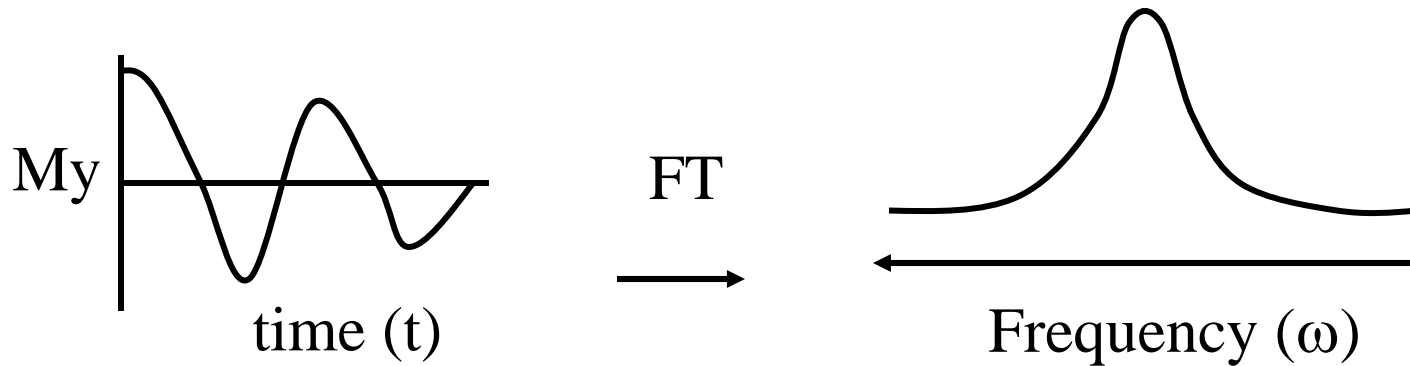


**BCMB/CHEM 8190**

**Data Acquisition and Processing**

**Fourier Transformation**

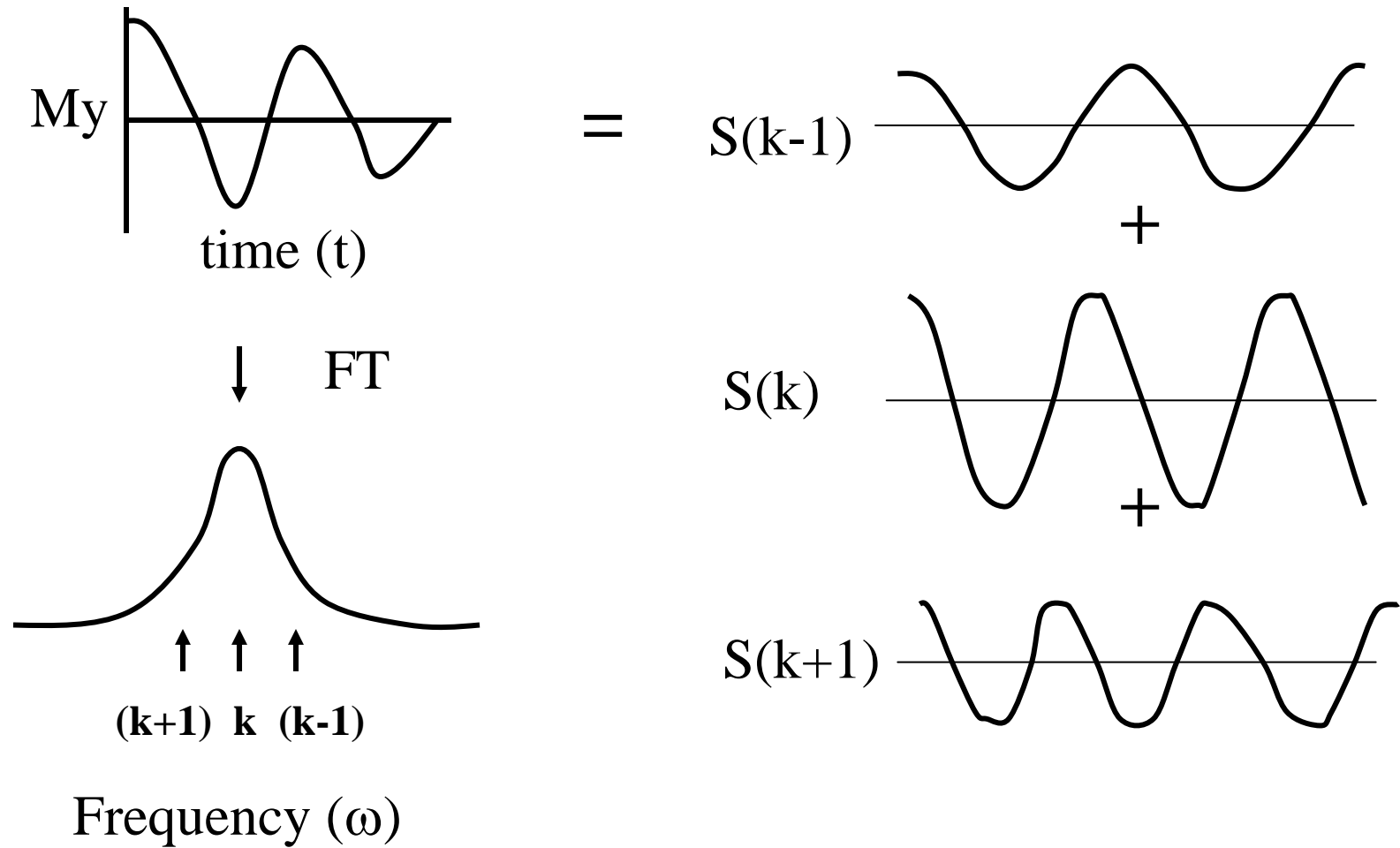
# Fourier Transformation



$$S(\omega) = \int_{-\infty}^{\infty} S(t) \exp(-i\omega t) dt = \int_{-\infty}^{\infty} S(t) (\cos(\omega t) - i \sin(\omega t)) dt$$

$$S(k/(dtN)) = \sum_{J=0}^{N-1} S(jdt) \exp(-i2\pi j (k/dtN)), \quad -N/2 < j < N/2$$

