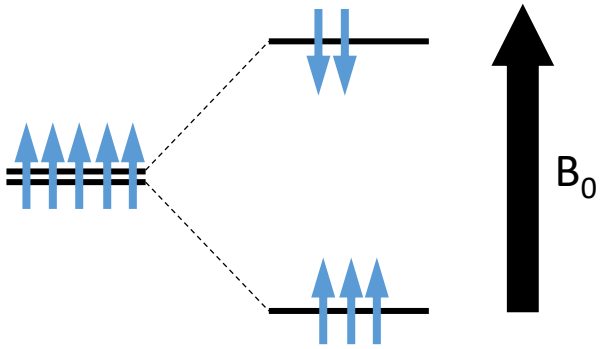
THE UNIVERSITY of EDINBURGH
School of Chemistry

The spectrometer is not a black box!

Andrew Hall & Juraj Bella

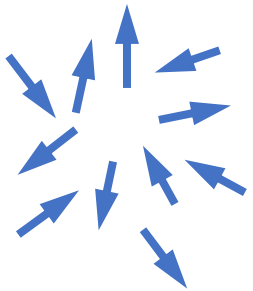
Magnetisation vectors

THE UNIVERSITY of EDINBURGH
School of Chemistry



No external field

With external field



Individual nuclear magnetic moments

μ_i

=

Bulk magnetisation vector

$\vec{M}$

Shopping list

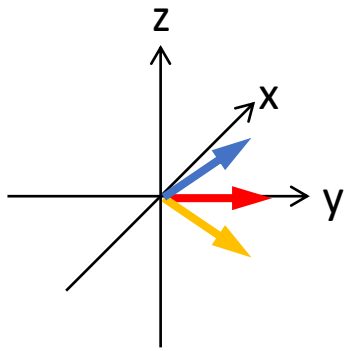
THE UNIVERSITY of EDINBURGH
School of Chemistry

NMR shopping list

1. Magnet (as big as possible)

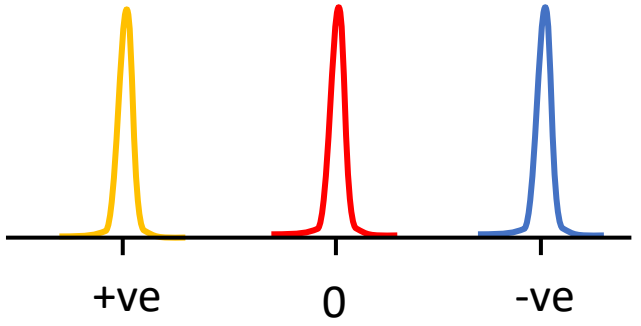
Frequency offset

Rotating frame



Positive chemical shifts rotate faster.
Negative chemical shifts rotate slower.

$$\omega_0 = -\gamma B_0$$



$\omega = +\Omega$ $\omega = 0$ $\omega = -\Omega$

$$\Omega = \omega_0 - \omega_{rot}$$

Shopping list

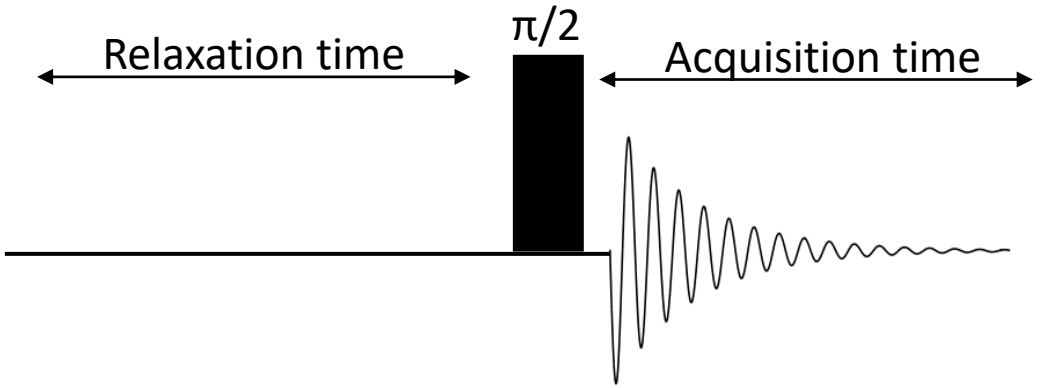
THE UNIVERSITY of EDINBURGH
School of Chemistry

