Field noise effects on NMR signals: FID's and 1D spectra

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Abstract

NMR (Nuclear Magnetic Resonance) FID instabilities due to the most common types of magnetic field and/or RF offset fluctuations are investigated. The study analyses quantitatively some of the artifacts due to such instabilities.

The effect of a random, normally distributed field noise on *averaged* FID's is shown to be their multiplication by a well-defined weighing function whose shape is intermediate between Lorentzian and Gaussian. While integral sensitivity of the instrument is not affected, there is a line shape distortion which might be easily mistaken for field inhomogeneity.

The effects of periodic/quasi-periodic field perturbations on FID's and spectra are also investigated in detail. The results are directly applicable to the effects of type A instabilities such as mains-related field brum and ripple (including environmental pick-up). Type B instabilities whose magnitudes have a non-uniform spatial distribution require an additional averaging over individual sample voxels. The study establishes the respective averaging procedures and shows that when the normalized self-correlation functions of the field fluctuations are the same for all voxels, the final effect on averaged FID's is still a simple weighting by a particular function. The results are applicable to effective field fluctuations induced by sample spinning (in HR-NMR), sample vibrations (all branches of NMR) and field gradients noise (in MRI and in PFG self-diffusion measurements).

I. Introduction

The free induction decay (FID) transient signals collected in nuclear magnetic resonance (NMR) are subject to a number of stochastic disturbances. Among these, the one most often discussed is the stationary 'receiver noise' which originates both in the sample and in the receiver system and determines the achievable signal-to-noise ratio. The Author has often carried out a statistical analysis of this noise either as a part of an instrument check-up or as a self-standing study, born out of the awareness that if it were not Gaussian, one could devise signal estimators superior to standard arithmetic averaging of repeated scans. Apart from situations linked to specific instrument defects, and apart from low-probability ‘spikes’ due to external disturbances, the receiver noise has always turned out to be normal, ruling out any conceptual improvement of the classical data accumulation.

There are, however, disturbances of other types which *always limit the performance of an instrument*.

In principle, these fall into two categories:

1) Random fluctuations of the main magnetic field and/or of the phase-detector reference frequency.

   These two effects can't be separated from each other because what one normally detects are just the relative beats between the RF reference and the field-dependent Larmor frequency of the nuclei. Since it is easy to carry out very precise bench tests of the *phase noise* of any RF source, this parameter can be kept in check much more easily than the magnetic field noise for which precise testing methods *other than NMR* do not exist. Consequently, the field noise is usually much more important than the RF phase noise (especially when using digital RF synthesis techniques).

2) Random fluctuations of magnetic field inhomogeneity across the sample.

For simplicity, the first type of fluctuations shall be called *field noise*, while the second type shall be referred to as *field inhomogeneity noise* or, in the presence of imposed gradients, *field gradient noise*.

One must keep in mind that, like the receiver noise, the field noise is *always* present. Hardware engineers and manufacturers of magnets and NMR instruments of course strive hard to produce magnetic fields as stable as possible and, wherever feasible, screen them from external disturbances. Over decades, such efforts have led to remarkable improvements in field stability which, however, have been more than matched by equally remarkable increases in the requirements imposed by the evolving NMR and MRI methodologies. Moreover, there are situations where field noise is inherently rather bad. The two situations which come to mind in his context are fast-field-cycling NMR relaxometry (FFC NMR) with its highly dynamic magnets and all kinds of ex-situ NMR techniques, including well-logging and the NMR MOUSE where, almost by definition, the field within the area of interest can be neither screened nor stabilized.

The question is therefore not whether the field is unstable but rather what are the quantitative characteristics of its fluctuations, how they affect the acquired data, and whether there are ways of suppressing such artifacts by suitable acquisition methods and/or post-acquisition corrections.

Terminology and assumptions

- At any moment, there is a distribution of the magnetic field induction $\mathbf{B}(\mathbf{r},t)$ across the constituent voxels of the sample. The average $\mathbf{B}(t) = \langle\mathbf{B}(\mathbf{r},t)\rangle_v$ over the sample volume is the *main magnetic field* while the deviations $\mathbf{H}(\mathbf{r},t) = \mathbf{B}(\mathbf{r},t)-\mathbf{B}(t)$ constitute the *magnetic field inhomogeneity*.

