proteins: CHIRP's for inversion only

What is the difference between smoothed CHIRP and composite smoothed CHIRP?

smoothed CHIRP: use for inversion only
comp. Sm. CHIRP: can be used for inversion and refocussing

Some ¨rules of thumb¨ for adiabatic pulses

How to calibrate an adiabatic pulse?

ShapeTool -> analyse -> „integrate adiabatic shape“

Power level for ^{13}C 0.5ms smoothed CHIRP and

^{13}C 2ms composite smoothed CHIRP ?

corresponds to 25 μsec ^{13}C pulse

adiabaticity Q-factor : 5 full adiabaticity

Power level for 1.5ms smoothed CHIRP 18-40kHz in CHIRP95 decoupling?

use GARP power level + 2-6 dB

adiabaticity Q-factor : 2-3 is sufficient (additional averaging due to the supercycles in the decoupling program)

Adiabatic pulses

1) Adiabatic pulses are included in XWIN-NMR, e.g.

- Crp60,0.5.20.1   for inversion
- Crp60comp.4   for refocussing

2) Many experiments are written with adiabatic pulses

3) Power of adiabatic pulses directly from ShapeTool

„integrate adiabatic pulse“ - option

Adiabatic inversion pulse

Crp60,0.5.20.1

size of shape	*1000*
total sweep-width	*60000*
length of pulse	*500*
% to be smoothed	*20*
low to high field	*-1*

power = same as 25us hard pulse

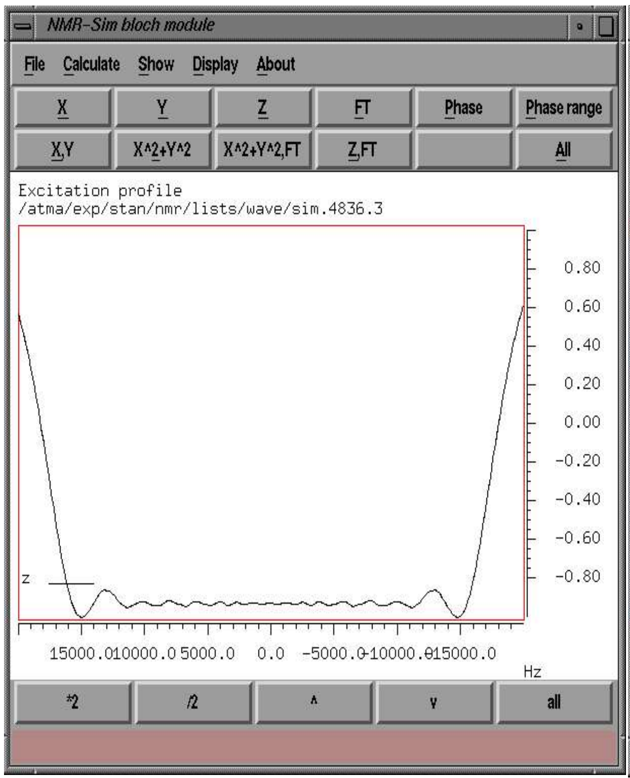
ShapeTool -> analyse-> integrate adiabatic shape
select Q-factor=5

