4. Imaging and Transport

The precession phase
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Spectroscopic imaging
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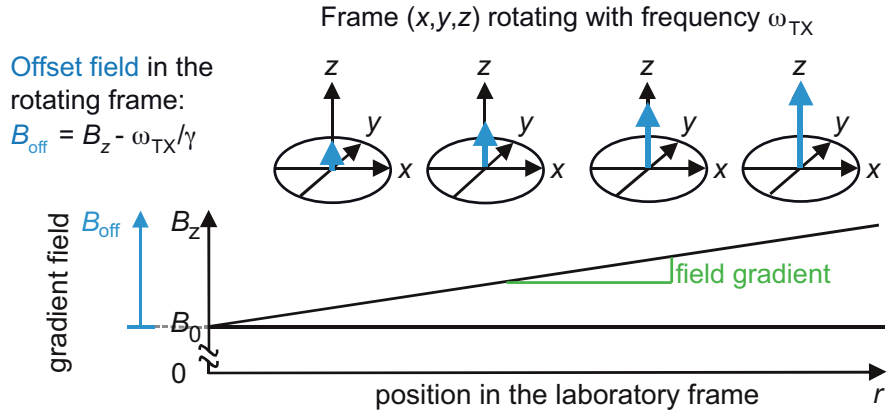
Projections and cross-sections

B. Blümich, *Essential NMR*,
https://doi.org/10.1007/978-3-030-10704-8_4

The Gradient-Field with a Constant Field-Gradient



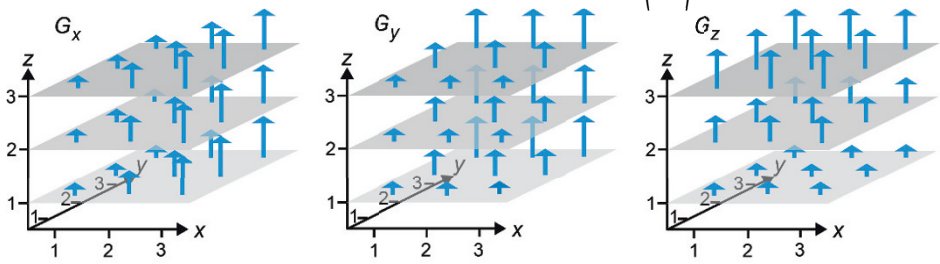
In the frame rotating with the transmitter frequency ω_{TX} in resonance with the Larmor frequency $\omega_0 = \gamma B_0$ of the homogeneous magnetic field B_0, the superimposed gradient field $B_z(r) - B_0 = B_{off}(r)$ leads to a precession of magnetization with the off-resonance frequency $\Omega(r) = \gamma B_{off}(r)$

Constant and Linear Magnetic Fields

- *NMR spectroscopy* requires magnetic fields sufficiently homogeneous across a typically 5-mm diameter sample tube to resolve differences in the *chemical shift* of 0.01 ppm = 10^{-8}
- *Magnetic resonance imaging* (*MRI*) does not primarily aim at resolving chemical shift differences
- The dominating signal in medical MRI results from water, which produces a single resonance line in the ^{1}H NMR spectrum
- The signals from different positions in an object are identified by means of their resonance frequencies $\omega = \gamma B$, provided the magnetic field $B(x,y,z)$ is different at each volume cell (*voxel*) in the object
- Along one dimension, the frequency is preferentially made to vary linearly with position r in the laboratory frame by assuring that the magnetic field scales linearly with position, for example, $B_z = B_0 + G\,r$, so that $\omega = \gamma\,(B_0 + G\,r)$
- The quantity $B_z - B_0 = B_{off} = G\,r$ is the offset-field in the coordinate frame rotating with the transmitter reference frequency $\omega_{TX} = \gamma B_0$
- With MRI instruments, linearly varying offset fields can be generated in all three dimensions of the laboratory frame by driving currents through *gradient coils* that produce magnetic *gradient fields* $G_x\,x$, $G_y\,y$, $G_z\,z$
- A linear variation of the magnetic field implies that the gradient is constant and not linear as often mistakenly stated in the literature

Static Magnetic Fields with Gradients

Magnetic gradient field in z direction: $\boldsymbol{B} = \begin{pmatrix} 0 \\ 0 \\ B_z \end{pmatrix}$



Field gradient in x direction | Field gradient in y direction | Field gradient in z direction

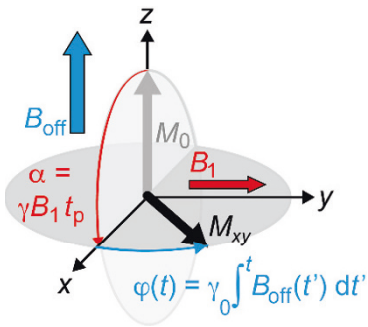
$\boldsymbol{G} = \begin{pmatrix} G_x \\ G_y \\ G_z \end{pmatrix}$

In high-field NMR the field gradient is approximated by a vector $\boldsymbol{G}$

In general the gradient vector $\boldsymbol{G}$ points into a direction different from the magnetic field vector $\boldsymbol{B}$

Gradient Fields and Field Gradients

- The direction of the *gradient field* generated by the *gradient coils* is aligned by default with the direction of the homogeneous magnetic field $\boldsymbol{B} = (0,0,B_0)^\dagger$
- The gradient field $B_{off} = G_x\, x + G_y\, y + G_z\, z = \boldsymbol{G}\, \boldsymbol{r}$ therefore adds to the z-component of the magnetic field producing the applied magnetic field $\boldsymbol{B} = (0,0,B_0 + \boldsymbol{G}\, \boldsymbol{r})^\dagger$
- In strict terms, the magnetic field gradient is a tensor or a 3 × 3 matrix in Cartesian coordinates with elements $G_{mn} = \partial B_m / \partial r_n$, and Maxwell's equations yield contributions B_x and B_y, which are due to the fact, that the magnetic field lines are curved and form closed loops
- At high magnetic field B_0, however, the B_x and B_y terms can be neglected so that in the high-field approximation the gradient is a vector $\boldsymbol{G} = (G_x, G_y, G_z)^\dagger$
- The direction of this vector is determined by the currents driving the three gradient coils that produce the gradient fields $G_x\, x$, $G_y\, y$, and $G_z\, z$, where each field is aligned with the $\boldsymbol{B}_0$ field direction
- In general, the directions of the *field-gradient vector* and the *gradient-field vector* are different and so are their units



The Acquired Signal

Following a 90° pulse and neglecting chemical shift, for each volume cell (voxel) at position $\boldsymbol{r}$ the transverse magnetization is given by

$M_{xy}(\boldsymbol{r},t) = M_z(\boldsymbol{r}) \exp\{-[1/T_2(\boldsymbol{r}) - i\,\Omega(\boldsymbol{r})]\, t\}$, where

$\Omega = \gamma\,(B_z - B_0) = \gamma\, B_{off}$, and

$M_{xy} = M_x + i\, M_y = M_z(\boldsymbol{r}) \exp\{-t/T_2(\boldsymbol{r})\} \exp\{i\varphi(\boldsymbol{r})\}$

In thermodynamic equilibrium $M_z(\boldsymbol{r}) = M_0(\boldsymbol{r})$

In general, Ω depends on time. Then $\varphi = \Omega\, t$ becomes $\varphi(t) = {}_0\int^t \Omega(t')\, dt'$ and

$$M_{xy}(\boldsymbol{r},t) = M_z(\boldsymbol{r}) \exp\{-t/T_2(\boldsymbol{r}) + i\, {}_0\int^t \Omega(\boldsymbol{r},t')\, dt'\}$$

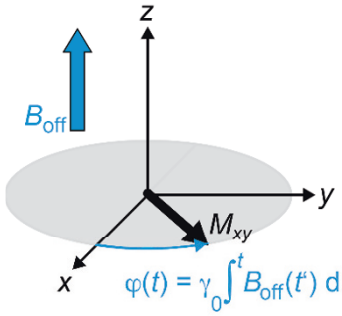
For non-exponential relaxation, the relaxation decay $\exp\{-t/T_2\}$ assumes the general envelope $a(t)$, and

$$M_{xy}(\boldsymbol{r},t) = M_z(\boldsymbol{r})\, a(\boldsymbol{r},t) \exp\{i\, \varphi(\boldsymbol{r},t)\} = M_z(\boldsymbol{r})\, a(\boldsymbol{r},t) \exp\{i\, {}_0\int^t \Omega(\boldsymbol{r},t')\, dt'\}$$

The NMR Signal in a Volume Cell

- In heterogeneous objects, the *longitudinal magnetization* M_z and the *transverse magnetization* $M_{xy} = M_x + i\, M_y \equiv M \exp\{i\varphi\}$ generated by a 90° pulse depend on the position $\boldsymbol{r}$ within the sample
- In thermodynamic equilibrium, the longitudinal magnetization $M_0(\boldsymbol{r})$ per volume element is the *spin density*
- Following an excitation pulse, the transverse magnetization $M_{xy}(\boldsymbol{r},t)$ of a voxel precesses with frequency Ω around the z axis in the *rotating coordinate frame*. Its magnitude ideally decreases exponentially with T_2
- The *precession frequency* Ω is determined by the *off-set field* in the rotating frame, which is approximated for a linear *gradient-field* by $B_{off} = B_z - B_0 = \boldsymbol{G}\, \boldsymbol{r}$, where $\boldsymbol{G}$ is the *field-gradient vector*, which collects the spatial derivatives of B_z
- For spins moving from one value B_{off} of the field to another, the precession frequency changes with time. So does the *precession phase*, so that the phase is written in integral form, $\varphi(\boldsymbol{r},t) = {}_0\int^t \Omega(\boldsymbol{r},t')\, dt'$
- For the sake of simplicity, Ω denotes a right-handed precession
- To accommodate transverse relaxation decays other than of exponential form, a generalized signal *attenuation function* $a(\boldsymbol{r},t)$ is introduced instead of $\exp\{-t/T_2(\boldsymbol{r})\}$

The Precession Phase



Off-set field in the rotating frame

$B_{off} = B_z - B_0$

NMR phase

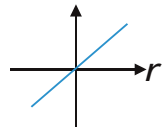
$\varphi(r,t) = {}_0\int^t \Omega(\boldsymbol{r},t')\, dt'$

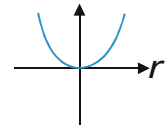
$= \gamma\, {}_0\int^t B_{off}(r,t')\, dt'$

Taylor series expansion in position *r*

$$B_{off}(r,t) = \left.\frac{\partial B_z(r,t)}{\partial r}\right|_{r=0} r(t) + \frac{1}{2}\left.\frac{\partial^2 B_z(r,t)}{\partial r^2}\right|_{r=0} r(t)^2 + \ldots$$

$$= G\,r + F\,r^2 + \ldots$$





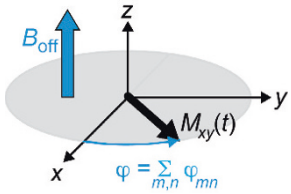
Taylor series expansion in time *t*

$$r(t) = r_0 + \left.\frac{\partial r}{\partial t}\right|_{t=0} t + \frac{1}{2}\left.\frac{\partial^2 r}{\partial t^2}\right|_{t=0} t^2 + \ldots = r_0 + v_0\, t + \frac{1}{2} a_0\, t^2 + \ldots$$

$$r^2(t) = r_0^2 + 2\, r_0 v_0\, t + (v_0^2 + r_0\, a_0)\, t^2 + \ldots$$

Dependence on Time and Position

- The fundamental quantity of importance for space encoding is the *phase* φ *of the transverse magnetization* $M_{xy}(\boldsymbol{r},t)$
- The variation of the *magnetization phase* with position ***r*** depends on the profile of the off-resonance field across the sample. If unknown, the magnetic field is expanded into a *Taylor series*
- For simplicity of notation, only one component *r* of position is considered in the following. Then associated parameters including the Taylor expansion coefficients of the magnetic field profile become scalar quantities
- For conventional imaging only the linear expansion coefficient, i.e. the *gradient G* of the field profile is important. The *curvature F* is usually made as small as possible by the spectrometer hardware. But it may assume significant values in unilateral NMR and in the pores of porous media
- If the nuclear spins are moving through the sample by random *diffusion* or *coherent flow*, their positions depend on time
- For motions slow compared to the time scale of the NMR experiment the time-dependent position is expanded also into a Taylor series, which involves initial *position* r_0, initial *velocity* v_0, and initial *acceleration* a_0



Moments and Fourier Pairs

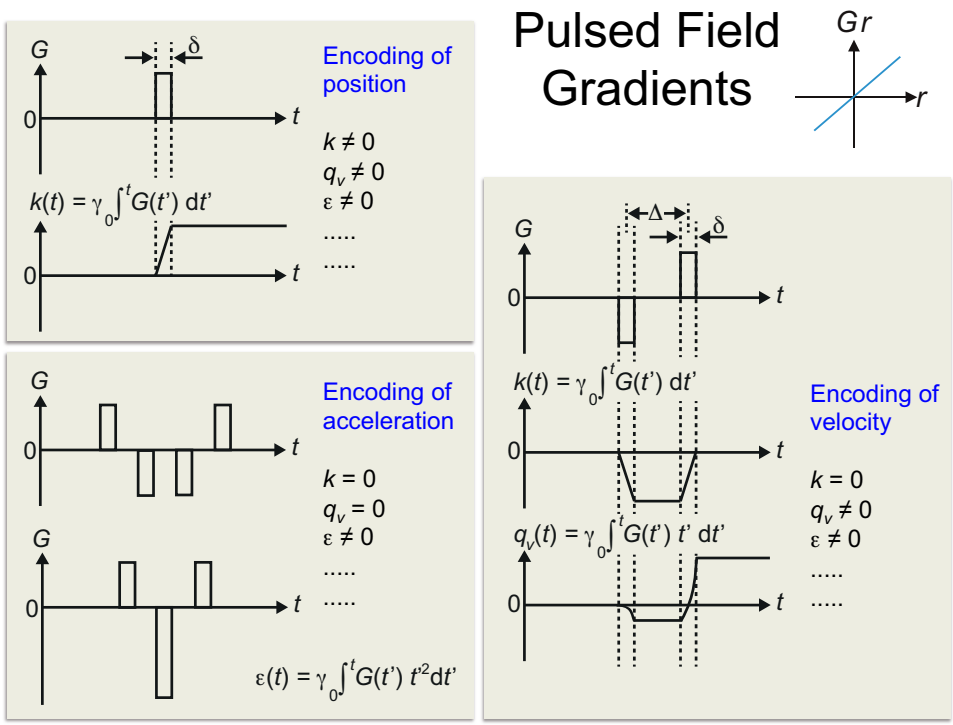
$$M_{xy}(t) = M_z(0)\,\exp\{-t/T_2 + i\,\gamma \int_0^t B_{off}(t')\,dt'\}$$
$$= M_z(0)\,\exp\{-t/T_2\}\,\exp\{i \sum \varphi_{mn}\}$$

