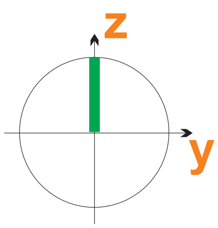
Nutation of Magnetization: *p1/pw*[†] *Array*

0°



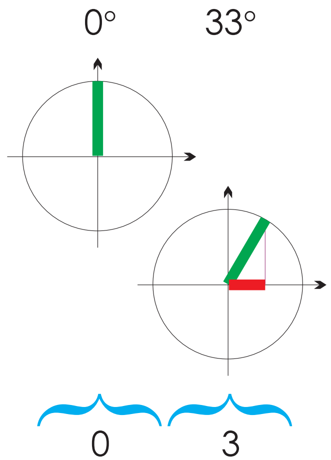
0

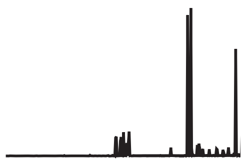
For p1/pw=0, the magnetization, **M**, is left along the +z axis (presuming sufficient time is allowed for longitudinal relaxation).

NMR spectrometers detect only magnetization transverse to the polarization (z) direction.

[†]**Bruker uses p1, Agilent uses pw**

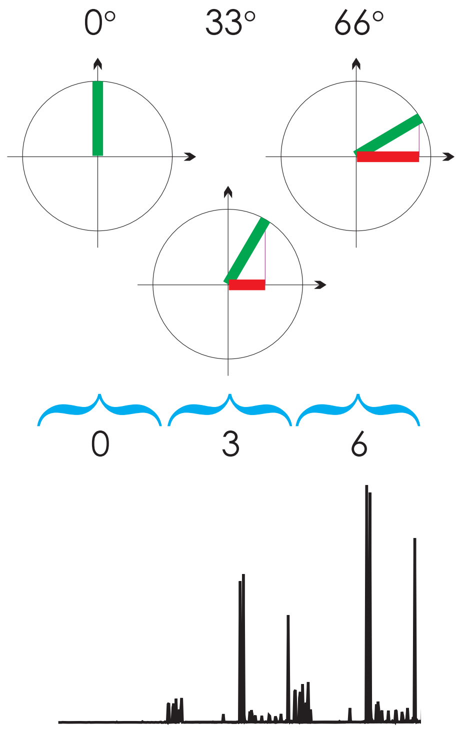
Nutation of Magnetization: *pw Array*





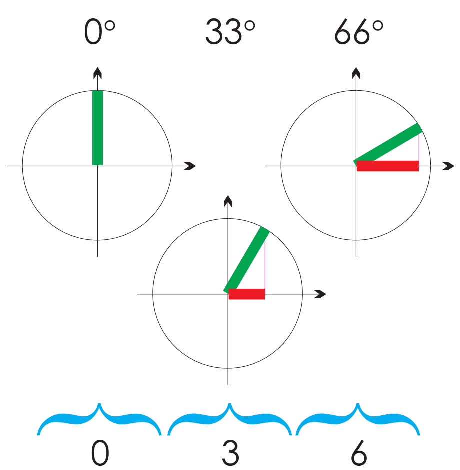
When pw = pw90/3 = 33°, we observe the transverse (**y**) component which equals sin(33°)×**M** = 0.54×**M**.