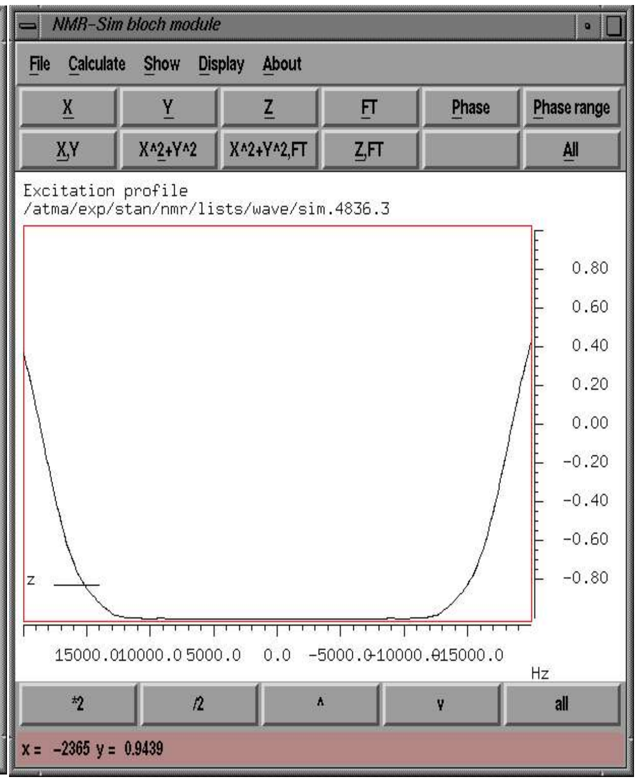
Simulation of inversion behaviour

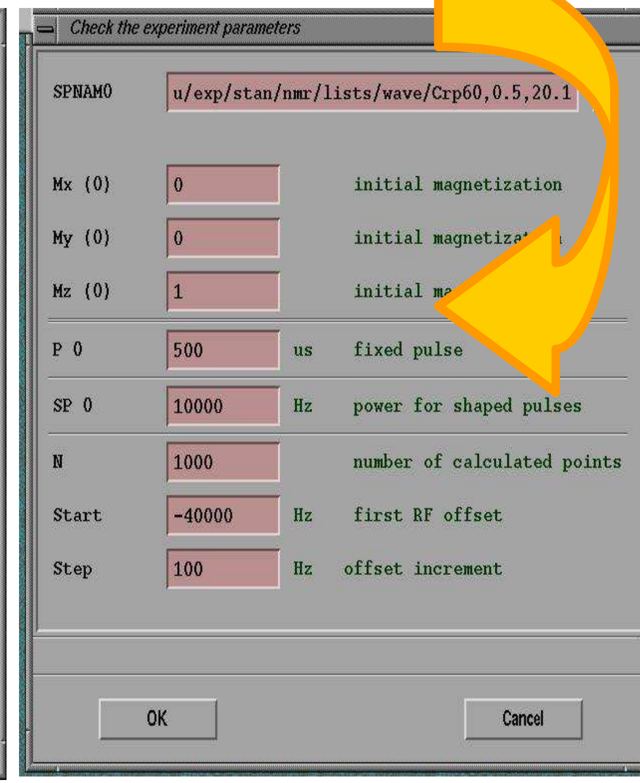
ShapeTool -> Analyse -> Simulate

power level=same as 25us hard pulse

power: 1/(4*0.000025s)=10000Hz







low adiabaticity
(Q-factor~2-3)

high adiabaticity
(Q-factor=5)

Adiabatic refocussing

Crp60comp.4

size of shape	*1000*
total sweep-width	*60000*
length of basic unit	*500*
% to be smoothed	*20*
low to high field	*-1*