Phases φ_{mn} acquired by spins moving in linear and quadratic fields

m \ n	0	1	2	.....
0	$\Omega_0\, t$	$\gamma \int_0^t G(t')\, t'^0\, dt'\, r_0$	$\gamma \int_0^t F(t')\, t'^0\, dt'\ r_0^2$	.....
1		$\gamma \int_0^t G(t')\, t'^1\, dt'\, v_0$	$\gamma \int_0^t F(t')\, t'^1\, dt'\, 2\, r_0\, v_0$	.....
2		$\gamma \int_0^t G(t')\, t'^2\, dt'\, ½\, a_0$	$\gamma \int_0^t F(t')\, t'^2\, dt'\, (v_0^2 + r_0\, a_0)$	.....
⋮		⋮	⋮	.....
0	$\Omega_0\, t$	$k\, r_0$	$\kappa\, r_0^2$	
1		$q_v\, v_0$	$\xi\, 2\, r_0\, v_0$	
2		$\varepsilon\, a_0$	$\zeta\, (v_0^2 + r_0\, a_0)$	

Truncated Phase Evolution

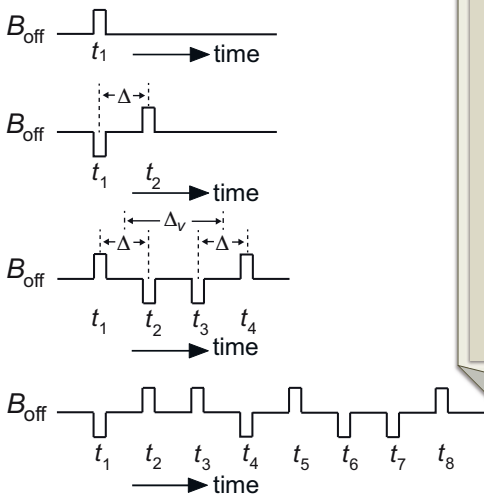
- The *Taylor expansions* in position and time are inserted into the expression for the *phase of the transverse magnetization* producing a sum of phase terms
- The overall precession phase becomes a sum of terms associated with linear and curved fields as well as with different parameters of motion
- *Linear field profiles* can readily be generated with many NMR instruments
- For irregular motions, and for motions with a spectrum of correlation times, a frequency domain analysis can be developed
- The truncated expansion of the time- and position-dependent phase involves the integrals of the time-dependent gradients $G(t)$ and curvatures $F(t)$
- $G(t)$ and $F(t)$ can be manipulated during the NMR experiment. Typically $F(t) = 0$, and $G(t)$ is modulated in terms of positive and negative, ideally rectangular pulses of variable amplitude
- The gradient integrals are the different time *moments of the gradient modulation function*
- Including the gyro-magnetic ratio γ, the products of the moments and the associated kinetic variables r_0, v_0, and a_0 form individual phase contributions
- Thus, the integrals denoted by k, q_v, ε are *Fourier conjugated variables* to r_0, v_0, and a_0, i.e. together with their partner variables they form *Fourier pairs*
- From a systematic variation of k, q_v, and ε with measurements of the associated values of the phases φ, the quantities r_0, v_0, and a_0 can be determined

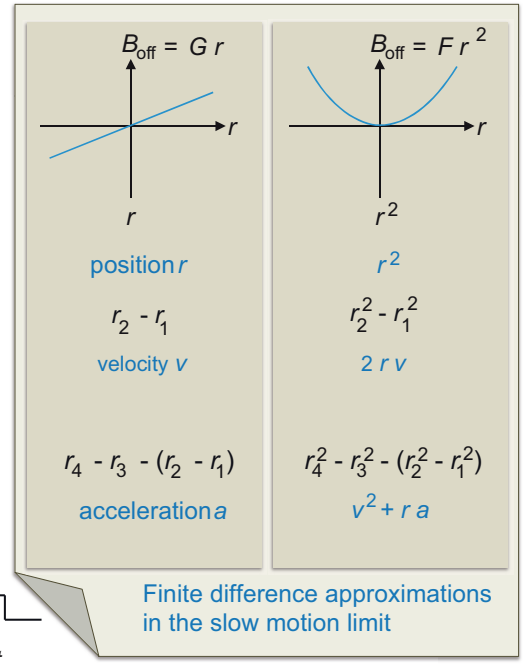


Manipulation of Gradient Moments

- *Gradient moments* are varied either by pulsing a magnetic gradient field, which is generated with current bearing coils near the sample, or by means of rf pulses
- In *pulsed field-gradient NMR* (*PFG NMR*) roughly rectangular gradient-field pulses are generated with durations of 10 μs to 100 ms and gradient strengths of 0.01 T/m to 10 T/m
- If the pulses are narrow, each of them generates a value for k at the particular time it is set
- On the other hand, a pair of gradient pulses with equal amplitudes but opposite phases separated by a time delay Δ generates a value for q_v while $k = 0$ at the end of the gradient-field pulse sequence
- Such a pair encodes a phase $\varphi = k\, r_2 - k\, r_1 = k\,(r_2 - r_1)$, where r_2 and r_1 are the final and initial positions of the magnetization component travelling for the time Δ in the direction of the field gradient
- Approximating velocity as $v = (r_2 - r_1)/\Delta$, the phase encoded by the anti-phase pulsed field-gradient pair becomes $\varphi = k\,\Delta\,(r_2 - r_1)/\Delta = q_v\, v$. It is identified as the phase term φ_{11} in the phase table
- Two anti-phase pairs of anti-phase gradient pulse pairs then generate a value for ε with $q_v = 0$ and $k = 0$ at the end of the sequence. Note that the two inner gradient pulses can be contracted into one to encode acceleration

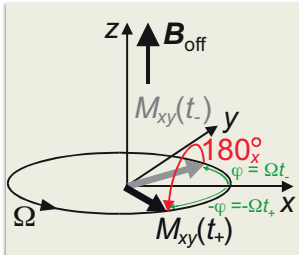
Phase Encoding with Linear and Quadratic Fields





Encoding Time Derivatives of Position

- A short pulse of a spatially *linear magnetic field* B_{off} marks *position*
- A short pulse of a *quadratic magnetic field* B_{off} marks position square
- An anti-phase pulse pair of a linear magnetic offset field B_{off} marks negative initial and positive final positions of a moving transverse magnetization component at times t_1 and t_2, respectively, separated by the pulse spacing Δ
- By dividing the marked position difference by the encoding time Δ, *velocity* is measured in a *finite difference approximation*
- Similarly, *acceleration* can be measured in a finite difference approximation
- Also other finite difference schemes known from numerical differentiation algorithms may be employed to encode these and other kinetic variables of translational motion
- This finite difference approach applies to arbitrary profiles of the offset field including the quadratic field profile



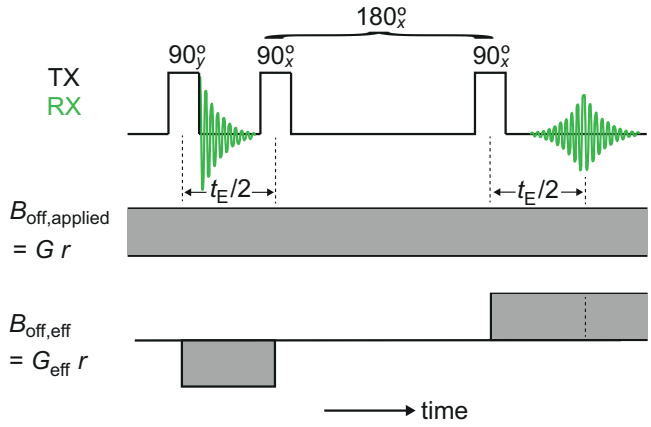
$\Omega = \gamma B_{off} = \gamma (B_z - B_0)$

A 180° pulse changes the sign of the precession phase φ. Example: $180°_x$ pulse at $t = t_E/2$:

Before:
$M_{xy}(t_-) = M_{xy}(0) \exp\{i \Omega t_-\}$
$= M_{xy}(0) (\cos \Omega t_- + i \sin \Omega t_-)$

After:
$M_{xy}(t_+) = M_{xy}(0) (\cos \Omega t_+ - i \sin \Omega t_+)$
$= M_{xy}(0) \exp\{-i \Omega t_+\}$

The Effective Gradient

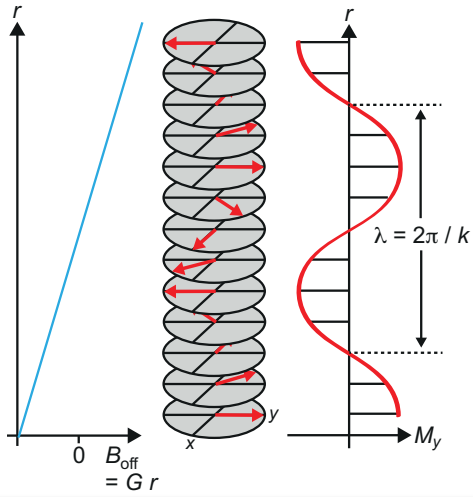


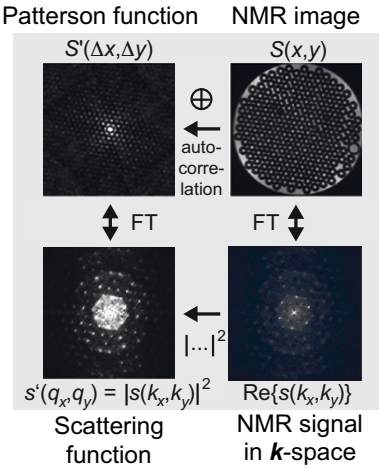
In the high-field approximation the spatial dependence of the off-resonance field B_{off} affects only transverse magnetization. This is used to generate pulses of effective gradients G_{eff} via rf pulses in time-invariant gradient fields $B_{off} = G r$

Time-Invariant Offset Fields

- In the magnetic resonance community, *pulsed field-gradient NMR* (*PFG NMR*) refers to NMR with *pulsed gradient fields* $B_{off} = G r$
- In pulse-sequence diagrams it is common practice to plot the time-dependence of the *field gradient* G and not of the applied *gradient field* $G r$
- The time-dependence of any off-set field affects only coherences but not the longitudinal magnetization as long as the offset field $B_{off} = G r$ is weak compared to the polarization field B_0
- Then the offset field affects the measured signal only during the evolution and detection periods, for example, when transverse magnetization evolves
- In consequence, time-invariant offset fields appear as pulses of an effective offset field B_{off} affecting transverse magnetization, for example, in the *stimulated echo* sequence
- For time-invariant linear offset fields $B_{off} = G r$ the time-dependent *effective gradient* G_{eff} is introduced
- Note, that the sign of any effective gradient in the past changes with each 180° rf pulse, because with each pulse the phase of the transverse magnetization changes sign
- In the maximum of the stimulated echo the first-order moment of the effective gradient modulation function ${}_0\int^{tE} G_{eff}(t)\, dt = k(t_E)/\gamma = 0$, which is the condition for a *gradient echo*

Transverse Magnetization in a Gradient Field





Position r and wave number k form a Fourier pair $\varphi(t) = \gamma \int_0^t G(t')\,dt'\, r = k\, r$

NMR is phase-sensitive and capable of mapping positions **r** by Fourier methods

From B. Blümich, *NMR Imaging of Materials*, **Clarendon Press**, Oxford, 2000, Figs. 2.2.4, 5.4.3 by permission of Oxford University Press

Interpretation of the Gradient Integral

- In a magnetic field, which varies linearly with position r, the spins precess with linearly varying *Larmor frequency*
- Following a gradient-field pulse the magnetization phase in adjacent voxels along the gradient direction then varies linearly with position
- The tips of the magnetization vectors lie on a helix, which winds around the direction r of the magnetic field gradient
- The projections of the magnetization vectors onto a transverse axis in the RCF produces a sinusoidal function with period $\lambda = 2\pi/k$ and phase $\varphi = k\, r$
- Therefore, k is the *wave number*, which specifies the spatial oscillation frequency of the transverse magnetization in analogy to ω, which specifies the temporal oscillation frequency
- An NMR image derives by Fourier transformation (FT) from transverse magnetization $M_{xy}(k_x,k_y) = s(k_x,k_y)$ acquired for a range of wave numbers along both image dimensions
- If the object has periodic structure, $s(k_x,k_y)$ shows *interference fringes*
- By forming the magnitude square of $s(k_x,k_y)$, the *scattering function* is obtained. The NMR phase is discarded but the interference fringes remain
- The Fourier transform of the scattering function is known as the *Patterson function*. It is the *auto-correlation function* of the image
- The Patterson function and $|s(k_x,k_y)|^2$ no longer give access to positions x, y but only to position differences Δx, Δy in analogy to X-ray *diffraction* data
- $\Delta x,\Delta y = \Delta r$ derive from the wave numbers $q_x,q_y = q$ of the peaks in the scattering function, because Δr and q form a Fourier pair corresponding to $\varphi = q\, \Delta r$