- Both $\mathbf{B}(t)$ and $\mathbf{H}(\mathbf{r},t)$ are time-dependent. The time-averages $\mathbf{B} = \langle\mathbf{B}(t)\rangle_t$ and $\mathbf{H}(\mathbf{r}) = \langle\mathbf{H}(\mathbf{r},t)\rangle_t$ are, respectively, the *static main magnetic field* and the *static field inhomogeneity*. The deviations $\mathbf{b}(t) = \mathbf{B}(t)-\mathbf{B}$ and $\mathbf{h}(r,t) = \mathbf{H}(\mathbf{r},t)- \mathbf{H}(\mathbf{r})$ are the respective *main field noise* and the *inhomogeneity noise*.

- We always intend the Z-axis to be aligned with the direction of the static main field **B**.

- The fluctuations $\mathbf{b}(t)$ and $\mathbf{h}(\mathbf{r},t)$ are random, time-dependent vector fields whose magnitudes are much smaller than **B**. Consequently, effects due to their x- and y-components can be neglected compared with those due to their z-components[1], denoted as $b(t) \equiv \mathbf{b}_z(t)$ and $h(\mathbf{r},t) \equiv \mathbf{h}_z(\mathbf{r},t)$.

- The static field inhomogeneity $\mathbf{H}(\mathbf{r})$ is related to magnet geometry and its imperfections, with additional corrections achieved in some applications by means of an active field-shim system. In all NMR applications, $|\mathbf{H}(\mathbf{r})|$ is supposed to be many orders of magnitude (typically 4 to 9) smaller than the main magnetic field **B**. By design, any small instability in $\mathbf{B}(t)$ originating *within* the magnet system is expected to to have a negligible effect on field inhomogeneity with its contribution to $h(\mathbf{r},t)$ being orders of magnitude smaller than its contribution to $b(t)$. *External* contributions to $\mathbf{B}(t)$, such as stray magnetic fields from distant sources, are expected to be quite homogeneous across the sample volume and thus unlikely to contribute appreciably to $h(\mathbf{r},t)$.

Throughout this study, we assume that $h(\mathbf{r},t)$ can be neglected with respect to $b(t)$. Even if this were not true, however, the two effects would be probably poorly correlated so that it would be possible to study their respective effects independently of each other. This study concentrates on the effects stemming from $b(t)$.

We shall find it convenient to distinguish between two types of field noise: those which are the same for every sample voxel (type A) and those which, despite a temporal coherence over the whole sample volume, have a non-uniform amplitude distribution (type B).

Typical sources of magnetic-field instabilities

a) Intrinsic (type A)

- Random noise in the current sources of air-coil magnets and electromagnets. For example, air-coil systems with top dynamic requirements such as those of fast field cycling relaxometers (FFC-NMR) are at present characterized by field noise of the order of 1 - 10 μT r.m.s. with correlation times of the order of 0.1 -1 ms. In a classical HR-NMR electromagnet the same parameters are likely to be of the order of 0.1 -1 μT and 1 - 10 ms.
- Residual brum and/or ripple in the current sources of air-coil magnets and electromagnets.
- Electronic noise in field stabilizers. In systems with active field-control systems such as flux stabilizers and/or NMR lock systems, the perturbations listed above are to a large extent

[1] This is justified by the fact that the perturbation of the *effective field* perceived by any nucleus is of first-order for the longitudinal components but of second-order for the transversal ones.

suppressed. Such control loops, however, are not always applicable[2] and, in any case, they have a noise of their own. They are often operated just below the limit of oscillations which makes them prone to fluctuations clustered around particular frequencies (quasi-periodic instabilities).

b) Environmental (type A)

- Stray alternating fields from mains power wiring[3], both external and internal to the instrument.
- Stray alternating fields from magnetic devices such as AC power transformers (including those located within the instrument's own power supplies!).

c) Motion induced (type B)

- Sample rotation in HR-NMR spectroscopy is a classic example of a periodic motion across an inhomogeneous field which subjects individual sample voxels to periodic field modulation.
- Sample motions induced by environmental vibrations (cooling pumps, acoustic waves, floor tremble, etc.) or by turbulence in the gas flows through auxiliary devices which involve the sample-assembly (spinner, temperature controller, decoupler coils cooling, etc.). Again, motion-induced field instabilities depend upon field inhomogeneity and affect different sample voxels in a different way.

