Improvement of the FID Signal in NMR by Phase Mirroring of the Electromagnetic Waves

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Abstract: In inhomogeneous magnetic fields, NMR produces only imprecise spectral lines. The cause is the rapidly growing phase difference between the many individual signals. These differences are reduced by briefly switching on two auxiliary magnetic fields, which increases the amplitude of the FID signal. Repeated phase inversions significantly improve the duration and SNR of the FID signal and reduce the half-width of the selected spectral line.

Intoduction

NMR spectroscopy is an indispensable tool for studying the structure of molecules. The usual principle of broadband excitation with subsequent Fourier analysis of the FID signal has been known for decades and will not be repeated here.

The known methods of NMR spectroscopy and NMR imaging require strong magnetic fields with extremely high homogeneity over macroscopic volumes. Only with a high technical effort it is possible to operate magnets whose field inhomogeneity is in the order of 10^{-9}. Smallest changes in the environment require a complex stabilization of the static magnetic field. The spatial homogeneity is optimized with a set of electromagnets, the so-called shims. The aim of the study is to reduce this effort.

The physical basis of NMR is the precession movement of the nuclear spin around the field lines of an external magnetic field ***B*** (Larmor precession). This movement induces an alternating voltage signal in a suitably oriented coil, the frequency of which is defined by the formula $\omega=\gamma\cdot|B|$. The signal from a single nuclear spin cannot be detected because it is far too weak. In order to achieve a sufficient signal-to-noise ratio, the FID signal of around 10^{20} nuclear spins is measured, which is composed of 10^{20} wave trains of similar frequency. But even then, the SNR is not very satisfactory. The inhomogeneity of the external magnetic field widens the spectral width and the amplitude of the FID signal quickly falls below the noise limit due to the increasing phase difference.

This is where the procedure described below comes into play: Each precessing nuclear spin is regarded as an isolated oscillator whose Larmor frequency is defined by the local magnetic field. Only the phase of the emitted electromagnetic wave can be changed from a macroscopic distance. If precisely dosed additional magnetic fields are switched on for a short period of time, the phase deviations change their sign and, as with Hahn's spin echo, the resulting overall amplitude then increases. This correction can be repeated several times in order to extend the duration of the FID signal.

The Bloch equations

70 years ago, Felix Bloch constructed a system of equations that describes the temporal course of a magnetization ***M*** = (M_x, M_y, M_z) in an external magnetic field ***B***. The equations are:

$$\frac{d\,\boldsymbol{M}(t)}{dt}=\gamma\cdot\boldsymbol{M}(t)\times\boldsymbol{B}(t)+relaxation\ terms$$, where γ is the gyromagnetic ratio of a nuclear spin.

The equation is a combination of the quantum mechanical quantity γ with an equation of motion from classical physics. It can be used, for example, to correctly calculate the duration of high-

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frequency pulses in order to influence the precession movement of nuclear spins in the magnetic field in a targeted manner.

In the absence of experimental facts, the “true” interpretation of the Bloch equation has been argued for decades. In particular, it is controversial whether ***M*** is to be understood as a single nuclear spin or whether ***M*** is the sum of very many nuclear spins (bulk magnetization of a whole sample). This question is unsolved because the induction voltage that a single precessing nuclear spin generates cannot be detected with current measurement technology. Therefore, all previous measurements are based on the FID signal of many millions of nuclear spins.

Without experimental knowledge of the reaction of individual nuclear spins, one remains in the area of doctrinal claims. The following proposed influencing of the precession movement by changes in the magnetic field ***B*** can be checked experimentally and could help to clarify. The proposal is based on the following assumptions:

- The Bloch equations apply to individual precessing nuclear spins.
- There are no non-linear couplings between adjacent precessing nuclear spins. The measurable total signal in the induction coil is the linear superposition of a large number of electromagnetic waves.
- Every precessing nuclear spin interacts with classical electromagnetic waves. Since the distance between the sample and the receiving antenna (coil) is much smaller than the generated wavelength, the formulas for the antenna's near field are to be used. Each precessing nuclear spin is a variable magnetic dipole and generates a magnetic field strength that decreases proportionally to $1/r^3$. This dependency has long been confirmed.
- From the reactive near field in the immediate vicinity of the antenna only little power is emitted into the far field. Considerably larger is the amount of reactive power that oscillates in the near field between the precessing nuclear spin and the near environment. Since a precessing nuclear spin radiates the total energy $h \cdot f$, some time passes until this amount is transferred from the near field to the far field and radiated. This explains the long duration of the FID signal.