# Visualization of FT



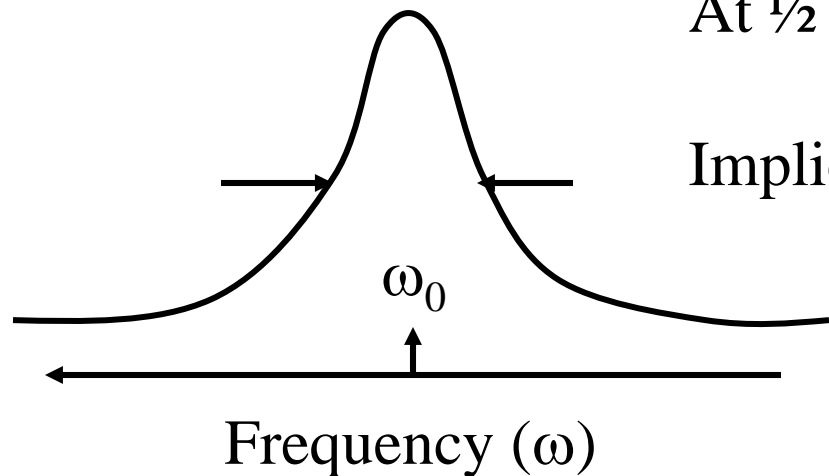
# Lorentzian Lines

$$S(\omega) = (M_0 T_2) / (1 + T_2^2(\omega_0 - \omega)^2)$$

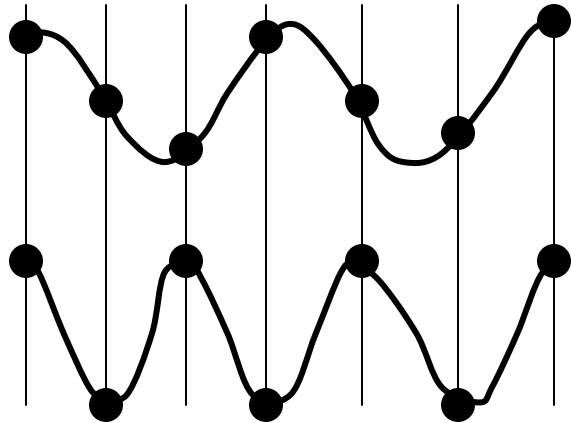
Signal is maximum at  $\omega_0$

At  $1/2$  height,  $T_2^2(\omega_0 - \omega)^2 = 1$

Implies  $\Delta\omega_{1/2} = 2/T_2$ ,  $\Delta\nu_{1/2} = 1/(\pi T_2)$

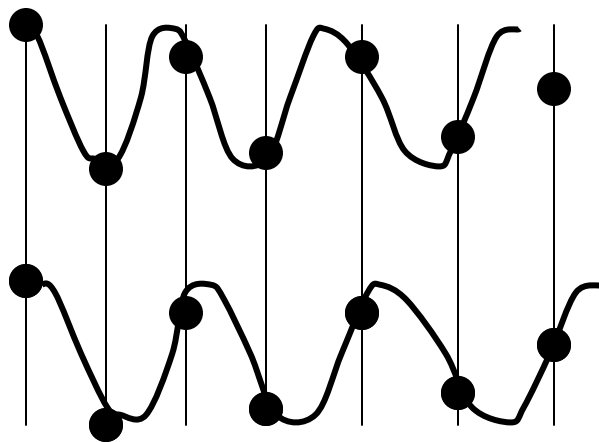