Just as it is impossible to completely suppress the receiver noise, no NMR instrument can be completely immune from field noise and from at least some of the other instabilities listed above. The resulting artifacts include:

* In high-resolution NMR spectroscopy (HRNMR):
  - Rotational sidebands.
  - Sidebands at integer multiples of the mains frequency.
  - Broadening of spectral peaks during repeated-scans averaging.
  - Reduced efficiency of noise suppression by repeated-scans averaging.
  - t1-noise in 2D spectra.
* In magnetic resonance imaging (MRI):
  - Image fringes related to the mains frequency.
  - Reduced efficiency of image improvement by repeated-scans averaging.
* In low-resolution NMR (LRNMR) and FFC relaxometry (FFC-NMR):
  - Irreproducibility of individual FID's.
  - Deformation of FID shapes[4] after repeated-scans averaging.

While all such artifacts are well known from practice, their statistical properties have rarely been analyzed in detail and there is only a limited empirical knowledge of their propagation during the data averaging process.

One point should be stressed before proceeding with the analysis. Since this Note deals only with the main field noise and not with field-inhomogeneity noise, the obvious way of avoiding its effects consists in using one of the signal-detection methods insensitive to RF phase and offset (diode detection, power detection, envelope detection). While this such approaches are not acceptable in HR-NMR and MRI where offset-sensitive signals are a must, they may be viable in LR-NMR and in FFC relaxometry.

II. Signal phase evolution during FID

The phase-detected NMR signal consists of two real-valued time series u(t) and v(t) revealed by the in-phase and out-of-phase outputs of an instrument's quadrature phase receiver, respectively. The two signals are burdened by two signal-independent components:

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[2] NMR techniques based on the use of pulsed field gradients (MR imaging, self-diffusion measurements) or pulsed main field (FFC-NMR) make the use of active field-control feedback problematic.

[3] A wire carrying 1A of AC current located 2m from an magnetically unshielded sample generates within the latter a field modulation of 0.1 μT, corresponding a proton Larmor frequency modulation of 4.25 Hz.

[4] This affects negatively those applications which might benefit from an accurate FID shape analysis such as relaxometry of multi-phase systems.

i) The stationary *receiver noise* which should have the same statistical properties in both channels though, at the same time, the two channels should be statistically independent of each other (in any case, the noise in both channels can be sampled and subject to statistical analysis).
ii) Mutually independent *DC offsets* [5].

We thus have

$$u(t) = U(t) + n_u(t) + c_u \qquad [1]$$
$$v(t) = V(t) + n_v(t) + c_v,$$

where U(t) and V(t) are the two signal components, n_u, n_v the two receiver noise series and c_u, c_v the two time-independent DC offsets.

The complex quantity U(t)+jV(t) can be viewed as a rotating complex vector describing a compounded spiral in the complex plane. Should the signal consist of a single spectral line, the amplitude of the spiral would start at some maximum value and decay toward zero, while its argument would start at a value Φ_0 (the *receiver phase*) and keep increasing or decreasing linearly with time at an angular rate equal to the instantaneous spectral line's offset which is a sum of the mean offset Ω (corresponding to the mean field value) and $\gamma b(t)$, where γ is the gyromagnetic ratio of the measured nucleus and b(t) is the above-defined deviation of the field from its mean value.

In the presence of many spectral components, one must keep in mind that i) at t=0 (just after the excitation RF pulse), all the components are synchronized and start with the same phase Φ_0, ii) field fluctuations affect all components in the same way and iii) the individual components add together linearly. Consequently, the composite signal can be expressed as

$$U(t) + jV(t) = \sum_k U_k(t) + jV_k(t) = \sum_k |s_k(t)| \exp\left[j\Phi_0 + j\int_0^t \{\Omega_k + \gamma b(\xi)\} d\xi \right], \qquad [2]$$

where the sum runs over all the present spectral components[6]. It follows that

$$U(t) + jV(t) = S(t)\exp(j\Phi_0)\exp[j\phi_f(t)], \qquad [3]$$

where

$$S(t) = \sum_k |s_k(t)| \exp[j\Omega_k t] = s_u(t) + js_v(t), \qquad [4]$$

is the 'true' in-phase signal void of any artifacts[7] and

$$\phi_f(t) = \gamma\int_0^t b(\xi)d\xi = \gamma\int_{-\infty}^{+\infty} \chi(t,\xi)b(\xi)d\xi, \qquad [5]$$

is a random phase contribution due to the field fluctuations. It is this quantity whose statistical properties we shall investigate. The auxiliary function $\chi(t,\xi)$ introduced in Eq.[5] is defined as

$$\chi(t,\xi) = 1 \text{ for } 0 \le \xi \le t \quad \text{and} \quad \chi(t,\xi) = 0 \text{ otherwise.} \qquad [6]$$