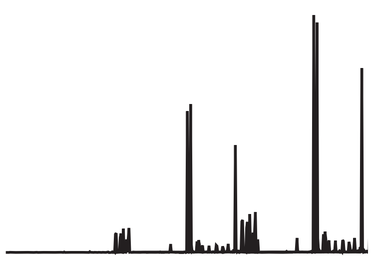
Nutation of Magnetization: *p1 Array*



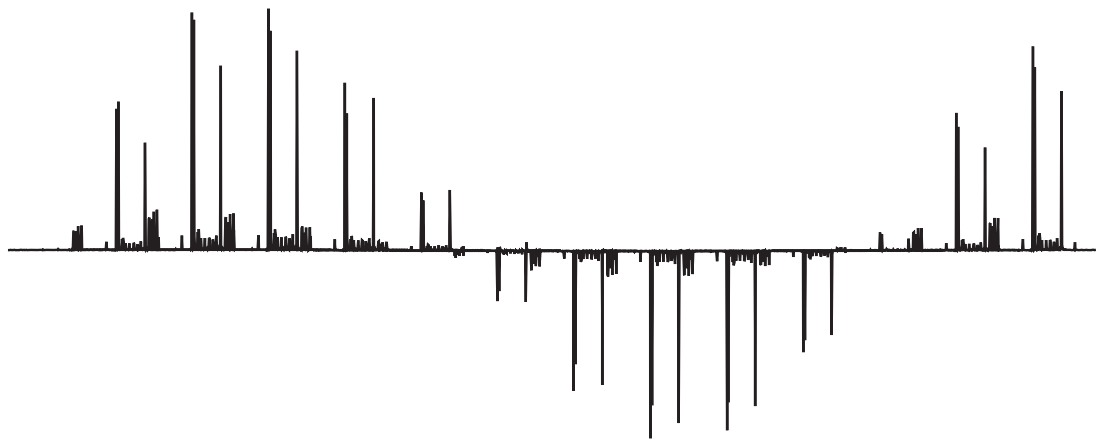
Now sin(66°) = 0.9. The horizontal stack (popt / dssh) pattern of intensities will be sinusoidal.

Nutation of Magnetization: *pw Array*

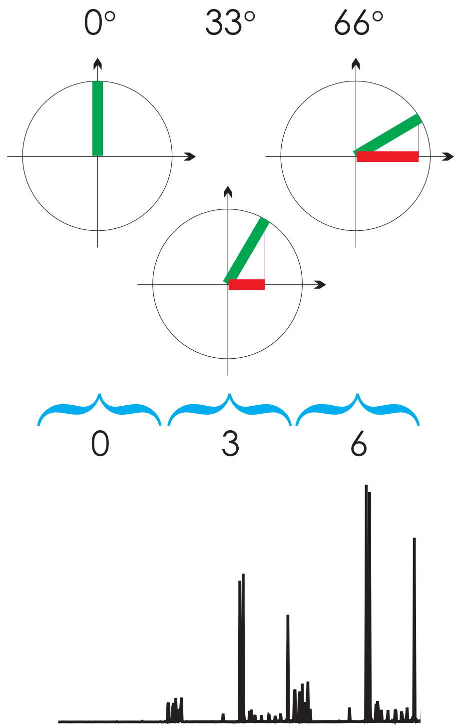




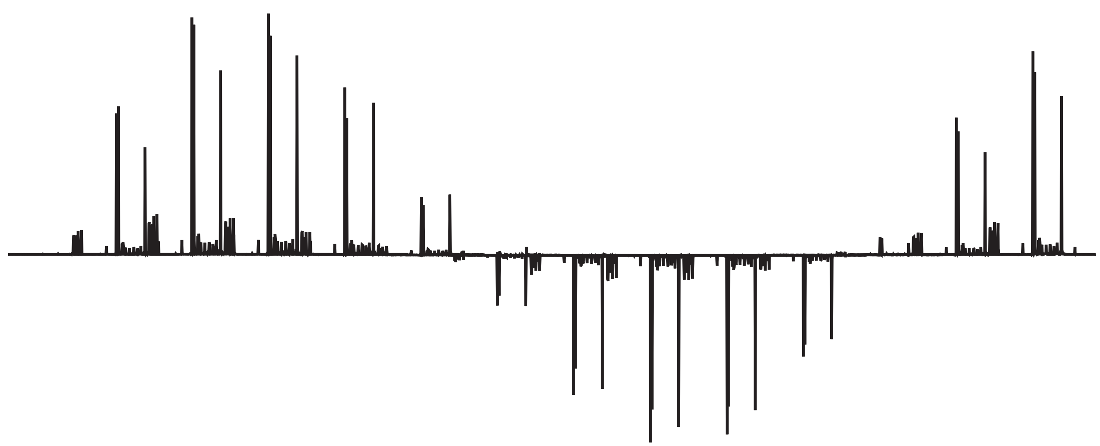
As the nutation angle is increased, the popt / dssh pattern of intensities should be sinusoidal.