Transverse Magnetization in Linear Fields

For simplicity of notation the indices '0' with r_0, v_0, a_0 are dropped form now on. Consider the signal from a single voxel at position $\boldsymbol{r}$:

$$M_{xy}(t, \varphi) = M_{xy0}(\boldsymbol{r},\boldsymbol{v})\, a(t,\boldsymbol{r}) \exp\{\mathrm{i}\, \varphi(t)\}$$
$$= M_{xy0}(\boldsymbol{r},\boldsymbol{v})\, a(t,\boldsymbol{r}) \exp\{\mathrm{i}\, [\Omega(\boldsymbol{r})t + \boldsymbol{k}(t)\boldsymbol{r} + \boldsymbol{q}_v(t)\boldsymbol{v}(\boldsymbol{r}) + ...]\}$$

The signal from the whole sample is the integral over all voxels:

$$M_{xy}(t,\boldsymbol{k},\boldsymbol{q}_v) = \iiint M_{xy0}(\Omega,\boldsymbol{r},\boldsymbol{v})\, a(t,\boldsymbol{r}) \exp\{\mathrm{i}\, [\Omega(\boldsymbol{r})t + \boldsymbol{k}(t)\boldsymbol{r} + \boldsymbol{q}_v(t)\boldsymbol{v}(\boldsymbol{r}) + ...]\}\, \mathrm{d}\Omega\, \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{v}$$

Spectroscopy: $\boldsymbol{k} = \boldsymbol{0} = \boldsymbol{q}_v$

$$M_{xy}(t) = \iiint M_{xy0}(\Omega,\boldsymbol{r},\boldsymbol{v})\, a(t,\boldsymbol{r}) \exp\{\mathrm{i}\, \Omega(\boldsymbol{r})\, t\}\, \mathrm{d}\Omega\, \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{v}$$

Imaging and flow: t_G << correlation time of motion; no dispersion in frequency Ω

Imaging with *phase encoding*: $t = t_E$, $\boldsymbol{k} = \gamma\, \boldsymbol{G}\, t_E$, $\boldsymbol{q}_v = \boldsymbol{0}$. Fix t_E, vary $\boldsymbol{k}$,

$$M_{xy}(\boldsymbol{k}) = \iiint M_{xy0}(\boldsymbol{r},\boldsymbol{v})\, a(t_E,\boldsymbol{r}) \exp\{\mathrm{i}\, \boldsymbol{k}(t_E)\, \boldsymbol{r}\}\, \mathrm{d}\Omega\, \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{v}$$

Imaging with *frequency encoding*: $\boldsymbol{k} = \gamma\, \boldsymbol{G}\, t$, $\boldsymbol{q}_v = \boldsymbol{0}$. Vary t and $\boldsymbol{k}$,

$$M_{xy}(t) = \iiint M_{xy0}(\boldsymbol{r},\boldsymbol{v})\, a(t,\boldsymbol{r}) \exp\{\mathrm{i}\, \gamma\, \boldsymbol{G}\, \boldsymbol{r}\, t\}\, \mathrm{d}\Omega\, \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{v}$$

Velocity distributions by phase encoding: $t = t_E$, $\boldsymbol{k} = \boldsymbol{0}$. Fix t_E, vary $\boldsymbol{q}_v$,

$$M_{xy}(\boldsymbol{q}_v) = \iiint M_{xy0}(\boldsymbol{r},\boldsymbol{v})\, a(t_E,\boldsymbol{r}) \exp\{\mathrm{i}\, [\boldsymbol{q}_v(t_E)\, \boldsymbol{v}(\boldsymbol{r})]\}\, \mathrm{d}\Omega\, \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{v}$$

Flow imaging by phase encoding: $t = t_E$. Fix t_E, vary $\boldsymbol{k}$ and $\boldsymbol{q}_v$,

$$M_{xy}(\boldsymbol{k},\boldsymbol{q}_v) = \iiint M_{xy0}(\boldsymbol{r},\boldsymbol{v})\, a(t_E,\boldsymbol{r}) \exp\{\mathrm{i}\, [\boldsymbol{k}(t_E)\, \boldsymbol{r} + \boldsymbol{q}_v(t_E)\, \boldsymbol{v}(\boldsymbol{r})]\}\, \mathrm{d}\Omega\, \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{v}$$

Information Accessible by PFG NMR

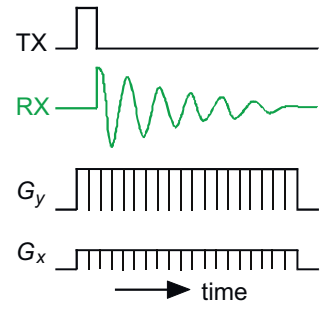
- Gradient fields are applied for a time t_G to identify the NMR signal from different voxels along the gradient direction
- The signal acquired from a heterogeneous sample is the integral of the signal from all voxels at positions $\boldsymbol{r}$
- For spins in motion, one also needs to integrate over all velocities $\boldsymbol{v}$
- In general the signal is acquired as a function of $\boldsymbol{k}$ and $\boldsymbol{q}_v$, where both variables depend on time t via the *moments of the gradient modulation function*
- The measured signal $M_{xy}(t,\boldsymbol{k},\boldsymbol{q}_v)$ derives from the longitudinal magnetization $M_z(\boldsymbol{r}_0,\boldsymbol{v}_0)$ following a 90° pulse
- Apart from the attenuation function $a(t,\boldsymbol{r}_0)$, $M_{xy}(\boldsymbol{r}_0,\boldsymbol{v}_0)$ is the *Fourier transform of the measured signal*
- Therefore, the signal is acquired for a sufficiently large number of values $\boldsymbol{k}$ and $\boldsymbol{q}_v$ and is subsequently Fourier transformed
- The *attenuation function* $a(t,\boldsymbol{r}_0)$ introduces a loss of image resolution, because the NMR image is the convolution of $M_z(\boldsymbol{r}_0,\boldsymbol{v}_0)$ with the Fourier transform of $a(t,\boldsymbol{r}_0)$
- The Fourier transform of $a(t,\boldsymbol{r}_0)$ is referred to as the *point-spread function*. It specifies the spatial resolution of the image
- When starting the imaging experiment from thermal equilibrium, $M_z(\boldsymbol{r}_0,\boldsymbol{v}_0) = M_0(\boldsymbol{r}_0,\boldsymbol{v}_0)$ is proportional to the *spin density* of the object

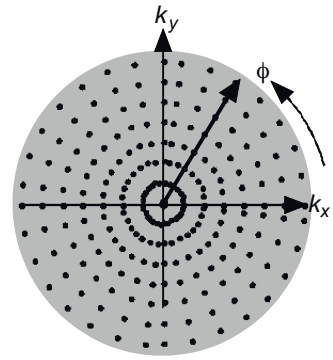
Sampling of *k* Space

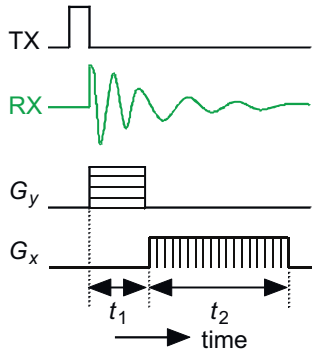
Cylindrical coordinates: Back-projection imaging: $\tan \phi = G_y/G_x$

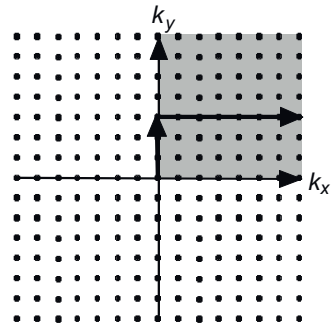
Data sampled at discrete points in time lead to discrete points in ***k***-space

Cartesian coordinates: Conventional Fourier imaging





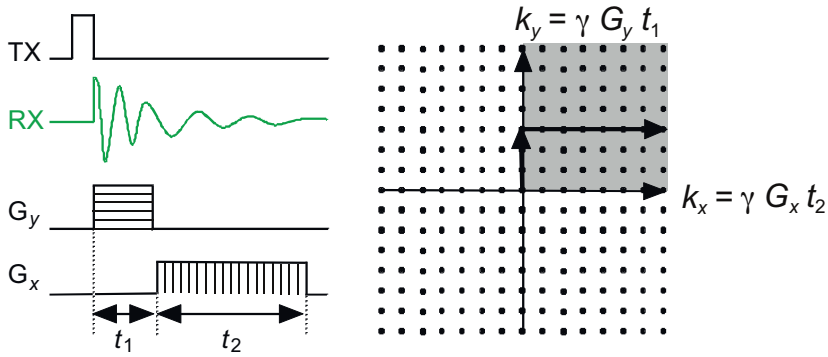




Principles of 2D Imaging

- With *Fourier NMR*, images are measured by acquiring the complex transverse magnetization $M_{xy} = M_x + iM_y$ as a function of $\boldsymbol{k} = (k_x, k_y, k_z)^\dagger$ and Fourier transforming the measured data over ***k***
- The values of ***k*** are scanned on a discrete grid in one, two, or three dimensions
- Historically, two principle approaches are discriminated: The ***k***-space grid can be defined on spherical/*cylindrical coordinates* and on *Cartesian coordinates*
- These schemes are commonly known as *back-projection* (BP) *imaging* and as *Fourier imaging*, although Fourier transformation is required in both cases
- The space-encoded data in one dimension are usually acquired directly in the presence of a time-invariant field gradient
- In BP imaging this scheme is used with repeated acquisitions under different gradient directions
- In Fourier imaging, the data for further space dimensions are acquired indirectly by pulsing gradient fields in orthogonal directions in *preparation periods* prior to data acquisition
- The Fourier transformation of BP imaging data involves the transformation from cylindrical to Cartesian coordinates because a fast *multi-dimensional Fourier transformation* is executed in Cartesian coordinates

Frequency and Phase Encoding



Frequency encoding: vary t_2 in n_2 steps

$M_{xy}(n_2) = \exp\{-[1/T_2^* - i\ \gamma\ G_x\ x]\ n_2\ \Delta t_2\}$

Spatial resolution limited by $\Delta\omega_{1/2}$

$\gamma\ G_x \Delta x\ \geq 2/T_2^* = \Delta\omega_{1/2}$

$1/\Delta x \leq \gamma\ G_x\ T_2^*/\ 2 = \gamma\ G_x\ /\Delta\omega_{1/2}$

Phase encoding: vary G_y in n_1 steps

$M_{xy}(n_1) = \exp\{-[1/T_2^* - i\ \gamma\ n_1\ \Delta G_y\ y]\ t_1\}$

Spatial resolution increases with $n_{1,\max}$

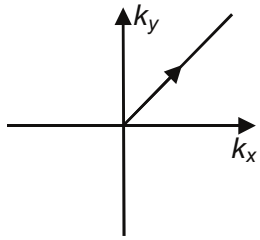
$\gamma\ n_{1,\max}\ \Delta G_y\ \Delta y\ t_1 \leq 2\pi$

$1/\Delta y \geq \gamma\ n_{1,\max}\ \Delta G_y\ t_1\ /\ 2\pi = k_{y,\max}/(2\pi)$

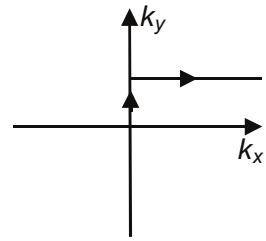
Space Encoding and Resolution

- The terminology of *phase encoding* and *frequency encoding* of the space information is historic
- The acquisition of the NMR signal in the presence of a time invariant field gradient is referred to as *frequency encoding* of the space information
- In frequency encoding k_x increases with the acquisition time t_2
- With increasing t_2 not only are higher values of k being encoded but also the signal attenuation by T_2^* increases, so that the *spatial resolution* $1/\Delta x$ is limited by the line width $\Delta\omega_{1/2} = 2/T_2^*$
- Modulation of the initial phase of the acquired magnetization in an *evolution time* t_1 prior to the *acquisition time* t_2 is referred to as *phase encoding*
- In phase encoding k_y is varied preferably by changing the gradient amplitude in steps ΔG instead of the gradient duration in steps Δt. This method is known as *spin-warp imaging*. It avoids variable signal attenuation from T_2 relaxation and signal modulations by the chemical shift and other spin interactions
- In spin-warp phase encoding the spatial resolution $1/\Delta y$ is limited by the maximum gradient strength $n_{1\max}\ \Delta G_y$
- Conventional 2D and 3D echo imaging methods combine spin-warp phase encoding and frequency encoding
- Pure phase encoding is used for *spectroscopic imaging*, *velocity encoding*, and for *imaging of solids*. It is referred to also as *single-point imaging* (*SPI*)

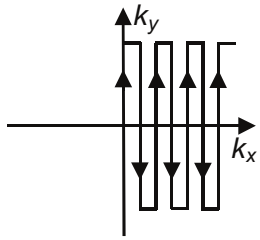
Scanning 2D ***k*** Space



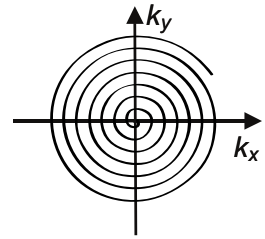
Back-projection imaging



Spin-echo imaging



Echo planar imaging (EPI)

