1. Practical aspects of pulse Fourier transform NMR spectroscopy

1.1 The basic NMR experiment: physical description

Spin

Component of the angular momentum of nuclei, electrons (and other elementary particles) that cannot be described as orbital momentum. Its origin is only understandable in terms of relativistic quantum mechanics.

The magnetic moment

The magnetic moment ($\mu$) associated with the orbital angular momentum ($L$) of a charged particle is given by:

$$\mu = \gamma L$$

Interaction between the magnetic moment und an external magnetic field

**Classical physics:**

The torque $T$ acts on $\mu$. In response, $\mu$

precesses around the direction of $B_0$ (analogous to a spinning top under the force of gravity) with the circular frequency $\omega_0$ [rad/s], which is called the Larmor frequency.

$$\omega_0 = -\gamma B_0$$

$$E_{pot} = -\mu \cdot B_0$$
**Quantum mechanics:**

Quantum mechanical description of the spin angular momentum $\vec{J} : \vec{J} = \hbar \vec{I}$

$\vec{I} :$ nuclear spin operator

$I :$ spin quantum number of the nucleus, a property of each isotope ($I = 1/2, n = 0, 1, 2...$).

The z-component (parallel to the external field) of the spin angular momentum can only assume certain values governed by the magnetic quantum number $m_i$:

$$J_z = \hbar m_i, \quad m_i = -I, -I+1, ..., 0, ..., I-1, I$$

This leads to $2I+1$ allowed states. For nuclei with $I = 1/2$, which are of predominant interest in organic chemistry, only the two states with $m_I = -1/2$ and $m_I = +1/2$ are possible.

The interaction energy for each state with a static external magnetic field along the z-axis is

$$E = -\mu_z B_0 = -\gamma J_z B_0$$

$$E = -\gamma \hbar m_i B_0$$

The energy difference between the two states is:

$$\Delta E = -\gamma \hbar \left(1/2 - (-1/2)\right) B_0 = -\gamma \hbar B_0$$

In order to achieve resonance, the energy of the irradiated radio frequency has to match the energy difference between the two states:

$$\Delta E = h\nu = \hbar \omega = -\gamma \hbar B_0$$

The Larmor (circular) frequency is:

$$\omega_i = -\gamma(1 - \sigma_i)B_{0z}$$

With $\omega_i =$ resonance frequency (rad/s) of spin $i$ with shielding constant $\sigma_i$

The resonance frequency for a given isotope is proportional to its gyromagnetic ratio and to the external magnetic field.

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a) The spin quantum numbers of nuclei follow the rules:

$$A = Z + N$$

A = mass number
Z = number of protons (nuclear charge)
N = number of neutrons

A even -> $I =$ integer
Z even, N even -> $l = 0$
Z odd, N odd -> $l = 1, 2, 3...$
A odd -> $l = 1/2, 3/2, 5/2...$
**Macroscopic magnetization $\mathbf{M}$**

Experimentally, only the total magnetization $\mathbf{M}$ of the sample inside the RF coil can be detected. $\mathbf{M}$ corresponds to the vector sum of the magnetic moments of all spins.

\[
\mathbf{M} = \sum_{i} \mathbf{\mu}_i \quad \text{sum over the total sample volume inside the coil}
\]

For $I = 1/2$, $\gamma > 0$ (e.g. $^1\text{H}$):

In the xy-components of the magnetic moments are distributed statistically. Hence, there is no net transverse magnetization. In the Boltzmann equilibrium and for $\gamma > 0$, the population of the $\alpha$ ($m_I = +1/2$) state is slightly larger than that of the $\beta$ ($m_I = -1/2$) state. This leads to a small residual $z$-magnetization parallel to the external field $B_0$.

The energy difference between the two states ($\alpha$: $m_I = +1/2$; $\beta$: $m_I = -1/2$) is very small.

For $^1\text{H}$ at 14.1 Tesla (600 MHz) the ratio of the two populations is only: $N_{+1/2} / N_{-1/2} = 1.0002$.

Because $\omega_0$ is proportional to $\gamma$ and $B_0$, nuclei with high $\gamma$ are more sensitive than those with low $\gamma$, and higher magnetic fields increase the sensitivity dramatically. In practice, the sensitivity of NMR spectrometers increases approximately according to $B^{3/2}$.

