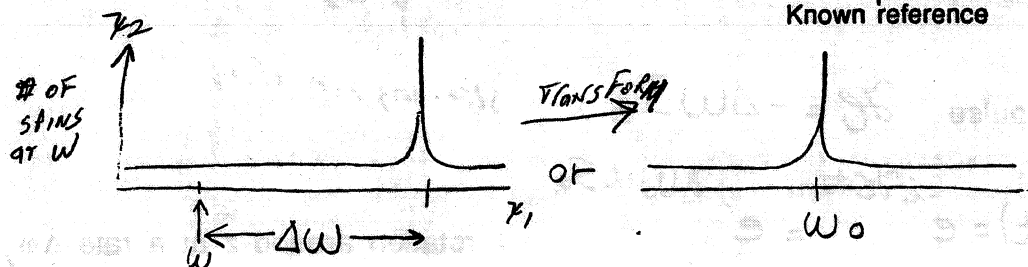
Bibliography – Ernst: 4.2 & 4.3 – Derome: Chs. 2 to 4
– Harris: 3.2, 3.3, 3.7 – 3.11
– Fukushima: II A, II B, II C

Section II: BASIC PRINCIPLES OF PULSED NMR

II.1 THE PULSED NMR EXPERIMENT

Our goal is to determine how many spins process at a frequency ω_0 or, equivalently, how many precess at an offset $\Delta\omega = \omega_0 - \omega$

Known reference



A simple way:

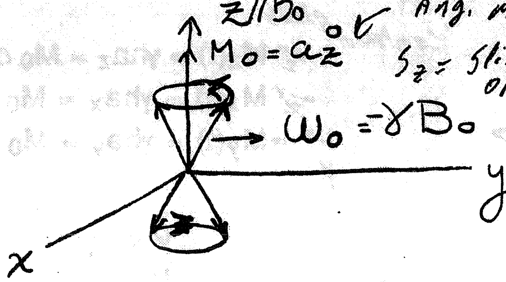
i) Let M_0 form in the presence of B_0

Lab frame Hamil'L:

$H = -\gamma B_0 S_z$

$= -\omega_0 S_z$

S_z = spin ang mom along z-axis



component of Ang. mom

S_z = spin ang. mom. op.

$\rho - \frac{\omega_0}{\beta} S_z$

or $M = (0, 0, M_0)/\beta = kT$

ii) Give a short but strong rf pulse in the neighborhood of ω_0 along the x axis of the rotating frame: much larger

During this pulse:

$$\mathcal{H}_r = -\Delta\omega S_z - \omega_1 S_x \approx -\omega_1 S_x$$

field along z & x

$\omega_{rf} - \omega_0$

$\omega_1 = \gamma B_1$ in Hz (gives rate of tilting)

$\bar{M} = (0, 0, M_0)$ $\quad \bar{a} = (0, 0, a_0)$

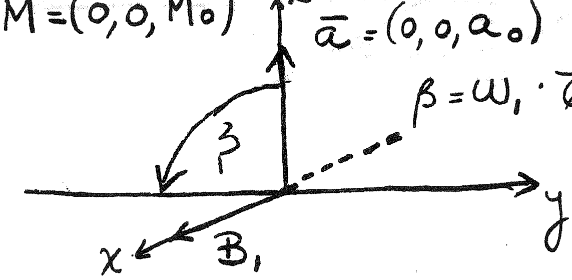
$\beta = \omega_1 \cdot \tau_{pulse}$ = pulse angle

eg) 20 kHz rotates once in 50 μs

$S_z|\alpha\rangle = \frac{\hbar}{2}|\alpha\rangle$

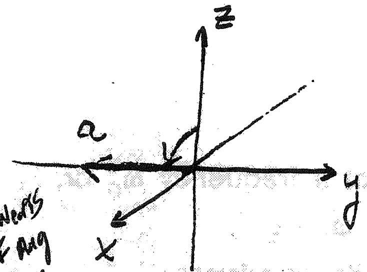
$S_z|\beta\rangle = -\frac{\hbar}{2}|\beta\rangle$

$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

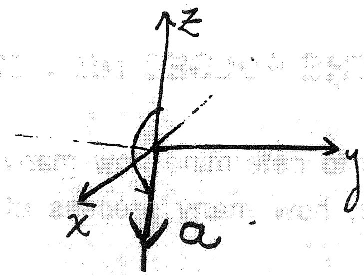


for $\rho_0 = a_0 \mathbb{1} + a_x \sigma_x + a_y \sigma_y + a_z \sigma_z$

If $\beta = \pi/2$



If $\beta = \pi$



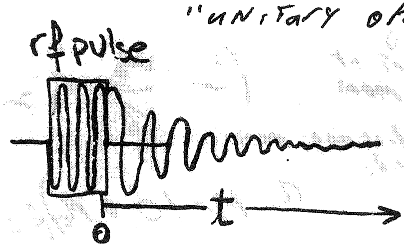
a_x, a_y, a_z components of ang mom

After the pulse $\mathcal{H} = -\Delta\omega S_z$. spin ang mom op S_z

$$\Rightarrow \mathcal{U}(t) = e^{-i\mathcal{H}t} = e^{i\Delta\omega t S_z}$$

: rotation around z at a rate $\Delta\omega$, which can be detected by a pair of coils placed in the lab frame

Time evolution operator "unitary operator"



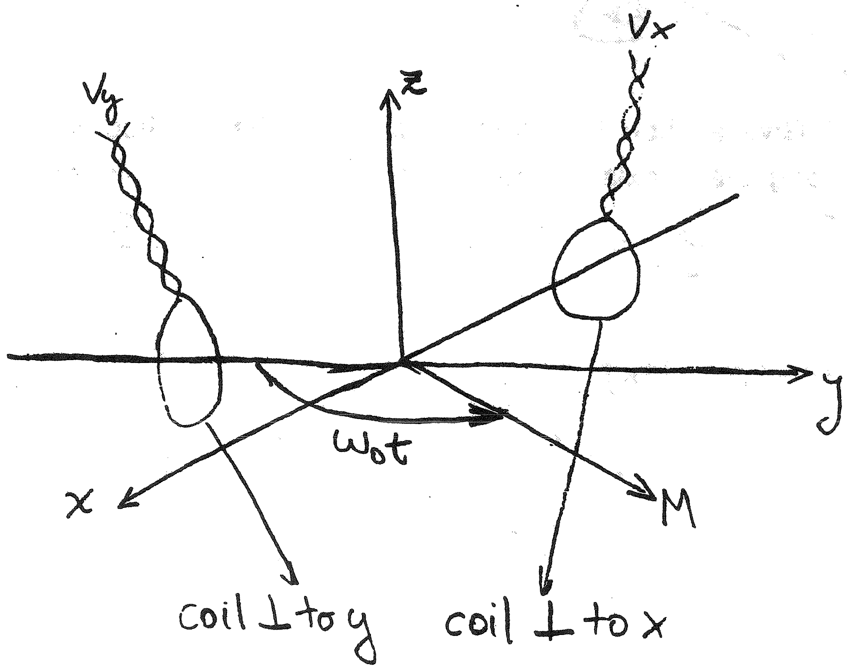
after pulse

component along

z: $M_z(t) = \gamma\hbar a_z = M_0 \cos\beta$

x: $M_x(t) = \gamma\hbar a_x = M_0 \sin\beta \cdot \sin(\omega_0 t)$

y: $-M_y(t) = \gamma\hbar a_y = M_0 \sin\beta \cdot \cos(\omega_0 t)$



(x, y, z): Lab frame

flux = Φ = Area $\cdot B_0$ = const $M(t)$
magnet

The oscillating magnetization will induce changes in magnetic flux, which will in turn induce emf's (voltages) in coils. The resulting signal **S**

Rotating magnet in coil inventor

$$\boxed{\vec{S} = \frac{d\vec{\Phi}}{dt} : \text{Faraday's Law}}$$

Φ: magnetic flux $\approx 10^{-4-5}$ volts

equil magnet — larger magnet → higher volts

look like 2 comp's of magnet

$$\left.\begin{array}{l} S_x \propto \dot{M}_x = M_0 \cdot \omega_0 \cos(\omega_0 t) \\ S_y \propto \dot{M}_y = M_0 \cdot \omega_0 \sin(\omega_0 t) \end{array}\right\} \text{Detected in Pulsed NMR}$$

twice the voltage between 2 & 1 looped coiled (but depends on Q factor)

It is convenient to express the rotating magnetization as a single quantity rotating in the complex plane:

express as single component

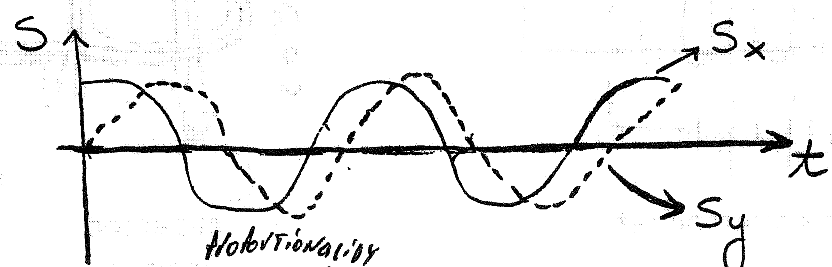
$$M_+ = M_x + i M_y \qquad (M_+ = \mathrm{Tr}(\rho \cdot S_+) \text{ in Quantum Mechanics}, \quad S_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix})$$

$$\Rightarrow \boxed{S_+(t) = S_x + i S_y \propto M_0 \cdot \omega_0 \cdot e^{i\omega_0 t}}$$

Signal detected
Not observable because not Hermite

If only know real, can't tell phase (+ or −)

detecting I-component of ρ, @ ω



Proportionality const

Note that $S_+(t) = i \cdot \omega_0 \cdot M_+(t) = \text{Constant} \cdot M_+(t)$

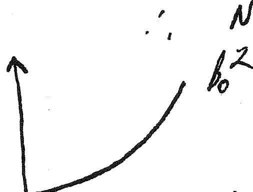
It is therefore usually said that NMR detects the magnetization in the x-y plane. Strictly speaking however, there is a $i \cdot \omega_0$ factor involved.

Moreover, since $M_0 = \dfrac{N \gamma^2 \hbar^2 B_0}{4kT}$ N = # of spins

* Curies law for nuclear induction
* describes anisotropy along z-axis for S = 1/2

Dec T → inc volt,
N ∝ signal
B_0^2 → inc B_0 → inc signal

$$\Rightarrow S_+ \propto \frac{\gamma^3 \hbar^2}{4k} \cdot \frac{N B_0^2}{T} \cdot e^{i\omega_0 t} :$$



one B_0 from Boltz
" " " inc ω

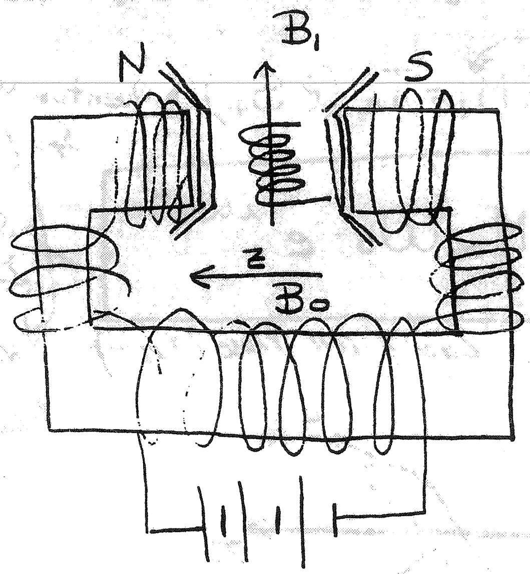
Bio det in S/N!

comes from electronics
* all comes down to a Q factor

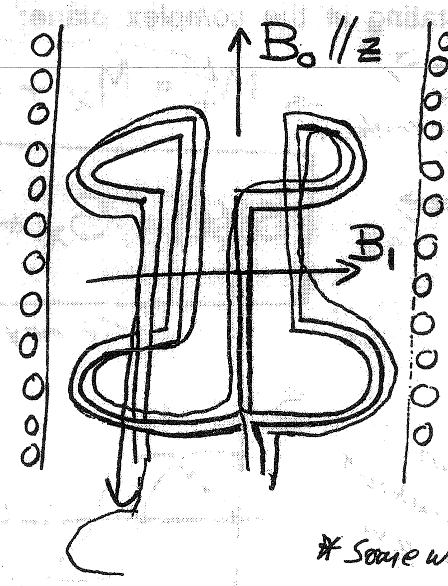
II.2 QUADRATURE DETECTION IN THE ROTATING FRAME

In pulsed NMR a single coil is used for → irradiation / → detection

The possible coil geometries:



electromagnet



supercon magnet

* Somewhat ineffective
* How do we make a turn H-H coil?

The irradiation pulse: $B_1 \cos(\omega t + \varphi_{Tx})$

T_x : Transmitter

The observed signal: $S_0 \cos(\omega_0 t + \varphi_{T_x})$

How do we get imag. part. (before had coil in q_y)

only one component * missing other s(ωt) w/ phase info

Can't use coils along x & y because they will have diff sens. ∴ can't (4.)

One can still observe S_x, S_y without using 2 orthogonal coils by using a **double balanced mixer** (DBM); the use of this approach leads to an experimental scheme called **phase-sensitive detection** or **phase-sensitive demodulation.**

A **DBM** is a device that takes in 2 signals S_1, S_2 and gives an output φ
out 'phi'

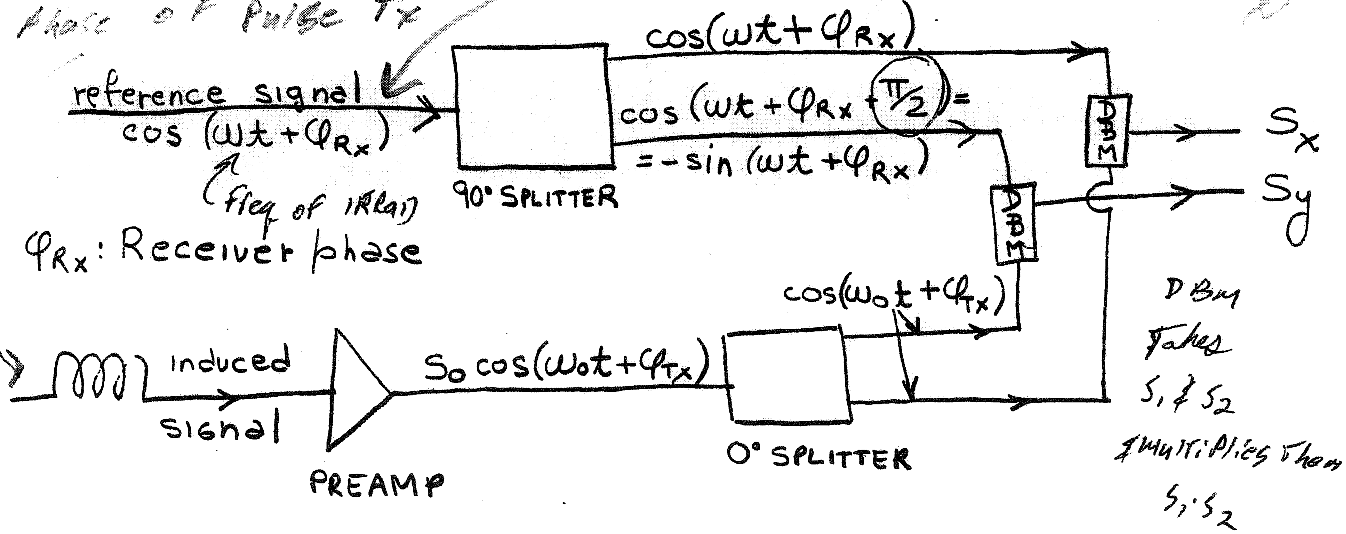
$$\varphi(t) \propto S_1(t) \cdot S_2(t)$$

A filter is chosen so that fast oscillating terms go away.

Jeener invention

In phase-sensitive detection experiments, the source used for irradiation is also used to demodulate the signal according to:

Can change phases by changing phase of pulse Tx or phase of modul. of Rec. ∴ after Ø



i.s = sine (of sum) + (diff)

$$S_x: \quad \underset{\text{Ref}}{\cos(\omega t + \varphi_{Rx})} \, \underset{\text{spins}}{\cos(\omega_0 t + \varphi_{Tx})} \propto c[(\omega - \omega_0)t + (\varphi_{Rx} - \varphi_{Tx})] + \text{fast osc. terms}$$

$$S_y: \quad s[(\omega - \omega_0)t + (\varphi_{Rx} - \varphi_{Tx})] + \text{fast osc. terms.}$$

$$S_x \propto \cos(\Delta\omega t + \varphi) \qquad \Delta\omega = \omega - \omega_0 : \text{offset}$$

= freq of spins in rotating frame & what is detected

$$S_y \propto \sin(\Delta\omega t + \varphi) \qquad \varphi = \varphi_{Rx} - \varphi_{Tx}$$

eg) $\omega_0 = 100.01$ MHz, $\omega = 10.00$ MHz } $|\omega_0 - \omega| \sim 10$ kHz

$|\omega + \omega_0| \sim 200$ MHz eliminate by low pass filter

We can therefore observe the two signals expected from orthogonal coils but **in the rotating frame**: **quadrature detection**

Note that whereas $\omega, \omega_0 \approx 100\text{'s MHz (rf)}$

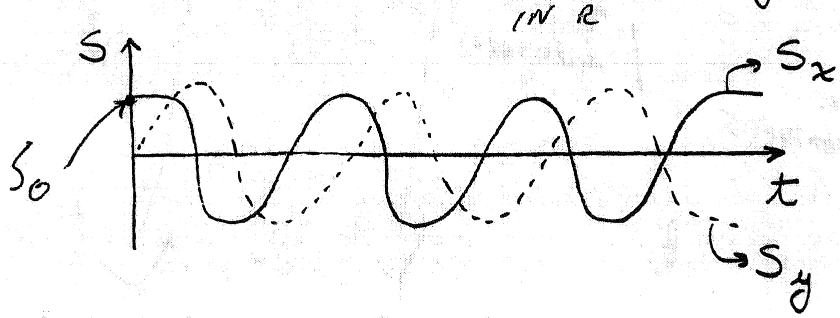
$$\Delta\omega \approx 0\text{–}100\ \text{KHz (audio)}$$

* all of NMR Detection Takes Place in the Rotating Frame.
* strange things happen in Rotating Frame

II.3 FOURIER ANALYSIS

Suppose that in the past example $\varphi = 0$

$$\Rightarrow S_+(t) = S_0 \left[\underbrace{\cos(\Delta\omega t)}_{S_x} + i\,\underbrace{\sin(\Delta\omega t)}_{S_y}\right] = S_0\, e^{i\Delta\omega t}$$



ROTATING Frame

100,01 MHz

or 99,99 MHz

Δw Now can disting w/ R & I

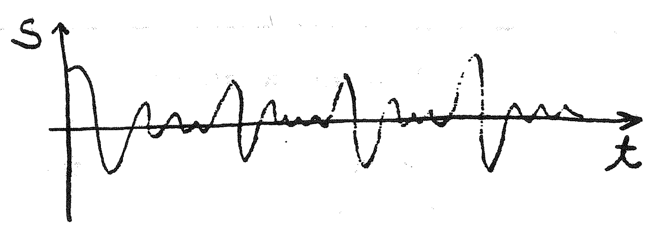
In these case, it is relatively simple to extract S_0, $\Delta\omega$

But, what happens if we have a superposition of several waves:

$$S(t) = f_1\, e^{i\omega_1 t} + \overset{\text{amp}}{f_2}\, e^{i\omega_2 t} + f_3\, e^{i\omega_3 t} + \ldots$$

$$\omega_1 < \omega_2 < \omega_3 < \ldots \quad ; \quad 0 \leq t \leq T$$

Now we want $f(\omega) = \begin{cases} f_1 \text{ at } \omega_1 \\ f_2 \text{ at } \omega_2 \\ \vdots \end{cases}$ from the interferogram S:



To extract each of these components, we multiply by $e^{-i\omega_j t}$ and integrate over t. In the case of ω_2 for instance

f's = pre-exponential factor relating relative contribution to FID (eg Area here)

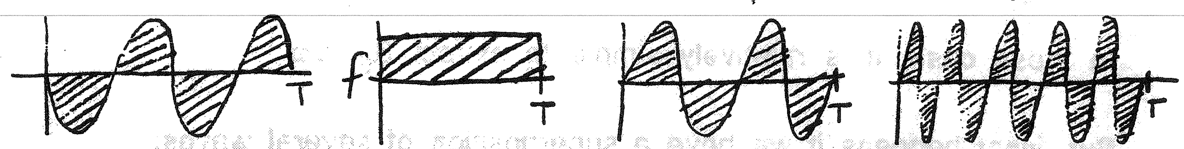
$$S(t)\cdot e^{-i\omega_2 t} = f_1 e^{i(\omega_1-\omega_2)t} + f_2 + f_3 e^{i(\omega_3-\omega_2)t} + f_4 e^{i(\omega_4-\omega_2)t} + \ldots$$

$e^{i(\omega_2-\omega_2)}$

amplitude

The real part:

time dependences



area = 0 area ≠ 0 area = 0 area = 0

area = $f_2 * t$

$$\Rightarrow \frac{1}{T}\int_0^T S(t)e^{-i\omega_2 t}\,dt = f(\omega_2):$$

The integral extracts the amplitude at ω_2

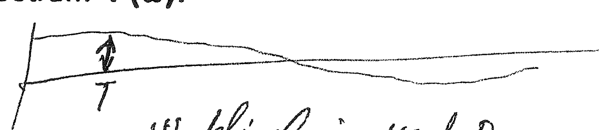
In general:

$$\boxed{F(\omega_k) = \frac{1}{T}\int_{-T}^{T} S(t)\, e^{-i\omega_k t}\,dt}$$

Fourier Analysis (T -> ∞)

This Fourier transformation relates the time-domain signal **S(t)** experimentally available with the desired spectrum **F(ω)**.

want $\int_{-\infty}^{\infty}$



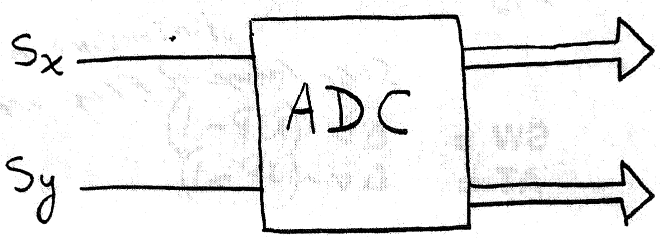
Ill defined ∴ need ∞

II.4 DISCRETE SAMPLING AND FAST FOURIER TRANSFORM

We had demodulated our NMR signal into 2 audio components. These voltages are now sampled at equal time intervals Δt by an analog-to-digital converter (ADC), whose output is a string of numbers

$\Delta W = |W_k - W_{k'}|$??

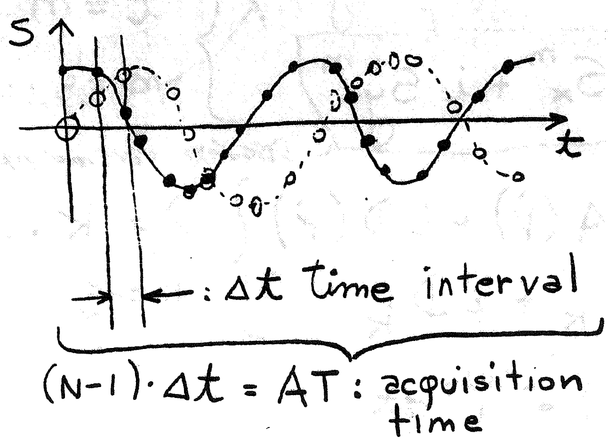
Need at least one IN ORDER TO KNOW WE DON'T have other



numbers (real part)

numbers (imaginary part)

This time-domain signal:



Δt: dwell time

N: number of complex data points acquired

The discrete sampling implies that the integral of the Fourier transformation has to be replaced by a discrete sum

$$\int_{-T}^{T} \longrightarrow \sum_{m=0}^{N-1}$$

The acquisition time determines the spectral resolution Δv of the spectrum:

$$\boxed{\Delta v \,.\, AT = 1}$$

same (time & ν domain)

Similarly, the dwell time Δt determines the spectral width (SW) of the spectrum:

$$\boxed{SW \,.\, \Delta t = 1}$$

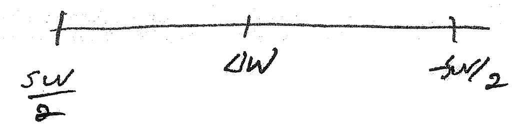
Nyquist Theorem

SW defined

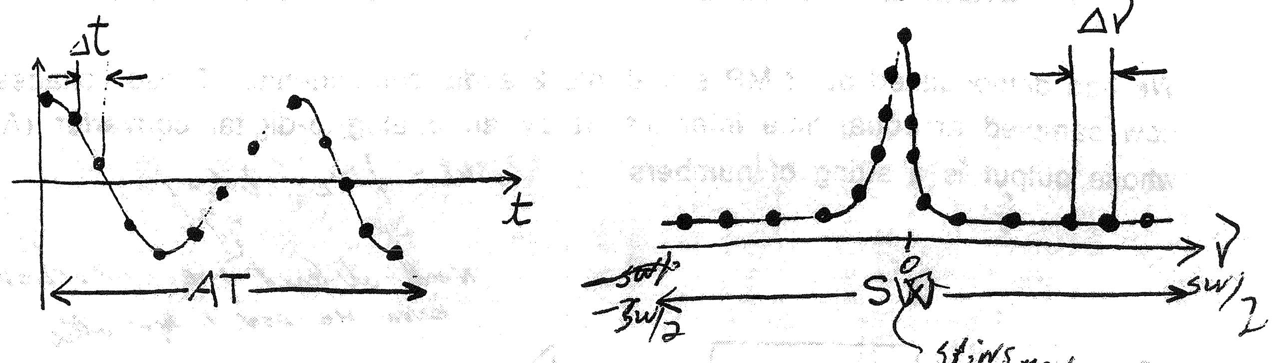
w_k w_l

$\int_{\Delta t} e^{i(w_k - w_j)t} \neq 0$

or $\int_{\Delta t} e^{i(w_k - w_j)t} \neq 0$



Time Domain **Frequency Domain**



spins moving at ref

SW = range of Freq we can observe

SW = $\Delta\nu \times (NP-1)$

AT = $\Delta t \times (NP-1)$

The detected signal $s(t) = S_x(t) + i\,S_y(t)$ $\quad t = m \cdot \Delta t$

$\mathcal{FT}\downarrow \quad \uparrow \mathcal{IFT} = (\mathcal{FT})^{-1}$ $\quad \boxed{S_m = S_x^{\,m} + i\,S_y^{\,m}}$ $\quad m = 0, \ldots, N-1$

Discrete version of this

The resulting spectrum $F(\nu) = A(\nu) + i\,D(\nu)$ $\quad \nu = k \cdot \Delta\nu$

$F_k = A_k + i\,D_k$ $\quad k = -\frac{N}{2}, \ldots, \frac{N}{2} - 1$

The $\mathcal{FT}$: $F(\omega) = \frac{1}{T}\int_{-T}^{T} s(t)\, e^{-i\omega t}\, dt$ $\quad T = T_{max} = (N-1)\Delta t$

(normalized)

$T = N\Delta t \; ; \; dt \rightarrow \Delta T \; ; \; \omega = 2\pi\nu \; ; \; -T = 0$

Discrete version $\quad F_k = \frac{1}{N}\sum_{m=0}^{N-1} S_m\, e^{-i 2\pi k \underbrace{\Delta\nu}_{1/AT} m \underbrace{\Delta t}_{AT/N}}$?

$$\Rightarrow \boxed{F_k = \frac{1}{N}\sum_{m=0}^{N-1} S_m\, e^{-i 2\pi km/N}}$$

dwell & AT are lost.

This is very convenient to program => computers can calculate Fk very fast if $N = 2^m$ using an algoritm called the fast Fourier transform (FFT)

F_k = complex #

or $s(t) = \int F(\omega)\, e^{i\omega t}\, d\omega$

Probability spins are resonating at W

So far assumed $S(t) = S_0 e^{i\omega t}$

an amplit x oscillating signal

II.5 EFFECTS OF RELAXATION: THE BLOCH EQUATIONS

So far we have that:

i) Before excitation $\vec{M} = M_0 \hat{z}$

ii) After excitation $\vec{M}(t) = M_0 \, (\cos(\omega t)\hat{x} + \sin(\omega t)\hat{y})$

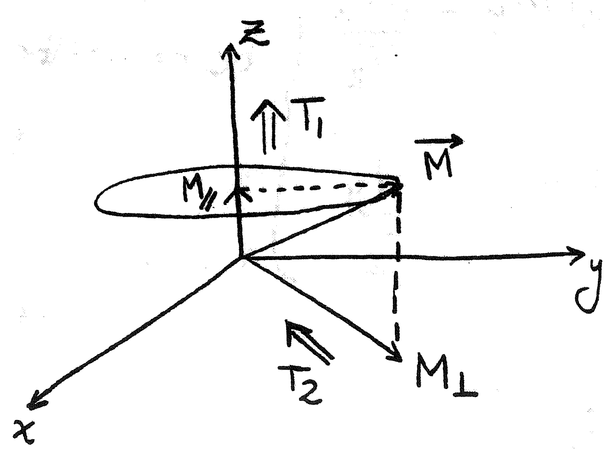
However, if one waits long enough, the magnetization is again parallel to $\hat{z}$. There is a mechanism that takes the system back from ii) to i): **Relaxation.**

Two relaxation times determine how this process takes place:

A "transverse" relaxation time T_2: Takes $M_y, M_x \rightarrow 0$

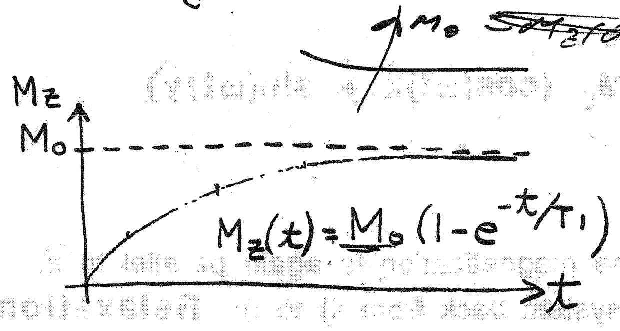
A "longitudinal" relaxation time T_1: Takes $M_z \rightarrow M_0$

t_2

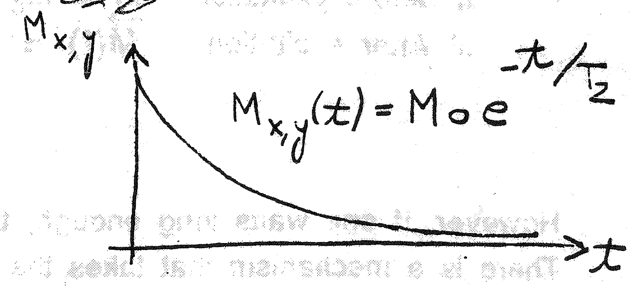


The longitudinal growth and the transversal decay are usually exponential.

T_1 or longitudinal relaxation



T_2 or transverse relaxation



These processes can be included into the equation of motion of **M** to give the **Bloch Equations:**

' x goes into y at ~~rate~~ Δw $\Rightarrow$ Precession

$$\dot{M}_x = -\Delta\omega M_y - \frac{M_x}{T_2}$$

'' y → x @ Δw ''

$$\dot{M}_y = \Delta\omega M_x - \frac{M_y}{T_2}$$

$$\dot{M}_z = \frac{M_0 - M_z}{T_1}$$

These 2 expressions can be rewritten as $M_+ = e^{i\Delta w t} M_+$

$$\dot{M}_+ = i\Delta\omega M_+ - \frac{M_+}{T_2}$$

where

$$M_+ = M_x + iM_y$$

~~$A = \ldots + i\Delta W$~~

$$\dot{M}_x = -\Delta w M_y - \frac{M_x}{T_2}$$

$$\dot{M}_+ = A \cdot M_+$$

$$\left(\frac{-1}{T_2} + i\Delta w\right.$$

$$M_+(t) = M_+(0)\, e^{At} \qquad e^{i\Delta w t} e^{-t/T_2}$$

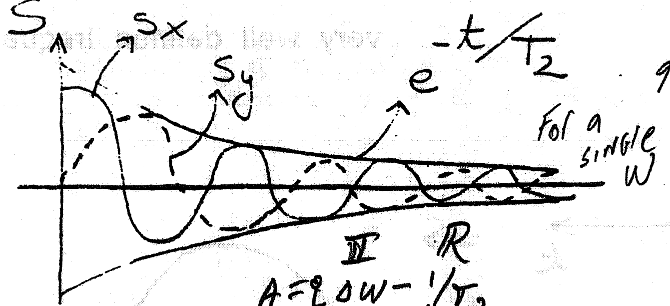
Rotate at same rate but w/ B_1 axes → Rec Trans

II.6 NMR LINESHAPES AND THE PHASE OF SPECTRAL PEAKS

Due to T_2 effects the actual **time-domain signal** looks like:

$$S(t) \propto e^{i\Delta\omega t}\, e^{-t/T_2}\, e^{i\phi}$$

$$\phi = \phi_{Rec} - \phi_{Trans}$$



The detected signal is referred to as **FID**

FID: Free Induction Decay

// absence of B_1 // Magnet. = Nuc. Induct Voltage

$A = i\Delta\omega - 1/T_2$ (Im, R)

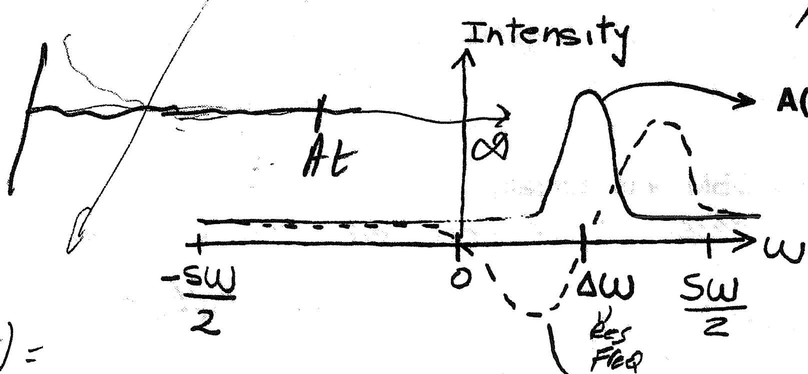
$S(t) = S_0 \cdot e^{At}\, e^{-i\omega t}$ A t + At here

$F(\omega) = \int_0^{At = \infty} e^{Bt}$ B = complex #

Complex FT:

Hmwk: $\int e^{Bt} = \frac{1}{B}$?

$At \to \infty$



A(ω): absorptive line shape

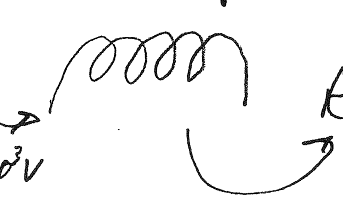
D(ω): dispersive line shape

S(t) =

$$A(\omega) = \frac{1 \cdot S_0 \cdot T_2}{1 + (\omega - \Delta\omega)^2 T_2^2} \qquad D(\omega) = \frac{T_2^2(\omega - \Delta\omega)}{1 + (\omega - \Delta\omega)^2 T_2^2}$$

Lorentzian Line Shape

T_x $B_1 = 10^3 V$



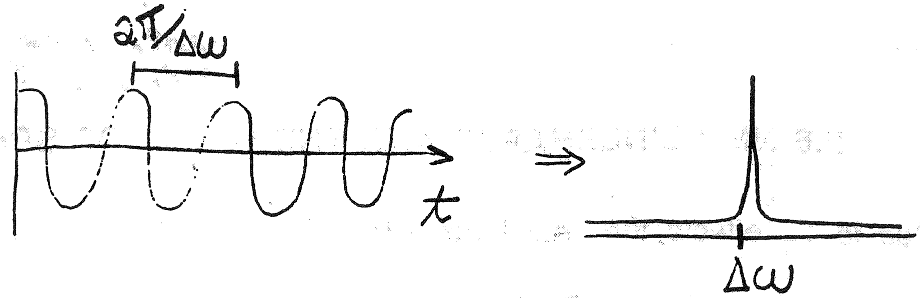
$R_x = 5 \cdot 10^{-5} V$

3) spins precess out before hitting z axis

Takes time for Voltage on Rec to die out

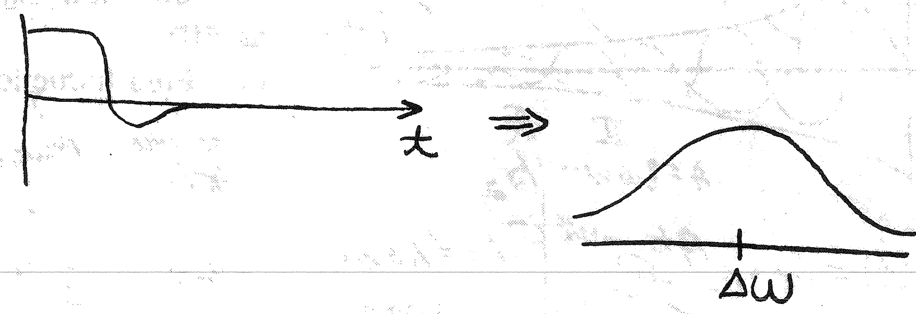
2) time it takes to ...