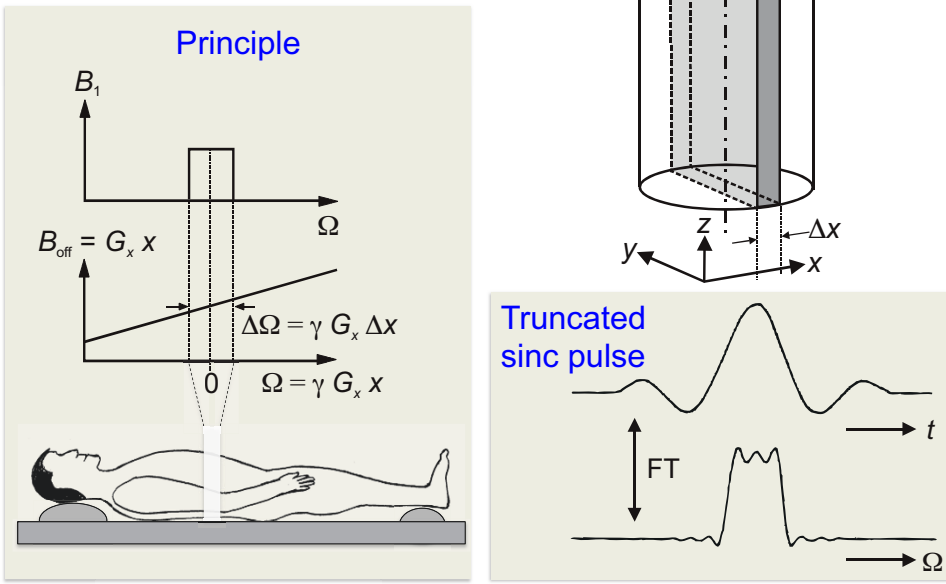


Spiral imaging

Walking Through ***k*** Space

- The information depicted in an NMR image centers at the ***k***-*space* origin
- To acquire the NMR signal with spatial resolution, it needs to be acquired for a region of ***k*** space centered at ***k*** = 0
- The signal in this region is defined on a discrete grid of points
- The sequence in which these points are addressed is determined in the imaging experiment
- The signal of a group of points is usually measured in one scan, which often includes the origin of one of the components of the ***k*** vector
- Typically many scans are needed to cover a complete region of ***k*** space
- Some *fast imaging* methods cover all relevant points of ***k*** space in one scan
- By *line-scan imaging* methods, the data from one line usually passing through the origin of ***k*** space are measured in one scan
- *Back-projection imaging* relies on several line-scans from different gradient directions
- *Spin-echo imaging* acquires data from parallel lines in subsequent scans
- *Echo planar imaging* (*EPI*) acquires the data of an entire image in a single shot following different traces through ***k*** space, e.g. meander and spiral traces
- *Sparse sampling* skips certain regions in ***k*** space to accelerate the data acquisition on the expense of image quality

Slice Selection

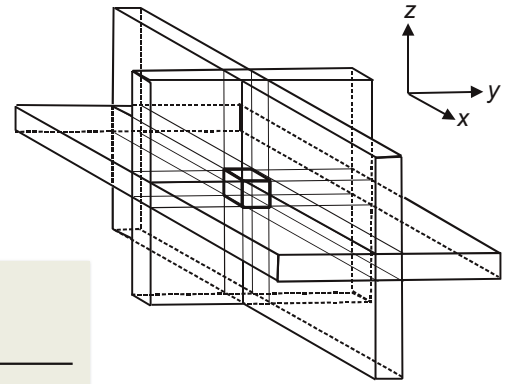


From P. G. Morris, *Nuclear Magnetic Resonance Imaging in Medicine and Biology*, **Clarendon Press**, Oxford, 1986, Fig. 3.8 by permission of Oxford University Press

Making 3D Objects Appear Like 2D Objects

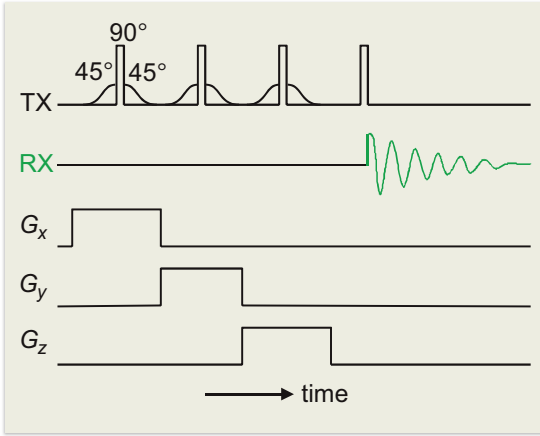
- To make 3D objects appear two dimensional in NMR, a *projection* must be measured or the magnetization of a 2D *slice* through the object
- Frequently images of 2D slices through 3D objects are measured
- To select a slice, a *frequency-selective pulse* is applied with the object exposed to an inhomogeneous magnetic field, which typically is a linear field with a space invariant gradient
- The linear field identifies different positions along the gradient direction by their NMR frequencies
- Constant frequencies are found in planes orthogonal to the gradient direction
- The frequency-selective pulse acts on the magnetization components within a limited frequency region only
- The width of the frequency region defines the thickness of the selected slice
- To a first approximation, the *Fourier transform* of the time-domain pulse shape defines the frequency-selection properties of the pulse
- A pulse with a *sinc* shape in the time domain exhibits a rectangular profile in the frequency domain
- To obtain pulses with finite durations, the lobes in the time domain are truncated on the expense of perfect *slice definition* in the frequency domain

Volume Selection



Principle

From S. Akoka in: J.D. de Certaines, W.M.M.J. Bovée, F. Podo, *Magnetic Resonance Spectroscopy in Medicine and Biology*, *Pergamon Press*, Oxford, 1992, p. 97, Fig. 5 with permission



Pulse sequence

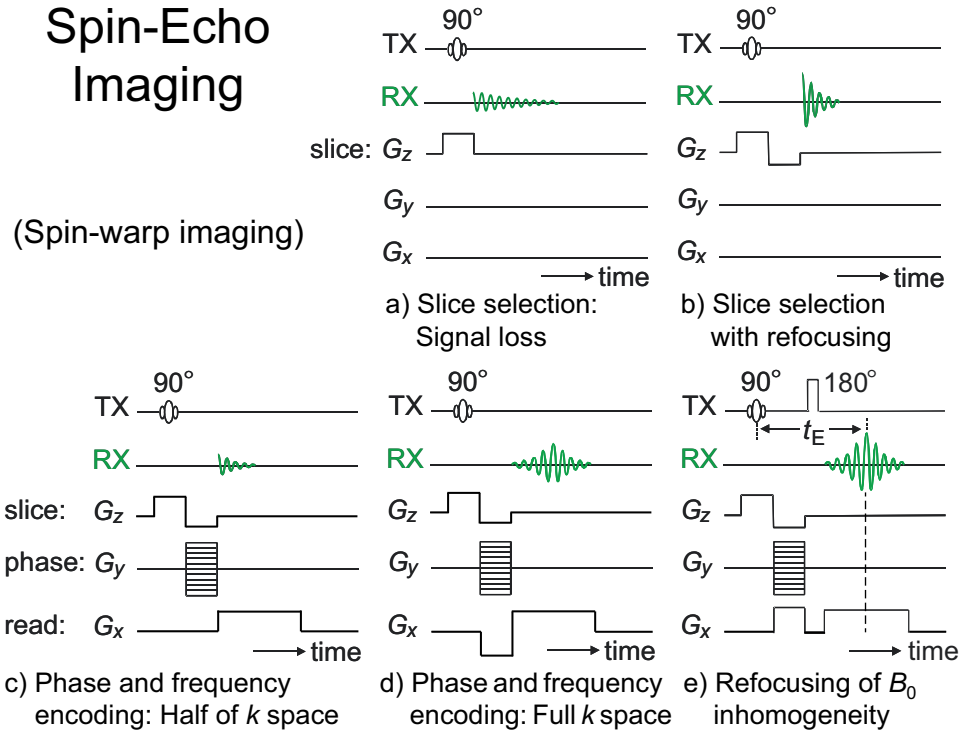
From W.P. Aue, S. Müller, T.A. Cross, J. Seelig, **J. Magn. Reson. 56** (1984) 350, Fig. 1 with permission

Restricting the Signal-Bearing Volume

- To investigate small regions within large objects by NMR imaging or to measure NMR spectra from well defined regions within the object (*volume-selective spectroscopy*), the magnetization within the selected volume must be accessed without crosstalk from magnetization in the surrounding volume
- Preferentially *longitudinal magnetization* is prepared because it relaxes slower than *transverse magnetization* in inhomogeneous fields
- Positions within the sample are labeled using magnetic field gradients in the same way as for slice selection of transverse magnetization
- The longitudinal magnetization outside the selected volume is eliminated
- The sensitive volume is defined at the intersection of three orthogonal *slices*
- Each pulse for selection of longitudinal magnetization consists of a package of three pulses, a selective 45° pulse, a nonselective 90° pulse, and another selective 45° pulse
- The first 45° pulse tips the magnetization within the selected plane by 45°
- The nonselective 90° pulse rotates the complete magnetization of the sample by 90°
- The last selective 45° pulse continues to rotate the magnetization of the slice through another 45°. In the end the magnetization of the slice has been rotated through a total angle of 180° and ends up as longitudinal magnetization
- The unwanted magnetization has been rotated by 90° only and dephases as transverse magnetization

Spin-Echo Imaging

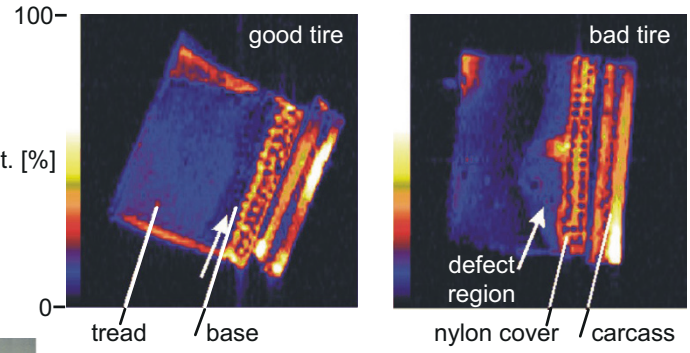
(Spin-warp imaging)



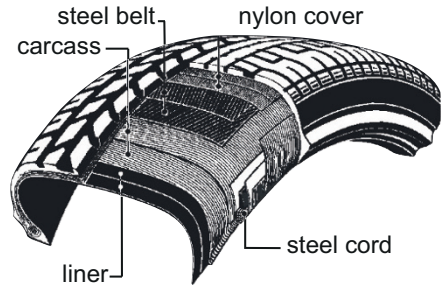
Slice-Selective 2D Spin-Echo Imaging

- A 2D imaging scheme starts by preparing the magnetization in a 2D *slice* selected with a suitably shaped pulse applied in the presence of a field gradient (a)
- The *slice-selective pulse* is long, and the magnetization dephases during the pulse in the inhomogeneous field
- This dephasing is refocused in a *gradient echo* generated by a second, negative field gradient pulse with an area half of that of the first gradient pulse (b)
- The 2D space information is inscribed into the *transverse magnetization* of the selected slice by *phase encoding* in an *evolution period* and by *frequency encoding* in the *detection period* (c)
- The *gradient switching times* are finite, and some signal is lost during these times. This signal needs to be recovered
- Also, components at negative ***k*** need to be encoded during the detection time
- Both demands are met by forming a *gradient echo* during the detection time (d)
- This echo is generated by starting the frequency-encoding gradient with an initial negative lobe having an area half of that of the succeeding positive lobe
- Signal dephasing from chemical shift distributions and inhomogeneity of the detection field can in addition be refocused in a *Hahn echo* by applying a 180° pulse separating evolution and detection periods (e)
- Then, the signs of the field-gradient pulses applied during the evolution time need to be inverted
- This method of 2D imaging is known as *spin-echo imaging*

Spin-Echo Imaging of Tire Samples



Pirelli pneumatico 1904

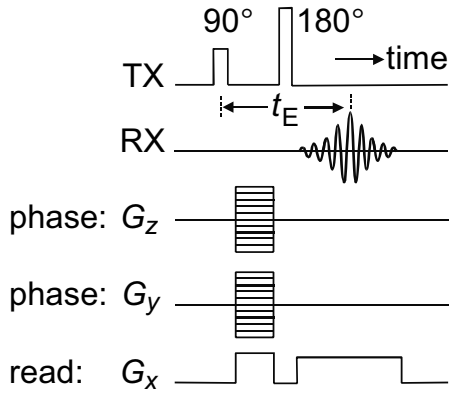


From A. Guthausen, G. Zimmer, S. Laukemper-Ostendorf, P. Blümler, B. Blümich, **Chemie in unserer Zeit 32** (1998) 73, Fig. 3 with permission

An Example of 2D Spin-Echo Imaging

- 2D *spin-echo imaging* used to be applied in clinical MRI. But imaging times are long, because the longitudinal magnetization needs to recover after each scan in preparation times approximately 5 T_1 long
- *Rubber* is an inhomogeneous product especially when filled with carbon black. Consequently signal lost from magnetization dephasing in local field distortions originating from changes of the magnetic susceptibility within the sample needs to be recovered in a *spin echo*
- Spin-echo imaging used to be employed in many tire development centers to probe the *vulcanization* state of different rubber layers in sample sections cut from test *tires*
- The *image contrast* is largely defined by differences in *transverse relaxation* during the *echo time* and by *longitudinal relaxation* during the *recovery period*
- Sample regions with soft rubber and mobile additives have long T_2, hard rubber has shorter T_2, and solid polymers like textile fibers have even shorter T_2
- The typical *spatial resolution* in such images is 1/(0.1 mm) in both dimensions
- The imaged slices are usually much thicker than 0.1 mm, of the order of 5 mm, in order to gain enough signal