**1.2 Excitation by radio frequency pulses**

**Rotating coordinate frame**: The Larmor frequencies in modern NMR spectrometers are in the order of 30 - 900 MHz. On the other hand, the differences between the individual spins of the observed nucleus (chemical shifts and scalar couplings) are typically in the 0 Hz to 20 kHz range. In order to make the description of the dynamics of the magnetization both mathematically and visually easier, it is usual to use a coordinate frame which rotates around the $B_0 = z$-axis with the circular frequency $\omega_0$. 
The resulting "stroboscope" effect allows to describe the precession in terms of frequency differences $\Omega = \omega - \omega_0$. In the following, we will use the rotating frame for all vector diagrams.

In modern NMR spectrometers with superconducting magnet coils, the magnetic field is parallel to the axis of the sample tube. The radiofrequency coil, which transmits the excitation pulses and the induced signal to and from the sample to the transmitter and detector, respectively, is a saddle coil that generates and detects RF fields having their magnetic component $B_1(t)$ orthogonal to the constant external field $B_0$. The relative orientation of $B_1$ vectors in the $xy$ plane can be controlled by changing the relative phase of the irradiating RF.

Irradiation by radiofrequency corresponding to the Larmor frequency of a given nucleus for a short time (an RF pulse of frequency $\nu = \omega_0/2\pi$ and duration $\tau$) induces a complicated "spiral" movement of the macroscopic magnetization $\overrightarrow{M}$ away from the $z$-axis towards the $xy$ plane. In the rotating coordinate frame this process, which is called nutation, is a simple rotation of $\overrightarrow{M}$ around the axis of the field $\overrightarrow{B}_1$. The nutation angle ($\xi$) is a function of both, the RF field strength $B_1$ and of the pulse duration (it is proportional to the integral of the RF pulse): $\xi = -\gamma B_1 \tau [\text{rad}]$. In practical work, the amplitude of the RF field is usually given as $\gamma B_1/2\pi [\text{Hz}]$. It can be calculated if the pulse length for a nutation of $\xi = 90^\circ$ is known:

$$\gamma B_1/2\pi = 1/(4\tau(90^\circ)).$$

**Note:** The spectrometer software uses parameters in the unit decibel (dB) attenuation from the maximal output in order to control the amplitude of RF pulses. Since these values are different for each instrument/amplifier/probe head combination, one should always use the absolute RF amplitude $\gamma B_1/2\pi [\text{Hz}]$ in publications.
Dependence of the excitation band width on the duration of the pulse

Because the nutational angle is proportional to the integral of the RF pulse, the same nutation can be achieved either with a long weak pulse or with a short intense one. However, this holds only for spins which resonate exactly at the frequency of the transmitter ($\Omega = 0$). The bandwidth of excitation (the frequency region in which spins are more or less equally excited) is directly dependent on the intensity of the pulse (peak to peak voltage, $B_1$ amplitude). The first zero crossing of the excitation function occurs at $\omega_0/2\pi \pm \gamma B_1/2\pi$ Hz. Short intense pulses (so called hard pulses) are non-selective and excite a broad region of the spectrum, long weak pulses (so called soft pulses) are selective and excite only a narrow region around the transmitter frequency. Continuous wave irradiation with very weak amplitude during 0.5-5s allows to irradiate a single line and is used for homodecoupling, in NOE difference spectroscopy and for presaturation of solvent signals.

Offset Effects

Spins resonating at frequencies different from the transmitter frequency experience an effective RF field $B_{1\text{eff}}$ that is the vector sum of $B_1$ and of a component along $B_0$:

$$\tan \theta = 2\pi (\nu - \nu_0)/\gamma B_1$$

Nutation around $B_{1\text{eff}}$ with $\tau(90^\circ)$ no longer follows a grand circle. For $90^\circ$ pulses, the longer path and slightly stronger field $B_{1\text{eff}}$ compensate each other. Therefore, $90^\circ$ pulses are much less sensitive to offset effects than $180^\circ$ pulses. Pulse sequences are usually based on the assumption that offset effects are negligible. In reality, offset effects lead to artifacts and loss of signal in pulse sequences.
such as DEPT and heteronuclear shift correlation, which depend on accurate 180° pulses. In order to minimize offset effects, high amplitude pulses for non-selective excitation are standard in modern instruments. In practice, probe heads and amplifiers (typically 300W for X-nuclei) on a modern high resolution spectrometer can deliver 90° pulses as short as ca. 7 μs ($\frac{B_1}{2\pi} = 35$ kHz). Higher power would lead to arcing in the probe and could destroy the probe head or amplifier. Practical example: 11.7 T (125 MHz for $^{13}$C / 500 MHz for $^1$H): chemical shift range $^{13}$C: -10 to 240 ppm = ±15.6 kHz. Offset of a carbonyl signal: 13.5 kHz. With $\frac{B_1}{2\pi} = 35$ kHz and transmitter frequency at 110 ppm -> $\theta = 21^\circ$.

**Offset effect**

![Offset effect diagram](image)

\[
\tan \theta = 2\pi (\nu - \nu_0) / \gamma B_1
\]

**Evolution of magnetization in the xy plane after excitation by an RF pulse**

If a system with equilibrium magnetization $M_z$ is excited by an RF pulse, transverse magnetization (with components along x and y) is created. This corresponds to a net promotion of $\alpha$ spins to the $\beta$ state and therefore to the generation of *single quantum coherence* (excitation of a $\Delta m_i = 1$ transition). After the pulse, the magnetization in the xy plane evolves due to the chemical shift and the scalar coupling between spins as shown below:
Evolution of transverse magnetization under chemical shifts and scalar couplings

In the coil of the probe head, the precession of magnetization in the xy plane induces a very weak RF signal (μV), the so called free induction decay (FID), which is amplified and recorded during the acquisition time $t_2$ (typically 0.1 s to 5 s). For practical reasons, the frequency of the transmitter and a so-called intermediate frequency are subtracted from the original signal such that the final signal entering the digitizer is in the kHz range (for details see 1.7).

Due to the transverse ($T_2$) and longitudinal ($T_1$) relaxation processes, the FID decays with time. $T_1$ is the characteristic time for recovery of z-magnetization (return to Boltzmann equilibrium), whereas $T_2$ is the characteristic time by which the coherence of transverse magnetization is lost because of dephasing of the individual spin vectors (for details see chapter 7.1). $T_2$ is correlated with the line width of a signal in the NMR spectrum. The time domain signal ($S(t)$, FID) is an interferogram of all frequencies corresponding to the individual lines of the NMR spectrum. The spectrum $S(\omega)$ has to be calculated from the time domain signal by the mathematical operation of a Fourier transform. Since computers can only do discrete Fourier transforms, the analog time domain signal has to be converted into a series of discrete numbers $S(t_0 + \Delta t)$ equidistant in time by the analog to digital converter (ADC, digitizer).
1.3 Digitization, window functions and Fourier transform

In order to allow reconstruction of a periodic signal such as a sine or cosine function from discrete data points, one has to digitize with at least twice the frequency of the periodic signal (Nyquist theorem). Therefore, the time interval between two data points, called dwell time ($t_{dw}$), has to be

$$t_{dw} \leq \frac{1}{2F} \quad [s]$$

when the signal most distant from the transmitter has a frequency $2\pi(\omega-\omega_0) = F$. Because single channel detection cannot distinguish between positive and negative frequencies, the transmitter has to be set at one of the edges of the spectrum. Practical example: $^1$H at 500 MHz. Transmitter at 16 ppm, TMS at 0 ppm. $F = 8000$ Hz, $t_{dw} < 62.5 \mu$s. With quadrature detection (standard nowadays), the transmitter can be set in the center of the spectrum which reduces the spectral width by half: $F' = F/2$ and $t'_{dw} = \frac{1}{2(F')} = 1/(F)$. However, because two data points have to be collected for each time increment (the ADC alternately digitizes the signals of the two channels), the dwell time allowed for each channel is again $1/(2F)$. Example: $^1$H at 500 MHz. Transmitter at 8 ppm, TMS at 0 ppm. F = $4000$ Hz, $t_{dw} < 125 \Rightarrow 62.5 \mu$s per channel. With the availability of faster digitizers, modern high-end instruments allow to digitize much faster then dictated by the Nyquist theorem (so called oversampling). The redundant data points are used for digital filtering, giving much sharper cutoffs than with analog filters.