The phase mirroring

Because of the inhomogeneity of the magnetic field ***B***, not all nuclear spins can generate electromagnetic waves with exactly the same frequency. The local magnetic field at the location of the nuclear spin defines the emitted frequency ω. The phase differences between the individual waves increase very quickly, mutual cancellation occurs and after a short time the resulting total amplitude drops below the noise limit (see Figure 1). There is no suggestion in the formula $\omega = \gamma \cdot |B|$ on how to synchronize the phases of the electromagnetic waves generated by different nuclear spins. This forces a different approach: the phase deviation of each precessing nuclear spin with respect to a freely selectable setpoint frequency is inverted at regular time intervals – independently of one another. This accelerates lagging phases and delays leading phases.

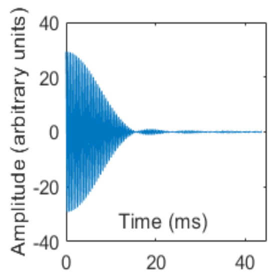

Fig 1: The FID signal without phase mirroring.

With 10^{20} nuclear spins in one sample, it is impossible to measure the phase of each nuclear spin individually and then influence it. A practicable method must act simultaneously on the phases of all radiated electromagnetic waves. The goal is a self-correcting procedure in which each nuclear spin detects and corrects its own phase deviation. The lower the inhomogeneity of the magnetic field, the less often the necessary corrections of the phases are necessary.

The simplified Bloch equation $\frac{d\,\boldsymbol{M}(t)}{dt} = \gamma \cdot \boldsymbol{M}(t) \times \boldsymbol{B}(t)$ offers various possibilities to influence the usually measured component M_x of a precessing nuclear spin. A numerical simulation shows that it is sufficient to change B_x and B_y during a precisely defined time interval. Phase errors of up to about ± 70^0 for a total of 10^{20} spins can thus be inverted simultaneously. The phase deviations do not disappear, only the signs change. In contrast to the well-known spin echo, the direction of the spins is not reversed (it does not change by 180^0), but is rotated by a much smaller angle (<80^0). The setpoint of the phase defines a freely selectable reference frequency. Figure 2 illustrates the process.

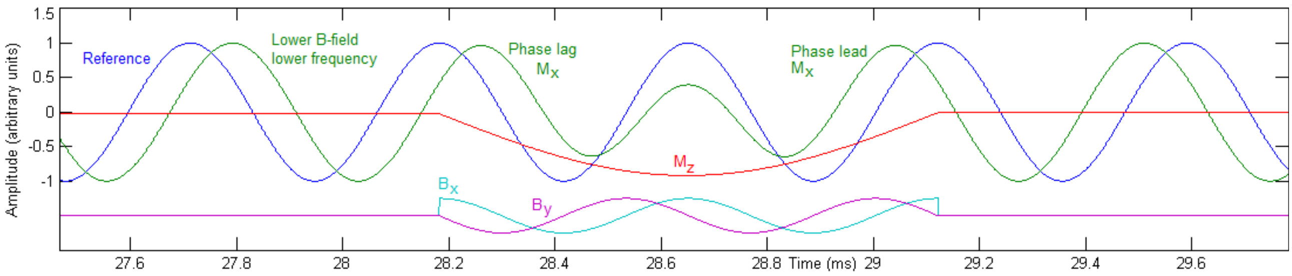

Fig. 2: Time sequence of the phase mirroring. The blue reference curve is the electromagnetic signal of a nuclear spin in a magnetic field with the setpoint B_0. If the actual field at the location of the nuclear spin is smaller than B_0, a delayed phase is measured (green curve). By precisely dosed activation of the auxiliary fields B_x and B_y, the delay is transformed into a lead of the phase.