For any given instant t, $\phi_f(t)$ is a random variable. Since $\phi_f(0)=0$, while this is not true when t>0, $\phi_f(0)$ is clearly non-stationary and all its statistical properties are a function of time.

We shall also need to evaluate the mean value <S(t)> which results from standard data-averaging in the limit of infinite number of scans. To do so, we start directly from Eq.[2], obtaining

$$< S(t) > = \sum_k |s_k(t)| < \exp[j\{\varphi_k(t) + \phi_f(t)\}] >, \qquad [7]$$

where $\varphi_k(t) = \Phi_0 + \Omega_k t$ is *not* random. In general, given a constant α and a random variable X,

$$<e^{j(\alpha+X)}> = <\cos(\alpha+X)+j\sin(\alpha+X)> = (\cos\alpha+j\sin\alpha)(<\cos X> + j<\sin X>) = e^{j\alpha}<e^{jX}> \qquad [8]$$

Applying this[8] to Eq.[7], we have

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[5] These may be negligible in case of over-sampled digital detector systems.
[6] Since an actual spectrum is never really discrete, the sum should be more appropriately replaced by a Lebesque-Stieltjes integral. In view of the fact that this does not affect our discussion, however, we shall keep the sum symbol, urging the reader to keep in mind the present comment.
[7] Except, of course, those due to field inhomogeneity.

$$<S(t)>=<e^{j\phi_f(t)}>S^0(t),\ \text{where}\ \ S^0(t)=\sum_k|s_k(t)|e^{j\varphi_k(t)}=U^0(t)+jV^0(t)\ \text{and} \qquad [9]$$

$$<U(t)>=<e^{j\phi_f(t)}>U^0(t),\ \ <V(t)>=<e^{j\phi_f(t)}>V^0(t)\,,$$

with the upper index (^{0}) indicating the signals one would have in the absence of field fluctuations. The equations show that field fluctuations, unlike the *additive* receiver noise, lead to a *multiplicative factor* <exp[jϕ_f(t)]>. The factor turns out to be *the same for both receiver channels* and, moreover, the result applies to samples of any spectral complexity since the factor is *the same for each spectral component*. Another corollary is the fact that the receiver phase Φ_0 can be taken out of the average, so that it makes no difference whether one adjusts Φ_0 by hardware *before* collecting the data or *afterwards* by means of software (e.g., by 'phasing' the spectra in HR-NMR).

Since the net effect of field fluctuations on the *averaged data* is the multiplication (weighing) of the final FIDs by the function

$$G(t) = <\exp[j\phi_f(t)]>, \qquad [10]$$

the latter plays a special role. Thus, for example, the effect of such a multiplication on HR-NMR spectra is the same as *convoluting them with the Fourier transform of* G(t).

The evaluation of G(t) is hindered by the fact that, while we shall derive reliable expressions for the variance <ϕ_f^2(t)>, the probability distribution function of ϕ_f(t) itself shall be often poorly defined. However, some generic assumptions appear to be quite safe and may help us with the task.

First, since there are no evident mechanisms leading to an asymmetry, the distribution of ϕ_f(t) can be assumed to be symmetric. In this case G(t) is a *real function* of time. Moreover, the first terms of its expansion are 1- <ϕ_f^2(t)>/2+..., showing that whenever the variance <ϕ_f^2(t)> is small with respect to 1, *any* function of <ϕ_f^2(t)> whose expansion starts in the same way is essentially acceptable.

Second, it is a common practice to assume that an unknown distribution is normal (Gaussian). Since for a random variable X with a centered normal distribution and variance ϕ^2 we have <e^{jX}> = exp(-ϕ^2/2), setting

$$G_n(t) = \exp(-<\phi_f^2(t)>/2) \qquad [11]$$

is exact whenever ϕ_f(t) has a normal distribution and amounts to a quite good approximation for any symmetric distribution even when the assumption of normality does not hold.