# Digitizing Data and Setting Sweep Widths (sw)



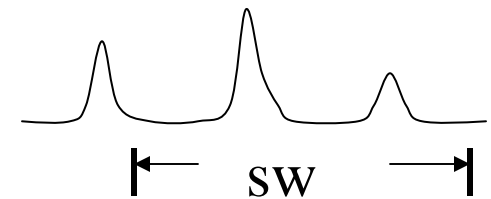
Data points define frequency well

Nyquist frequency – minimum points

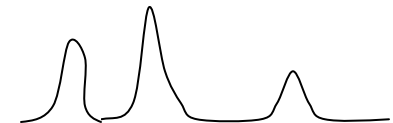


Ambiguities arise at higher frequencies  
Note: pattern of points is the same

real spectrum



observed spectrum



# Phase Cycling Reduces Artifacts

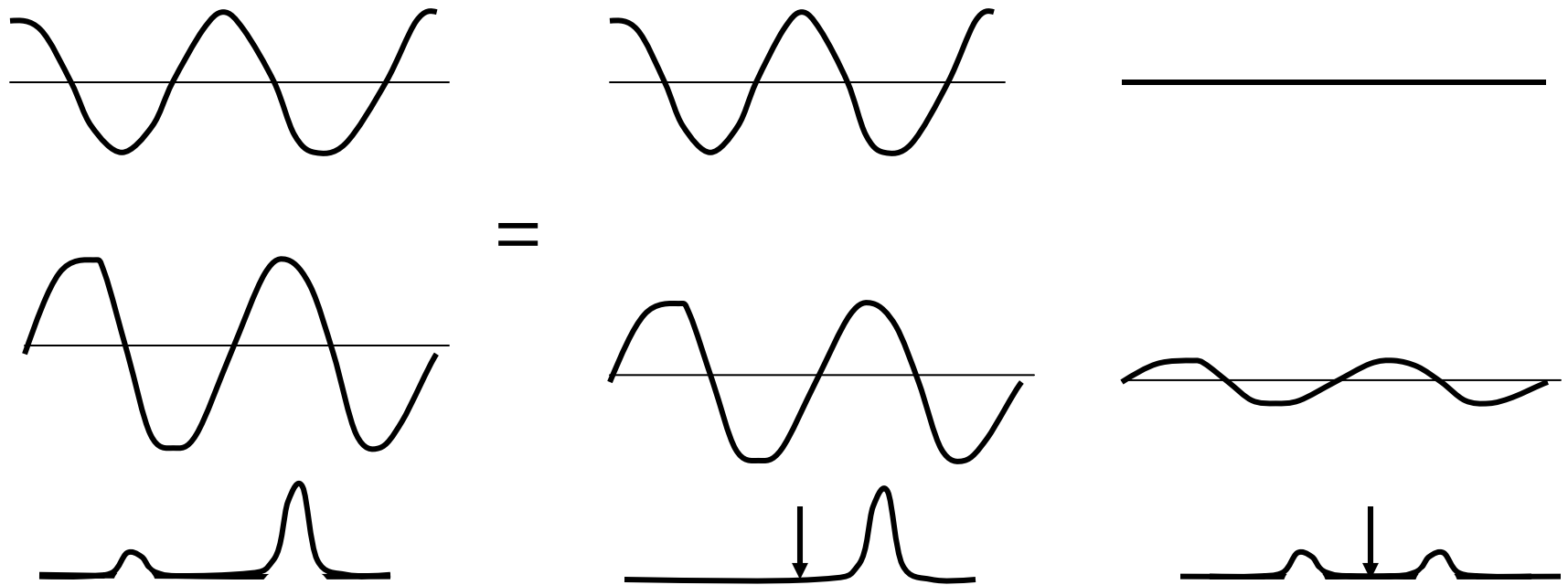
One artifact is a glitch at zero frequency (middle of spectrum).