**Folding (Aliasing):** Illustration of the Nyquist theorem:

![Nyquist theorem illustration](image)

Solid line: $\cos(2\pi vt)$ with $v=300$ Hz; broken line: $\cos(2\pi(N-v)t)$ with $N = 1000$ Hz, $v = 300$ Hz.

The dwell time is $t_{dw}=1$ms, corresponding to a Nyquist frequency ($2F$) of 1000 Hz. Both signals give identical digitized data and the signal from the broken line would be folded into the spectrum after FT. With these parameters, the highest correctly digitized frequency would be ± 500 Hz.
Signals that are outside the limits given by the Nyquist theorem \( |v - v_o| > 1/(2t_{sw}) \) will be folded around the edges of the spectrum. Not only signals, but also noise is folded into the spectrum from regions outside the spectral width. This makes it necessary to use computer settable analog cutoff filters that are set to ca. ±(1.25*SW/2).

For real FT, folding occurs around the nearer edge of the spectrum, for complex FT around the far edge (see quadrature detection). Because no analog filters act in the artificial time domain \( t_1 \) of 2D spectra, folding is of particular importance in the \( \omega_1 \) dimension of 2D spectra.
Fourier transform

After single channel detection, the time domain array of data points is transformed by a discrete real FT (cos-transform). With quadrature detection the data in the two channels are used as the imaginary and real part of a complex FT. The algorithm used is FFT which, using precompiled sine tables and coefficient swapping instead of multiplications, is very fast on today's computers.

Complex analytical FT:

\[ s(\omega) = \int_{-\infty}^{\infty} \{f_r(t) + if_i(t)\} e^{-i\omega t} dt \]

Complex discrete FT

\[ S(\omega) = \sum_{k=0}^{N-1} \{S_r(k\Delta t) + iS_i(k\Delta t)\} \exp(-i2\pi k / N) \]

Phase correction

After the Fourier transform, the real and imaginary parts both contain the spectrum but with a phase difference of 90°, in other words, orthogonal linear combinations of the absorption \( A \) and the dispersion spectrum \( D \). During the process of zero order phase correction, a mixing coefficient \( \theta \) is determined interactively such that the "real" part of the spectrum (the one displayed on the screen), contains the pure absorption spectrum.

\[ R = A \cos \phi + D \sin \phi \rightarrow A = R \cos \theta + I \sin \theta \]

Frequency dependent phase errors are approximately corrected according to \( \theta = \theta_0 + c \nu \) in the 1st order phase correction. Frequency dependent phase errors are typically the result of delayed acquisition after the end of the pulse sequence.

Digital resolution

The acquisition time corresponds to the dwell time multiplied by the number of data points acquired in the time domain \( t_{aq} = t_{dw} n_{aq} \). After the Fourier transform, the number of data points of the real spectrum is half the acquired points \( n_{aq} = n_{aq} / 2 \), evenly distributed over the spectral width \( sw \).

Therefore, the digital resolution in the frequency domain is \( 2sw/n_{aq} \) [Hz/pt]. Because \( t_{dw} = 1/(2sw) \) the digital resolution is \( 1/t_{aq} \). In order to correctly digitize a well-resolved spectrum with natural line widths of 0.2 Hz, one has to acquire for 10 s (at least 2-3 data points per line).
Zero filling

Extension of the measured time domain signal by an arbitrary number of zero data points before Fourier transformation leads to an interpolation of data points in the frequency spectrum. This gives smoother data but can not recover resolution that was lost by too short an acquisition. Since, in 2D experiments, the number of acquired points in the time domain t is directly proportional to the experiment time, zero filling by at least a factor of two is standard in the t/ω dimension.

Convolution and window functions

The natural envelope of a (strictly: single spin) FID is an exponential function according to:

\[ I(t) = I_0 e^{i \omega t} e^{-t/T_2} \]

The effective line width 1/T* is the sum of the natural line width 1/T_2 and the instrumental line broadening 1/T* (e.g. due to a inhomogeneous magnetic field)

\[ 1/T* = 1/T_2 + 1/T* \]

Fourier transformation of an exponential function gives a Lorentz function, the natural line shape of a single spin NMR signal. Multiplication of the time domain signal with another exponential function before the FT does not change the Lorentz nature of the frequency domain signal but changes the apparent line width: multiplication with e^{-t/a} leads to line broadening concomitant with improved S/N whereas multiplication with e^{t/a} narrows the lines and drastically deteriorates the S/N.