length of pulse	*2000us*

power level= 25us hard pulse

ShapeTool -> analyse-> integrate adiabatic shape

select Q-factor = 5

Create a pulse for adiabatic decoupling

Crp40,1.5.20.1

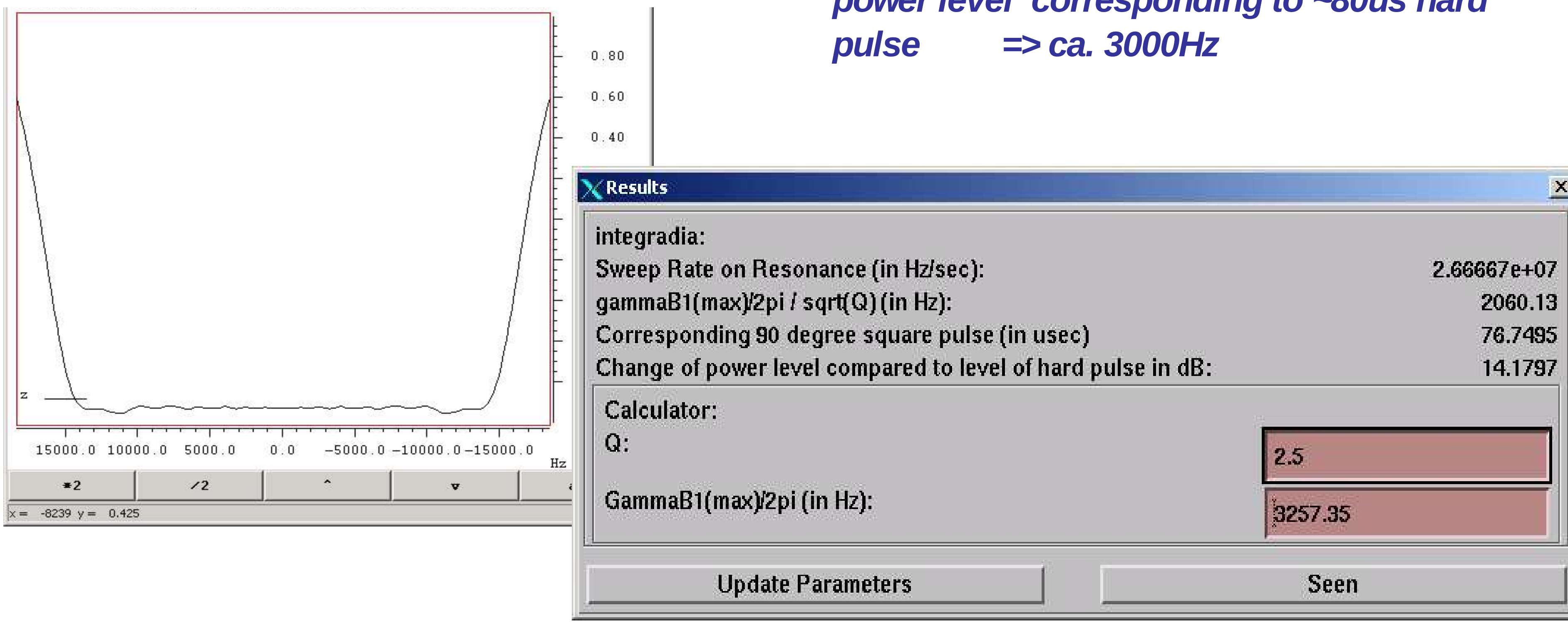
size of shape	*1000*
total sweep-width	*40000*