NMR shopping list

1. Magnet (as big as possible)
2. Shims

NMR signal generation

THE UNIVERSITY of EDINBURGH
School of Chemistry



Pulses cause a rotation of the magnetisation vector

Magnetic field induced by pulse

Pulse angle

$$\theta = 2\pi\,\gamma\,B_1 t_p$$

Gyromagnetic ratio

Pulse length

Shopping list

THE UNIVERSITY of EDINBURGH
School of Chemistry

NMR shopping list

1. Magnet (as big as possible)
2. Shims
3. Probe

Shopping list

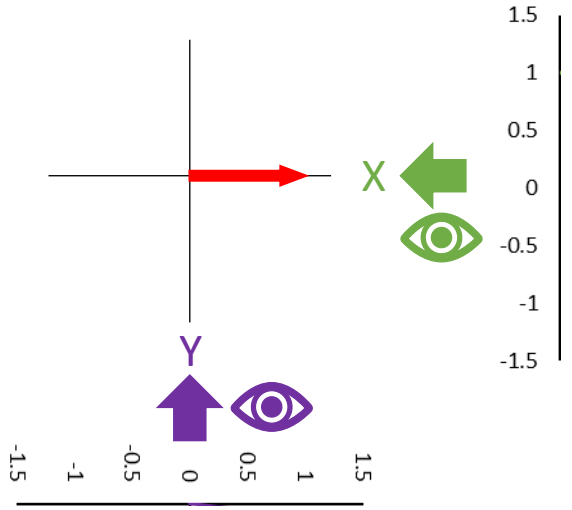
THE UNIVERSITY of EDINBURGH
School of Chemistry

NMR shopping list

1. Magnet (as big as possible)
2. Shims
3. Probe
4. Pulse generator
    a. Signal generator
    b. Amplifier

The NMR signal (FID)

THE UNIVERSITY of EDINBURGH
School of Chemistry

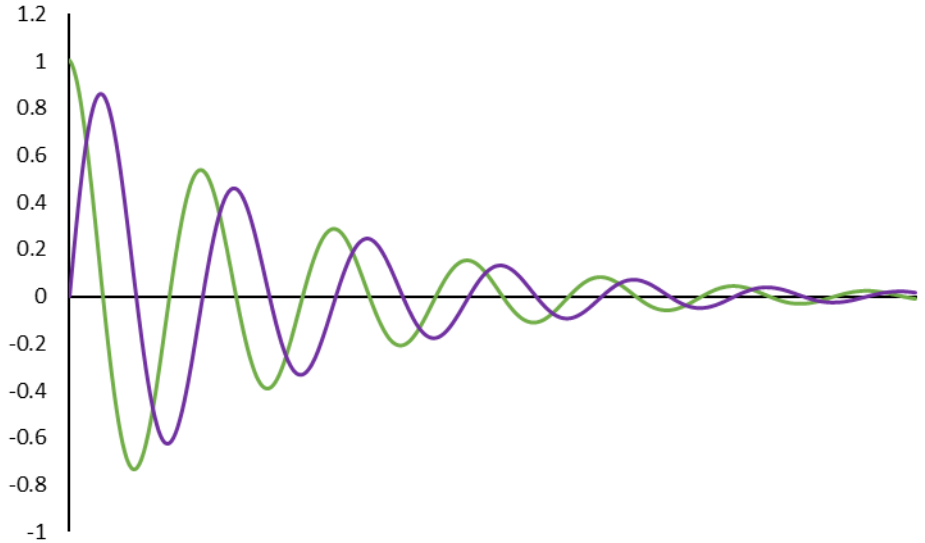


'Real'