Nutation of Magnetization: *p1/pw Array*

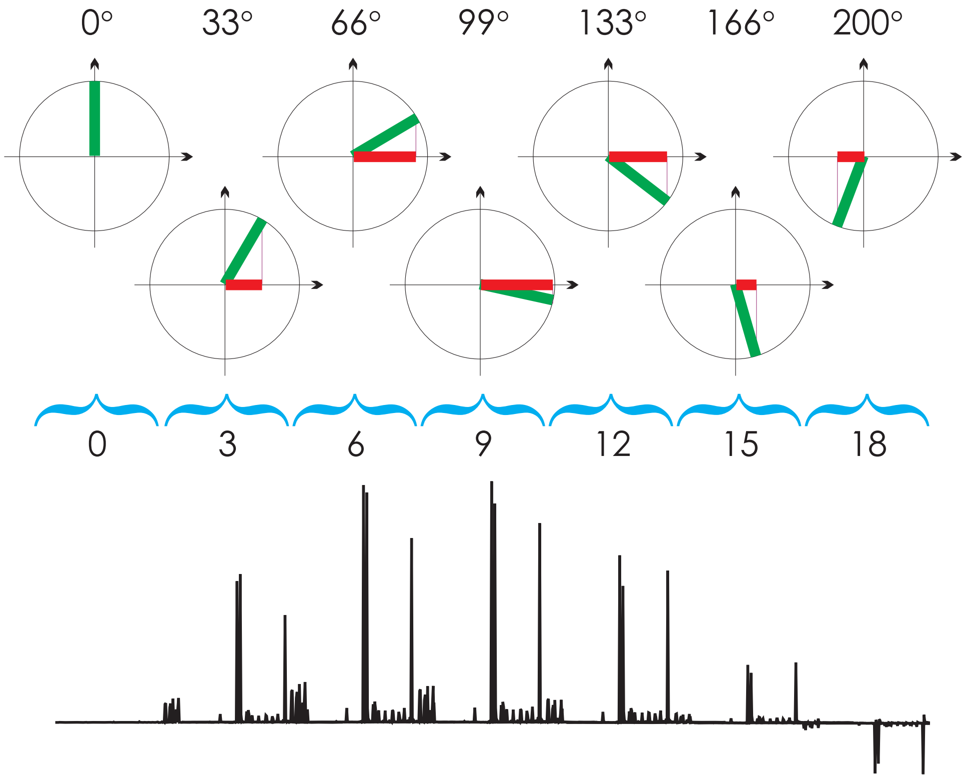


Now sin(66°) = 0.9. The dssh pattern of intensities should be sinusoidal.



If the popt / dssh pattern is highly non-sinusoidal:
check probe definition / tuning and plw1 / tpwr.
The most common reason, however, is too fast a repetition in running thru the array: increase d1.