length of pulse	*1500*
% to be smoothed	*20*
low to high field	*-1*

cpd-program p5m4sp180

sweep-width (decouples ~80% of40 000Hz)

length of pulse 1500us

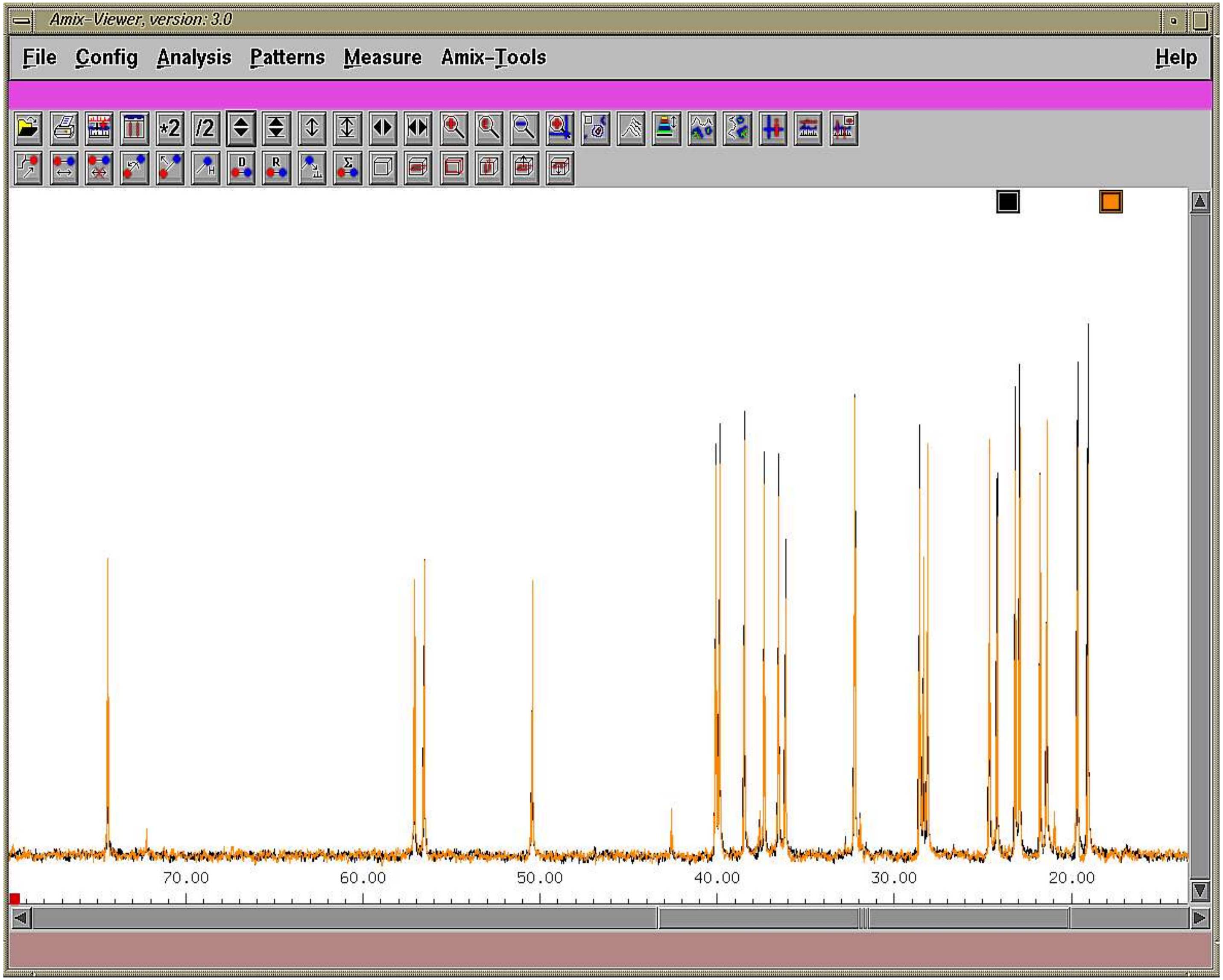
power level corresponding to ~80us hard pulse => ca. 3000Hz