$S_{real} = \cos(\Omega t)$

'Imaginary'

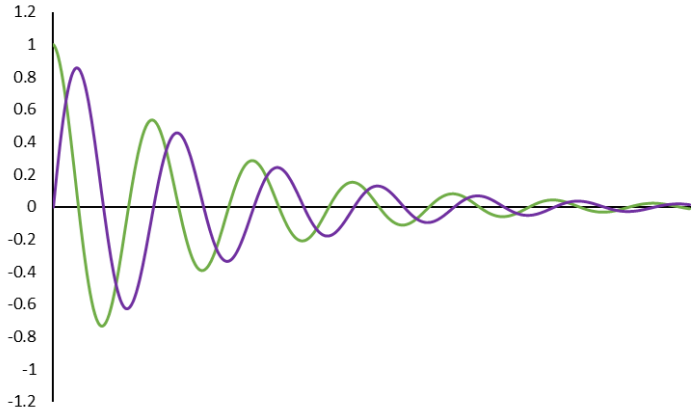
$S_{imag} = i.\sin(\Omega t)$

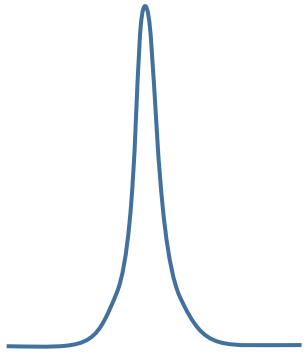


Receiver gain

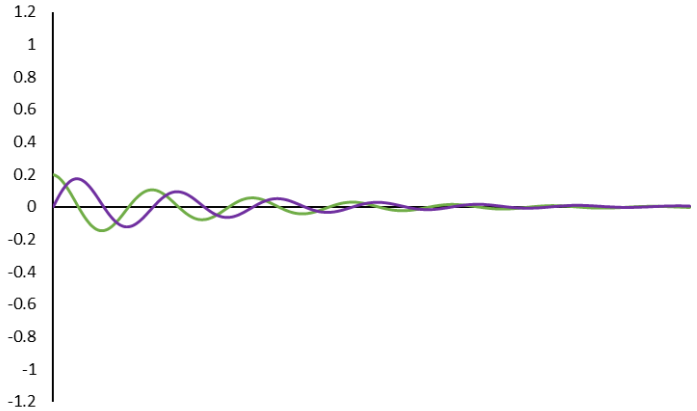
THE UNIVERSITY of EDINBURGH
School of Chemistry