One important aspect of the above equation is the fact that G(t)≠1 even though <ϕ_f(t)>=0, meaning that phase noise introduces a *bias which does not average out* during the standard data accumulation process.

III. Phase error variance

According to our conventions <b(t)>=0 so that the mean value <ϕ_f(t)> of the random function ϕ_f(t) is also null. For the variance of ϕ_f(t) we have

$$<\phi_f{}^2(t)>=\gamma^2\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\chi(t,\xi)\chi(t,\xi')<b(\xi)b(\xi')>\,d\xi d\xi'\,. \qquad [12]$$

Assuming the field fluctuations to be stationary, one can define their autocorrelation function

$$C(\zeta) = <b(t)b(t+\zeta)> \qquad [13]$$

which is independent of t and whose value at ζ=0 is the variance of b(t).
Denoting the latter as σ, it is convenient to write

$$C(\zeta) = \sigma^2 c(\zeta), \qquad [14]$$

where c(ζ) is the normalized correlation function with c(0)=1. Eq.[12] then becomes

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[8] One might factorize the complex exponential and right away average both of them separately. However, since the complex notation is just a shorthand for signals which, by themselves, are all real, the actual applicability of such an approach to the *physical* problem at hand needs to be proved - which is the essence of the apparently redundant Eq.[8].

$$<\phi_f^2(t)> = (\gamma\sigma)^2 \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} c(\xi'-\xi)\chi(t,\xi)\chi(t,\xi')\,d\xi\, d\xi' . \qquad [15]$$

After a transformation from the coordinate system $\{\xi,\xi'\}$ to $\{\xi,\zeta\}$ with $\zeta=\xi'-\xi$, this gives

$$<\phi_f^2(t)> = (\gamma\sigma)^2 t \int_{-\infty}^{+\infty} c(\zeta)\, w(t,\zeta)\, d\zeta , \qquad [16]$$

where $w(t,\zeta)$, defined as:

$$w(t,\zeta) = t^{-1} \int_{-\infty}^{+\infty} \chi(t,\xi)\chi(t,\xi+\zeta)\, d\xi , \qquad [17]$$

is a symmetric function of ζ which, using Eqs.[6], turns out to have the explicit values

$$w(t,\zeta) = 1-|\zeta|/t \quad \text{for } |\zeta| \le t, \text{ and } \quad w(t,\zeta) = 0 \quad \text{otherwise.} \qquad [18]$$

IIIa. Special cases: random field noise

One of the most important special cases is an a-periodic, random *field noise* with a single characteristic correlation time T_m (the index m stands for *magnet*) which can be described by a normalized correlation function of the ubiquitous type

$$c(\zeta) = e^{-|\zeta|/T_m}. \qquad [19]$$

Carrying out the integration in Eq.[11], one obtains

$$<\phi_f^2(t)> = (\gamma\sigma)^2 T_m^2\, r\, F(r), \qquad [20]$$

where $r = t/T_m$ is a reduced-time argument and (Fig.1)

$$F(x) = 2(1-g(x)) \quad \text{with} \quad g(x) = (1-e^{-x})/x. \qquad [21]$$

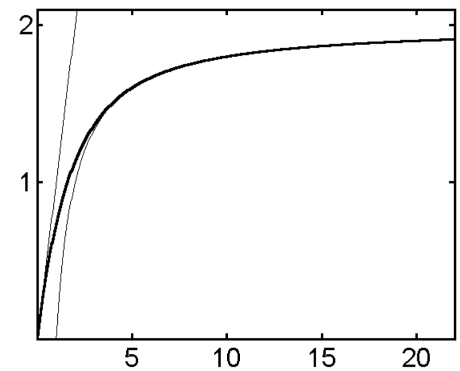

Fig.1.
Function F(r) plotted against $r = t/T_m$. The thin lines are the approximations F(r)=r (upper) and F(r)=2-2/r (lower).

For $t \ll T_m$ we have $F(r) \approx r$ and therefore $<\phi_f^2(t)> \approx (\gamma\sigma)^2 t^2$, reflecting the fact that any field/offset excursion γb present at t=0, provided it remains approximately constant, generates a phase excursion of about γbt at time t.