If $T_2 \to \infty$



very well defined frequency

If $T_2 \to 0$



ill defined frequency

Recall that the signal from the DBM was actually

x-y axes of Transmitter & Rec. are not coincident

$$S(t) = S_0 e^{i\Delta\omega t} e^{i\varphi}$$

$\Delta\omega$: offset

$\varphi = \varphi_{Rx} - \varphi_{Tx}$

$$\therefore S(t) = \underbrace{S_0 e^{i\Delta\omega t} e^{i\varphi}}_{\phi} \; \underbrace{e^{i\Delta\omega t_{dead}} e^{-t/T_2}}$$

Moreover, if one takes into account that:

i) the magnetization starts to precess as soon as it departs from the z-axis

ii) after we turn off the rf-pulse, we have to wait some time ("dead time") until we can start to digitize the signal

Rec $10 \mu V$

Trans $10 V$

QUIZ ON WED
1ST 1/2 T.6.

$$\Rightarrow S(t) = S_0\, e^{i\Delta\omega t}\, e^{i\phi}$$

FT

$$\phi = \varphi + \Delta\omega \cdot \tau$$

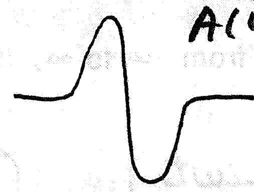
constant phase correction

linear phase correction (proportional to the frequency)

D(W) Pure

$$F(\omega) = \left[A(\omega)\cdot\cos\phi - D(\omega)\sin\phi\right] + i\left[D(\omega)\cos\phi + A(\omega)\sin\phi\right]$$

A(W) Pure



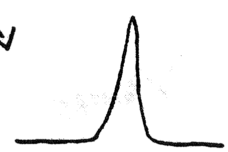
: $\mathbb{R}$

: $\mathbb{I}$

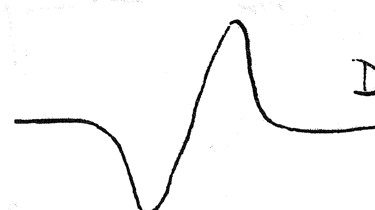
Phase correction

$$\mathbb{R}' = \cos\phi\cdot\mathbb{R} + \sin\phi\cdot\mathbb{I} \qquad \mathbb{I}' = \cos\phi\,\mathbb{I} - \sin\phi\,\mathbb{R}$$

$A(\omega)$

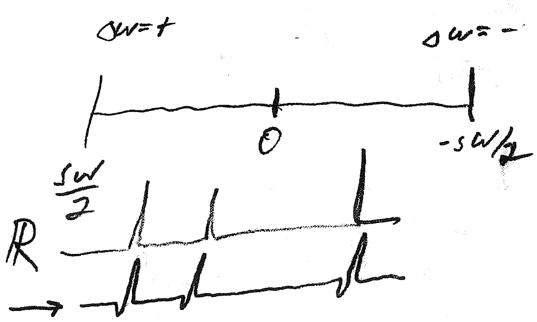


purely absorptive

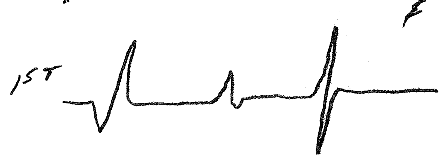


$D(\omega)$

purely dispersive



1ST effect $\xrightarrow{\text{INC}}$ Further away from Zero & opposite sign



Note: The fact that we have dispersive components is a consequence of the impossibility of knowing the signal for t < 0 (causality of NMR).

$$F(w) - [A(w) + i\,D(w)]\cdot e^{i\phi} = \mathbb{R} + i\,\mathbb{I}$$

$\cos\phi + i\sin\phi$

Informal Proof: We know that given a signal S

$$S(t>0) = S_0\, e^{i\omega t}$$

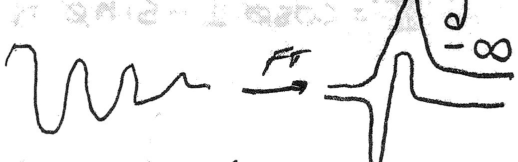
$$\Rightarrow \; F_{OLD}(\omega) = \int_0^{\infty} S(t)\, e^{-i\omega t}\, dt = A(\omega) + i D(\omega)$$

only positive times

$\int_0^{\infty} e^{Bt}$

If the signal goes from -∞ to ∞, the new spectrum

$$F_{NEW}(\omega) = \int_{-\infty}^{\infty} S(t)\, e^{-i\omega t}\, dt = \int_0^{\infty} S(t)\, e^{-i\omega t}\, dt + \underbrace{\int_{-\infty}^{0} S(t)\, e^{-i\omega t}\, dt}$$



$t' = -t$

$-dt' = -dt$

"Kramers - Kroenig" = relates A with disp

$$= \underbrace{\int_0^{\infty} S(t)\, e^{-i\omega t}\, dt}_{F_{OLD}(\omega)\ a+id} + \underbrace{\int_0^{\infty} S(-t')\, e^{i\omega t'}\, dt'}_{F^*_{OLD}(\omega)\ a-id}$$

complex conj.

* Does not work for 2D NMR!!

$$= 2A(\omega)$$

Q.E.D.

∴ adding

$a + id$

$a - id$

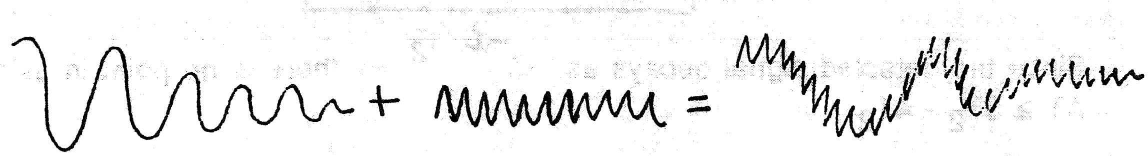
$2a$

* means that if we

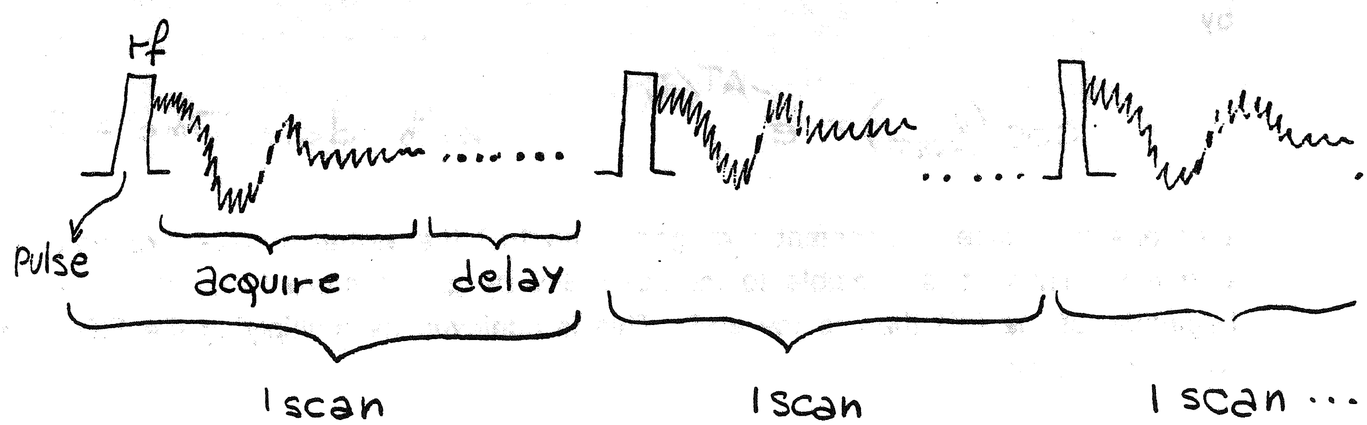
II.7 SIGNAL-TO-NOISE (S/N) RATIO IN PULSED NMR

NMR relies on M_0 = excess of α spins (↑) over β spins (↓). This is a very small fraction, and therefore a normal FID looks like

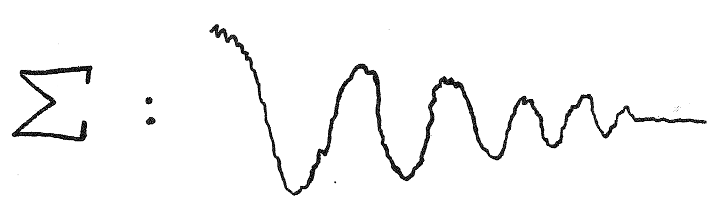
$T_2 \gtrsim 1$ sec



Noise is the main drawback of NMR spectroscopy. NMR spectroscopy bypasses this problem by **signal averaging**



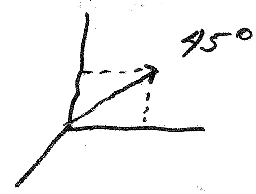
The acquisition computer adds the data digitized in each scan point by point



The intensity of the **signal** adds up coherently => $S \propto$ # of scans

The intensity of the **noise** adds up randomly => $N \propto \sqrt{\text{\# of scans}}$

$$\Rightarrow \quad \boxed{S/N \propto \sqrt{\text{\# of scans}}}$$



$\sin(45°) \cong 70\%$

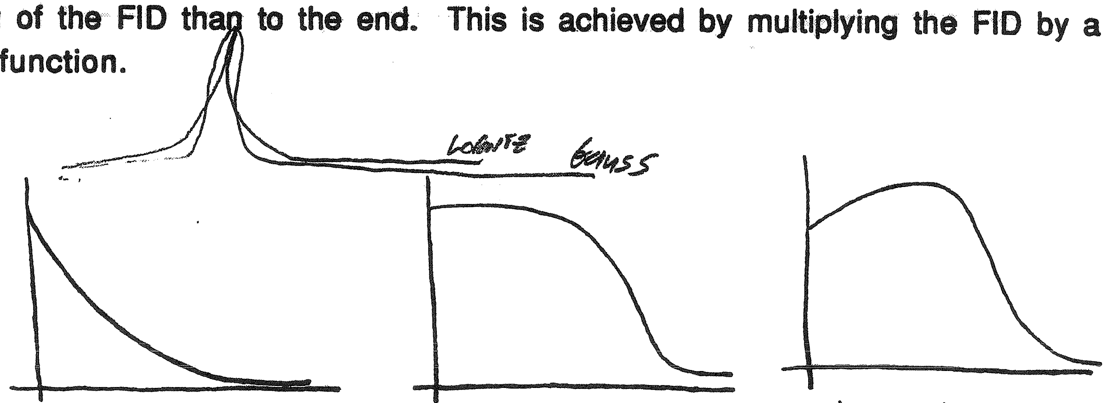
Since the detected signal decays as e^{-t/T_2} => there is no point in using $AT \geq 3T_2 - 4T_2$

The spin system starts to relax right after the rf pulse. If the excitation pulse is $\pi/2$ no M_0 is left parallel to z; if the excitation pulse is $\pi/4$ we get only 70% of the maximum possible signal, but 70% of M_0 is still parallel to z => $\pi/2$ pulses do not necessarily afford the best S/N

In general, if $T_1 \approx T_2$ (most liquids) => the optimum excitation angle β_{opt} is given by

$$\cos(\beta_{OPT}) = e^{-AT/T_1} \quad ; \text{ with delayTime} = 0$$

Whereas the noise is constant throughout the FID the signal decays exponentially with time. Thus, it is possible to increase S/N by giving more "weight" to the beginning of the FID than to the end. This is achieved by multiplying the FID by a window function.



exponential $e^{-t \cdot LB}$

gaussian $e^{-t^2 \cdot GB}$

Lorentz-Gauss $e^{t \cdot LB} \cdot e^{-t^2 \cdot GB}$

Growing Decay

The optimal window function matches the shape of the FID envelope

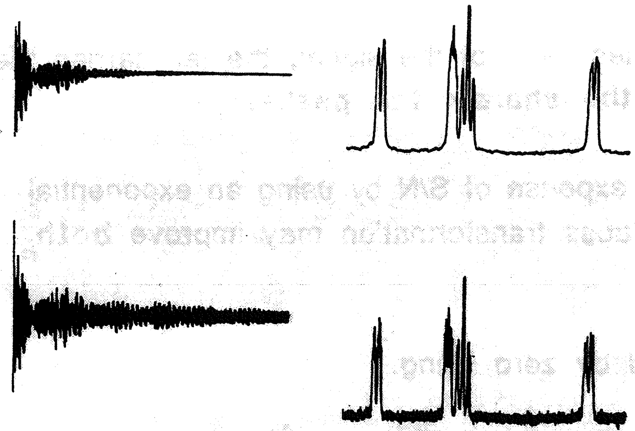


Figure 2.18 Application of the matched filter improves sensitivity.

T/off
WINDOW

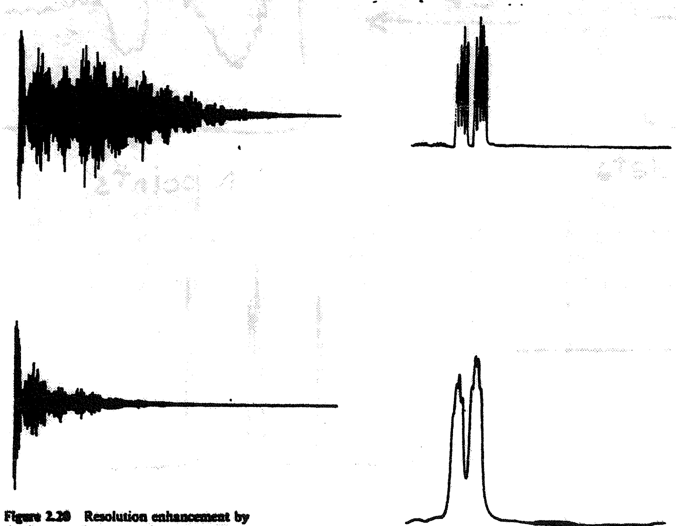


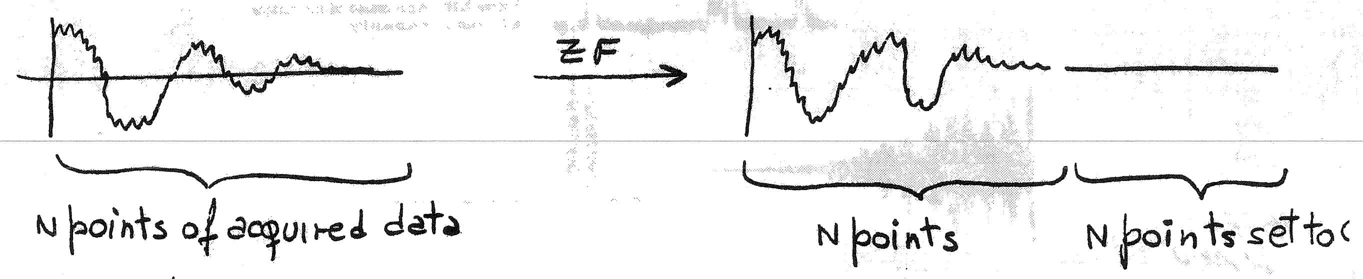
Figure 2.20 Resolution enhancement by the Lorentz-Gauss transformation. The lower traces show the natural FID and its transform, while in the upper trace the early part of the decay has been cancelled by the window function (whilst still ensuring apodisation). Such strong manipulation as this can only be applied to data with a very high signal-to-noise ratio.

II.8 RESOLUTION CONSIDERATIONS

Although the head of the FID carries most of the signal, the tail carries the resolution: **the longer the FID, the sharper the peaks.**

Resolution can be improved at the expense of S/N by using an exponential weighting with LB < 0. Lorentz-Gauss transformation may improve **both** resolution and sensitivity.

Digital resolution can be improved by zero filling.



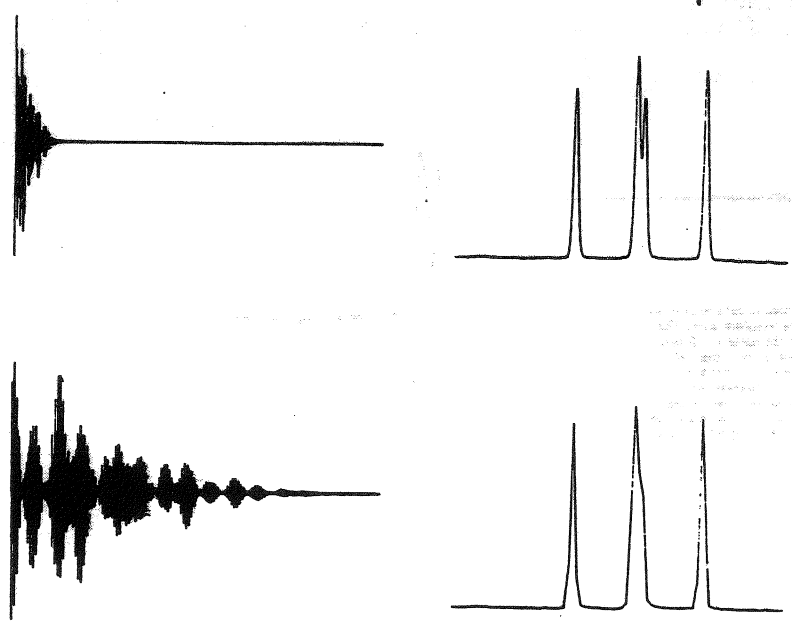
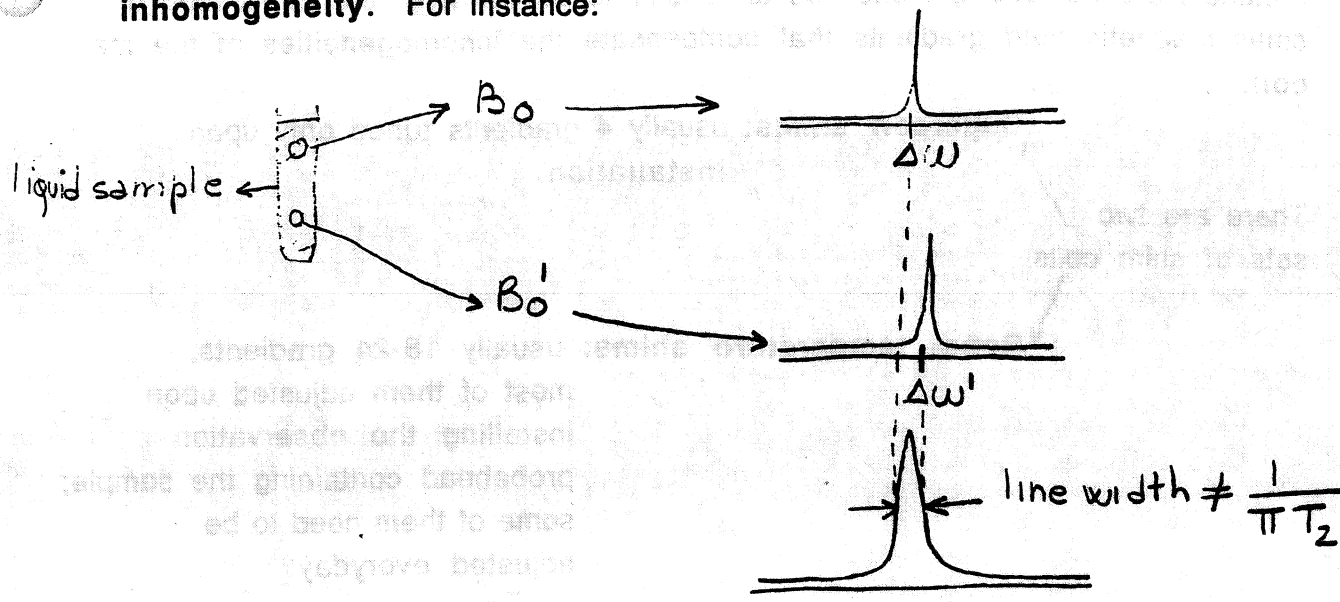


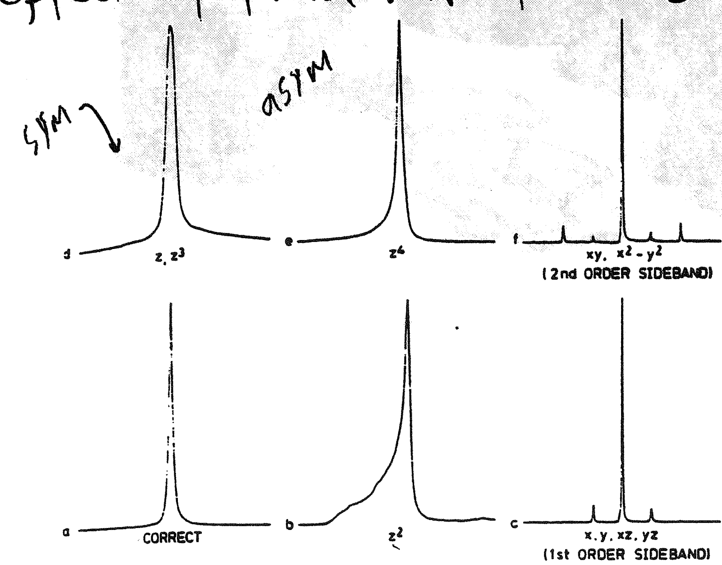
Figure 2.14 Zero-filling the time domain data interpolates extra points into the frequency spectrum, improving its appearance.