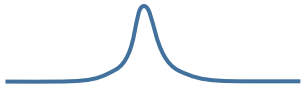
RG = 10



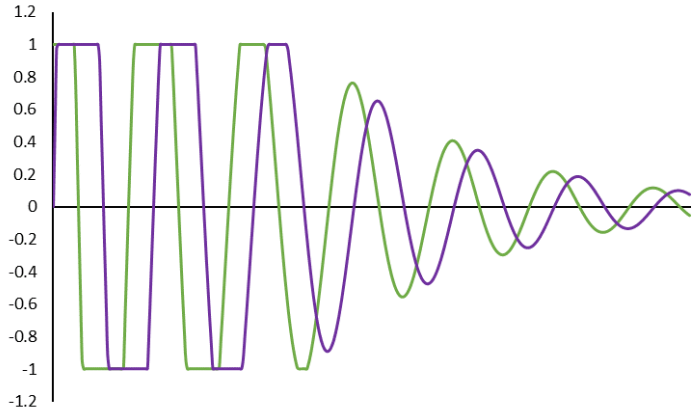


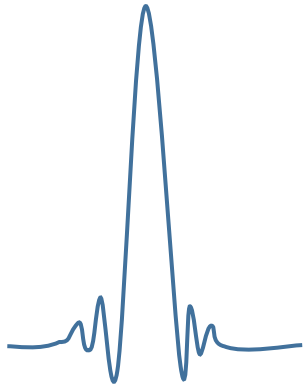
RG = 2





RG = 50





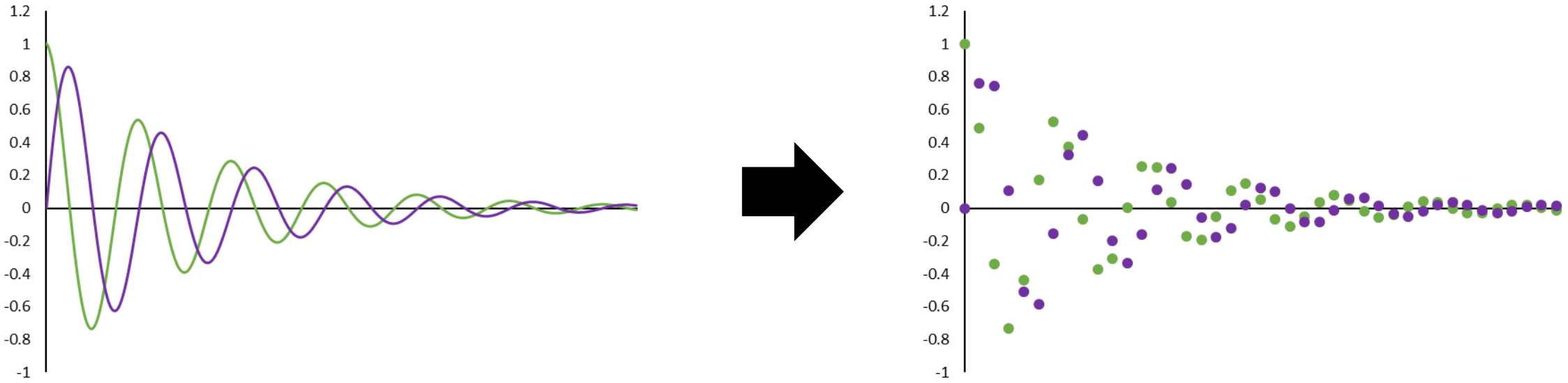
Shopping list

THE UNIVERSITY of EDINBURGH
School of Chemistry

NMR shopping list

1. Magnet (as big as possible)
2. Shims
3. Probe
4. Pulse generator
    a. Signal generator
    b. Amplifier
5. Receiver
    a. Amplifier

Digitisation



Shopping list

THE UNIVERSITY of EDINBURGH
School of Chemistry

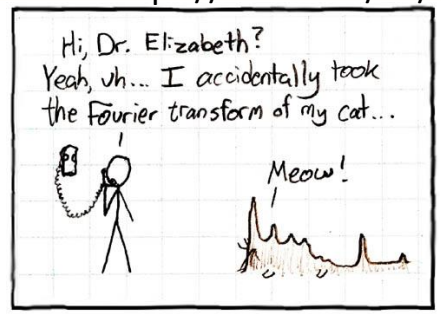
NMR shopping list

1. Magnet (as big as possible)
2. Shims
3. Probe
4. Pulse generator
    a. Signal generator
    b. Amplifier
5. Receiver
    a. Amplifier
    b. Digitiser