ShapeTool: analyse-> integrate adiabatic shape

select Q-factor= 2-3 sufficient (supercycles!)

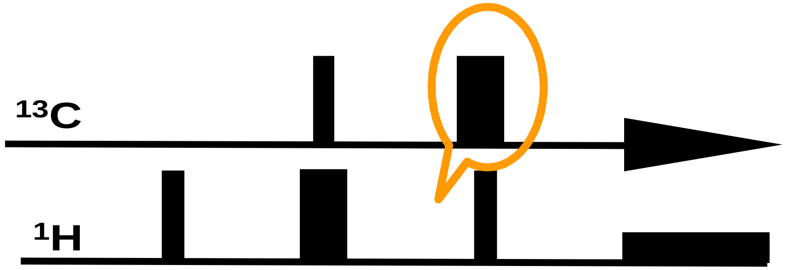
Adiabatic refocusing pulse in DEPT



yellow = standard DEPT45

black = DEPT45 with adiabatic inversion

Adiabatic refocusing pulse in DEPT



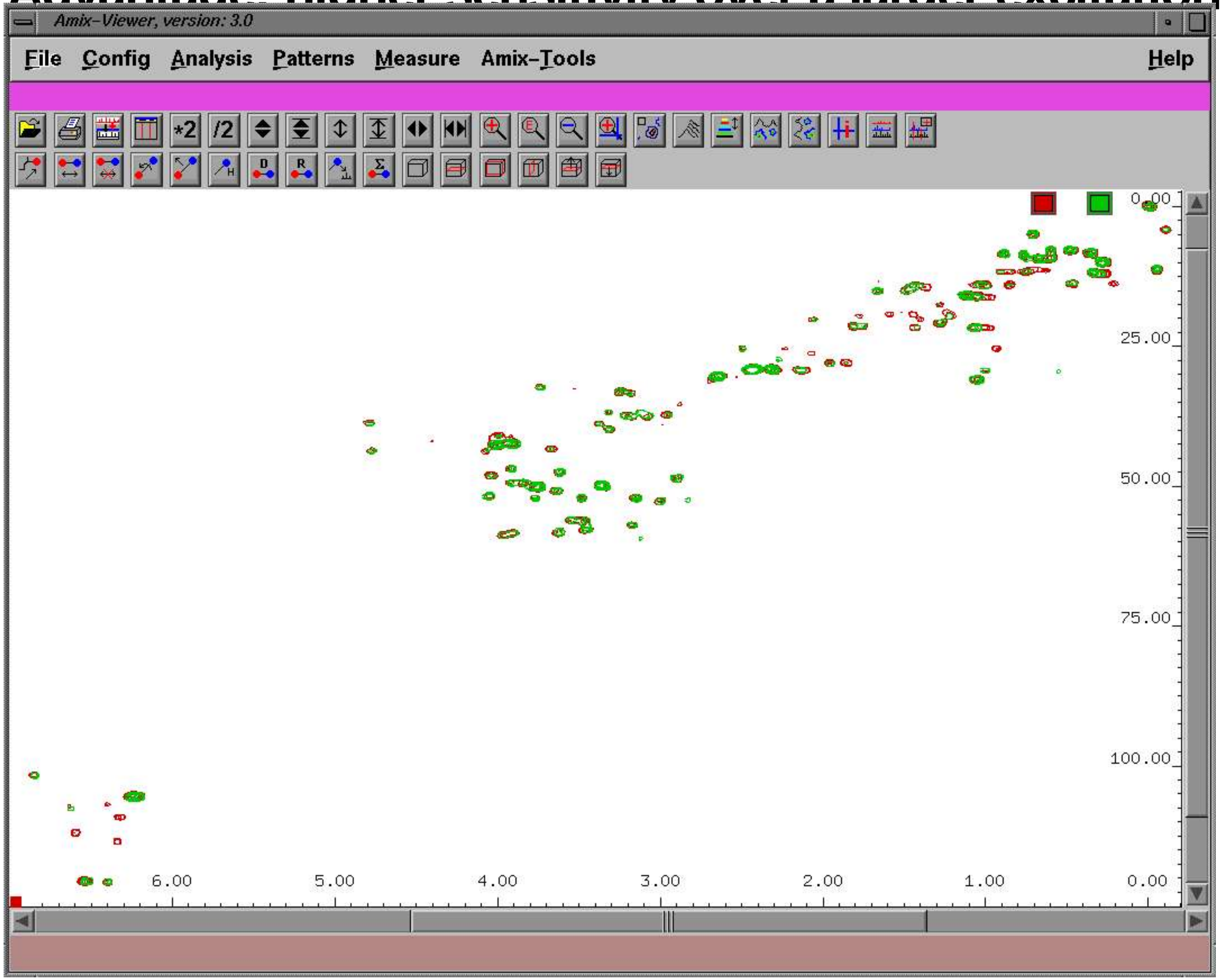
Refocusing pulse
Crp60comp.4

Adiabatic refocussing pulse in DEPT experiments:

pulprog	deptsp45 / deptsp90 / deptsp135
spnam2	Crp60comp.4
sp2	power level corresponding to 25us 90°-^{13}C-pulse
p12	2000us