This can come from a DC imbalance of quadrature channels.

Adding scans with  $180^\circ$  phase shift of pulse and receiver eliminates

Another artifact is a quadrature image. Cycling x and y channels

Along with a  $90^\circ$  phase shift of the pulses eliminates this (cyclops)

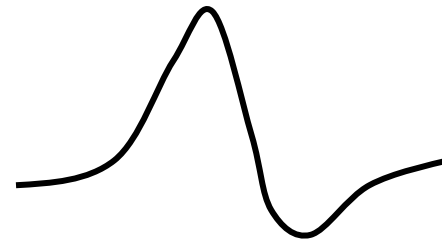


# Zero Order Phase Correction

Phase of reference frequency is arbitrary:

$M_y$  is not pure cos and  $M_x$  is not pure sin

Observe:



In general:

$$M_y = M_r(\cos \phi) + M_i(\sin \phi)$$

$$M_x = M_i(\cos \phi) - M_r(\sin \phi)$$

To recover:

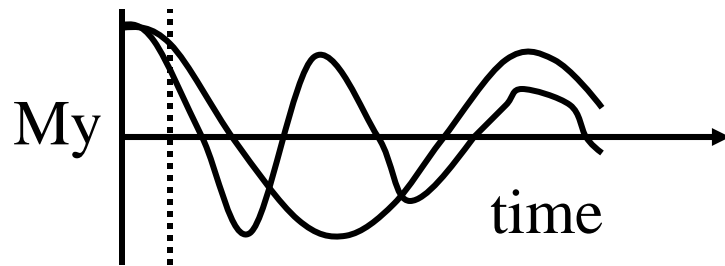
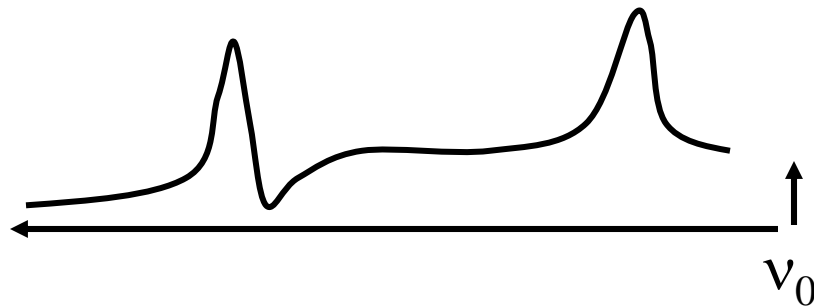
$$M_r = M_y(\cos \phi) - M_x(\sin \phi)$$

Done interactively to get:



# First Order Phase Correction

Phi ( $\phi$ ) can be frequency dependent:  $\phi_0 + v \phi_1$

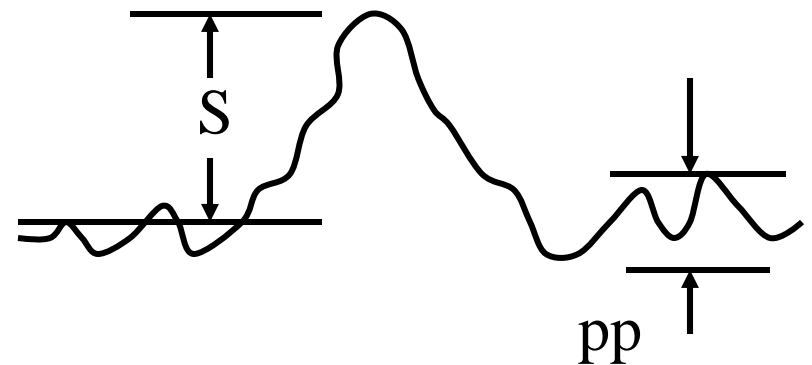


Actual start of collection: phase is not zero  
and error is greater for higher frequencies