Fourier transforms

THE UNIVERSITY of EDINBURGH
School of Chemistry

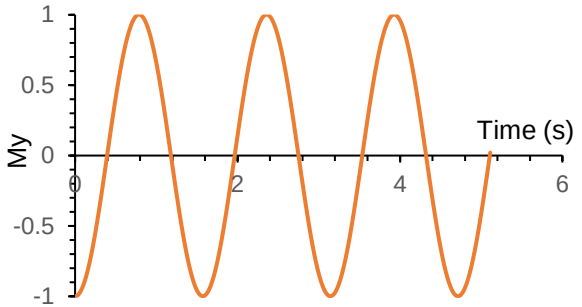
https://xkcd.com/26/



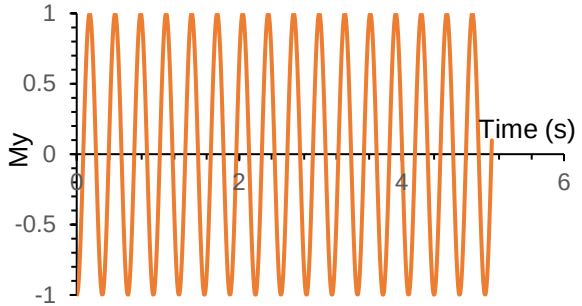
Fourier transforms convert time domain data to frequency domain:

Step 1:
Make a guess at the frequency that the signal is precessing:

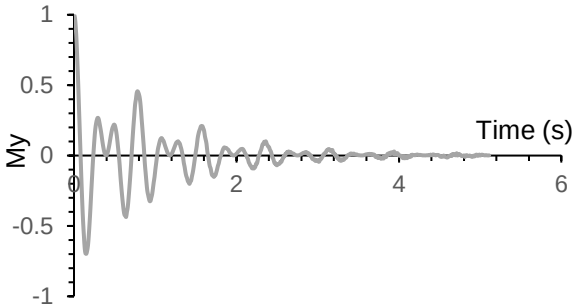
Ω_{guess} = 4 Hz

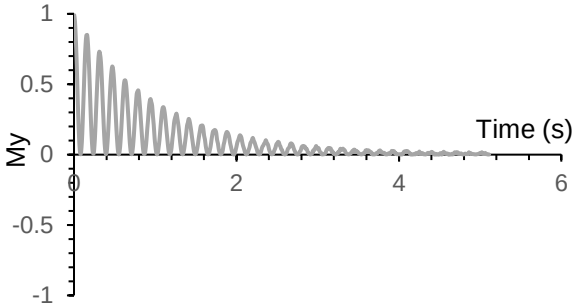


Ω_{guess} = 20 Hz



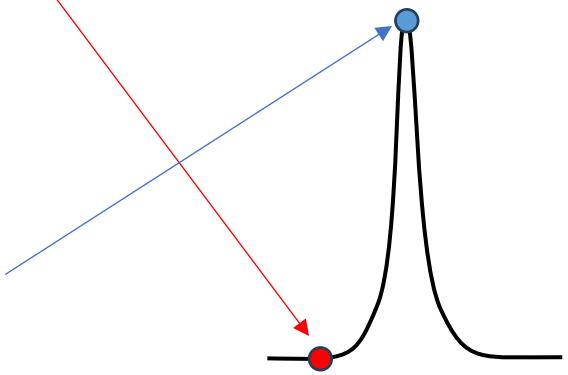
Step 2:
Multiply the guess signal with the FID