In liquid NMR, the main factor conspiring against resolution is **field inhomogeneity**. For instance:



Due to the field inhomogeneity the decay of the FID is usually given by a $T_2^* < T_2$.
The homogeneity required from an NMR magnet is extremely high: Over the sample volume (≈ 1 cm diameter x 1 cm height cylinder), the linewidth at ≈ 500 MHz should be ≈ 0.05 Hz => Inhomogeneity ≈ $\frac{5 \cdot 10^{-2}}{5 \cdot 10^{8}} =$ 1 part in 10^{10}

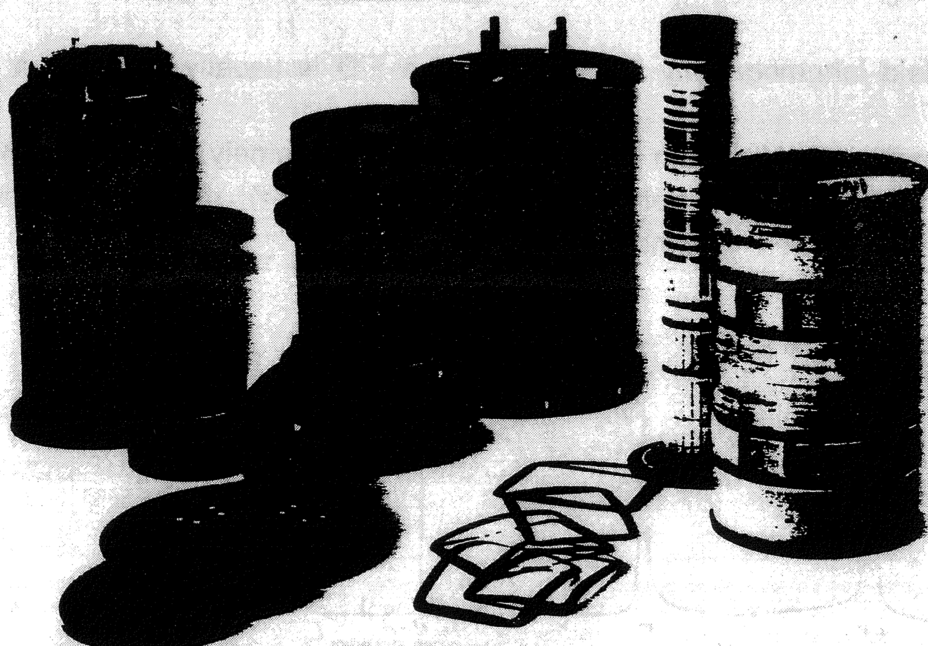
The effects of field imperfections:



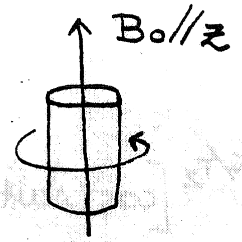
To achieve such resolution a "perfect" magnet and completely non-magnetic materials are not enough, one has to resort to **shimming**: the application of small magnetic field gradients that compensate the inhomogeneities of the main coil.

There are two sets of shim coils:

- **Supercon shims**: usually 4 gradients tuned only upon installation.
- **Room temperature shims**: usually 18-24 gradients, most of them adjusted upon installing the observation probehead containing the sample; some of them need to be adjusted everyday.

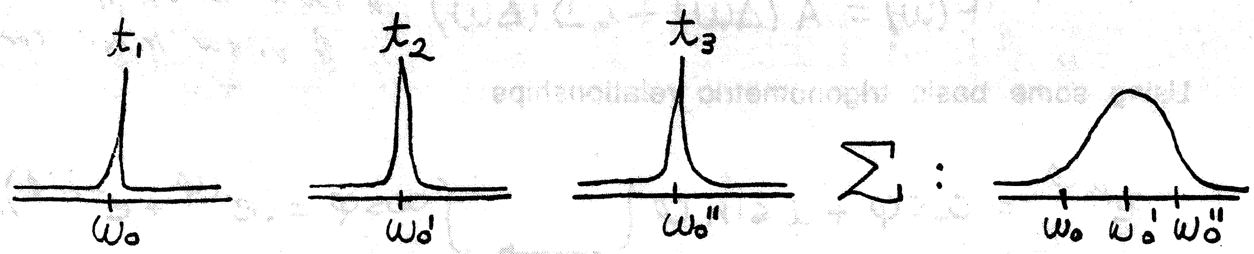


Even shims are not enough, the highest homogeneity is achieved by **spinning** the sample at ≈ 20-40 Hz.

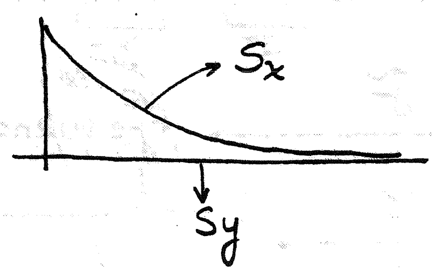


Spinning averages out inhomogeneities in the x-y plane => attention is focussed on the z-axis shims.

Although shimming and spinning can eliminate instantaneous inhomogeneities, sharp lines also require the elimination of long term drift:

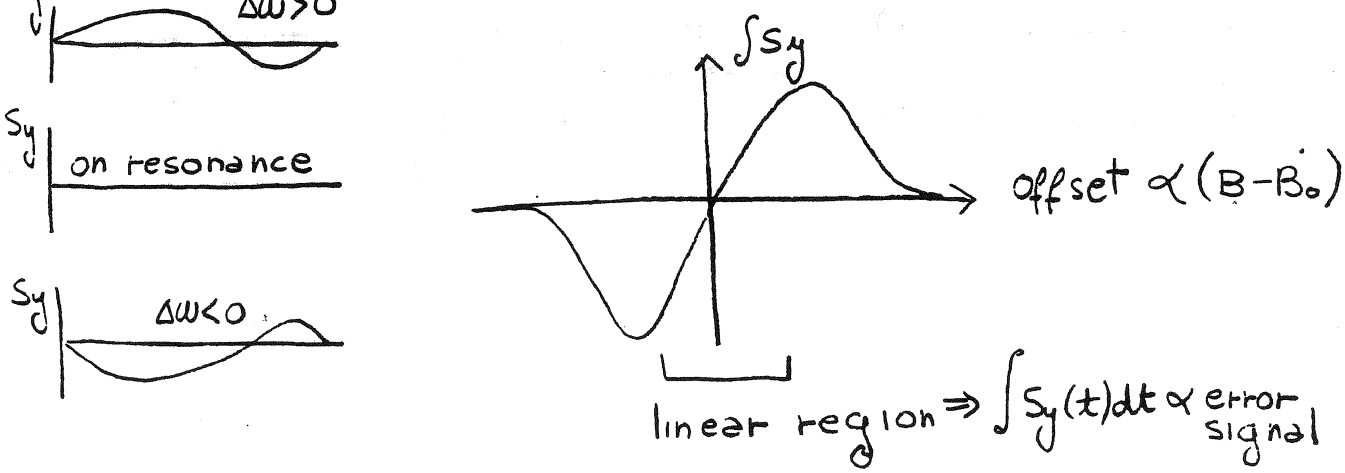


This is achieved using a **deuterium lock**: a system which keeps the magnetic field locked (on-resonance) on a ^2H NMR signal.
At the ^2H NMR frequency



:^2H NMR FID

The deuterium lock system keeps B_0 constant by monitoring $\int S_y(t)\,dt$



II.9 NON-QUADRATURE DETECTION AND QUADRATURE GHOSTS

We saw that given a signal

$$S(t) = S_0 e^{i\Delta\omega t} e^{-t/T_2} = S_0 e^{-t/T_2}\left[\cos(\Delta\omega t) + i\sin(\Delta\omega t)\right]$$

$$\downarrow \mathcal{F}T$$

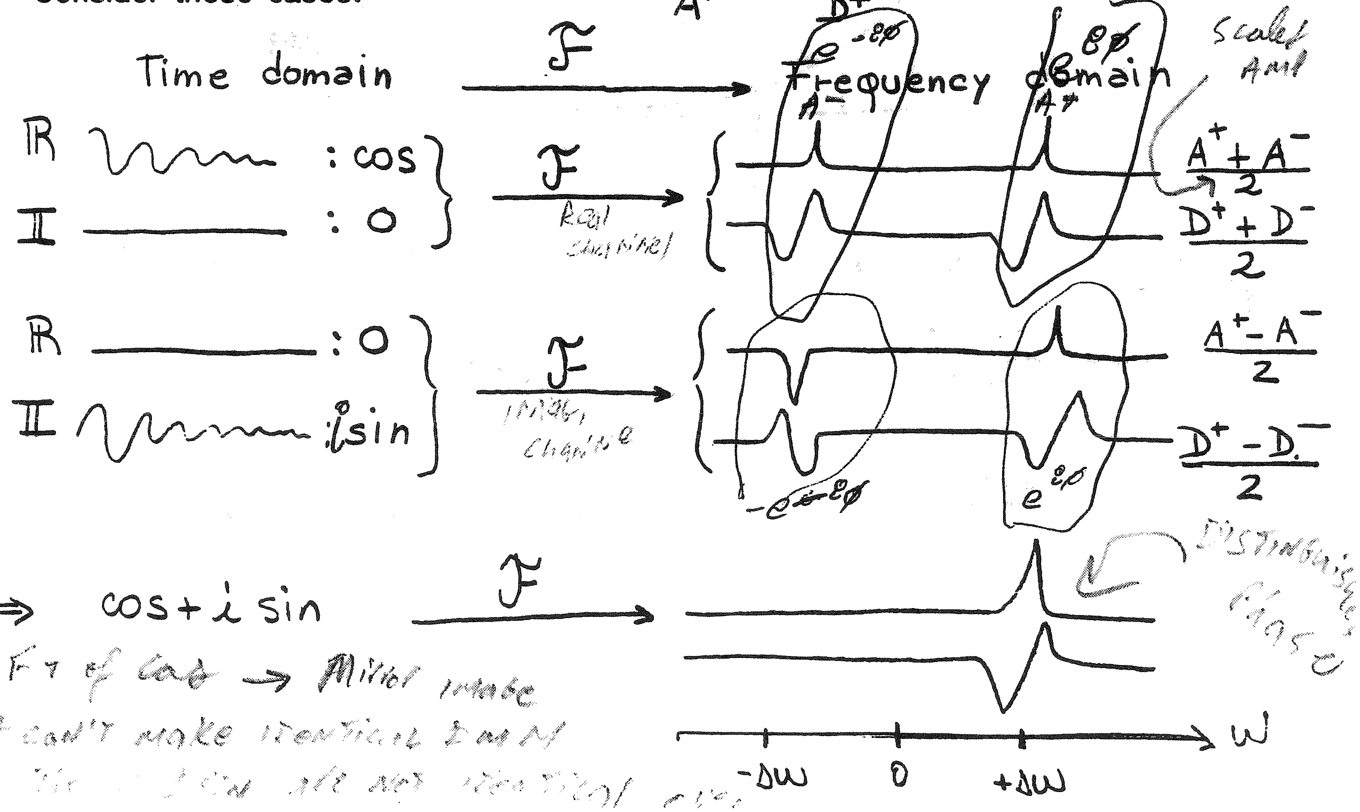
$$F(\omega) = A(\Delta\omega) + i\,D(\Delta\omega)$$

& now break up & view indiv. comp.

Using some basic trigonometric relationships

$$\left.\begin{aligned} e^{i\varphi} &= \cos\varphi + i\sin\varphi \\ e^{-i\varphi} &= \cos\varphi - i\sin\varphi \end{aligned}\right\} \longrightarrow \left\{\begin{aligned} \cos\varphi &= (e^{i\varphi} + e^{-i\varphi})/2 \\ \sin\varphi &= -i(e^{i\varphi} - e^{-i\varphi})/2 \end{aligned}\right.$$

One can get further insight into how the $\underbrace{A(\Delta\omega)}_{A^+} + i\,\underbrace{D(\Delta\omega)}_{D^+}$ line shape is obtained. Consider these cases:



Old systems used non-quadrature detection ($\mathbb{R}$ = cos; $\mathbb{I}$ = 0). In these cases one always has to work off-resonance and throw away half the points, but even though peak folding can be avoided noise folding cannot.

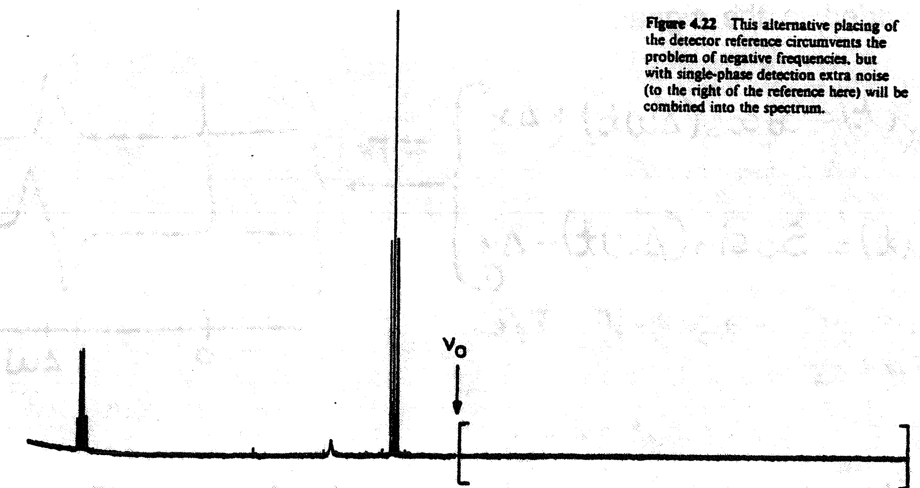
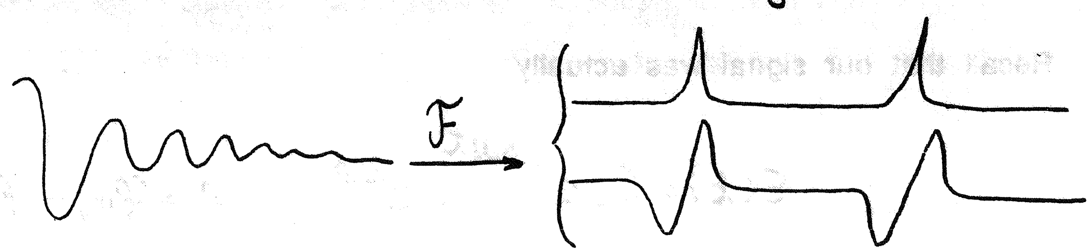


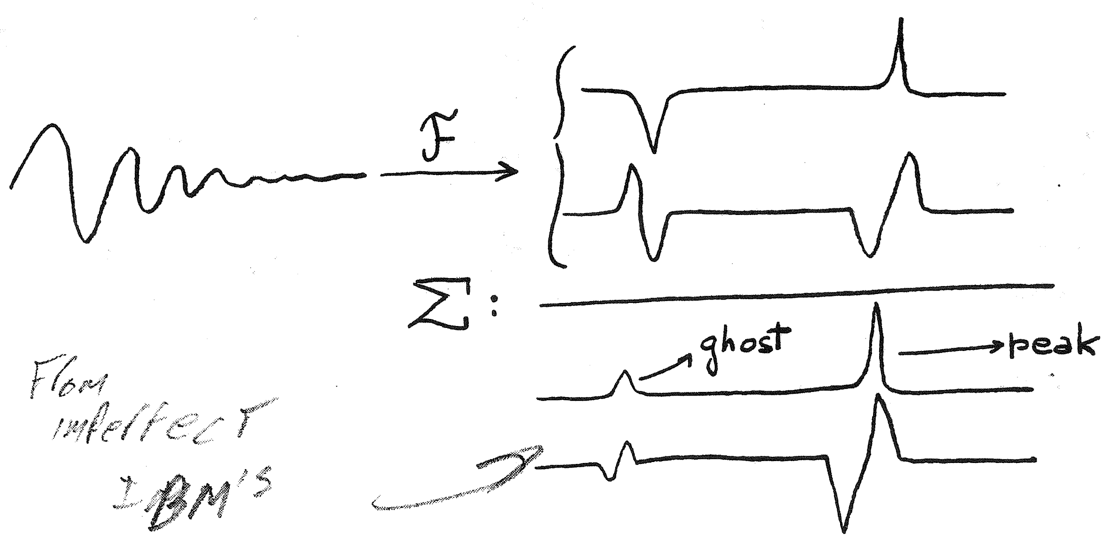
Figure 4.22 This alternative placing of the detector reference circumvents the problem of negative frequencies, but with single-phase detection extra noise (to the right of the reference here) will be combined into the spectrum.

Even in quadrature detection it is impossible to make the gain of both channels identical; this artifact appears as a quadrature ghost. E.g.:

Larger
in $\mathbb{R}$



Smaller
in $\mathbb{I}$



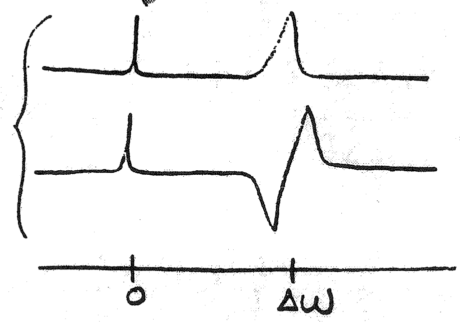
From imperfect
IBM's

II.10 PHASE CYCLING

DC OFFSET

An additional potential artifact that affects pulsed NMR experiments is a small DC offset added to the signal:

$$\left.\begin{aligned} S_x(t) &= S_0\cos(\Delta\omega t) + \Delta x \\ S_y(t) &= S_0\sin(\Delta\omega t) + \Delta y \end{aligned}\right\} \xrightarrow{FT}$$



center of mass of the 2 voltages

* IF overall BC.

If known, subtraction of the average baseline noise from the FID ("baseline correction") can eliminate the peak at zero. A more general procedure which can eliminate **both** baseline and quadrature problems is **phase cycling**

Recall that our signal was actually

$$S(t) = S_0 e^{i\Delta\omega t} \cdot e^{i\varphi} \; ; \quad \varphi = \varphi_{Rx} - \varphi_{Tx}$$

Consider four signals arising from 4 independent experiments:

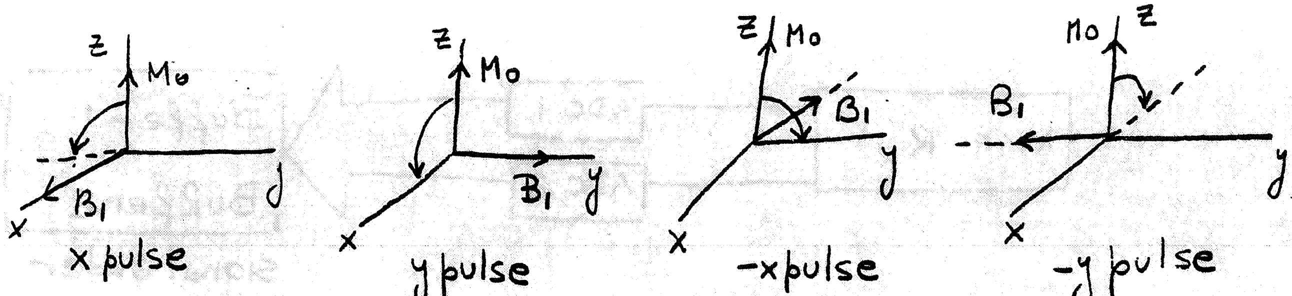
	1	2	3	4
Phase of pulse:	φ_{Tx}	$\varphi_{Tx} + \pi/2$	$\varphi_{Tx} + \pi$	$\varphi_{Tx} + 3\pi/2$
Phase factor:	$e^{i\varphi}$	$e^{i\varphi}e^{i\pi/2} = ie^{i\varphi}$	$e^{i\varphi}e^{i\pi} = -e^{i\varphi}$	$e^{i\varphi}e^{i3\pi/2} = -ie^{i\varphi}$
R signal:	$\cos(\Delta\omega t+\varphi)$	$-\sin(\Delta\omega t+\varphi)$	$-\cos(\Delta\omega t+\varphi)$	$\sin(\Delta\omega t+\varphi)$
I signal:	$\sin(\Delta\omega t+\varphi)$	$\cos(\Delta\omega t+\varphi)$	$-\sin(\Delta\omega t+\varphi)$	$-\cos(\Delta\omega t+\varphi)$

how the S(t) changes

add them up while changing Rx phase.