Multiplication of the time domain signal with a Gaussian \( e^{-t^2/a} \) leads to Gaussian instead of Lorentzian line shapes in the spectrum. Since Gaussians have a much more narrow base than Lorentz lines, this improves the apparent resolution of multiplets without serious costs in S/N.

Stopping the acquisition before the analog signal has fully decayed into the noise is equivalent to multiplication of a step function into the FID. After the FT, this gives spectra with wiggles on both sides of each signal (the FT of a step function is a sinc (sin x / x) function). This can be avoided if the end of such an FID is multiplied with a half Gaussian function (apodization).
Simultaneous acquisition of the signal by two detectors that are 90° out of phase allows to distinguish between positive and negative frequencies. The signals from the two channels are combined as the real and imaginary part of the integrand in the FT.

\[ s(\omega) = \oint_{-\infty}^{\infty} \left[ f_x(t) + if_y(t) \right] e^{-i\omega t} dt \]  
complex FT
Illustration of the principle:

\[ \cos(-\omega t) = \cos(\omega t) \]

\[ \sin(-\omega t) = -\sin(\omega t) \]

\[ \text{sum} \]
Redfield method of quadrature detection

The digitizer rate is doubled: $t_{dw} = 1/(2SW)$

This gives the same number of data points as with true two channel detection but in a single file. The time domain signal is the integrand of a real (cos) Fourier transform:

$$s(\omega) = \int_{-\infty}^{+\infty} f_t(t)e^{-i\omega t} dt$$

This method is also called TPPI (time proportional phase increments), in particular, if used in the $t_1$ dimension of a 2D spectrum.
1.5 Phase cycles and z-gradients

Cyclops

<table>
<thead>
<tr>
<th>Pulse #</th>
<th>Transmitter</th>
<th>Phase</th>
<th>FID Channels A, B</th>
<th>Memory</th>
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<tr>
<td>1</td>
<td>-x</td>
<td>-y</td>
<td>A:</td>
<td>+</td>
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<td>2</td>
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</table>

A-B-A+B = 4 x \cos \omega t

B+A-B-A = 4 x \sin \omega t

Channels A and B are fully equalized
Phase cycles are not only used to balance the contributions of the two detector channels but also in order to select desired coherence transfer pathways and to eliminate undesired contributions to the signal. This is possible because zero- and multi-quantum coherence respond differently to a phase shift than single quantum coherence. A phase shift of 90° leaves zero quantum coherence unshifted, shifts single quantum coherence by 90° and double quantum coherence by 180°. That allows constructing phase cycles that lead to coherent addition of the desired signal but eliminate the undesired components by subtraction (a 180° phase shift on alternate scans is equivalent to a difference spectrum).

Disadvantage of phase cycles:

1. The undesired components are eliminated by subtraction. Therefore, the full signal, including the unwanted components, is entering the receiver and the receiver gain has to be set to accommodate the full signal. Good subtraction requires very high spectrometer stability over the length of the experiment; otherwise, non-perfect subtraction of large unwanted signals gives residual artifacts in the spectrum.

2. Suppression of unwanted coherence transfer pathways requires a certain minimal length of the phase cycle (e.g. 16 or 32 scans per FID). This imposes a lower limit on the experiment time even if the signal to noise ratio of a sample would allow recording the spectrum with only one or two scans per FID.

Gradients

The disadvantages of phase cycling mentioned above can be avoided if coherence transfer pathways are selected using z-gradients. A gradient coil in the probe head generates a linear field gradient along the z-axis that adds itself to the main field $B_0$. If such a gradient of amplitude $g$ (usually given in Gauss/cm) is applied for the time $t_g$, the frequency of precession of $xy$-magnetization depends not only on $\Omega$ and $J$ but also on the location of the spin along the z-axis of the sample. If the gradient is strong...
and long enough (it is the integral under the gradient pulse that counts), the frequencies of individual spins will be spread according to their z-coordinate and the net xy-magnetization is no longer detectable. Application of a gradient in the opposite direction with equal length and amplitude reverses the dephasing process and leads to a gradient echo when the spins in all volume elements reach the original phase coherence.