From a defined point in time (e.g. maximum of the blue reference curve) and during a short interval (exactly two oscillation periods), the auxiliary magnetic fields $B_x = ¼ \cdot B_z \cdot \cos \omega_0 t$ and $B_y = -¼ \cdot B_z \cdot \sin \omega_0 t$ are switched on. This changes the spin $\boldsymbol{M}$ of each nuclear spin in such a way that the sign of the phase deviation is reversed. For example, the lagging phase $\Delta\varphi = +70^0$ is transformed into the leading phase $\Delta\varphi = -70^0$. If the two auxiliary magnetic fields are to start at a different point in time, the curve shapes of B_x and B_y must be adapted accordingly.

Repeated phase mirroring in an inhomogeneous field.

In the earth's magnetic field (B_z = 50 µT, $B_x = B_y = 0$) protons precess with 2129 Hz around the direction of the z-axis. We assume that at t = 0 all spins point in the direction of the positive x-axis. The damping is negligible, the T2 relaxation is ignored. If the magnetic field were homogeneous, all spins would move synchronously and their M_x component would be described by the reference curve (blue color in Fig. 2 and Fig. 3). The 10^{20} protons in the sample would generate an FID signal of constant amplitude in the receiver coil.

Now we consider a nuclear spin at a point where the magnetic field B_z is 1% smaller than the average value. Since the spin precesses with a Larmor frequency that is too low, the phase of the electromagnetic wave generated is more and more delayed in comparison with the reference wave. In this example the phase of the signal generated by this nuclear spin is already delayed by about 70^0 after t_1 = 9 ms (green color in Fig. 2 and Fig. 3) and it is time to correct the phase deviation.

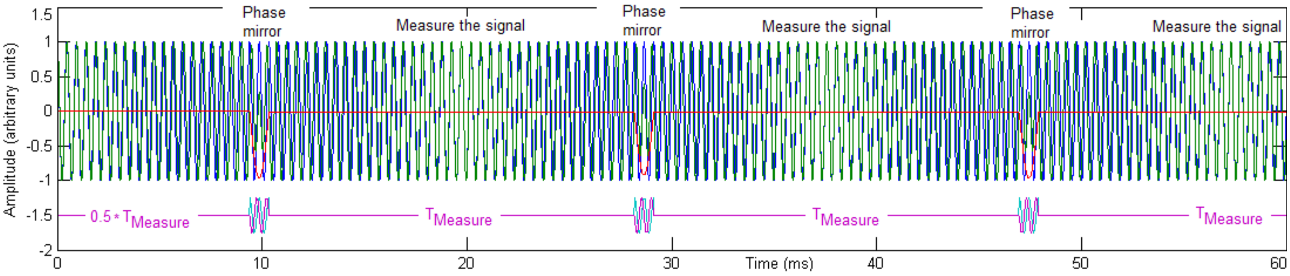

Fig 3: Repeated phase mirroring by briefly switching on the two auxiliary fields B_x and B_y. In between there are longer periods of time in which the FID signal can be measured undisturbed. Colors as in Figure 2.

This method works the same way (with reversed signs) if the local magnetic field ***B*** at the location of the nuclear spin is higher than the average value.

The phase mirroring is repeated at regular intervals. The optimal period for measuring the weak induction voltage of the precessing nuclear spins starts after the auxiliary magnetic fields are switched off and ends shortly before they are switched on again. The more homogeneous the magnetic field ***B***, the less frequently the measurement intervals have to be interrupted. Since all switching times are synchronized with the reference frequency, the signal-to-noise ratio is improved by adding up the partial measurements.