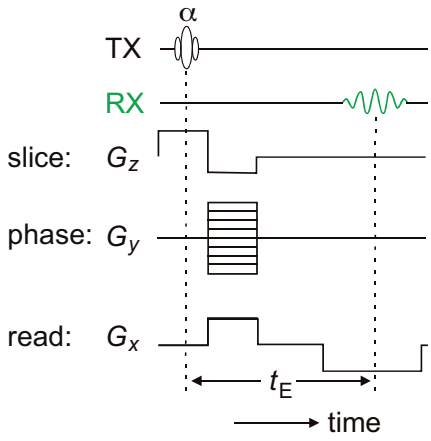
3D Spin-Echo Imaging



3D Imaging

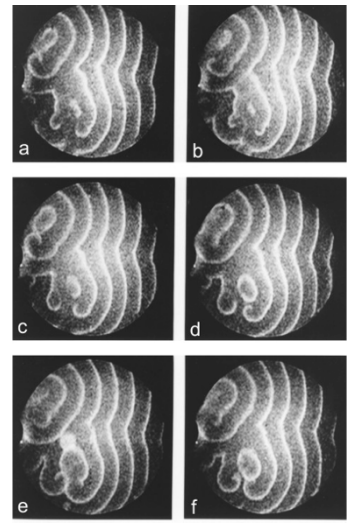
- *3D images* can be obtained in different ways
- Successive 2D slices measured by *slice-selective 2D imaging* can be combined into a 3D image
- Here, the spatial resolution perpendicular to the slice plane is low. During acquisition, the signal comes from one selected slice only, while the noise comes from the entire sample
- In *3D Fourier imaging*, the signal is acquired at all times from the same volume, which also produces the noise, and the resolution can be high in all three dimensions
- For 3D Fourier imaging the slice-selective pulse from 2D MRI is replaced by a non-selective pulse
- A further *phase-encoding gradient* pulse is introduced and stepped through positive and negative values independent of the other gradient pulses
- The image is obtained by *3D Fourier transformation* of the acquired data set

Gradient-Echo Imaging



FLASH: Fast low-angle shot

From A. Haase, J. Frahm, D. Matthei, W. Hänicke, K. D. Merboldt, **J. Magn. Reson. 67** (1986) 258, Fig. 1 with permission



Mn catalyzed Belousov-Zhabotinsky reaction: Images taken at 40 s intervals

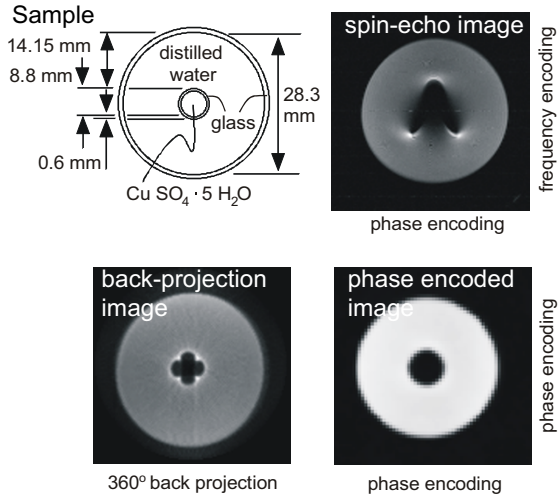
From A. Tzalmona, R. L. Armstrong, M. Menzinger, A. Cross, C. Lemaire, **Chem. Phys. Lett. 174** (1990) 199, Fig. 1 with permission

Reducing the Measurement Time

- The measurement time for a *spin-echo image* is determined by the number of lines in the image data matrix and the duration of the *recycle delay* to recover the longitudinal magnetization
- Due to the fact that in a spin echo the entire longitudinal magnetization is perturbed, the recycle delay is of the order of 5 T_1
- Shorter recycle delays can be employed if the longitudinal magnetization is only slightly perturbed from its thermodynamic equilibrium value
- This is achieved by discarding the 180° refocusing pulse in the imaging sequence. In particular, if a *small flip-angle pulse* is used instead of the initial 90° pulse to rotate the longitudinal magnetization only partially into the transverse plane, the recycle delay can be shortened considerably
- Following Richard Ernst, the optimum flip angle α_E and the optimum recycle delay t_0 are determined by the longitudinal relaxation time T_1 according to $\cos\alpha_E = \exp\{-t_0/T_1\}$, where α_E is the *Ernst angle*
- The resultant imaging method is called *gradient echo imaging* or fast low-angle shot (*FLASH*) *imaging*
- It is a standard method in *clinical imaging*
- It has also been used for imaging slow dynamic processes in soft matter, such as chemical waves in oscillating reactions

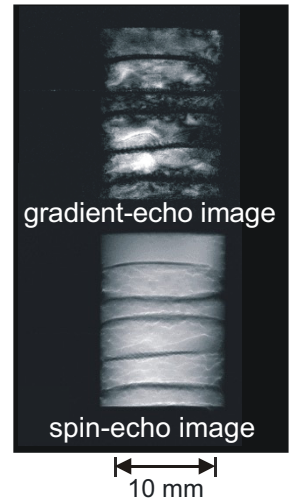
Susceptibility Contrast

Susceptibility distortions



From O. Beuf, A. Briguet, M. Lissac, R. Davis, **J. Magn. Reson. B 112** (1996) 111, Figs. 2, 5 with permission

Stacked EPDM sheets

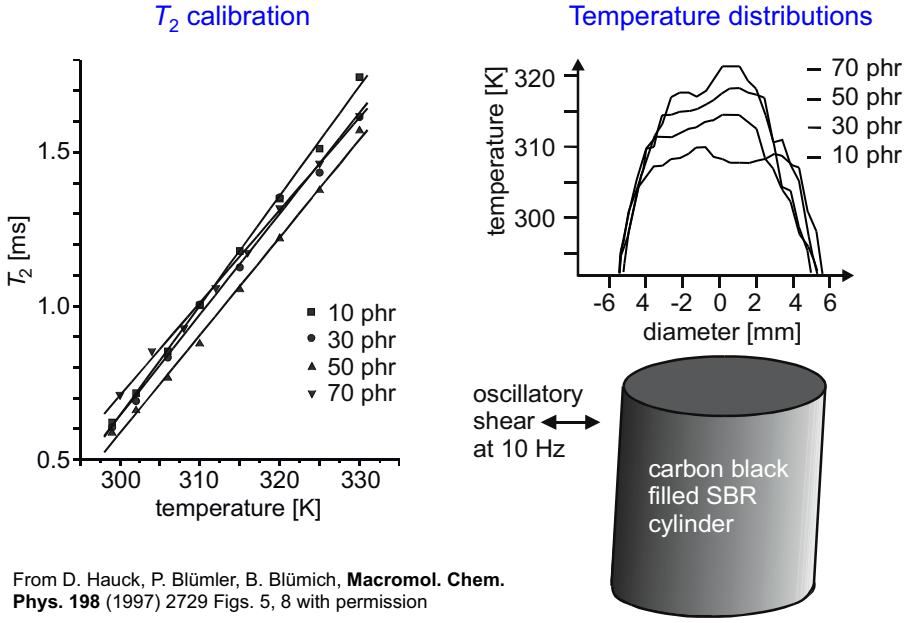


From P. Blümler, V. Litvinov, H.G. Dikland, M. van Duin, **Kautschuk Gummi Kunststoffe 51** (1998) 865, Fig. 1 with permission

Contrast and Artifacts

- In spin-echo imaging, the image *contrast* is determined by three factors
- 1) The *spin density*, i.e. the number of nuclei at position $\boldsymbol{r}$ contributes $M_{z0}(\boldsymbol{r})$
- 2) *Transverse relaxation* during the echo time t_E contributes $\exp\{-t_E/T_2(\boldsymbol{r})\}$
- 3) *Partial saturation* due to short recycle delays t_0 contributes $1-\exp\{-t_0/T_1(\boldsymbol{r})\}$
- In total, the image amplitude is given by $M_{z0}(\boldsymbol{r})\ \exp\{-t_E/T_2(\boldsymbol{r})\}\ [1-\exp\{-t_0/T_1(\boldsymbol{r})\}]$
- In addition, the contrast is enhanced by *magnetic field distortions* in sample regions, where the *magnetic susceptibility* changes
- Examples are carbon-black filler clusters embedded in a rubber matrix and the glass interface between distilled water and water doped with copper sulfate
- In *gradient-echo imaging*, the magnetization dephasing due to *magnetic field inhomogeneity is* not refocused, so that susceptibility distortions are enhanced in the frequency-encoding direction
- These distortions do not appear in the *phase-encoding dimension* because the encoding time t_1 is kept constant
- In *back-projection imaging* with frequency encoding in both dimensions, the artifacts appear symmetrically in both dimensions
- In pure *phase-encoding imaging*, they are not observed at all
- In standard spin-echo imaging, the dephasing from magnetic field inhomogeneity is refocused for the phase-encoding dimension in the echo maximum
- *Susceptibility effects* can be considered artifacts in images, but can also be used to generate image contrast, e.g. in carbon-black filled *elastomers*

Temperature Imaging from Relaxation Maps

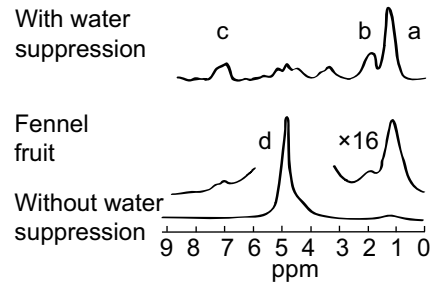


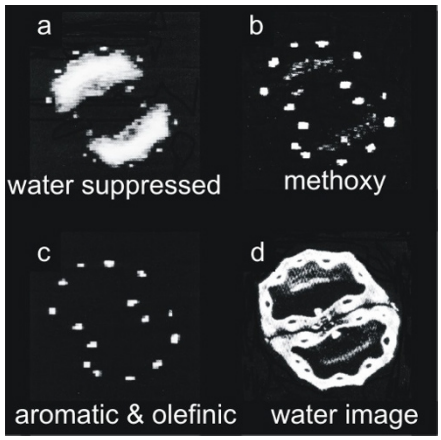
From D. Hauck, P. Blümler, B. Blümich, **Macromol. Chem. Phys. 198** (1997) 2729 Figs. 5, 8 with permission

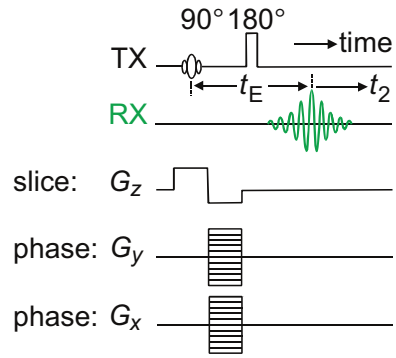
Parameter Images

- Images of the spin density $M_{z0}(\boldsymbol{r})$, which are weighted by a function of other NMR parameters, for example by $\exp\{-t_E/T_2(\boldsymbol{r})\}$, are called *parameter-weighted spin-density images*
- By acquisition of several images with different echo times, the parameter $T_2(\boldsymbol{r})$ can be extracted for every voxel at position $\boldsymbol{r}$ from the set of images
- The resultant map of $T_2(\boldsymbol{r})$ is called a T_2 *image* or in general a *parameter image*
- In elastomers, T_2 is often found to be proportional to temperature within small temperature ranges
- Then, a T_2 parameter image $T_2(\boldsymbol{r})$ can be calibrated into a *temperature map*
- Such a temperature map has been determined by NMR for a carbon-black filled rubber cylinder undergoing small oscillatory shear deformation at a frequency of 10 Hz
- Due to the dynamic loss modulus, some deformation energy is dissipated as thermal energy
- The heat gain inside the sample competes with the heat loss through the sample surfaces
- The resultant *temperature distribution* exhibits a peak in the center of the sample
- Dynamic mechanical load thus leads to dynamic sample heterogeneity

Spectroscopic Spin-Echo Imaging





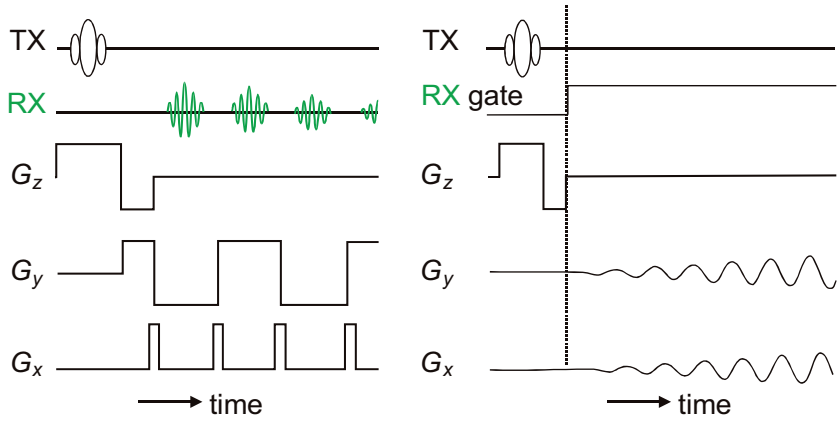


From H. Rumpel, J. M. Pope, **Magn. Reson. Imag. 10** (1992) 187, Fig. 8 with permission

Incorporating a Spectroscopic Dimension

- An *NMR spectrum* can be acquired in each voxel either indirectly or directly
- Indirect acquisition of the spectrum demands stepping point by point through the FID in an evolution time with different scans while the field gradient is off
- Direct acquisition corresponds to sampling the FID in a homogeneous field during the detection period
- The typical *digital resolution* of an NMR image is 256 points in each dimension
- A 1D NMR spectrum consists of roughly 1024 = 1k to 64 k data points
- On account of short measuring times, the spatial information is encoded for all dimensions indirectly in the signal phase during an evolution period t_1, and the spectroscopic information is acquired directly during the detection period t_2
- From such *spectroscopic images*, other images can be derived, where the *contrast* is defined by the integral of a given line in the NMR spectrum
- In this way, the concentration distributions of different chemical compounds can be imaged, for example, in plants, muscles, and the human brain