Nutation of Magnetization: *p1 Array*

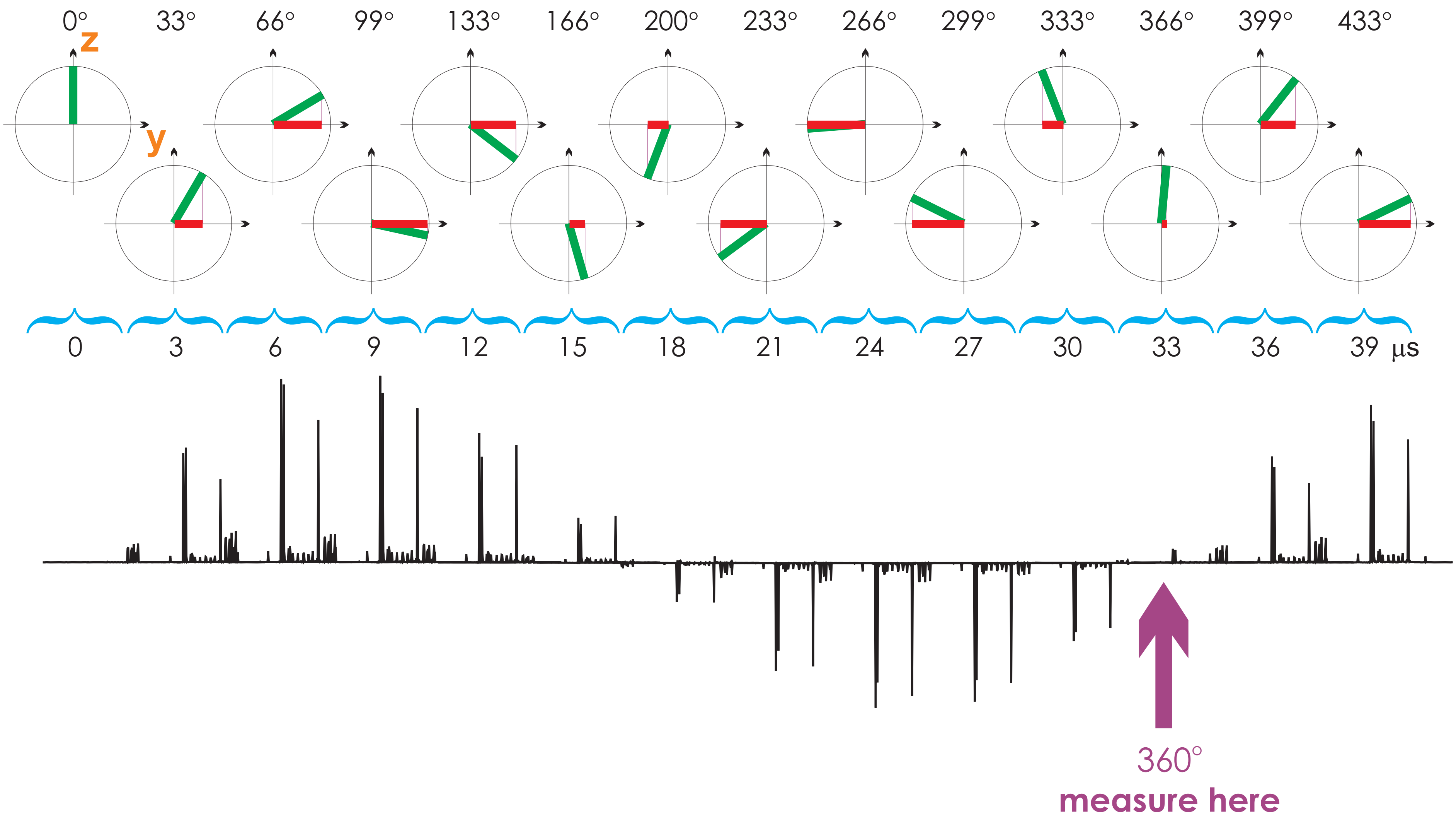


When p1 = 180°, **M** is along the –**z** axis. For slightly longer pw, the transverse component, **sin(θ)×M** is along the –**y** axis.