Really changing phase of Tx → changes phase of B_1

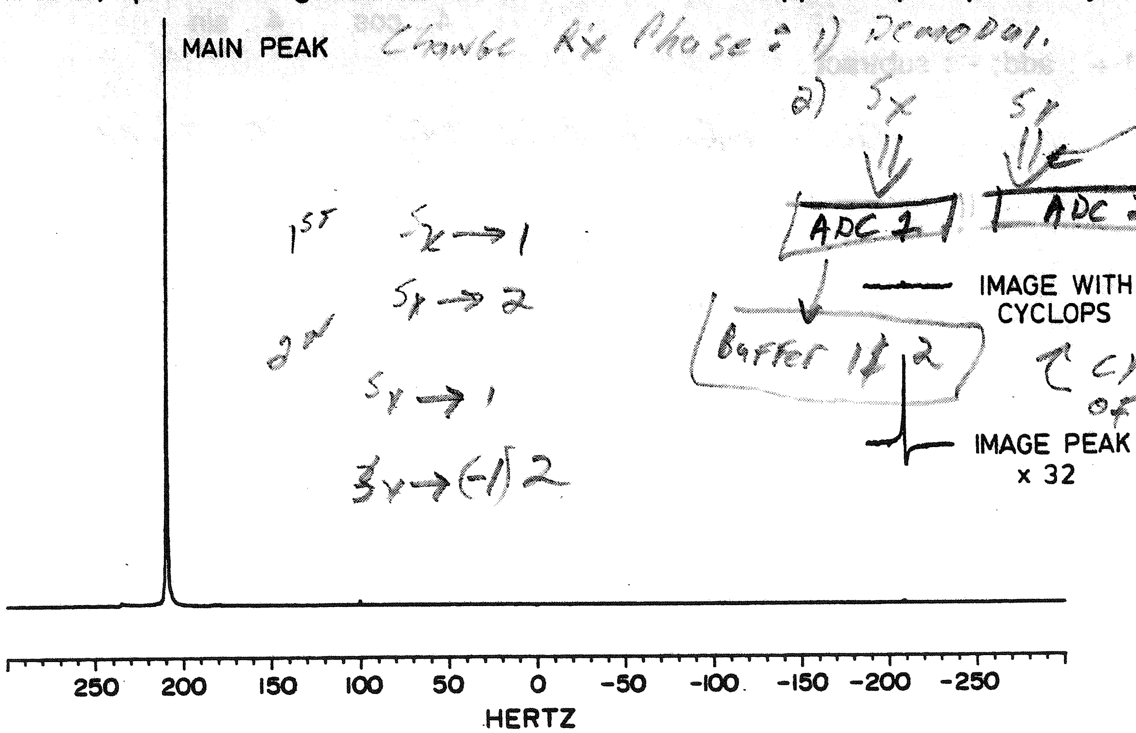
The signals that can be expected from these experiments:



If these signals are added with φ_{Rx} = constant, the result is 0, but if the receiver phase is incremented by $\pi/2$ in each experiment, the signals add up coherently:

$$\varphi_{Rx} - \varphi_{Tx} = \varphi = \text{constant}$$

However, quadrature ghosts and baseline offsets disappear upon phase cycling.



Change Rx Phase: 1) Demodul.

2) S_x S_y cables

ADC 1 ADC 2

Buffer 1 & 2

cycle of phases

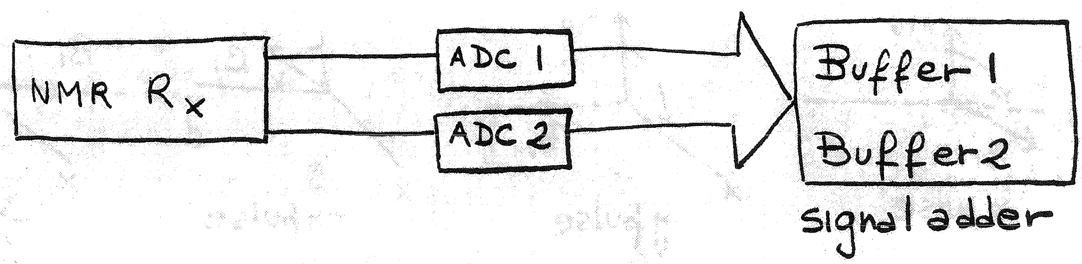
1st $S_x \to 1$

$S_y \to 2$

2nd $S_y \to 1$

$S_x \to (-1)\,2$

Changing φ_{Tx} requires 90° phase shifts of the T_x rf; changing φ_{Rx} however can be done by software:



Experiment #	ADC1 (R)	ADC2 (I)	Buffer1(*)	Buffer2(*)
1	cos	sin	+ADC1	+ADC2
2	-sin	cos	+ADC2	-ADC1
3	-cos	-sin	-ADC1	-ADC2
4	sin	-cos	-ADC2	+ADC1 GOD
			4 . cos	4 . sin

(*) + : add; - : subtract

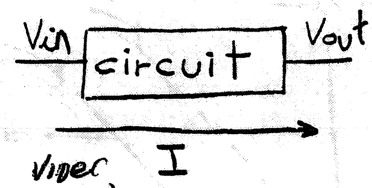
hmwk Quad Ghosts & DC off are elim

ADC 1 : DC off 1
ADC 2 : DC off 2 } 1

Quiz next Fri

II.11 REVIEW OF ELECTRONICS

When dealing with DC currents or voltages, circuits are described by their resistance **R**:



$$V_{in} - V_{out} = R \cdot I$$

Video

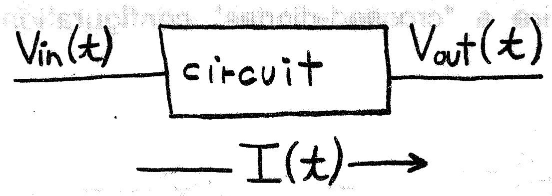
In AC (Audio⟷kHz, rf⟷MHz or microwave⟷GHz) circuits, voltages and currents are time-dependent functions $A \cdot \cos(\omega t + \varphi)$, usually described by complex functions:

Only keep Real Part. Not like quantum

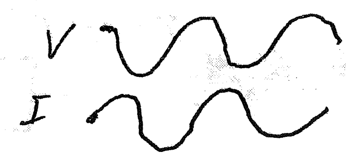
$$V = V_0 e^{i(\omega t + \varphi)} \quad ; \quad I = I_0 e^{i(\omega t + \varphi)}$$

Ohm's law is still valid in this context,. but instead of resistances we now talk about **impedances** (**Z**):

Z = a complex quantity



$$V_{in}(t) - V_{out}(t) = Z \cdot I(t)$$



The three basic linear components of a circuit are:

Resistor: $Z_R = R$ *(Real)* R: resistance (Ω)

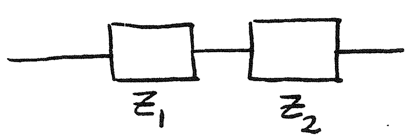
Capacitor: $Z_C = -i/\omega C$ *(complex)* C: capacitance (μF, pF)

Inductor: $Z_L = i\omega L$ *(complex)* L: inductance (μH)

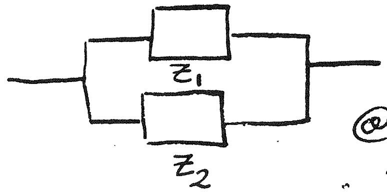
reactances   *i → indicate phase shift*   *90° out of phase*

The impedance of a complex circuit can be expressed in terms of the impedance of its components according to:

at high freq e⁻s don't move essentially



; series circuit $Z_{eq} = Z_1 + Z_2$

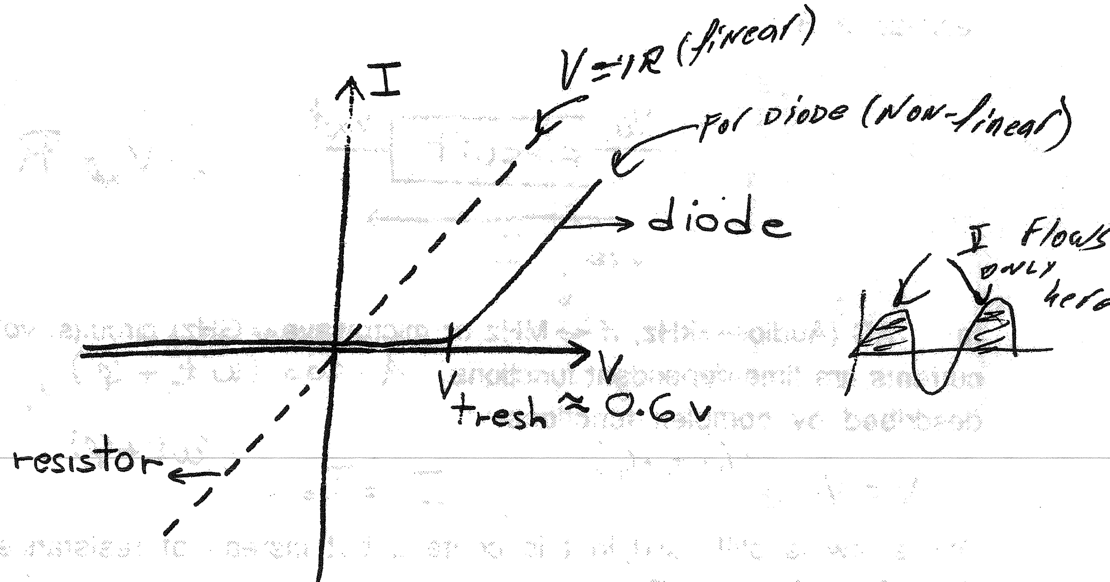


; parallel circuit $\dfrac{1}{Z_{eq}} = \dfrac{1}{Z_1} + \dfrac{1}{Z_2}$

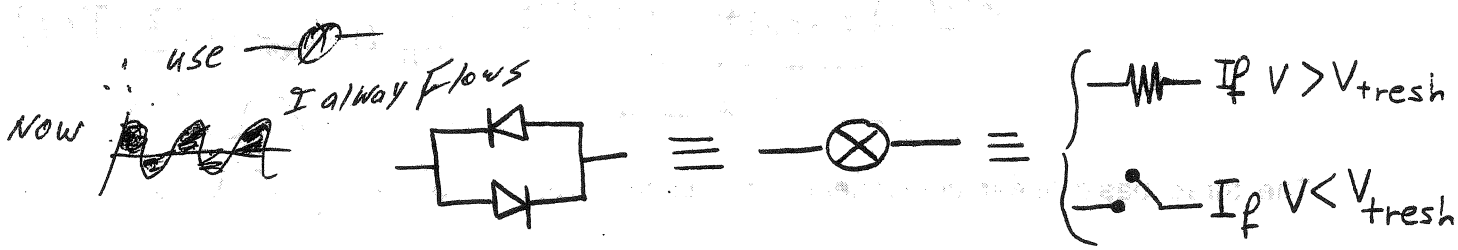
@ 600 MHz have to take into account inductance of Res. (~~S~~ negligible @ low freqs)

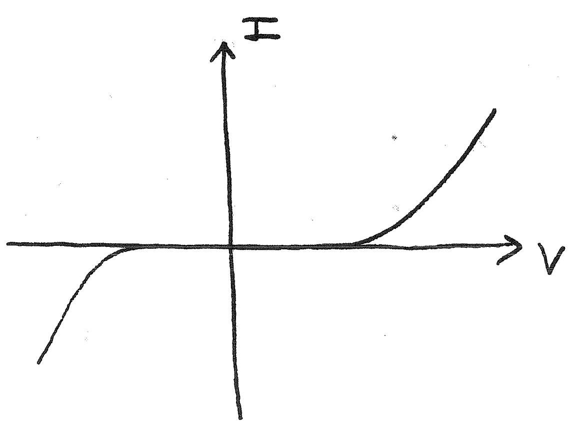
@ 100's MHz, parasitic stuff ... important

An important non-linear element is the diode →|— . A diode behaves like a resistor when a large enough voltage is applied ⟶, but does not let current flow when voltage is applied ⟵ :



Many applications require a "crossed-diodes" configuration

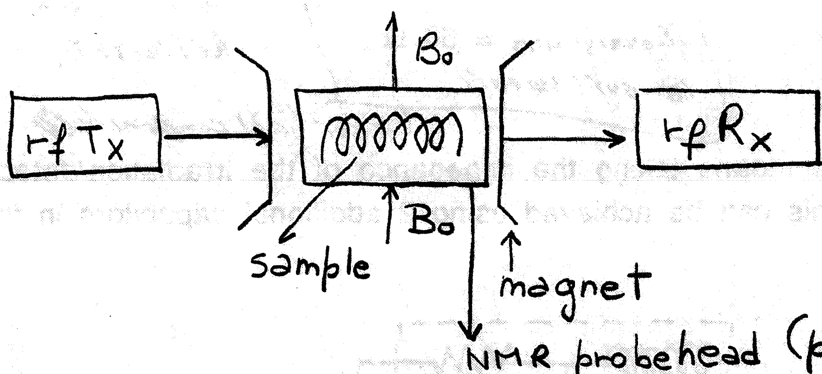


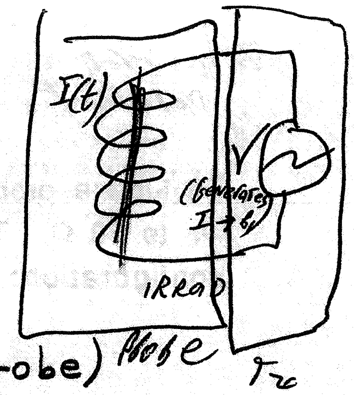


II.12 NMR PROBES

both T_x & R_x
connected to coil

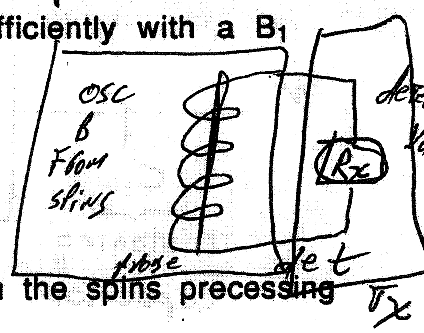
A basic NMR experiment requires:





In an NMR experiment we need a probehead capable of

- Irradiating the sample efficiently with a B_1 oscillating at ω_0
- Detecting the signal from the spins precessing at ω_0



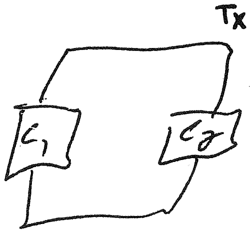
Most effic transfer from $T_x \rightarrow$ ~~coil~~ Probe

Need $Z_{probe} = Z_{Tx}$ (Impedances must be same at Larmor Freq. Forget other Freqs)

If the same coil is used for irradiation and detection these 2 conditions are equivalent: a system capable of delivering rf efficiently, will also detect small signals efficiently.

The electronic properties of the probe are described by the probe's impedance Z_{probe}. To achieve maximum efficiency in the

rf transmission: $Z_{Tx} = Z_{probe}$ at $\omega = \omega_0$ rf detection: $Z_{Rx} = Z_{probe}$ at $\omega = \omega_0$



HMWK; show max power transfer

$Z_{TX} = Z_{prob} = Z_{RX}$

For maximum flow want R of C_1 = R of C_2

Similar problems arise in other situations involving rf, where it was realized that things could become simpler if everyone uses devices with the same impedance. This was chosen as:

Z is Freq Dependent

$$\boxed{Z_{everything} = 50\ \Omega}$$

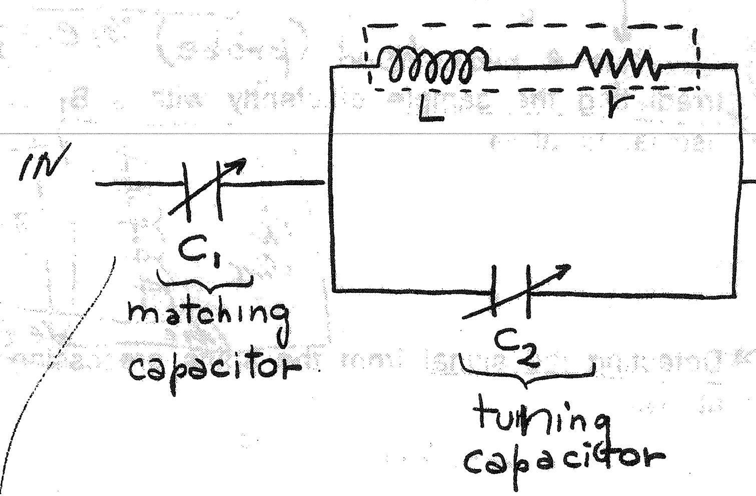
@ our Larmor

For all components

If Impedances are diff then get signal Reflected,

eg) amp DSM of 50 Ω

To tune a probe means taking the impedance of the irradiation/detection coil at ω_0 to 50 Ω. This can be achieved using 2 additional capacitors in the following configuration:



L, r: inductance and parasitic resistance of sample coil

Need 2 capacitors because)
1) need R = 50 Ω
2) " " X = 0 Ω

If for such a circuit

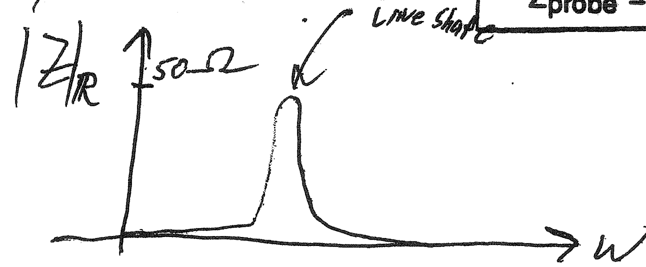
$$C_1 = \frac{\sqrt{r/50}}{\omega_0^2 L} \quad ; \quad C_2 = \frac{1 - \sqrt{r/50}}{\omega_0^2 L}$$

Values of 2 capacitors → 50 Ω = Z_R

Then,

$$\boxed{Z_{probe} = 50\ \Omega}$$

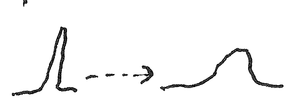
Resonance Line Shape



Match effects height

tune effects W

eg)

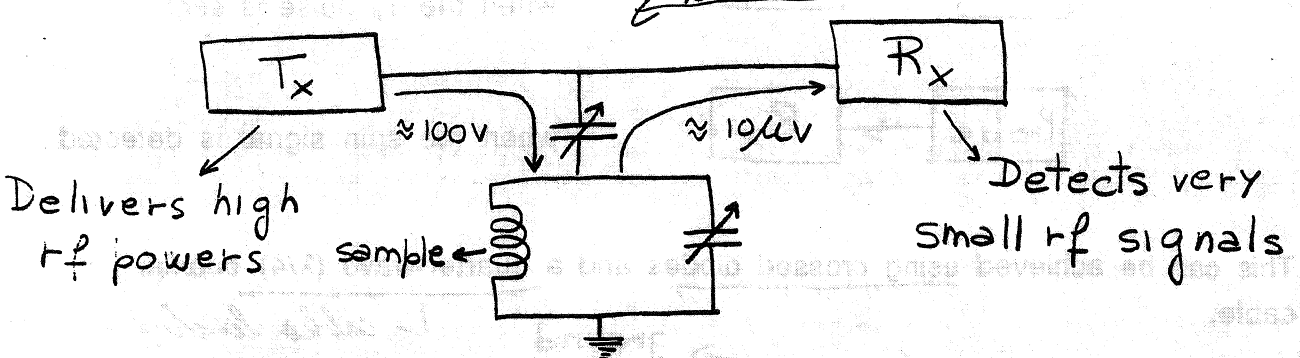


changes shape ∴ match changes it . .