Reduction of possible interference from transients

The two auxiliary magnetic fields B_x and B_y have to be switched on again and again in order to mirror the different phase deviations of all nuclear spins in the sample. The sudden switching of strong electrical currents creates electromagnetic interference that can degrade the signal-to-noise ratio of the very weak FID signals. Possible disturbances are reduced if the two auxiliary fields B_x and B_y are gently switched on and off. In order to compensate for the lower currents at the beginning and at the end, one has to double the current in the middle part of the interval. Figure 4 shows the time course of M_x and M_z when the magnetic field B_z at the location of the nuclear spin is 1% greater than the average value and the envelope H for B_x and B_y is modulated in a bell shape:

$$H = 1 - \cos(\tfrac{1}{2}\omega_0 t) \quad \text{with} \quad 0 \le \omega_0 t < 4\pi \quad .$$

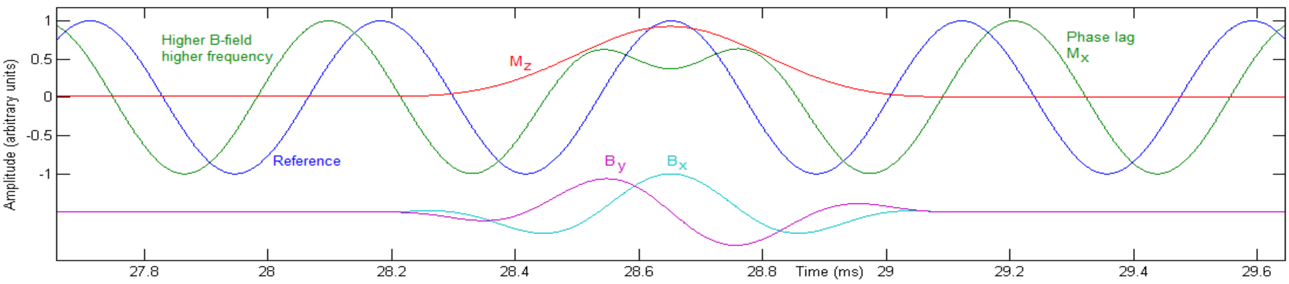

Fig 4: Soft switching of the auxiliary magnetic fields B_x and B_y reduces interference, but requires stronger magnetic fields.

Signal improvement with an inhomogeneous magnetic field

So far, the effect of phase reflection on the signal of a single precessing nuclear spin has been discussed. However, real measurements are always the response of a large number of nuclear spins in an inhomogeneous magnetic field of strength B ± ΔB. With the method described, the inhomogeneity ΔB/B can be up to 2%. The frequencies of the electromagnetic waves emitted by the nuclear spins differ accordingly, and instead of a sharp spectral line, a wide frequency range is measured (blue curve in Fig. 5). The phase mirroring only changes the phases, but not the frequency ω of the electromagnetic waves generated. Since the phase deviation always remains smaller than about 70^0, the half-width of the measurable spectral line is reduced and the spectral resolution increases. The signal-to-noise ratio improves by at least one order of magnitude. The primary cause is the considerably longer measurability of the FID signal despite the inhomogeneous magnetic field. Only the inevitable T2 relaxation limits this duration.

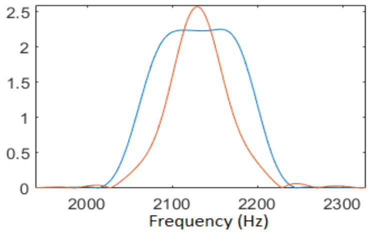

Fig 5: Blue: spectrum of the FID signal without phase mirroring. Red: spectrum with phase mirroring.

Figure 6 shows that the diverging phases of the many individual signals together with the repeated phase reflections produce an amplitude modulation of the FID signal. If the amplitude falls below a minimum value (for example half the maximum value), phase mirroring ensures that the amplitude increases again. This can be repeated several times until the signal disappears in the noise.

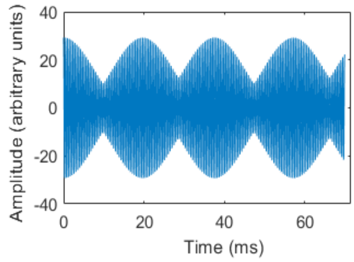

Fig 6: FID signal with repeated phase mirroring.

The period of time Δt after which phase mirroring should take place depends on the relative inhomogeneity ΔB/B of the magnetic field ***B*** and can be estimated using the following empirical formula:

$$\Delta t \cdot B \cdot \frac{\Delta B}{B} \approx 10^{-8}\, T \cdot s$$

. Δt is measured in seconds and B in Tesla.