As with phase shifts, coherences of different order respond to gradients in a different way. Zero quantum coherence precesses with the difference of the frequencies, double quantum coherence with the sum. Accordingly, magnetization that was dephased by a gradient as single quantum coherence, and then transformed into double quantum coherence by a pulse, will not be refocused by a gradient of opposite sign and equal amplitude and length. Application of gradients at suitable places in the pulse sequence is therefore an alternative method for selection of desired coherence transfer pathways.

\[ \theta_{tg} = -\gamma p \int_{0}^{t_g} \Delta B_2(t) dt \]

\( p = \) coherence order; ±1 for SQC, ±2 for DQC, 0 for ZQC; \( \theta_{tg} = \) dephasing angle

**Advantages of gradients for coherence transfer pathway selection**

Since the unwanted magnetization is not refocused, the receiver does not detect it at all. This allows setting the receiver gain according to the desired signals only and eliminates the necessity for subtraction and the artifacts related to it. Since phase cycling is no longer mandatory, samples with a good S/N ratio can be measured with only one or two scans per FID, which reduces the experiment time dramatically.
Disadvantages of gradients

Because the refocusing of magnetization that was dephased by a gradient depends on the z-coordinate of a given molecule to remain constant during the experiment, diffusion leads to a loss of refocusable signal. This imposes an upper limit on the duration of the pulse sequence. Gradient spectroscopy requires additional hardware: the probe head has to be equipped with a gradient coil and a gradient amplifier that can deliver stable and high currents (typically 10A) is needed. Because of the enormous advantage of using gradients, this equipment is now standard for high end spectrometers.

1.6 Dynamic range and solvent suppression

Dynamic range = ratio between the strongest signal and the weakest signal to be digitized.

Example: 1 mM protein in H₂O; (110 M in protons) dynamic range = 110/0.001 = 10^5
**Accumulation:**

Modern instruments have 16Bit ADCs for high resolution work and 32 or 64 Bit computer words. This corresponds to a dynamic range of $\pm 32768 : \pm 1$.

The signal is accumulated according to $S(N) = N \cdot S(1)$. Correctly digitized noise will accumulate as $N = N^{10} \cdot N(1)$. Therefore, S/N improves with the square root of the number of accumulations. However, this requires that the noise is digitized correctly. Because, in samples of very high dynamic range, the receiver must be set to accommodate the largest signal, there is a risk that the smallest signals (including noise) are no longer correctly digitized because the corresponding voltage is below the least significant bit of the ADC. In this situation, accumulation does not improve the S/N.

**Solvent suppression**

If the molecules to be analyzed have exchangeable protons (NH, OH) and have to be measured in protic solvents such as water or methanol, the exchangeable protons are replaced by $^2\text{H}$ of the deuterated solvent (D$_2$O or CD$_3$OD) and are no longer detectable. In particular with oligopeptides and oligonucleotides, the NH protons are very important for the structure analysis. Therefore, one usually measures the spectra in H$_2$O / D$_2$O 9:1 or in CD$_3$OH, which makes it necessary to suppress the extremely intense solvent proton signal in order to be able to measure the analyte signals correctly.

Depending on the exchange rate of the NH (OH) protons, two strategies are used:

If the exchange is relatively slow on the time scale of $T_1$ (ca $< 0.01 \text{ s}^{-1}$), the solvent signal is saturated by a highly selective cw-irradiation of 1-5 s duration at the beginning of the pulse sequence. This so-called presaturation method can be used successfully for most amide NH in oligopeptides. The imino- and amino-NH protons in oligonucleotides, however, exchange too fast for this method: presaturation of the solvent signal leads to transferred saturation of all NH signals as well. In this situation, one has to use a method that does not excite the solvent signal, but all other signals as uniformly as possible. The corresponding methods include jump-return, WATERGATE and excitation sculpting. The last two methods use pulsed z-field gradients and are among the best water suppression techniques available today.
1.7 NMR spectrometer hardware

Block diagram of a modern high resolution liquids NMR spectrometer

Radio frequency unit
Magnet and probe head

Further reading