# Signal Averaging

NMR is not a high sensitivity technique:  
signal averaging improves the signal to noise ratio

S/N defined as:  $2.5 \times S/pp$



On averaging signal adds as number of scans,  
noise adds as the root of the number of scans

$$S/N \propto N/\sqrt{N} = N^{1/2}$$

$$4 \times \text{scans} = 2 \times S/N$$

# Best Single Scan Parameters

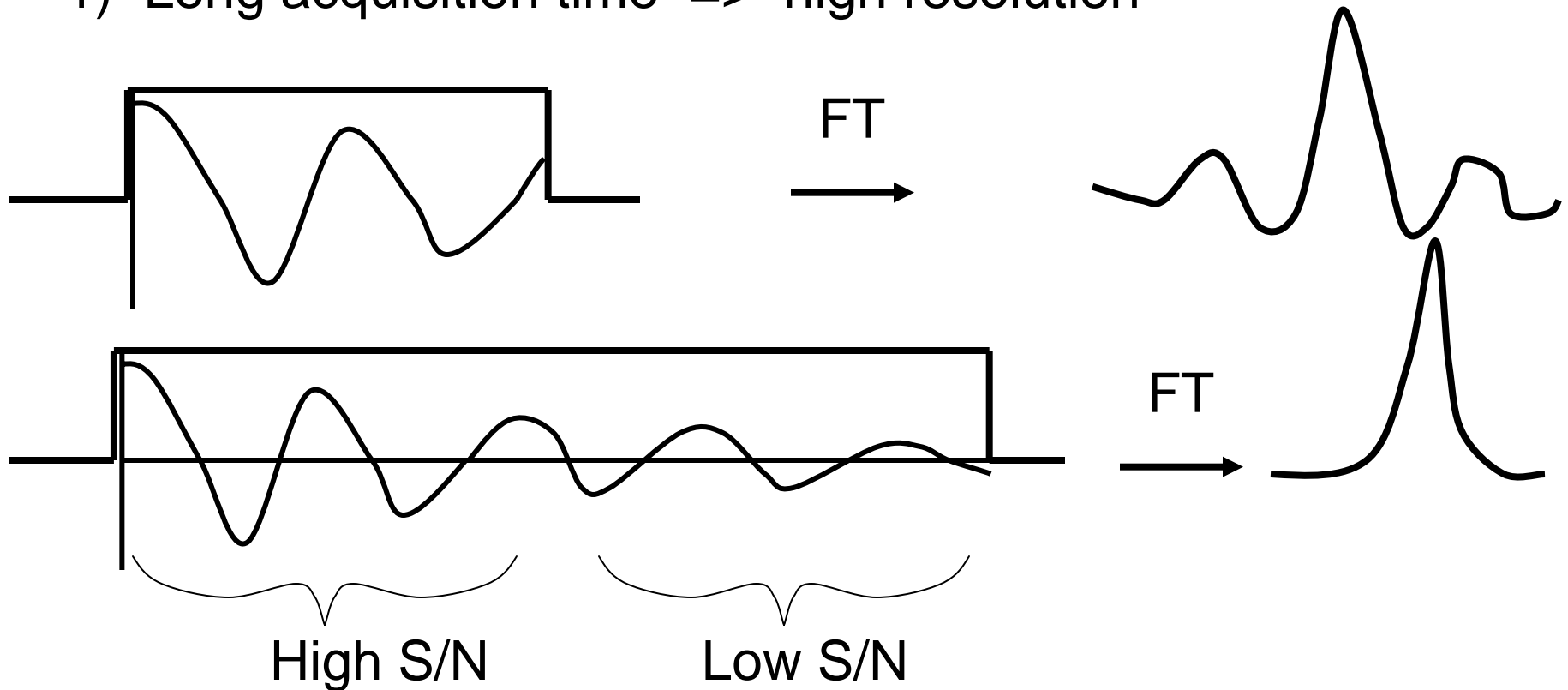
- Recycle times? Pulse angle?
- These are opposing factors
  - recovery of magnetization:  
$$M_z(T) = M_0(1 - \exp(-T/T_1))$$
  
3 X  $T_1$  for 90% recovery
  - more scans / unit time:  
$$S/N \propto N^{1/2}$$
- Compromise: use  $\beta < 90^\circ$ 
  - Ernst angle:  $\cos\beta_{\text{opt}} = \exp(-T/T_1)$