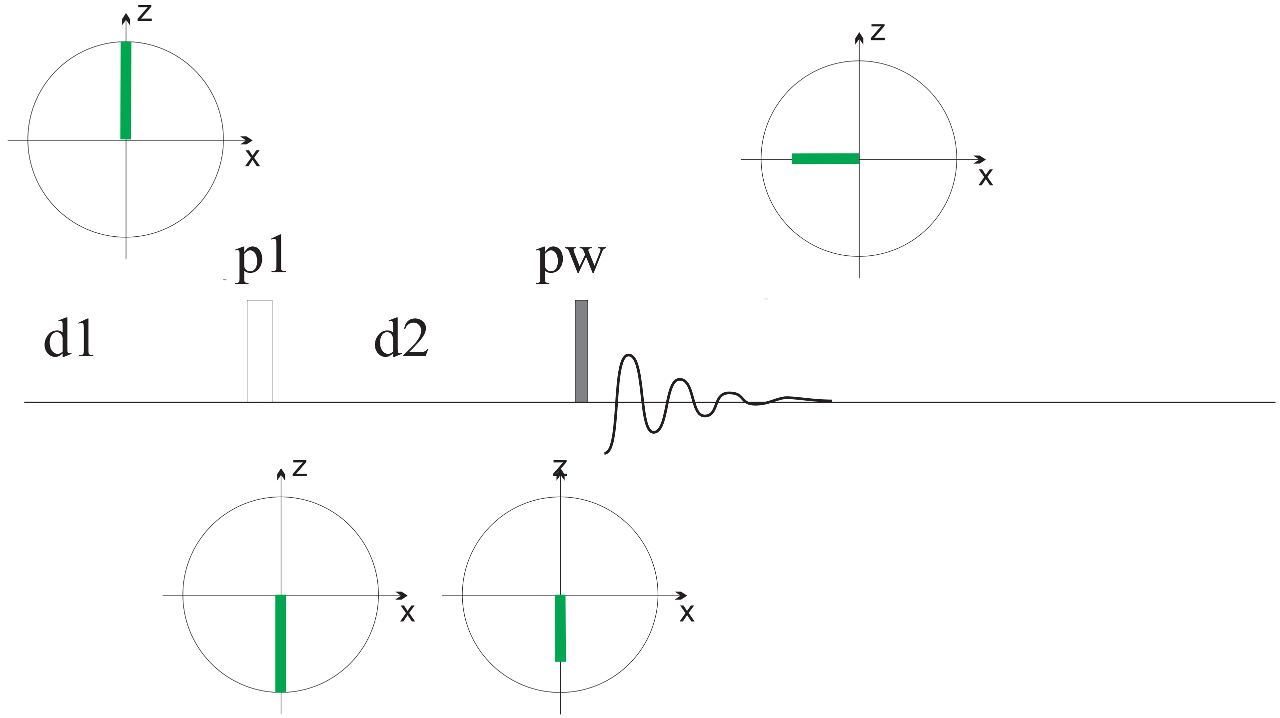
This + to - crossover is simple to observe, but **M** is far from equilibrium. This part of the arrayed experiment is the most sensitive to repetition rate (d1+aq) [the crossover here will tend toward larger values].

When p1 = 360°, d1 has the least effect, so we use that crossover instead.