Echo-Planar Imaging (EPI)



Cartesian EPI

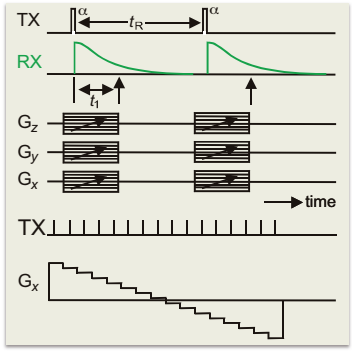
Spiral imging

$k_x(t) = k_{max}\ (t/t_{max})\ \sin \omega_k t$
$k_y(t) = k_{max}\ (t/t_{max})\ \cos\omega_k t$
$\gamma\ G_{xy}(t) = \mathrm{d/d}t\ k_{xy}(t)$

Acquiring Images in a Single Scan

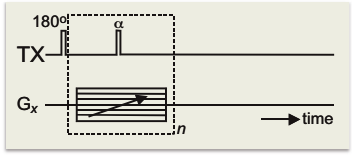
- Fast imaging methods can be designed in different ways
- In the *steady-state free precession* method the transverse magnetization stays in dynamic equilibrium with the excitation and with relaxation
- Other methods use multiple scans in rapid succession with short or without recovery time by avoiding Hahn echoes in favor of gradient echoes. One such method is the *FLASH imaging* method
- But an entire 2D image can also be acquired in one shot by generating multiple echoes, where each echo encodes a different trace through ***k***-space
- Methods of this type are referred to as *echo planar imaging* (*EPI*)
- In clinical imaging, they are usually pure gradient-echo methods to avoid excessive rf exposure
- In the original EPI method, ***k***-space is scanned in either a zig-zag trace or in parallel traces on a Cartesian grid by rapidly pulsing field gradients
- When the gradient echoes are replaced by Hahn echoes, the *RARE* (Rapid Acquisition with Relaxation Enhancement) method is obtained
- A method less demanding on hardware and with less acoustic noise is *spiral imaging*, where the trace through ***k***-space forms a spiral

Single-Point Imaging (SPI)

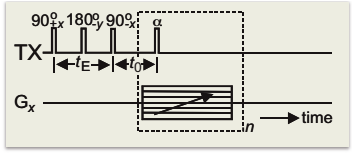


Basic pulse sequence

SPRITE: Single-point ramped imaging with T_1 enhancement

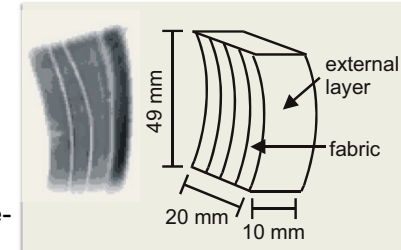


T_1 filter

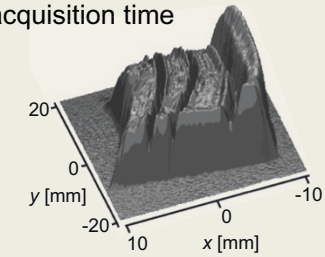


T_2 filter

From P. Prado, B. J. Balcom, M. Jama, **J. Magn. Reson. 137** (1999) 59, Fig. 1 with permission



Tire section: 200 s acquisition time



From P.J. Pablo, L. Gasper, G. Fink, B. Blümich, V. Herrmann, K. Unseld, H.-B. Fuchs, H. Möhler, M. Rühl, **Macromol. Mat. Eng. 274** (2000) 13, Fig. 3 with permission

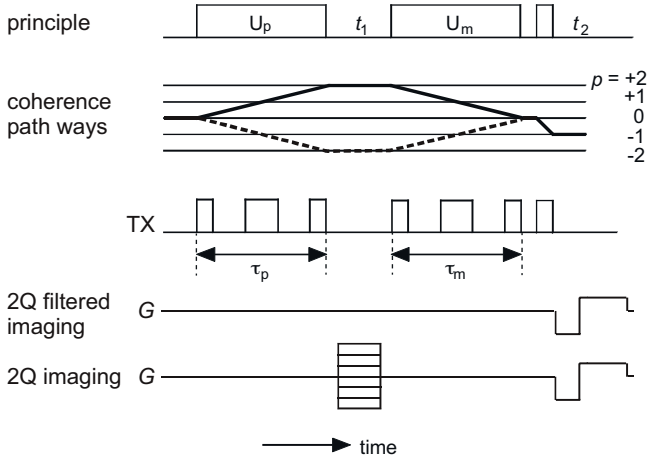
Imaging with Pure Phase Encoding

- The most successful technique for imaging objects with short transverse relaxation times such as solids or fluid-filled porous media is *single-point imaging* (SPI)
- ***k***-space is sampled by pure phase encoding
- A short rf pulse with a small flip angle is applied in the presence of a field gradient
- A single point of the FID is sampled after a short dead time t_1
- The gradient is ramped to a different value and the experiment is repeated
- Depending on the flip angle and the repetition time, T_1 contrast is generated
- Different *magnetization filters* can be introduced to generate contrast by preparing the initial longitudinal magnetization in a particular way. Examples for such filters are the inversion-recovery sequence for T_1 contrast and the spin-echo sequence for T_2 contrast
- Despite the pure phase-encoding procedure, images can be acquired rather fast, such as 50 s for a single scan of an image with 128 × 64 data points

Imaging of Double-Quantum Coherences

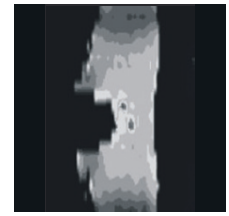
Application to strained rubber bands with a cut

Pulse sequences:

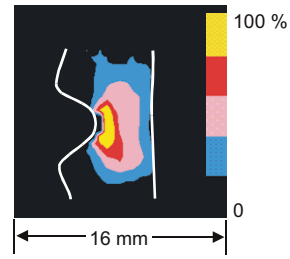


From M. Klinkenberg, P. Blümler, B. Blümich, **Macromolecules 30** (1997) 1038, Fig. 5 with permission

^{1}H 2Q-filtered image



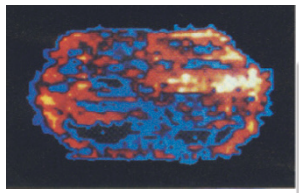
^{2}H 2Q image

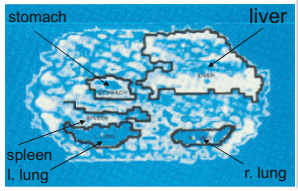


Tricks with Coupled Spins

- Systems of coupled spins ½ and *quadrupolar spins* give rise to *multi-quantum coherences*
- The dephasing angle of coherences by precession in magnetic fields is proportional to the *coherence order p*
- *Double-quantum coherence* (p = 2) dephases twice as fast as *single-quantum coherence* (p = 1)
- Phase encoding of multi-quantum coherences effectively multiplies the strength of the field gradient with the coherence order *p*
- This can be made use of for imaging if the multi-quantum relaxation time is long enough, as in the case of the double-quantum coherence of deuterated oligomers incorporated into elastomers
- In other cases, the multi-quantum coherence can still be exploited in a magnetization filter preceding the image acquisition to separate signals from uncoupled and coupled spins or from isotropic and anisotropic material regions
- *Double-quantum imaging* and *double-quantum filtered imaging* have been applied to image local stress and strain in strained rubber bands by contrasting the signals from differently deformed regions of the rubber network

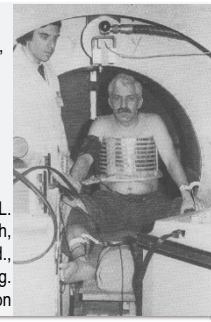
FONAR and Spin Warp Imaging

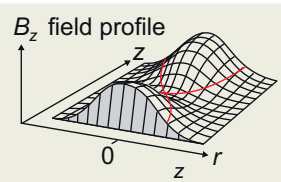




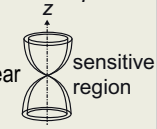
R. Damadian, L. Minkoff, M. Goldsmith, **Physiol. Chem. & Physics 10** (1978) 561, Fig. 1, private communication, 15 August 1979

From R. Damadian, L. Minkoff, M. Goldsmith, in: R. Damadian, ed., **NMR 19** (1981) 1, Fig. 10 with permission

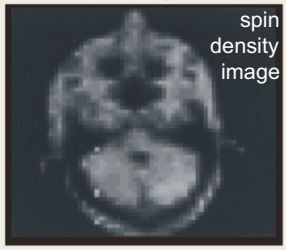


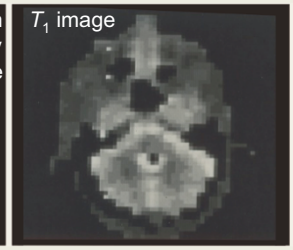


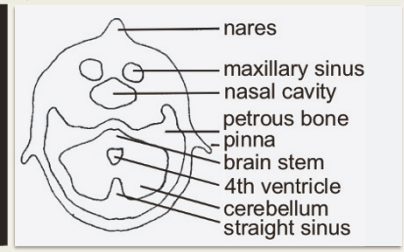
FONAR: Field Focused Nuclear Magnetic Resonance



Spin-warp imaging: Head section, 25 mm below the eyes





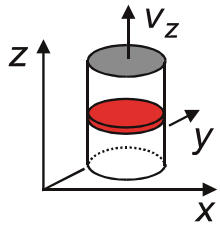


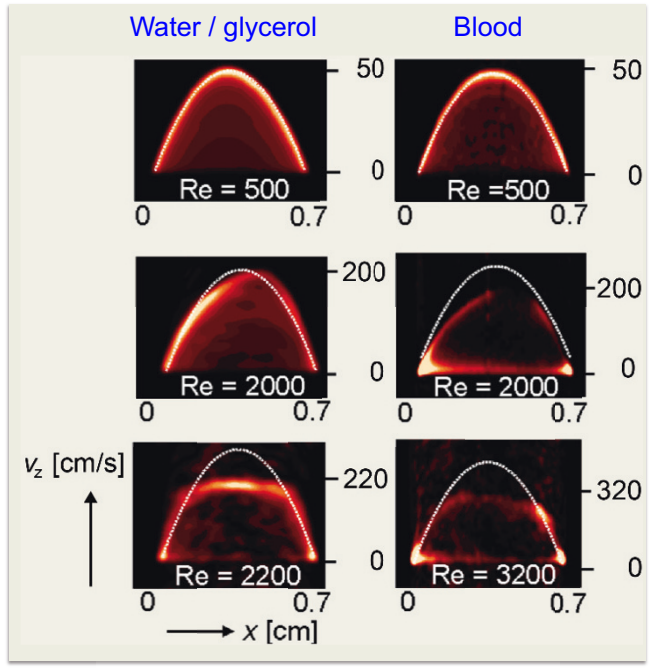
From W. A. Edelstein, J. M. S. Hutchison, G. Johnson, T. Redpath, **Phys. Med. Biol. 25** (1980) 751, Fig. 2 with permission

Early Medical Images

- The first medical images were measured in 1978 by Raymond Damadian and co-workers with the *FONAR* method
- They acquired images point-by-point in real space by shifting the patient through the sweet spot of an inhomogeneous field
- The sweet spot was generated by a saddle point in the $\boldsymbol{B}_0$ field profile
- Within the sweet spot the field is less inhomogeneous than outside, so that the NMR signal from this region in space decays not as fast as outside
- The acquisition time was several hours, and the image quality was low
- Yet, 10 years later NMR imaging was already an indispensable diagnostic tool in hospitals all around the world
- However, it was not the FONAR method reaching the finishing line, but the *spin-warp imaging* technology developed at General Electric by W. Edelstein and collaborators
- Spin-warp imaging is spin-echo imaging with a fixed evolution time in which the gradients and not the evolution time t_1 are incremented to scan $\boldsymbol{k}$-space
- Already the original spin-warp publication reported promising *parameter images* of the spin density and of T_1 from slices through different parts of the human body

Flow Imaging of Blood



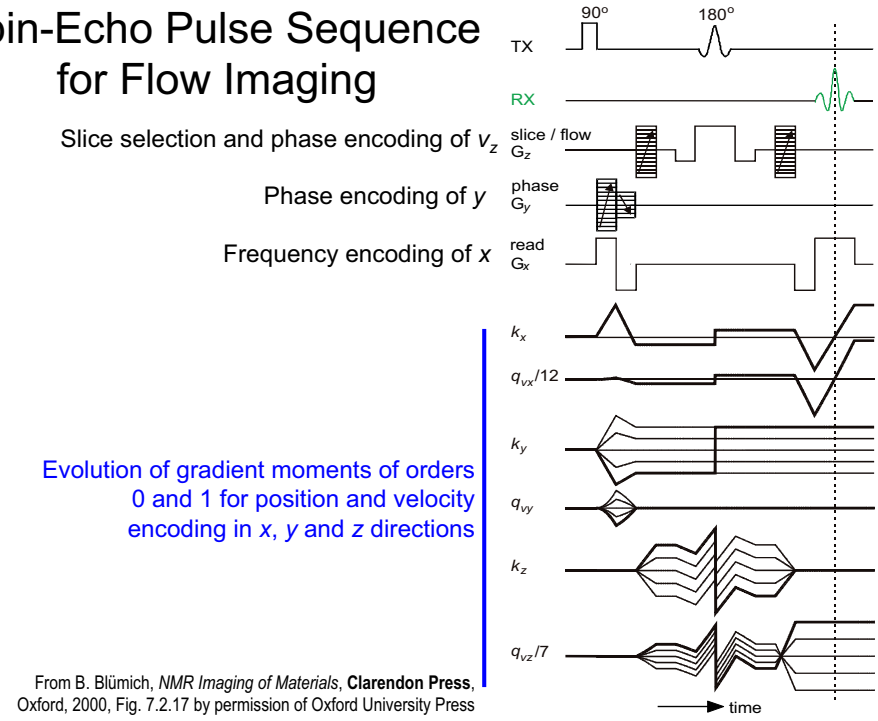


From S. Han, O. Marseille, C. Gehlen, B. Blümich, **J. Magn. Reson. 152** (2001) 87, Figs. 3, 5 with permission