When $t \gg T_m$, F(r) approaches its limit of 2 and $<\phi_f^2(t)> \approx 2(\gamma\sigma)^2 T_m t$ becomes proportional to the elapsed time t. This is a behavior characteristic of a diffusion process with the 'diffusion constant' $D = (\gamma\sigma)^2 T_m$.

Notice, however, that we can talk about a pure diffusion only when t is be greater than at least $10T_m$. For t greater than about $3T_m$, F(r) is reasonably approximated by the asymptotic formula $F(r) \approx 2(1-1/r)$.

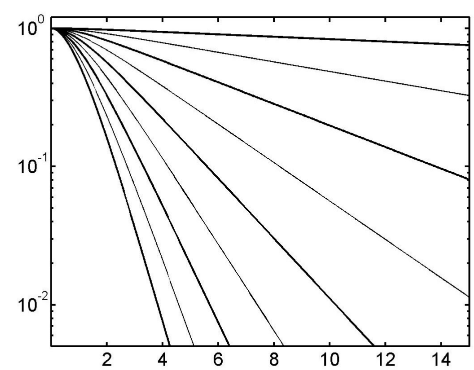

Fig.2.
A semi-log plot of $g_n(r)$ as a function of $r = t/T_m$ for $w = \gamma\sigma T_m = 0.1$ (top), 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8 and 0.9 (bottom).

The difference in behavior between the two extreme cases may be quite important to a system engineer. When the duration of the FID's is much shorter than T_m, additional filtering of the field noise improves the FID phase stability since it reduces σ^2 and T_m is irrelevant. On the other hand, when the FID's last much longer than T_m, additional simple filtering is of little help because it generally increases T_m and keeps the product $\sigma^2 T_m$ constant. Since the duration of the FID's depends upon the nature of the sample (solid, gel, tissue, liquid), this has straightforward application-related implications.

One can reasonably expect the amplitude of a random field noise to have a normal distribution so that Eq.[11] should be exactly applicable. After standard data averaging, the effect of the field noise on the averaged FID's is therefore a multiplication by the function

$G_n(t) = g_n(r) = \exp\{-(\gamma\sigma T_m)^2\, r\, F(r)\}$, [22]

where again $r = t/T_m$ (see Fig.2).

When $t<T_m$, one has approximately $G_n(t) \approx \exp\{-(\gamma\sigma)^2\, t^2/2\}$, corresponding to spectral convolution with a Gaussian line of standard width $\Delta = 2(\gamma\sigma)$ [rad]. In the opposite extreme, when the FID lasts longer than about $10T_m$ and the function $G_n(t)$ still has an appreciable value, the Gaussian part of $G_n(t)$ is ineffective (very close to 1) and the FID is in essence multiplied by the exponential $G_n(t)= \exp\{-(\gamma\sigma)^2 T_m t\}$ which corresponds to spectral convolution with a Lorentzian line of half-height width $\Delta = 2(\gamma\sigma)^2 T_m$.[rad]. In the intermediate region we have a spectral line-shape deformation tending towards a Lorentzian central peak with a broader Gaussian 'hump'. The transition between the two regions, however, is too smooth for a neat visual distinction of the two components.

In terms of the reduced-time parameter $r = t/T_m$ the shape of the weight function (and thus also the shape of the convolution line) is described by the dimensionless parameter $w = \gamma\sigma T_m$. This family of shapes ranges from exponential (Lorentzian) for $w\to 0$ to Gaussian for $w\to\infty$. While the *shape* depends only upon w, the total line broadening depends also on the T_m, being $2w/T_m$ in the Gaussian limit and $2w^2/T_m$ in the Lorentzian limit.

IIIb. Special cases: periodic field modulation

Periodic perturbations are encountered in practice quite often. The most common ones are related to the mains-power frequency of the country in which the measurements are taken. Denoting the mains power period as T_0, one is likely to encounter periods of T_0 (*brum* fields from single-phase transformers and from environmental power wiring), $T_0/2$ (*ripple* fields from single-phase DC power supplies with full-wave rectifiers), $T_0/3$ (three-phase transformers and power wiring) and $T_0/6$ (ripple from three-phase DC power supplies with full-wave rectifiers).

Another very common source of a periodic modulation is the sample rotation in HR-NMR whose frequency is freely adjustable anywhere between ~5 to ~50 Hz. Unlike all the mains-related modulations, sample rotation is a disturbance of type B, i.e., it does not affect all voxels of the sample in the same way.