1) Disconnect Tx during detection
2) Disconnect Rx during pulse.

II.13 DUPLEXING

We have the system connected in such a way that (reflects (burns Tx))



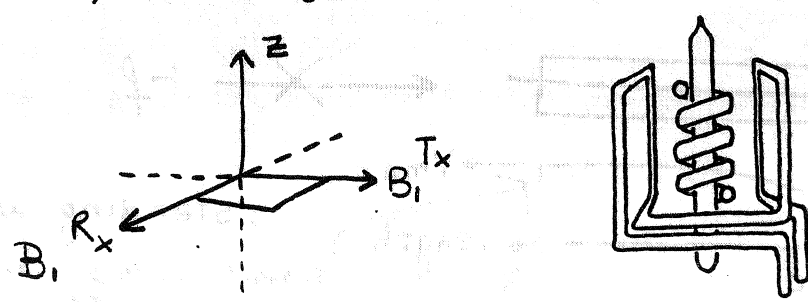
If the Rx is not isolated from the Tx, the rf burst will burn it.

There are 2 ways of isolating (**duplexing**) the rf on such a system:

a) Use 2 orthogonal coils, each with its own set of capacitors:

* This decouples Tx from Rx

Dis



Advantage: By construction, the Tx and Rx don't see each other.

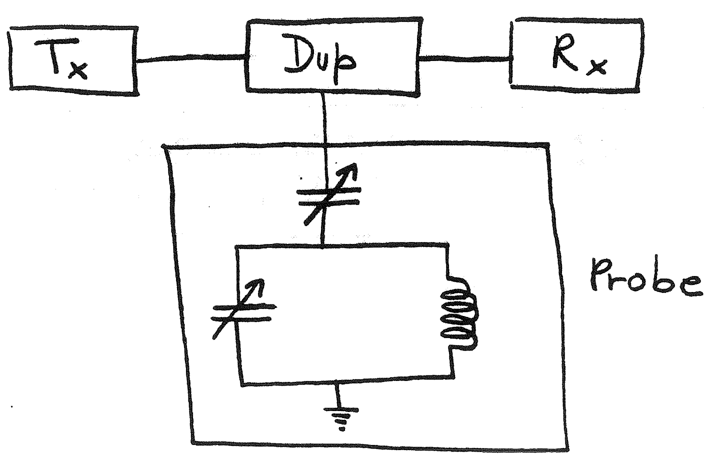
Disadvantages: i) The Tx coil is larger => less efficient (coil far from sample)

ii) Only works for Helmholtz coils (≈ 1/3-1/2 as efficient as solenoid coils)

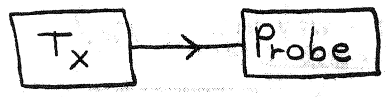
of use

b) Use an active or passive duplexing system

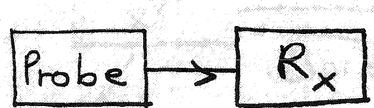
Too many diodes & transistors add noise.



that looks like



when the T_x pulse is sent

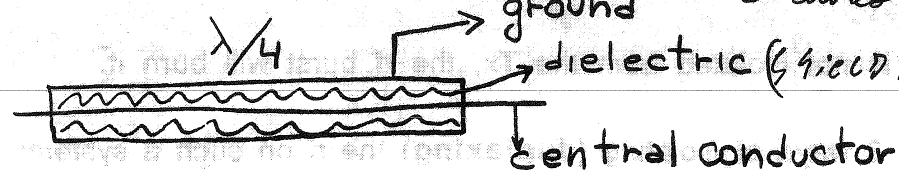


when the spin signal is detected

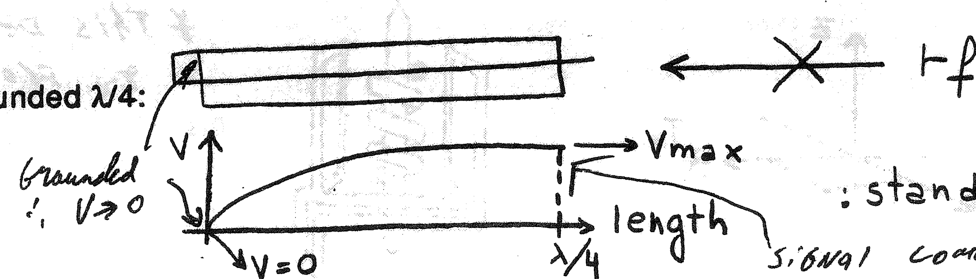
This can be achieved using crossed diodes and a quarter-wave ($\lambda/4$) coaxial cable.

L cables length =

A coax:



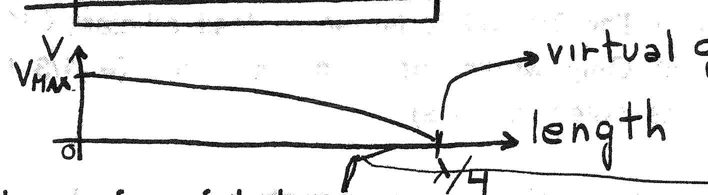
grounded $\lambda/4$:



: standing wave

signal comes in the e-s can't flow because at Vmax!

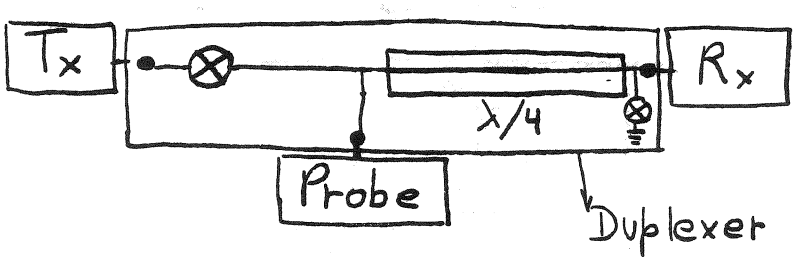
open $\lambda/4$:



: standing wave

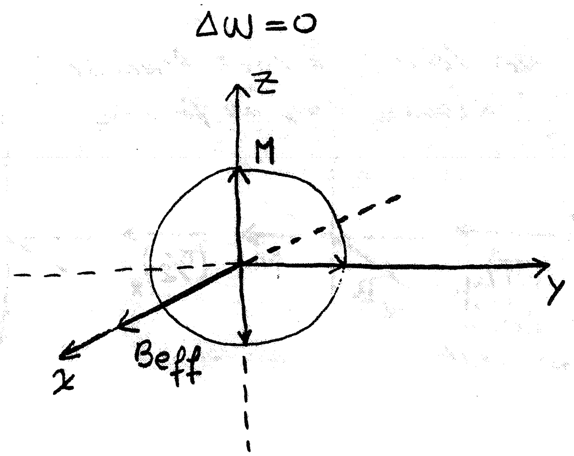
A simple scheme of an rf duplexer:

1st) Pulse builds standing wa[ve]
∴ Goes to Prob[e]

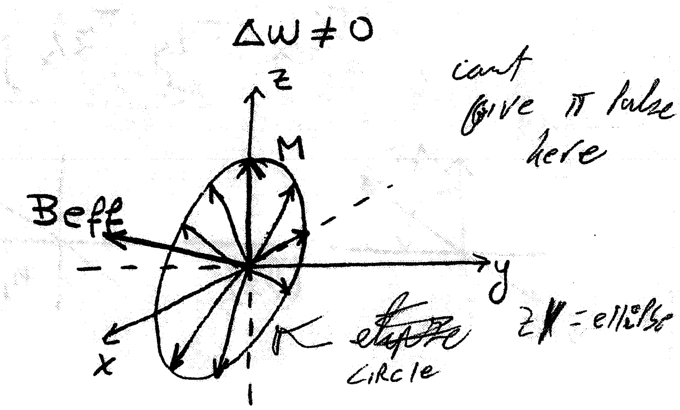


II.14 BROADBAND IRRADIATION (using classical magnet Desc.)

In general, an NMR experiment is done off-resonance. Under these conditions it is difficult to apply accurate $\pi/2$ or π pulses:



circle on the z-y plane



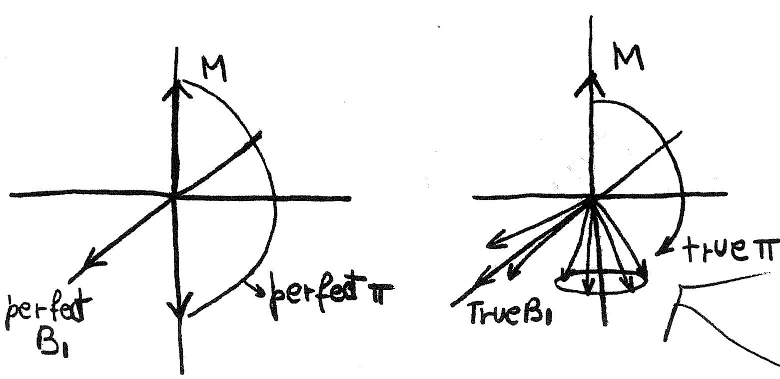
can't give π pulse here

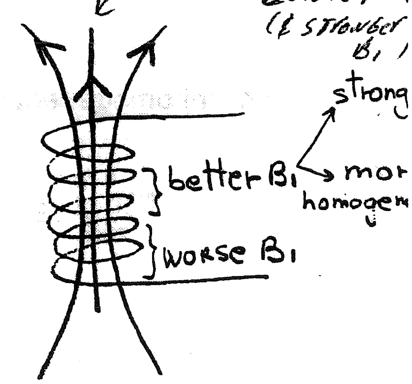
elipse: – crosses the x-y plane but not the y-axis
– does not touch the –z axis

Even if $\Delta\omega = 0$, spatial inhomogeneities of the rf field produce problems

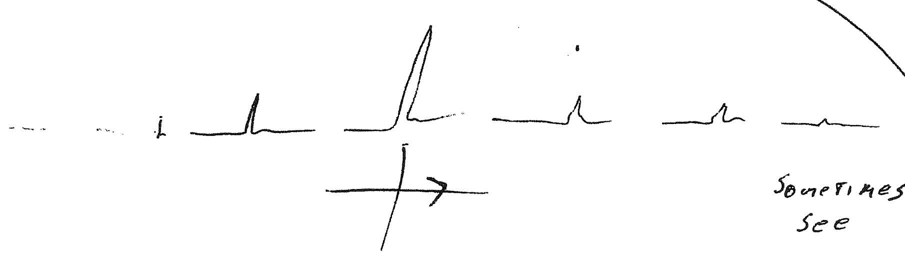
B_1 inhomogeneity much larger then B_0's

1×10^9 for B_0

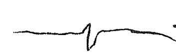




10 mm can't give Pi pulses



Sometimes see



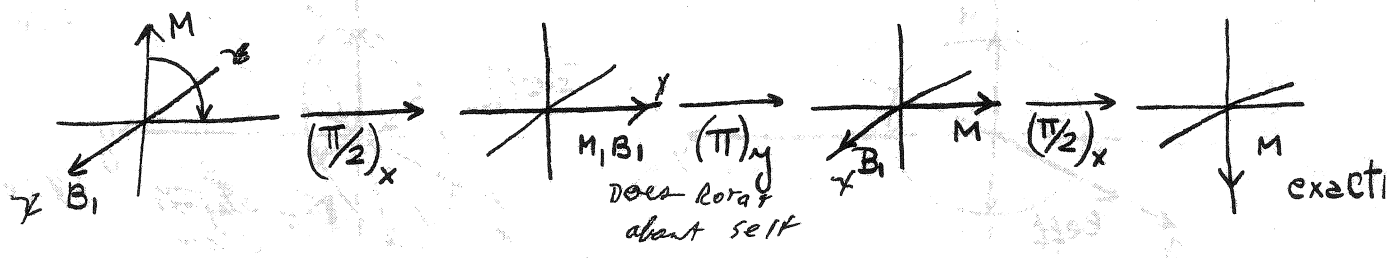
Because of we are then

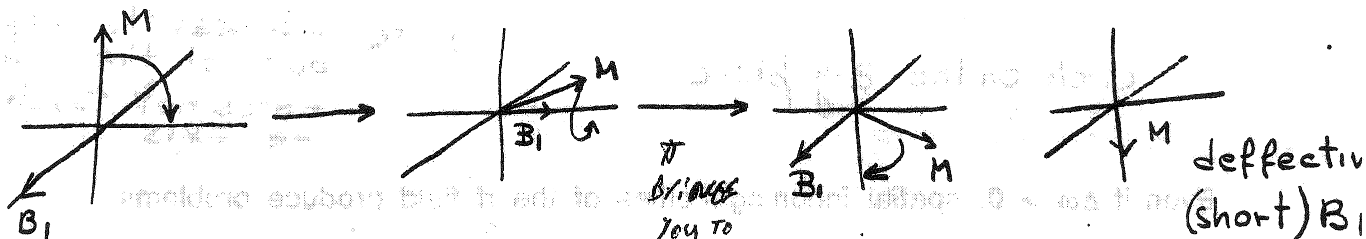
It is possible to minimize these imperfections by replacing $\pi/2$ or π pulses by **composite pulses**: sequences of rf irradiation whose net effect are those of an ideal $\pi/2$ or π pulse.

E.g. : if we have inhomogeneity in B_1, we can replace a π_x pulse by

$$\left\{ \left(\tfrac{\pi}{2}\right)_x \left(\pi\right)_y \left(\tfrac{\pi}{2}\right)_x \right\}$$

Not really exact Remember assume they are for now





a self compensating effect.

& Malcolm Levy technique called MLEV

For inhomogeneous B_1:

For a 90° pulse
$$\left(\tfrac{\pi}{2}\right) \equiv \left\{ \left(\tfrac{\pi}{4}\right)_{-y} \left(\tfrac{\pi}{2}\right)_x \left(\tfrac{\pi}{2}\right)_y \left(\tfrac{\pi}{4}\right)_x \right\}$$

For offset $\Delta\omega$:

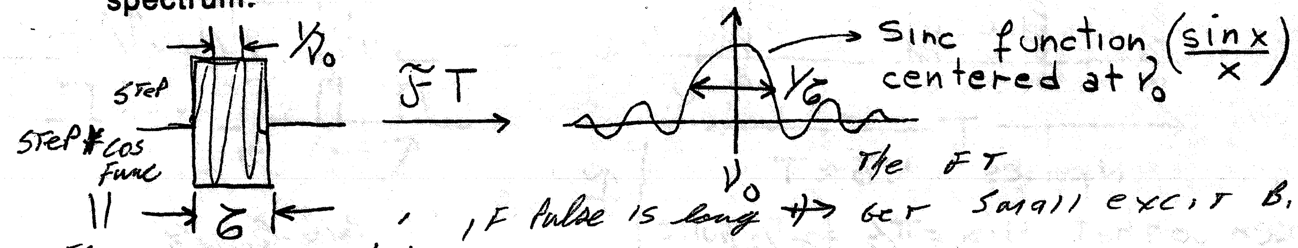
For 180's w/ some offset
$$\pi \equiv \left\{ \left(\tfrac{\pi}{2}\right)_x \left(\tfrac{4\pi}{3}\right)_y \left(\tfrac{\pi}{2}\right)_x \right\}$$

II.15 SELECTIVE IRRADIATION

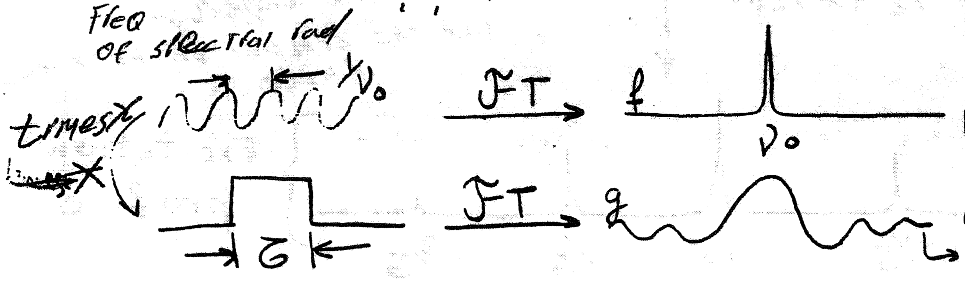
whats the irrad BW eq)

The excitation spectrum of an rf pulse is approximately ~~given by its Fourier~~ spectrum:

will these be excited too



The FT ∴ if pulse is long → get small excit B.W.

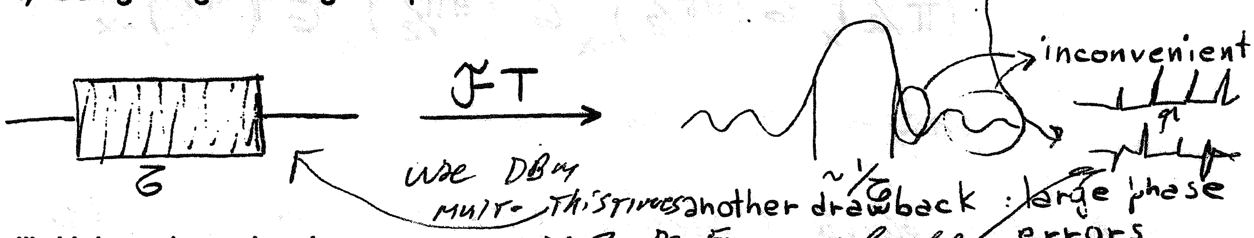


$* :$ convolution $(\nu) = \int_{-\infty}^{\infty} f(\nu-\omega)g(\omega)d\omega$

Sometimes, one wants to restrict excitation to a narrow region of the frequency domain. There are several ways of achieving this :

These wiggles can also be neg, can give

i) Using long rectangular pulses:

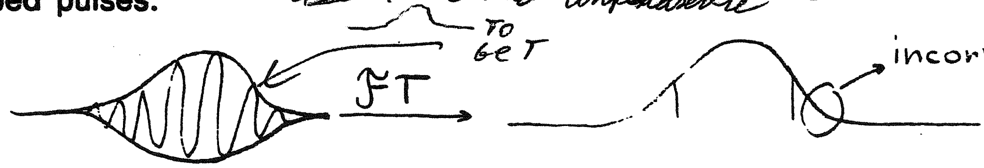


use DB by mult. This is times another drawback : large phase errors

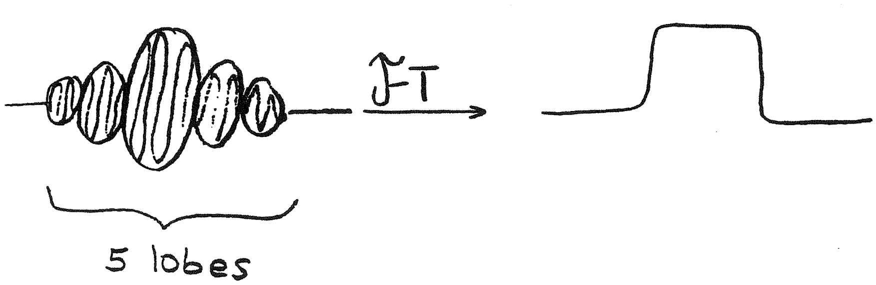
ii) Using shaped pulses:

a DC func unreachable to get

Gaussian (relatively easy)

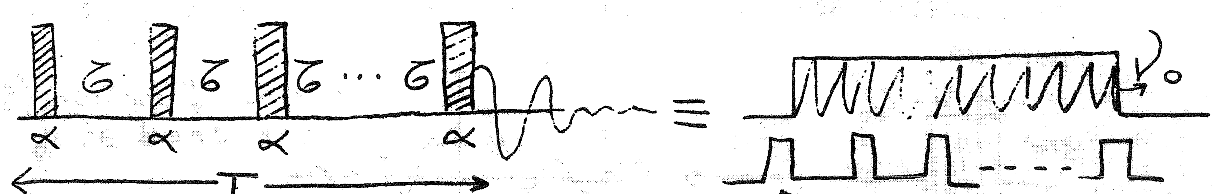


Sinc (more difficult)



IV

iii) Using a **DANTE** (Delays Alternating with Nutations for Tailored Excitation) sequence: train of short rectangular pulses of angle α



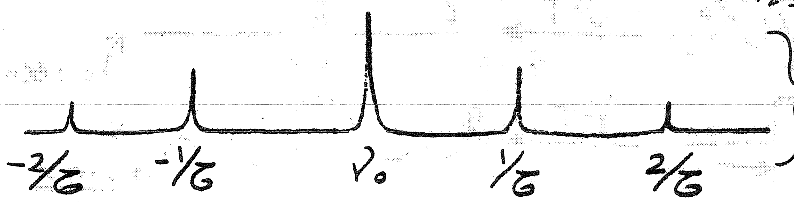
N pulses ; $N\tau \approx T$

chosen so that $N\cdot\alpha = \pi/2$ for $\pi/2$ pulse

$\mathcal{F}$

1-2° pulse lengths

Get the conv of very long pulse



Excitation profile

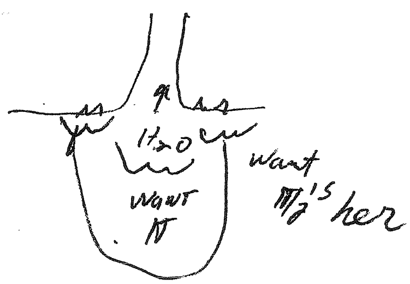
iv) Using composite pulses; e. g.