Imaging Flowing Liquids

- The most important application areas of non-medical imaging are in *chemical engineering* and *materials science*
- An important application field is the characterization of *transport phenomena* like fluid and granular flow or molecular self- and inter-diffusion in technical devices and porous media, which are optically non-transparent
- As long as the set-up is non-magnetic and radio-frequency transparent, the transport properties can be measured by NMR
- Usually, the phenomenon in question has to be reproduced inside the magnet unless stray-field NMR techniques are employed and the object is investigated from one side
- An important, optically opaque fluid is blood. Its rheological properties are of interest in medical engineering for building devices like artificial arteries and veins, heart valves, hemodialyzers, and blood pumps. Only the blood substitute water/glycerol is sufficiently transparent for optical velocity analysis
- With pulsed field-gradient NMR, *velocity-vector fields* can be imaged
- For quantitative MRI a slice of the moving fluid is selected, which stays inside the resonator for the durations of the space and velocity encoding periods as well as the detection period
- A complete velocity image has six dimensions: 3 for space and 3 for velocity
- Also, the velocity distribution can be determined in each voxel

Spin-Echo Pulse Sequence for Flow Imaging

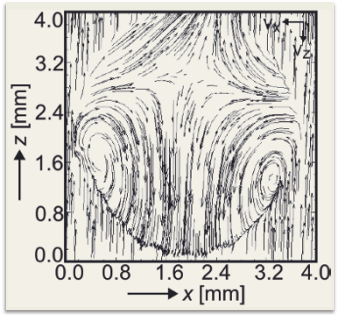


From B. Blümich, *NMR Imaging of Materials*, **Clarendon Press**, Oxford, 2000, Fig. 7.2.17 by permission of Oxford University Press

Pulse-Sequence Design

- Pulse sequences for *velocity imaging* have to incorporate *space encoding* by scanning $\boldsymbol{k}$ space and *flow encoding* by scanning $\boldsymbol{q}_v$ space
- The $\boldsymbol{k}$ and $\boldsymbol{q}_v$ spaces must be encoded independently
- For example, one $\boldsymbol{k}$ component is frequency encoded for direct acquisition and the other components of $\boldsymbol{k}$ and $\boldsymbol{q}_v$ are phase encoded in the acquired signal
- A compromise has to be made for the velocity component in direction of the frequency encoded space component. Here, complete decoupling of phase evolutions is not possible
- For example, to image $v_z(x,y)$, an xy slice is selected, and the transverse magnetization is acquired as a function of k_x, k_y, and q_{vz}
- The components q_{vx}, q_{vy}, and k_z should be zero during data acquisition
- If frequency encoding is used for k_x, then q_{vx} also varies during the detection time
- The gradient-modulation sequences for such imaging modalities are numerically optimized
- For accelerated flow the acceleration phase needs to be considered as well
- After Fourier transformation over k_x, k_y, and q_{vz}, the relaxation-weighted spin density $M_z(x,y,v_z)$ is obtained from which $v_z(x)$ and $v_z(y)$ can be extracted

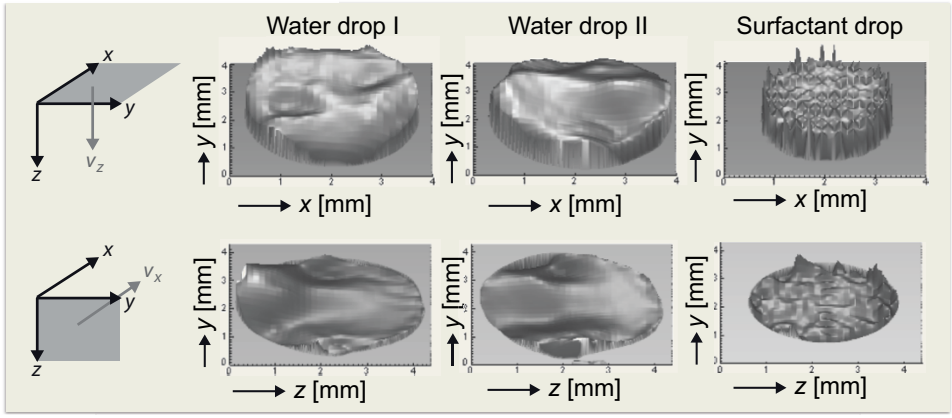
NMR Imaging of Falling Water Drops



zx projection of the velocity vector field

From S. Han, S. Stapf, B. Blümich, **Phys. Rev. Lett. 87** (2001) 145501, Figs. 2, 3 with permission

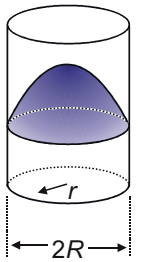
Velocity-component images



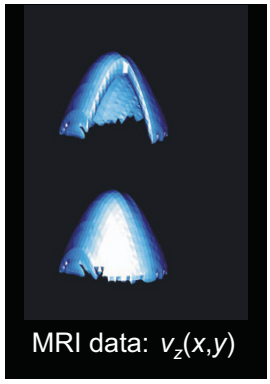
Imaging Velocity Fields

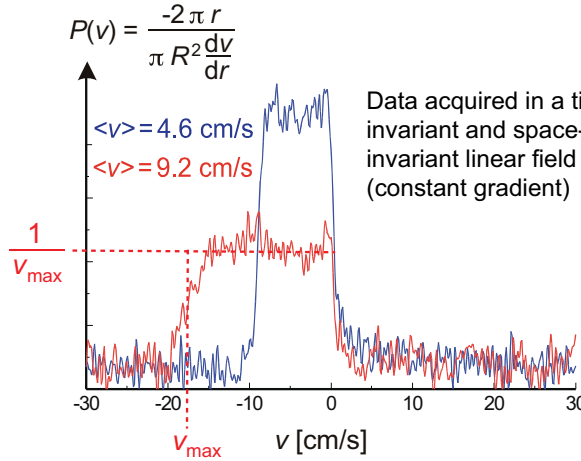
- Straight forward *flow encoding* in MRI requires long acquisition times ranging from several minutes to several hours
- Fast flow imaging schemes use echo trains to encode different components of $\boldsymbol{k}$ and $\boldsymbol{q_v}$ in each echo time and employ sparse sampling of the $\boldsymbol{k}$ and $\boldsymbol{q_v}$ spaces
- Due to long acquisition times, most flow processes suitable to conventional NMR imaging are either stationary or repetitive
- An example of a repetitive process is the *vortex motion* in water drops falling through the NMR magnet
- Due to the short residence time of the drop in the receiver coil, *single-point acquisition* is necessary for all points in $\boldsymbol{k}$ and $\boldsymbol{q}_v$ space
- Drops from different dripping experiments show different velocity profiles
- A *water drop* covered with a surfactant does not show internal motion
- A 2D velocity vector field is composed of two data sets, each providing one of the two in-plane velocity components
- If $\boldsymbol{k}$ or $\boldsymbol{q}_v$ space is traced in only one or two dimensions without line or slice selection, a projection is acquired in real space or in velocity space (see *projection – cross-section theorem* at the end of this chapter), i.e. the signal is integrated over the hidden space or velocity components

Laminar Flow in a Circular Pipe



Theory: $v(r) = \frac{v_{max}}{R^2}(R^2 - r^2)$, $P(v)\,dv = \frac{-2\,\pi\,r\,dr}{\pi\,R^2}$

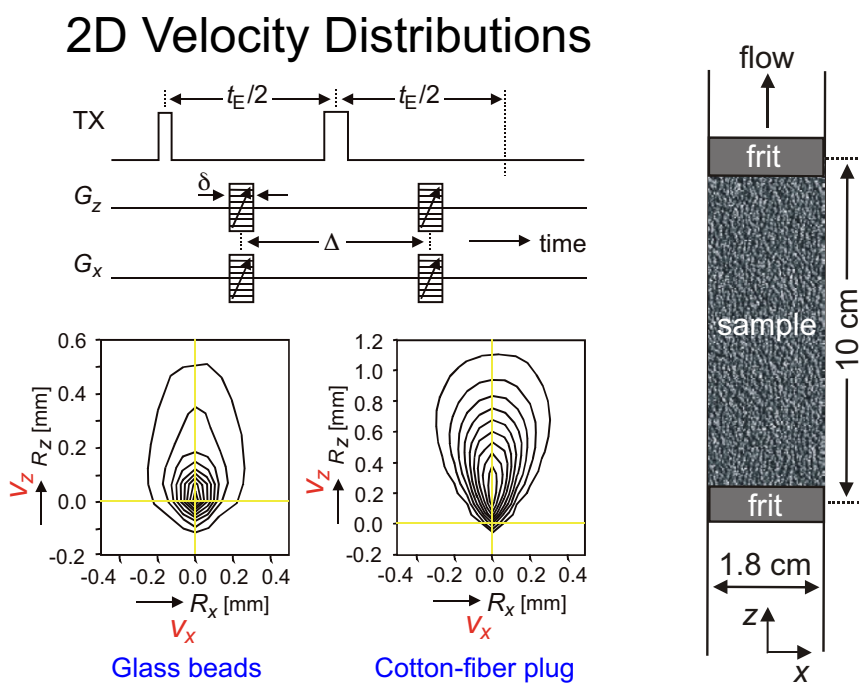




From B. Blümich, S. Han, C. Heine, R. Eymael, M. Bertmer, S. Stapf, in: J. Fraissard, O. Lapina, eds., *Magnetic Resonance in Colloid and Interface Science*, **Kluwer**, Dordrecht, 2002, p. 3, Fig. 2c with permission

Probability Densities of Velocity

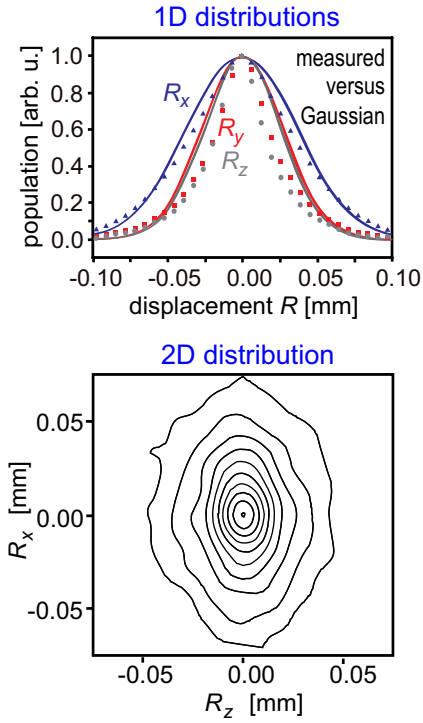
- *Probability densities* are called *distributions* in short
- A *distribution of velocities* is the Fourier transform of the NMR signal as a function of $\boldsymbol{q}_v$
- In the simplest experiment one component of $\boldsymbol{q}_v$ is varied and the distribution is plotted against *displacement R* in a given time Δ
- This notation is also applied to diffusive motion. In the NMR community, the corresponding *distribution of displacements* is called the *propagator*
- The distribution of velocities is most simply measured with a pair of anti-phase field-gradient pulses, and the amplitude of the associated echo is recorded as a function of the gradient amplitude
- In principle, the experiment can be conducted also with time-invariant field gradients by varying the echo time t_E in an echo experiment
- For *laminar flow through a circular pipe* the *velocity profile* is parabolic
- The velocity distribution is obtained by equating the probability $P(v)\,dv$ of finding a velocity component between v and $v + dv$ with the relative area of the annulus at radius r with width dr in which this velocity component is found
- The distribution is constant for all velocities between 0 near the tube wall and v_{max} in the center, and zero elsewhere. It has the shape of a hat
- *Velocity distributions* are very sensitive against slight imperfections in the experimental set-up. They may provide better fingerprints of a flow process than *velocity images* and are faster to measure



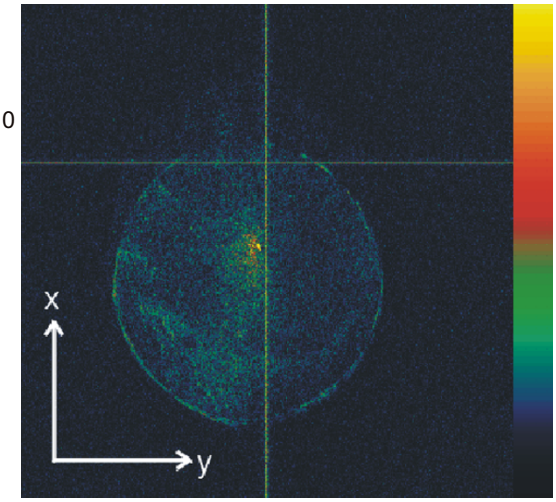
From B. Blümich, *NMR Imaging of Materials*, **Clarendon Press**, Oxford, 2000, Fig. 5.4.7 by permission of Oxford University Press

Velocity-Vector Distributions

- 1D *velocity distributions* are *projections* of 3D velocity distributions obtained by integration over the unresolved velocity components
- *2D velocity distributions* provide more detailed information than 1D distributions
- They are obtained by measuring the transverse magnetization as a function of two components of the wave vector $\boldsymbol{q}_v$ and subsequent 2D Fourier transformation
- Flow through circular pipes filled with glass beads or cotton fibers can readily be distinguished by the associated 2D distributions of radial and axial velocities
- For the cotton fibers, strong radial dispersion is observed at high axial flow
- For the glass beads, considerable axial backflow is observed at zero radial flow
- The observed velocities are *finite difference approximations* of velocities corresponding to displacements R experienced during the encoding time Δ
- For field gradient pulses with durations δ no longer short compared to the characteristic times of motion, the *slow-motion approximation* fails and the finite difference interpretation can no longer be applied