Adiabatic pulses in ^{13}C-HSQC

Advantage: higher sensitivity over a larger excitation bandwidth



green = standard HSQC

red = HSQC with adiabatic inversion

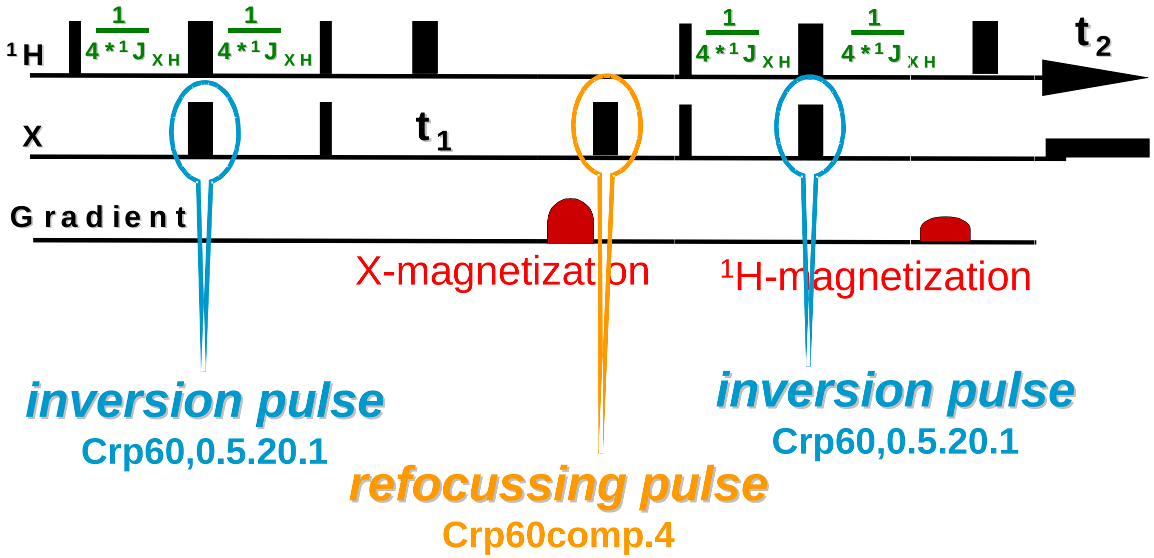
Adiabatic pulses in ^{13}C-HSQC

Two options:

1) hsqcetgpsp with adiabatic inversion
(proteins, ^{13}C labeled)

2) hsqcetgpsp.2 with adiabatic inversion and refocussing
(^{13}C at natural abundance)

HSQC with gradients



Adiabatic pulses in ^{13}C-HSQC

^{13}C labeled - only adiabatic inversion:

pulprog	hsqcetgpsisp
spnam3	Crp60,0.5.20.1
sp3	power level corresponding to 25us 90°-^{13}C-pulse
p14	500us

non labeled - adiabatic inversion und refocussing:

pulprog	hsqcetgpsisp.2
spnam3	Crp60,0.5.20.1
sp3	power level corresponding to 25us 90°-^{13}C-pulse
p14	500us
spnam7	Crp60comp.4
sp7	power level corresponding to 25us 90°-^{13}C-pulse
p24	2000us

Adiabatic decoupling programs

/NMRhome/exp/stan/nmr/lists/cpd/p5m4sp180

Note: this cpd-program uses sp15

cpdprg2	***p5m4180***
pcpd2	***1500us***
spnam15	***Crp40,0.5.20.1***
sp15	***power (with Q-factor 2-3)***
pl12	***= sp15***

```
#setphase
1 pcpd:sp15:0
  pcpd:sp15:150
  pcpd:sp15:60
  pcpd:sp15:150
  pcpd:sp15:0
  pcpd:sp15:0
  pcpd:sp15:150
  pcpd:sp15:60
  pcpd:sp15:150
  pcpd:sp15:0
  pcpd:sp15:180
  pcpd:sp15:330
  pcpd:sp15:240
  pcpd:sp15:330
  pcpd:sp15:180
  pcpd:sp15:180
  pcpd:sp15:330
  pcpd:sp15:240
  pcpd:sp15:330
  pcpd:sp15:180
  jump to 1
```

Adiabatic bilevel decoupling programs

/NMRhome/exp/stan/nmr/lists/cpd/
bi_p5m4sp_4pl

- this cpd-program uses sp15

cpdprg2	***bi_p5m4sp_4pl***
pcpd2	***1500us***
spnam15	***Crp40,0.5.20.1***
sp15	***power at Q-factor 2-3***
pl30	***= sp15***
pl31	***= sp15 minus 6dB***

Note - use synchronous mode, cpd2s:f2

```
#setphase
bilev "l31=(nsdone+ds)%4+1"
1 pcpd*0.5:0 pl=pl31
  lo to 1 times l31
2 pcpd:sp15:0 pl=pl30
  pcpd:sp15:150
  pcpd:sp15:60
  pcpd:sp15:150
  pcpd:sp15:0
  pcpd:sp15:0
  pcpd:sp15:150
  pcpd:sp15:60
  pcpd:sp15:150
  pcpd:sp15:0
  pcpd:sp15:180
  pcpd:sp15:330
  pcpd:sp15:240
  pcpd:sp15:330
  pcpd:sp15:180
  pcpd:sp15:180
  pcpd:sp15:330
  pcpd:sp15:240
  pcpd:sp15:330
  pcpd:sp15:180
```