SIDE bands depend on $1/\tau$

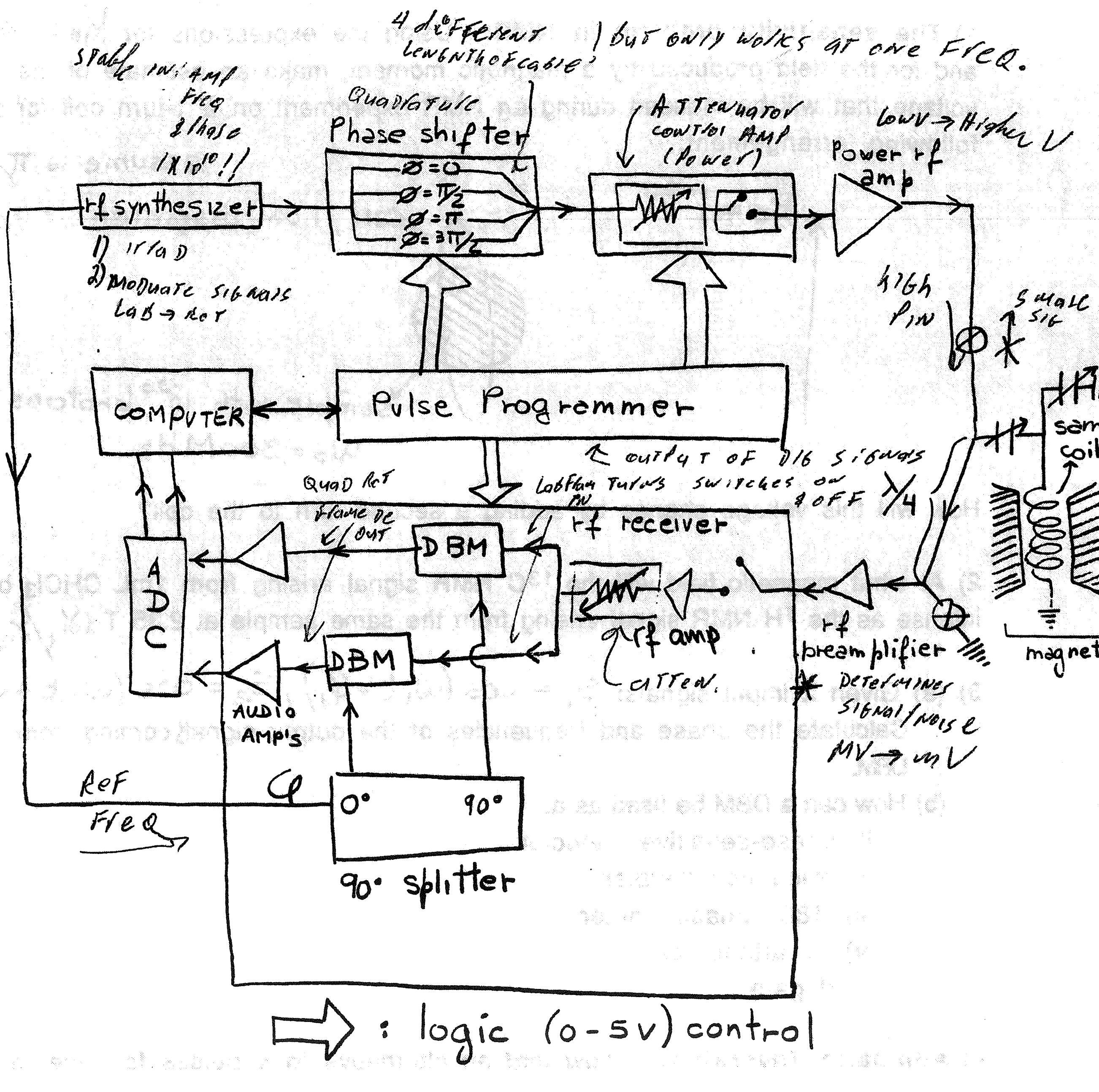
$$(\pi/2)_x\ \tau\ (3\pi/2)_{-x}\ \tau\ (3\pi/2)_x\ \tau\ (\pi/2)_{-x}$$

vary τ then vary excit

why use dante (selective excit) eg) a prot in H_2O



II.16 BLOCK DIAGRAM OF A BASIC NMR SPECTROMETER

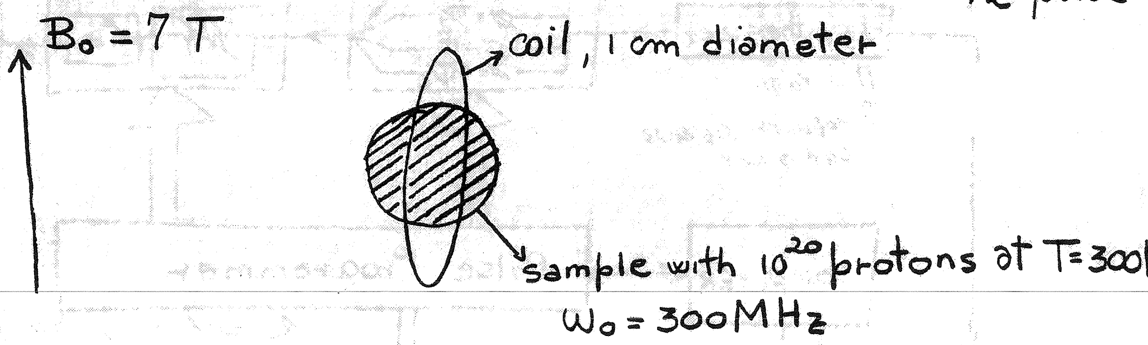


⇨ : logic (0-5V) control

II.17 PROBLEMS

1) **The sensitivity problem in NMR:** Using the expressions for $M_0 = M_0(\gamma, B, T)$ and for the field produced by a magnetic moment, make an estimate of the voltage that will be induced during an NMR experiment on a 1-turn coil for the following arrangement.

assume a $\pi/2$ pulse



How will this voltage change by adding a second turn to the coil?

2) At what magnetic field will the ^{13}C NMR signal arising from 1mL $CHCl_3$ be as intense as the ^1H NMR signal arising from the same sample at 2.35 T ($\gamma_{^1H}/\gamma_{^{13}C} = 4$).

3) (a) Given 2 imput signals: $S_1 = \cos(\omega_1 t + \varphi_1)$, $S_2 = \cos(\omega_2 t + \varphi_2)$ Calculate the phase and frequencies of the output signals coming from a DBM.

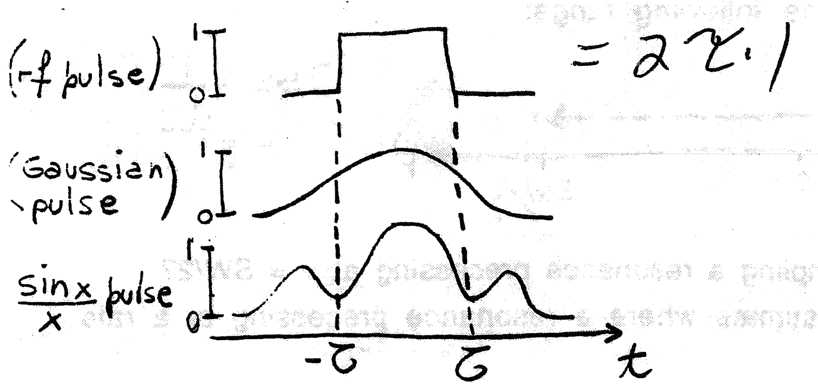
(b) How can a DBM be used as a:

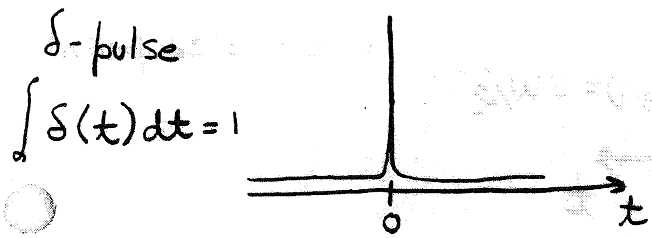
i) phase-sensitive detector
ii) frequency doubler
iii) 180° phase shifter
iv) rf attenuator
v) rf gate

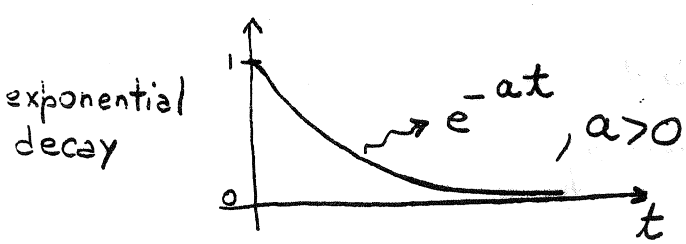
4) **Adiabatic Inversion:** Show that an alternative to π pulses for inverting a magnetization vector is to sweep slowly enough a B_1 field from well-above to well-below exact resonance.

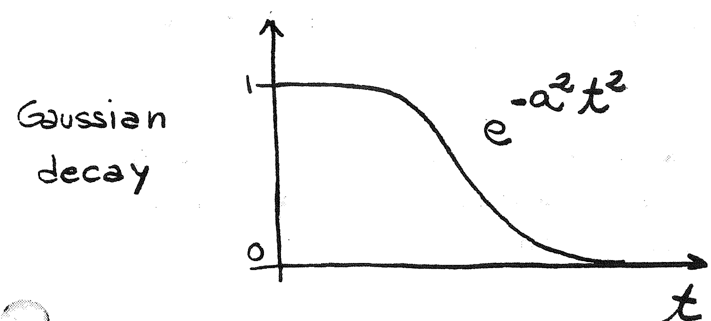
5) **The time- vs the frequency-domain:** Calculate the Fourier transforms of the following functions:

Time-domain **Frequency-domain**





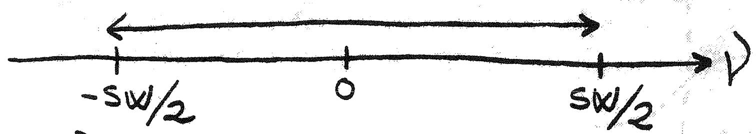




6) What are the mathematical expressions of the inverse Fourier transform in continuous and in discrete sampling cases.

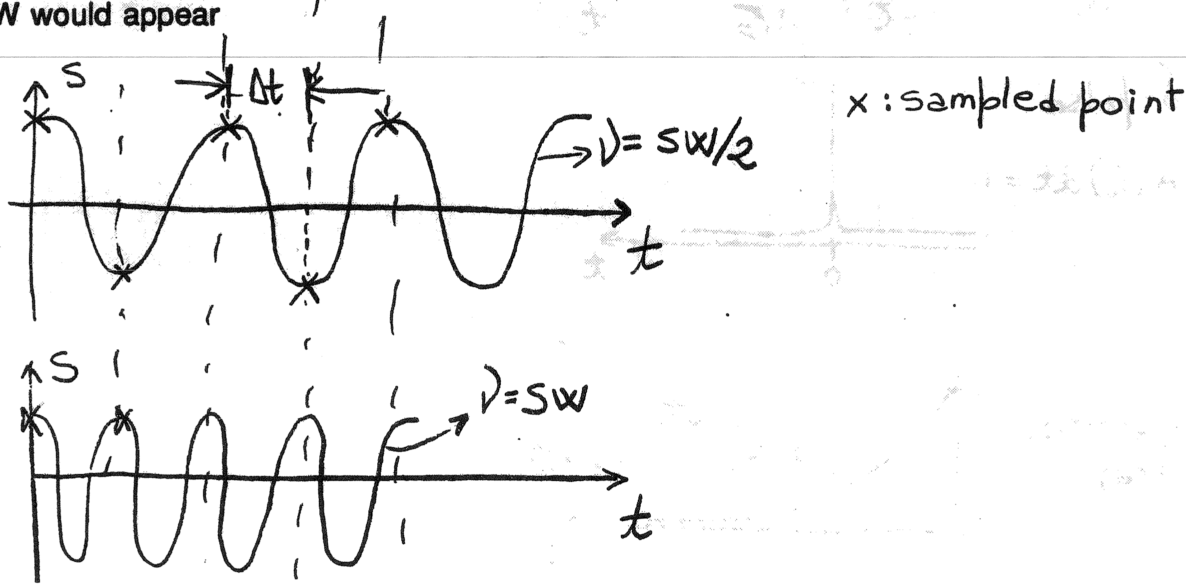
7) **Peak folding:** Nyquist theorem states that given a dwell time Δt, we can only characterize peaks within the following range:

$$SW = \frac{1}{\Delta t}$$



i) How many points per cycle would be sampling a resonance precessing at $\nu = SW/2$?

ii) Use the following picture to estimate where a resonance precessing at a rate $\nu = SW$ would appear



iii) Where would a $\nu = -SW$ resonance appear? On which region of the spectrum would a resonance precessing between $\nu = sw/2$ and $\nu = sw$ appear?
Cases ii) and iii) are examples of peak folding: if Δt is not chosen correctly, peaks appear where they shouldn't.

8) What dwell time should be used and how many points should be acquired to obtain a spectrum characterized by a spectral window of 10 kHz and a digital resolution of 0.5 Hz? (recall that usually the # of points = 2^m)

9) Calculate the first 8 points of an NMR signal arising from a site whose

resonance offset is 1000 Hz and line width = 1 Hz; assume a dwell time of 0.5 ms

10) How does the **total length** of a magnetization vector change with time after a $\pi/2$ pulse in the case of $T_1 = T_2$?

11) Give the expression for the Bloch equations in the presence of a B_1 field placed at an arbitrary orientation along the x-y plane.

12) **NMR line shapes:** Calculate the $\mathcal{F}$T of $S(t) = e^{i\Delta\omega t} e^{-t/T_2}$

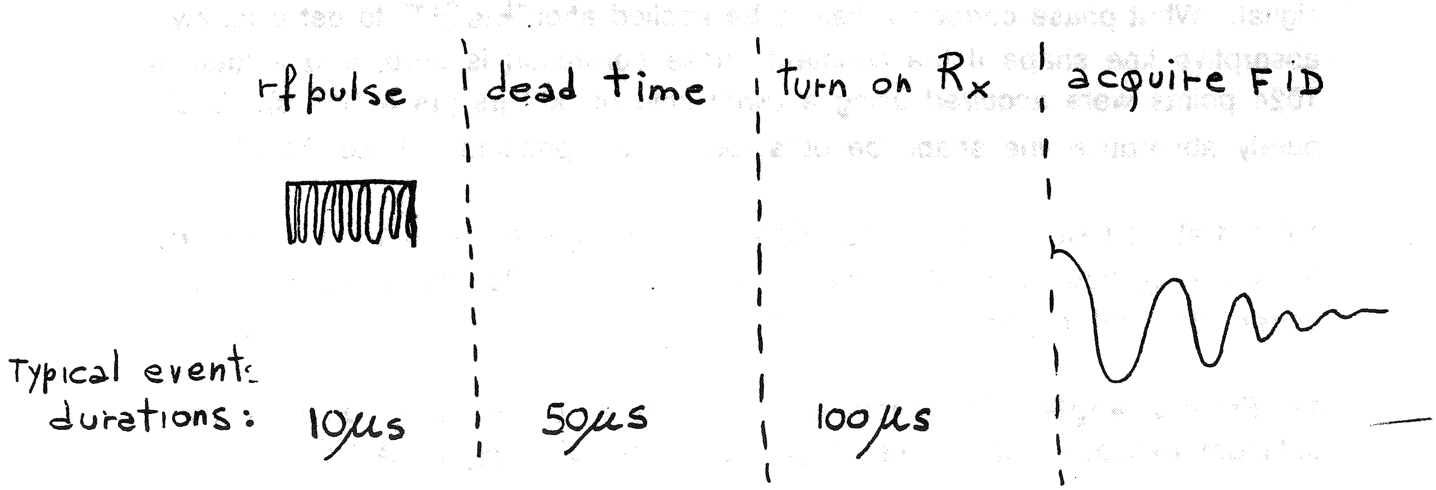
13) **The justification of phasing:** Find the expression for the full-width at half-height of:

i) a lorentzian line shape $A(\omega)$

ii) a magnitud representation of the signal $= \sqrt{A(\omega)^2 + D(\omega)^2}$

On the basis of this analysis, justify the use of phasing.

14) The sequence of events involved in a 1-pulse NMR experiment:



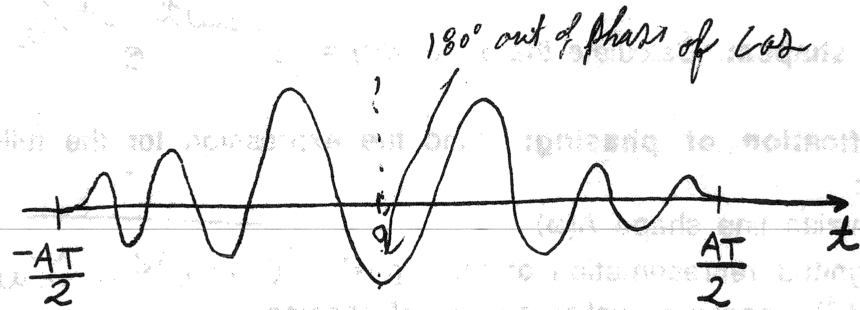
If an experiment carried on-resonance affords a peak that requires a phase-correction of $\varnothing = 45°$ to become purely absorptive, what phase correction will be needed if the transmitter is moved

i) +5 kHz off-resonance

ii) -5 kHz off-resonance

Use the typical time delays listed above.

15) **Echo experiments:** An NMR echo affords a time-domain FID of the type



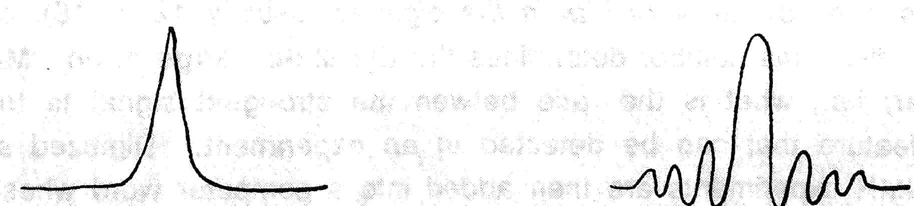
Schematize the real and imaginary parts of the spectrum obtained by $\mathcal{F}$T-ing this signal. What phase correction has to be applied after this $\mathcal{F}$T to get a purely absorptive line shape if the constant phase correction is zero, and a total of 1024 points were acquired using a dwell time of 500 µs (µs = 10^{-6} s). Could a purely absorptive line shape be obtained without phasing? If so, how?