# Ernst Angle Example

- Small molecule:  $T_2$  limited by shimming  
 $T_2^* = 0.3\text{s}$  (1 Hz);  $T_1 = 2.0\text{s}$
- Collect 0.6s to optimize resolution
- $\cos\beta_{\text{opt}} = \exp(-0.6/2) \Rightarrow \beta_{\text{opt}} = 42^\circ$
- Cost: may not have unit intensity for all resonances since  $T_1$ s differ
- Comparison to waiting 3 X  $T_1$ :  
10 scans / min @ unit intensity =  $\sqrt{10} = 3.2$   
100 scans / min @ 0.67 intensity = 6.7

# How long should acquisition time be?

1) Long acquisition time => high resolution

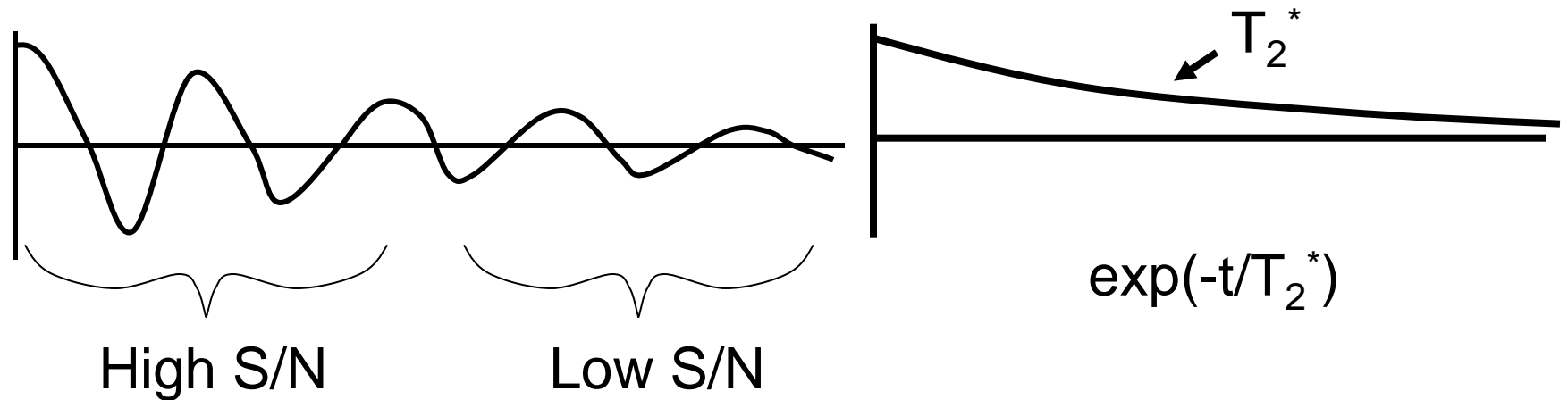


2) Long acquisition time => low S/N

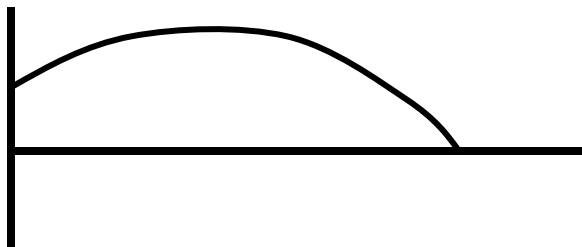
3) Compromise"  $T = (1-2) \times T_2$

# Some other processing details

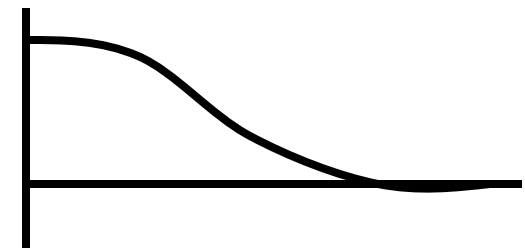
- Matched Filters – maximize S/N



- Other Filters: sine-bell



- kaiser



# Alternate Processing Methods

- What is wrong with FT?
  - no assumption about max # lines
  - no assumption about line shape
  - FFT uses a uniform distribution of pts
- Alternatives
  - Maximum entropy
  - Linear prediction
  - non-linear sampling
- Reference: Rovnyak, D Hoch, JC Stern, AS Wagner, G, (2004) J. Biomol. NMR, 30, 1-10.