Nutation of Magnetization: *p1/pw Array*



Relaxation in NOE Expts: T_1 Array



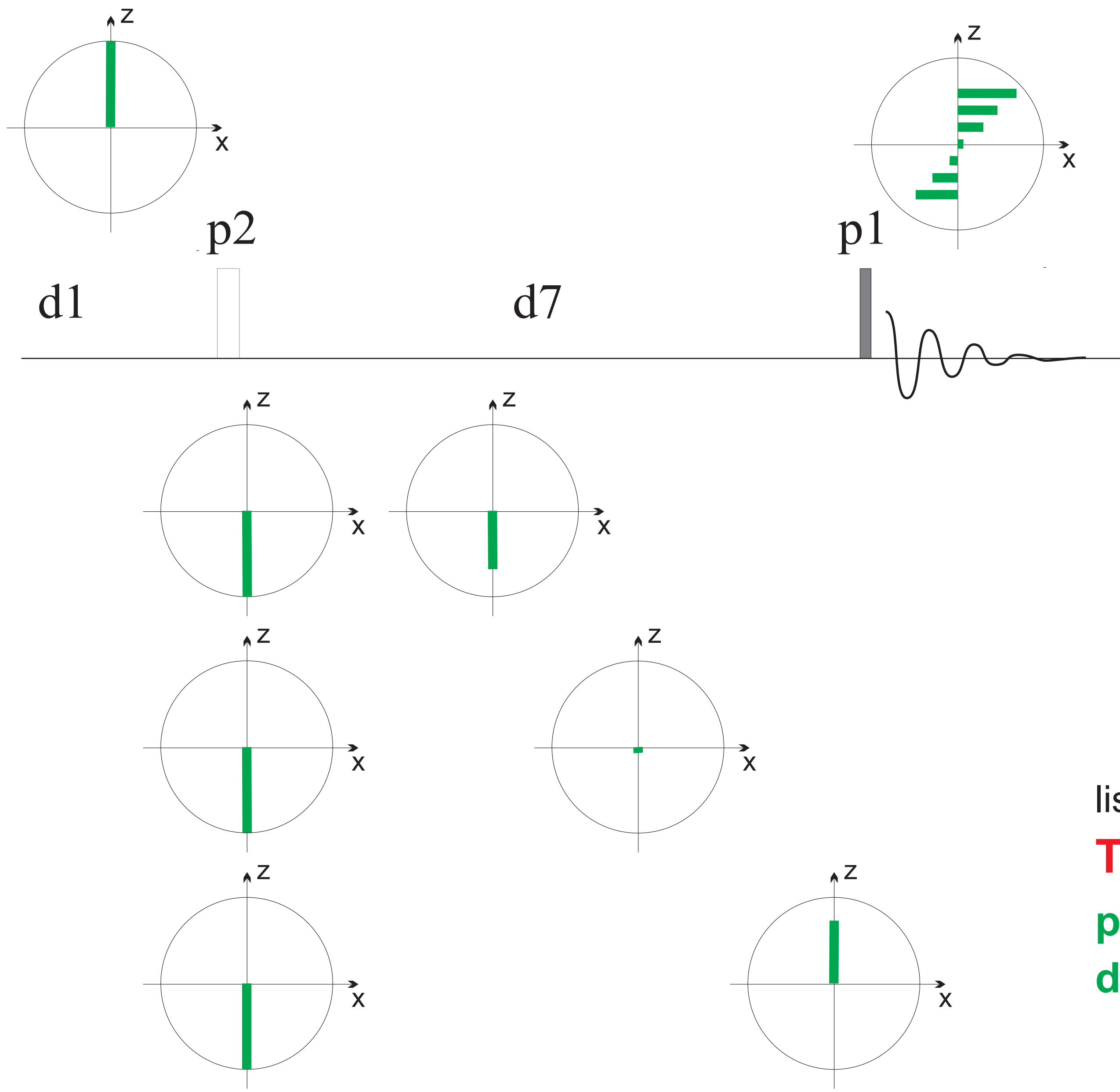
psglib: s2pul

T1est :

p1=pw90×2

d2=”arrayed”

Relaxation in NOE Expts: T_1 Array



lists/pp: t1ir1d

T1est :

p2=p1×2

d7="one-by-one"

Overview of Spin-Lattice Relaxation

$$\frac{1}{T_1^I} \equiv R_1^I \propto \sum_S \frac{\langle \tau_c \rangle}{r_{IS}^6}$$

T_1	=	relaxation time
R_1	=	relaxation rate
Σ	$\rightarrow$	over all neighboring protons (within 0.6 nm)
r_{IS}	=	distance between protons I and S
τ_c	=	rotational correlation time (roughly average time to undergo 360º isotropic rotation)

T_1 Array for Unknown A18

$$\frac{1}{T_1^I} \equiv R_1^I \propto \sum_S \frac{\langle \tau_c \rangle}{r_{IS}^6}$$

$$T_1 \simeq d2_{null} / \ln 2$$