16) If 1mL of $CHCl_3$ gives a ^{13}C NMR spectrum with a S/N = 10 in 1 scan (total AT = 1 sec), how long will it take to reach a S/N = 100 with a 0.2 mL of sample under identical experimental conditions? ← Should be conc.

17) **Ernst's angle:** Demonstrate the validity of the equation defining the optimum excitation conditions (β_{opt} = Ernst angle). See page 55.

18) **Truncation:** The number of acquisition points used in an NMR experiment has to be chosen large enough to let the signal decay to ca. the level of the noise. Calculate the line shape obtained if only one quarter of this number of points is

acquired. Hint: The result is the convolution of the normal line shape with the FT of a step function:



from normal signal from truncated signal

How can the wiggles originating by truncating the signal be eliminated without increasing the number of acquired points? At what cost?

19) Why isn't it convenient to spin the sample faster than ca. 50 Hz when recording a high-resolution NMR spectrum?

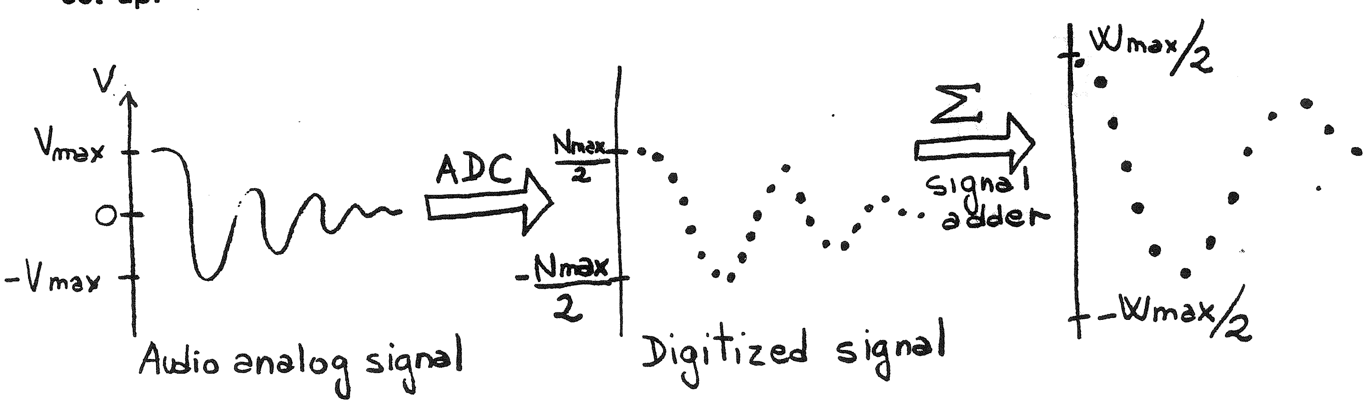
20) Calculate the signals arising from an FID whose real and imaginary components are

i) $\Re \longrightarrow \sin(\omega t)\ ;\ \Im \longrightarrow 0$

ii) $\Re \longrightarrow 0\ ;\ \Im \longrightarrow \cos(\omega t)$

21) **Coherence selection:** from a quantum mechanical point of view, an NMR experiment detecting a signal $S(t) = Tr(\rho I_+) = const.\ e^{i\Delta\omega t}$ is said to be detecting the -1 coherence (the I_- component of ρ). How is it necessary to rearrange the NMR data so as to detect the +1 coherence (i.e., to obtain a peak at $-\Delta\omega$ from the same spin system).

22) **Dynamic Range:** Final digitization of an NMR signal involves the following set up:



An ADC is characterized by the largest voltage (V_{max}) that it can represent and by the largest digit ($N_{max}/2$) assigned to this voltage. A typical value for V_{max} = 5V; N_{max} is given by the *# of bits in the digitizer* (usually 12 or 16), according to $N_{max} = 2^{\#\text{of bits}}$. This number determines the **dynamic range** of an NMR spectrometer; i.e., what is the ratio betwen the strongest signal to the smallest significant feature that can be detected in an experiment. Digitized signals from succesive NMR experiments are then added into a computer word whose maximum value $W_{max}/2$ is given by the # of bits in the word (usually 20 or 24: $W_{max} = 2^{20}$ or 2^{24}).

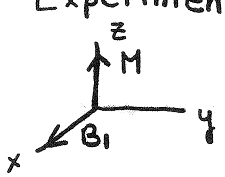
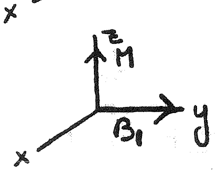
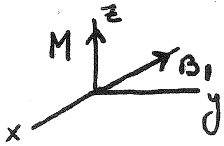
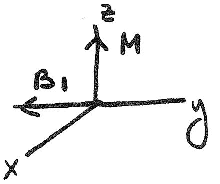
i) What is the dynamic range of a 12 bit digitizer? And of a 16 bit digitizer?

ii) What should the voltage of the acquired signal be set to in order to observe a weak NMR resonance under optimal conditions?

iii) Given the acquisition conditions of item ii), calculate how many scans can be acquired using a 16-bit digitizer before overflowing (i.e., reaching the maximum value) of a 24-bit word for a system where (a) the S/N $= \infty$; (b) the S/N $\approx$ 0. (Remember that noise adds up randomly)

23) Demonstrate that an imbalance ΔG in the gain of the real and imaginary audio channels gives origin to a quadrature ghost. Calculate the intensity of the ghost as a function of $\Delta\omega$, ΔG.

24) Fill out the following table:

Experiment	φ_{Tx}	$\mathbb{R}$ signal	$\mathbb{I}$ signal
	0	$\cos \Delta\omega t$	$\sin \Delta\omega t$
	$\pi/2$	$-s(\Delta\omega t)$	$\cos(\Delta\omega t)$
	π	$-c(\Delta\omega t)$	$-\sin(\Delta\omega t)$
	$3\pi/2$	$s(\Delta\omega t)$	$-\cos(\Delta\omega t)$

25) Given n phase-shifted experiments characterized by transmitter rf phases

$$\varphi_{Tx} = \varphi^{\circ}_{Tx} + 2\pi(i-1)/N \; ; \quad i = 1, 2, \ldots, N \; ; \quad \varphi^{\circ}_{Tx} = \text{any} \; ;$$

i) Calculate the coefficients $c_1^i, \ldots c_4^i$ of the linear combinations

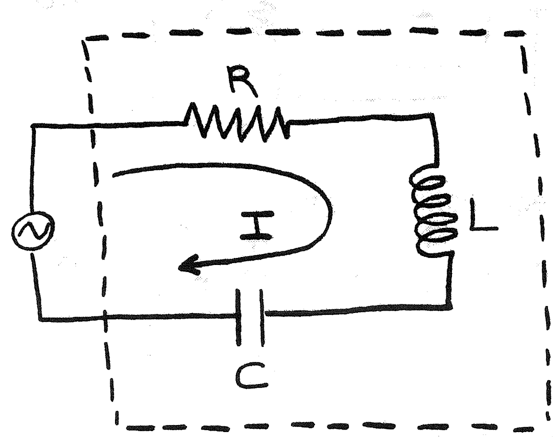
$$c_1^i \cdot \text{ADC}\,1 + c_2^i \cdot \text{ADC}\,2 \longrightarrow \text{memory buffer } 1,$$
$$c_3^i \cdot \text{ADC}\,1 + c_4^i \cdot \text{ADC}\,2 \longrightarrow \text{memory buffer } 2,$$

that are needed to add the signals of the different experiments coherently.
ii) Find the minimum N that will eliminate DC offsets. Will this phase cycle also cancel quadrature ghosts?
iii) Find the minimum N that will eliminate quadrature ghosts. Will this phase cycle also cancel DC offsets?

26) Calculate the equivalence impedance of:
   i) 2 resistors in parallel/series
   ii) 2 capacitors in parallel/series
   iii) 2 coils in parallel/series

27) Calculate the impedance $Z(\omega)$ of
   i) A series R-L-C circuit

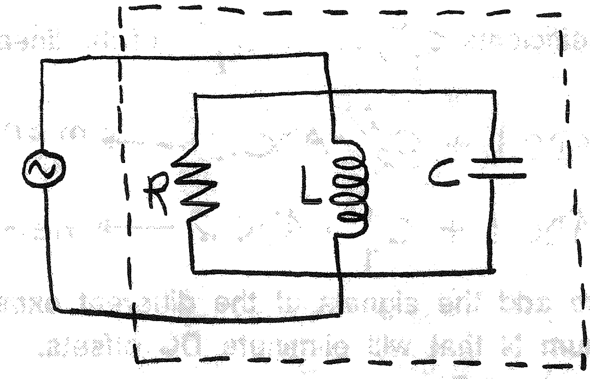
$V = V_0 e^{i\omega t}$



$Z_{eq} = ?$

ii) A parallel R-L-C circuit

$V = V_o e^{i\omega t}$

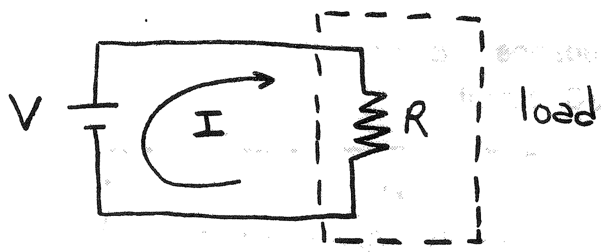


$Z_{eq} = ?$

Graph the behavior of Z_{eq} as a function of ω (i.e., the frequency response of the system). Note what happens at the resonance condition $\omega = (LC)^{-1/2}$?

28) In DC systems, the power delivered to a load R is given by

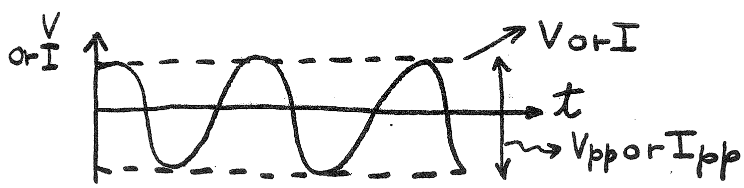
$$P = V^2/R = I^2R:$$



In AC systems, these equations become

$$P = V_{rms}^2 / R = I_{rms}^2 \cdot R,$$

Where



rms : root-mean-square

pp : peak to peak

$$V_{pp} = 2 \cdot V \qquad V_{rms} = V/\sqrt{2} \qquad I_{pp} = 2 \cdot I \qquad I_{rms} = I/\sqrt{2}$$

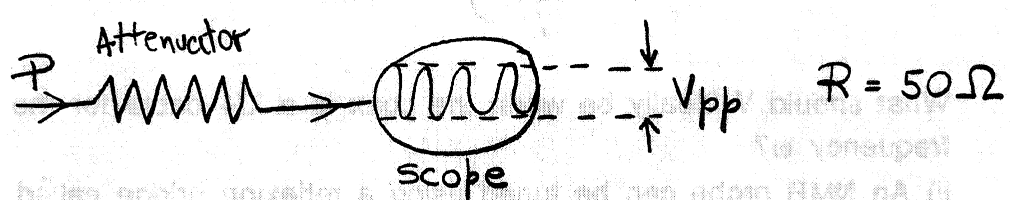
$[P] = \text{Watts}$; $[V] = \text{volts}$; $[I] = \text{amps}$; $[R] = \text{ohms}$

A measure of *relative power* is the decibel or db:

$$(db): \text{relative power} = 10 \cdot \log \frac{P_{in}}{P_{out}} = 20 \cdot \log \frac{V_{in}}{V_{out}}$$

i) What V_{pp} corresponds to 100 mw sent to a 50 Ω load?

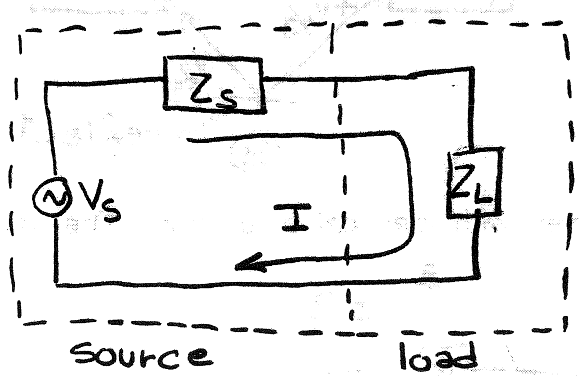
ii) What's the relationship between the measured V_{pp} and the incoming power P in the following setup



30 db attenuator $\longrightarrow$ $V_{pp}(P) = ?$

40 db attenuator $\longrightarrow$ $V_{pp}(P) = ?$

29) **Maximum power transfer theorem:** Consider the following setup, analogous to the one characterizing the transmission of rf to the probe or the reception of rf from it:



In transmission $\begin{cases} \text{source} = T_x \\ \text{load} = \text{probe} \end{cases}$

In reception $\begin{cases} \text{Source} = \text{spins} \\ \text{load} = R_x \end{cases}$

Demonstrate that the condition of maximum power transfer from the source to the load is given by $\boxed{Z_S = Z_L}$ Z_{eq}, Z_s $\quad Z_{eq} = Z_S + Z_L$

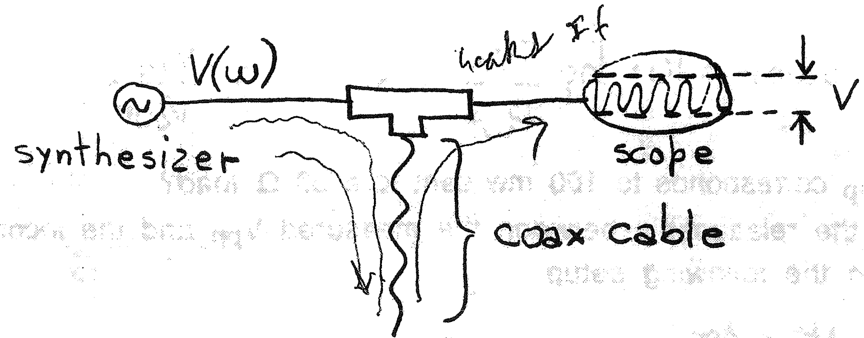
Hint: Power $P_L = I \cdot V_L$; $I = V_S/Z_{eq}$ $\quad Z \cdot$ $\quad P = IV$

$V = IR \quad P = V^2/R = P_{out} = I^2 R \quad I^2 Z_L$

$I^2 = \quad I^2 = \frac{V^2}{(Z_S + Z_L)^2}$

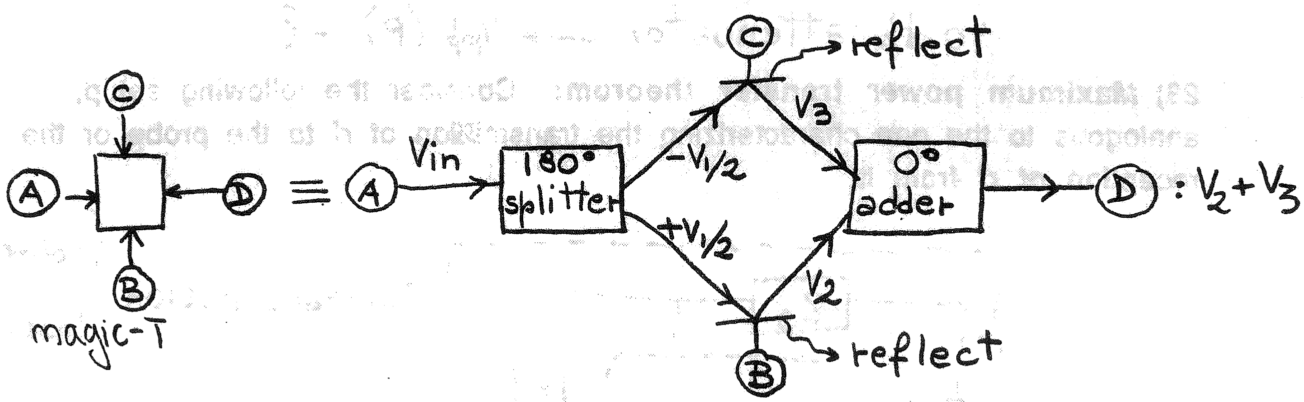
I

30) i) A $\lambda/4$ cable can be measured using the following setup:

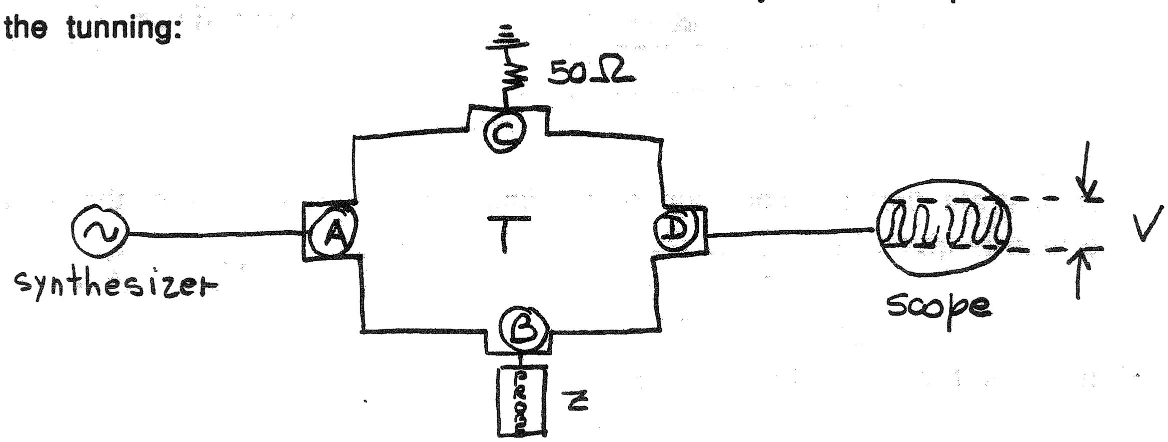


What should V ideally be when the coax is a $\lambda/4$ cable for the proper frequency ω?

ii) An NMR probe can be tuned using a reflexion bridge called "magic-T". It is a device with 4 ports whose equivalent circuit is

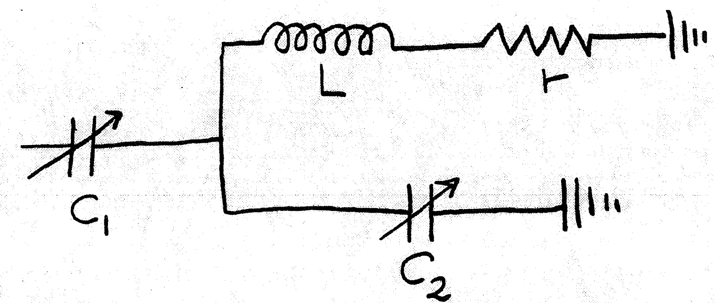


At B and C, rf is reflected with identical efficiency. The setup involved in the tunning:



What will V be when $Z_{probe} = 50\ \Omega$?

31) Calculate the C_1, C_2 values that take the impedance of the following arrangement to 50 Ω, as a function of L, r:



32) Explain the operation of the quarter-wave-based duplexer shown in page 65.

33) **Composite pulses:** Calculate the direction of the magnetization in the x, y, z, sphere after

i) A $(\pi)_x$ pulse

ii) A $\left(\frac{19\pi}{20}\right)_x$ pulse (i.e., an imperfect π-pulse)

iii) A composite $(\pi)_x$ pulse that takes the imperfection into account:

$$\left(\frac{19\pi}{40}\right)_x \left(\frac{19\pi}{20}\right)_y \left(\frac{19\pi}{40}\right)_x$$

Use the rotations that were worked out in the problems of Section I.