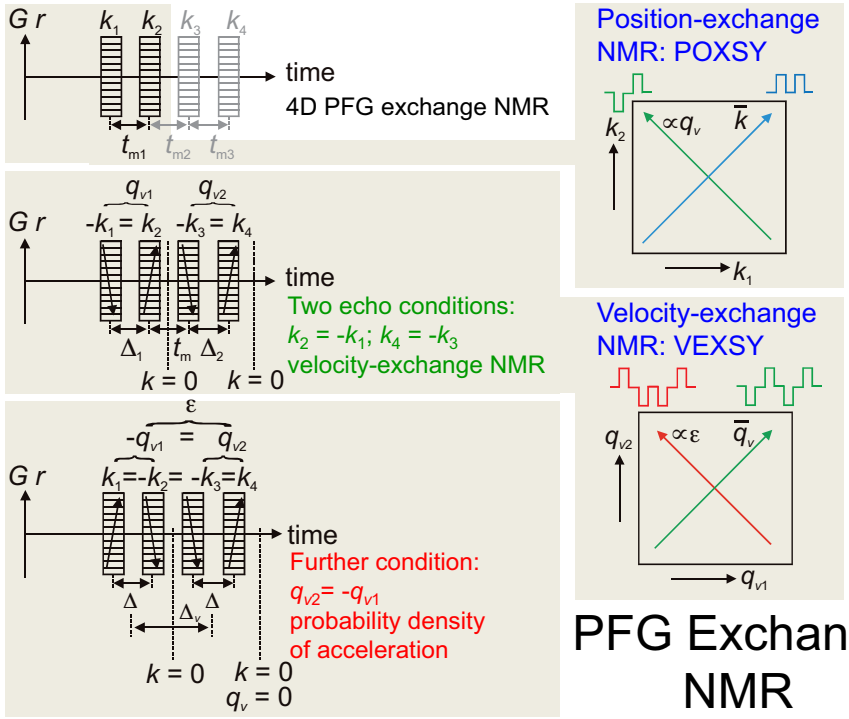
Oriented Ice from Freezing Salt Water



From M. Menzel, S.-I. Han, S. Stapf, B. Blümich, **J. Magn. Reson. 143** (2000) 376, Figs. 2, 3, 4 with permission

Diffusion in Anisotropic Media

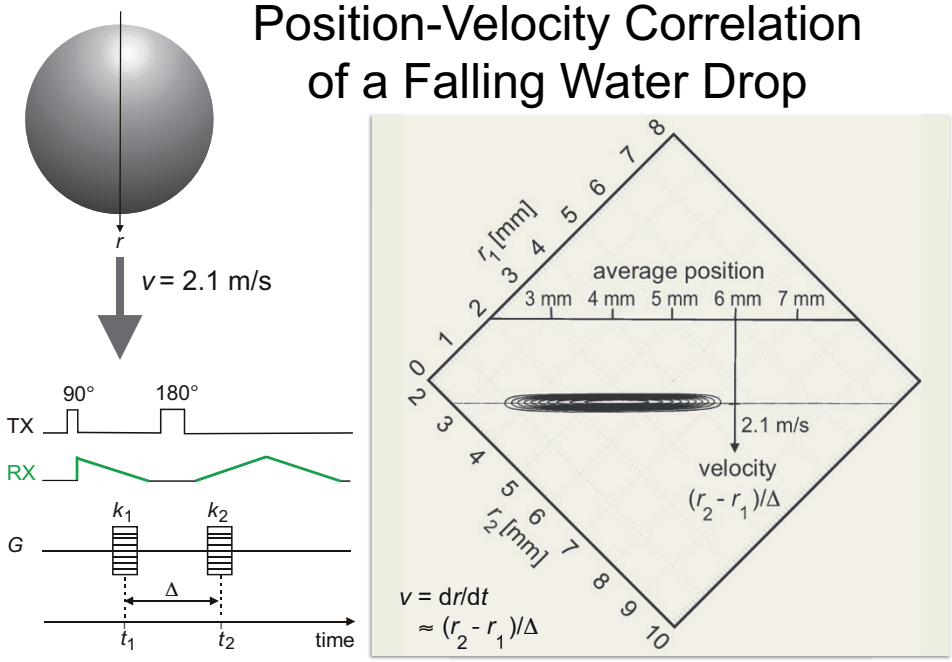
- *Translational diffusion* leads to *incoherent displacements* of molecules as opposed to *coherent displacement* by flow
- To probe incoherent motion, displacements R_x, R_y, R_z are measured in given time intervals Δ with PFG NMR using the same pulse sequences as for flow encoding in a first approximation
- For free diffusion, the *distribution of displacements* (*propagator*) has a Gaussian form, and the mean diffusion length $\langle \boldsymbol{R}^2 \rangle^{1/2}$ scales with the square root of the diffusion time Δ
- For free 3D diffusion, one obtains $\langle \boldsymbol{R}^2 \rangle = \langle (\boldsymbol{r}_2 - \boldsymbol{r}_1)^2 \rangle = 6\, D\, \Delta$, where D is the diffusion coefficient. For 1D diffusion on obtains $\langle R^2 \rangle = 2\, D\, \Delta$
- For *restricted diffusion* in the narrow pores of rocks and heterogeneous catalysts, the confining pore walls limit the diffusion length
- For short diffusion times, a *Gaussian distribution* is observed. For long diffusion times, the confinements lead to deviations from a Gaussian distribution
- Macroscopic anisotropy of porous media, such as oriented biological tissue and ice formed from salt water can be identified by comparing the 1D distributions of displacements in different space directions at long diffusion times
- Another method consist of analyzing *2D distributions of displacements* for deviations from circular symmetry



Position-Exchange NMR

- *Flow* or *displacements* in given times are typically measured with short, anti-phase gradient-pulse pairs. The second, positive pulse marks final position and the first, negative pulse initial position
- For measurements of displacements, both gradients pulses are locked to equal magnitude in each amplitude step, i.e. $k_2 = -k_1$ at all times
- Stepping both gradient pulses independently leads to a 2D experiment
- The Fourier transform of the acquired data is the joint probability density of finding a magnetization component at a particular initial position and a time Δ later at a particular final position
- On the principal diagonal, the average of the initial and final positions is identified. On the secondary diagonal, the difference between final and initial positions, i.e. displacement or velocity, is identified
- The experiment is called *position-exchange spectroscopy* (*POXSY*) in analogy to *frequency exchange-spectroscopy* (EXSY) in NMR spectroscopy
- A 4D exchange experiment results with four gradient pulses
- Conditions on the gradient variations, such as the formation of a *gradient echo* for detection, reduce the dimensionality of the experiment
- The conditions $k_2 = -k_1$ and $k_4 = -k_3$ imposed on the 4D POXSY sequence lead to *velocity-exchange spectroscopy* (*VEXSY*)
- Here, *average velocity* is identified along the principal diagonal and velocity difference or *acceleration* along the secondary diagonal
- The additional condition $k_4 = -k_3 = -k_2 = k_1$ leads to a 1D experiment by which the *distribution of accelerations* can be measured

Position-Velocity Correlation of a Falling Water Drop

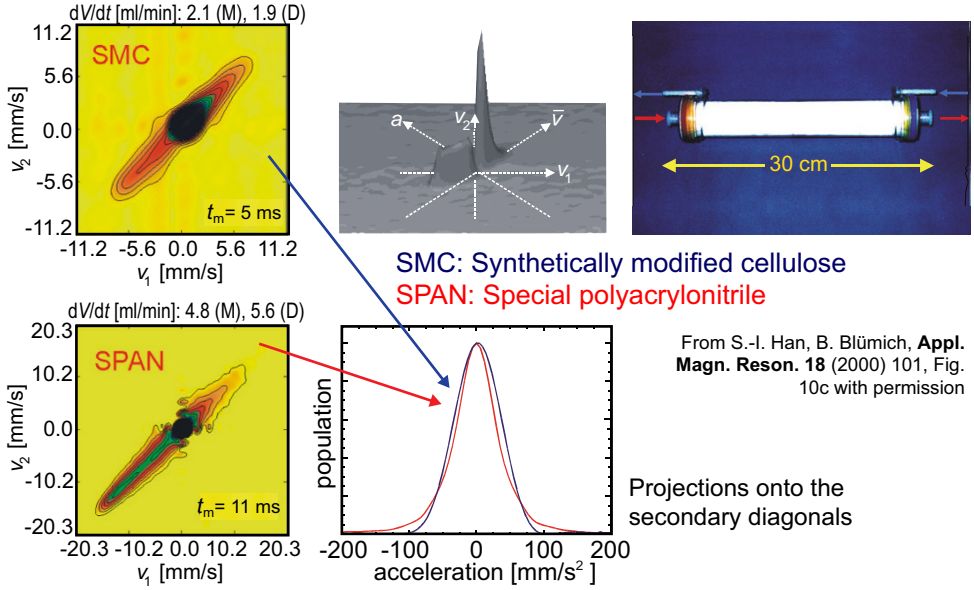


From S.-I. Han, S. Stapf, B. Blümich in: J. Fraissard, O. Lapina, eds., *Magnetic Resonance in Colloid and Interface Science*, **Kluwer**, Dordrecht, 2002, p. 327, Fig. 5 with permission

Demonstration of Position-Exchange NMR

- An instructive example of a *position-exchange experiment* is that performed on a falling *water drop*
- Initial and final positions are marked in the Fourier domain by the wave numbers k_1 and k_2
- The maximum of a Hahn or a stimulated echo with one gradient pulse in each free evolution period is recorded for all values of k_1 and k_2
- The 2D Fourier transform of the experimental data set is the position-exchange map
- The principal diagonal identifies average position and the secondary diagonal position difference
- Along the principal diagonal, the projection of the drop onto the gradient direction is observed
- Along the secondary diagonal, the drop displacement during the encoding time Δ corresponding to the *velocity* of the falling drop is observed

Cross Filtration by VEXSY



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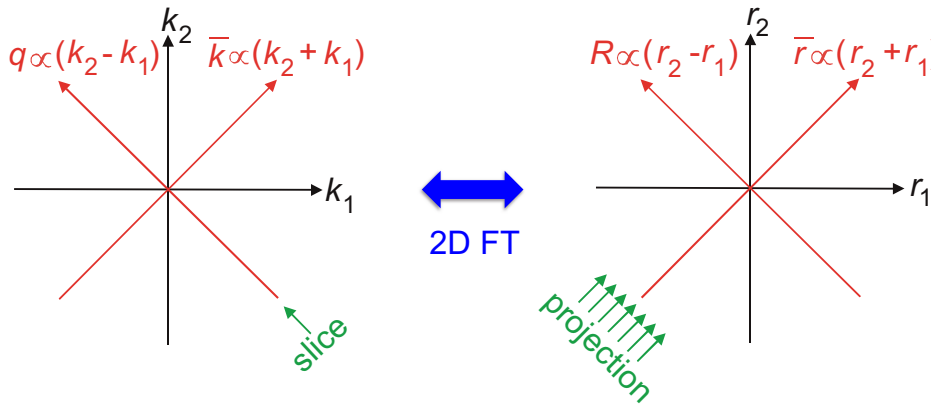
Velocity-Exchange NMR

- Similar to the *position-exchange NMR* experiment, initial and final velocities can be encoded in terms of q_{v1} and q_{v2} along the axes of a 2D data matrix, leading to the *velocity-exchange NMR* experiment (*VEXSY*)
- Velocity-exchange NMR has been used to study *cross-filtration* in hollow-fiber filtration modules which are used in hemodialysis as artificial kidneys
- Water was passed inside and outside the hollow fibers in counter flow
- Water molecules crossing the membrane must change their direction and lead to off-diagonal signal in a velocity-exchange map
- On the diagonal, the distribution of *average velocity* is observed
- For negative velocities one finds the hat function corresponding to *laminar flow* within the round membrane fibers. For positive velocities, the distribution maps the interstitial flow and depends on the packing of the fibers
- The projection along the principal diagonal and onto the secondary diagonal of the velocity-exchange map eliminates average velocity from the data set, and the remaining variable is velocity difference or *acceleration*
- For two different membrane materials (SMC, SPAN) and operating conditions, the velocity exchange spectra are different, and so are the projections onto the secondary diagonals, i.e. the *distributions of accelerations*
- SPAN shows signal at high accelerations corresponding to more efficient interactions of the molecules with the membrane walls than the SMC

Projection - Cross-Section Theorem



Projections in Multi-Dimensional Fourier NMR

- In *multi-dimensional Fourier NMR* the data are acquired in the space of one set of variables (t, $\boldsymbol{k}$, $\boldsymbol{q}_v$) and subsequently Fourier transformed into the space of the set of *Fourier-conjugate variables* (ω, $\boldsymbol{r}$, $\boldsymbol{v}$) appropriate for data interpretation
- A *slice* in one space corresponds to a *projection* in the Fourier-conjugate space
- For example, a 1D slice in (k_1,k_2) space along the secondary diagonal corresponds to a projection in Fourier-conjugate space along the principal diagonal so that the data are projected onto the secondary diagonal
- The term “projection” means “integration” of the multivariable function so that the number of variables is reduced and the variable in the direction of the projection is the variable of the integration
- This relationship can readily be derived from the expression for the *multi-dimensional Fourier transformation*
- It is known as the *projection – cross-section theorem*
- The projection – cross-section theorem is helpful in relating 1D distributions to 2D distributions and designing fast experiments with reduced dimensionality