Step 3:
Integrate the signal over time

$$S(\Omega) = \int_0^\infty S_{guess}(t) \times FID(t)\, dt$$



Shopping list

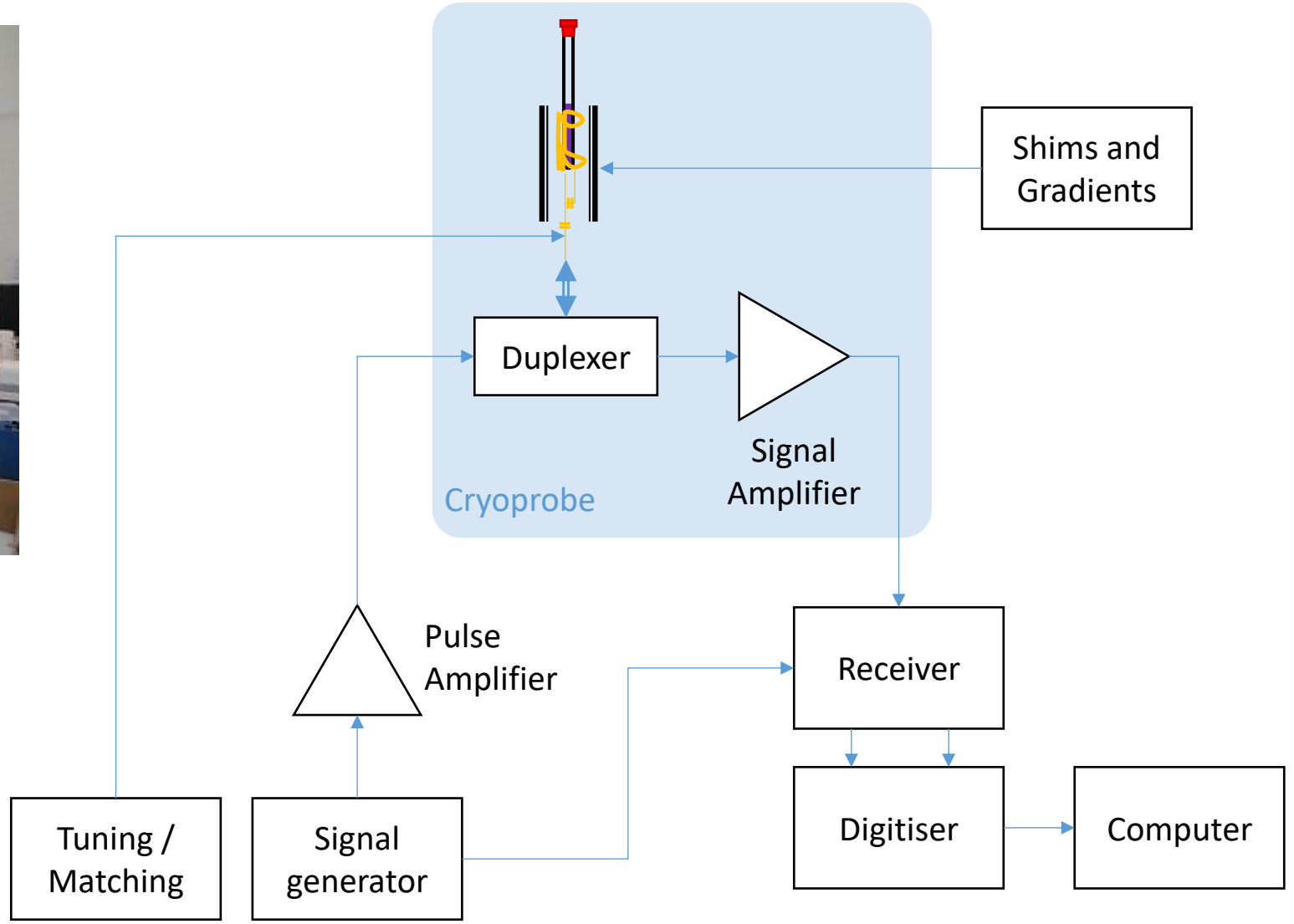
THE UNIVERSITY of EDINBURGH
School of Chemistry

NMR shopping list

1. Magnet (as big as possible)
2. Shims
3. Probe
4. Pulse generator
    a. Signal generator
    b. Amplifier
5. Receiver
    a. Amplifier
    b. Digitiser
    c. Computer

The NMR spectrometer

THE UNIVERSITY of EDINBURGH
School of Chemistry



Shopping list

THE UNIVERSITY of EDINBURGH
School of Chemistry

NMR shopping list

1. Magnet (as big as possible)
2. Shims
3. Probe
4. Pulse generator
    a. Signal generator
    b. Amplifier
5. Receiver
    a. Amplifier
    b. Digitiser
    c. Computer
6. Gradients
7. Temperature control