In the presence of a single harmonic perturbation, we have $b(t) = b.\cos(\omega t+\alpha)$, where b is the amplitude of the z-component of the oscillatory magnetic field, ω is its frequency (we shall also use its period $T=2\pi/\omega$) and α is its initial phase just after the excitation pulse. Since the disturbance is usually not synchronized with the RF pulses, α is a random variable distributed uniformly over the interval $[0,2\pi)$. The starting phase causes differences between subsequent scans and thus, though there is nothing stochastic in a single passage, we still have to face the statistics associated with repeated scans. Following the reasoning associated with Eqs.[5], the signal phase at time t is given by

$$\phi_f(t) = \gamma\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\chi(t,\xi)b(\xi)d\xi = (\gamma b)\int_{-\infty}^{+\infty}\chi(t,\xi)\cos(\omega\xi+\alpha)d\xi\,. \quad [23]$$

Since $<\cos(\omega\xi+\alpha)>_\alpha = 0$, we have $<\phi_f(t)>_\alpha = 0$ (notice that we are now averaging with respect to α). Consequently, the variance of $\phi_f(t)$ with respect to α is

$$<\phi_f^2(t)>_\alpha = (\gamma b)^2\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} <\cos(\omega\xi+\alpha)\cos(\omega\xi'+\alpha)>_\alpha \chi(t,\xi)\chi(t',\xi)\,d\xi d\xi'\,, \quad [24]$$

which, putting $\xi' = \xi+\zeta$ and considering that

$$<\cos(\omega\xi+\alpha)\cos(\omega\xi'+\alpha)>_\alpha = $$
$$= <\cos^2(\omega\xi+\alpha)>_\alpha \cos(\omega\zeta) - <\cos(\omega\xi+\alpha)\sin(\omega\xi+\alpha)>_\alpha \sin(\omega\zeta) = (1/2)\cos(\omega\zeta) \quad [25]$$

gives

$$<\phi_f^2(t)>_\alpha = \frac{(\gamma b)^2}{2}\, t\int_{-\infty}^{+\infty}\cos(\omega\zeta)\, w(t,\zeta)\,d\zeta\,, \quad [26]$$

where $w(t,\zeta)$ is the function defined by Eq.[17]. This corresponds to Eq.[16] provided that the r.m.s. deviation σ and the normalized autocorrelation function $c(\zeta)$ are defined as

$$\sigma^2 = b^2/2,\quad c(\zeta) = \cos(\omega\zeta). \quad [27]$$

Carrying out the integration in Eq.[26], one obtains

$$<\phi_f^2(t)> = (\gamma\sigma)^2\, T^2\, P(\rho), \qquad [28]$$

where $T=2\pi/\omega$ is the period of the harmonic perturbation, $\rho = t/T$ is a reduced time parameter, and

$$P(\rho) = (1/\pi^2)\, \sin^2(\pi\rho). \qquad [29]$$

We see that, despite the randomization of the starting-phase α, the variance of the FID phase fluctuations oscillates between zero at times t which are integer multiples of the period and a maximum of $(\gamma\sigma)^2\,(T/\pi)^2$ attained whenever t is an odd multiple of T/2.

Considering the factor T^2 in Eq.[22], shorter periods are preferable. This regards all those cases where the period can be controlled (sample rotation) as well as comparisons between countries with different mains frequency.

We shall now face the problem of evaluating the weight function G(t) for the averaged FID's. Unlike in the preceding case, the assumption of normal distribution of $\phi_f^2(t)$ would not be justified here. The amplitude b is a constant and the only randomization parameter is the starting phase α. Since α obeys a uniform circular distribution, $b(t)/b = \cos(\omega t+\alpha)$ follows the distribution function of the random variable $Y = \cos(\alpha)$. It is then evident from Eqs.[23] that, apart from a non-random, time-dependent proportionality factor, the same distribution applies to $\phi_f(t)$.

The random variable Y, defined on the interval [-1,1], has the probability density $(1-X^2)^{-1/2}dX$ and the variance of 1/2. A random variable X proportional to Y and having a variance ϕ^2 is therefore defined on the interval $[-\phi\sqrt{2},+\phi\sqrt{2}]$ and distributed as

$$dP(X) = \frac{1}{\phi\sqrt{2}}\,\frac{dX}{1-(X/\phi\sqrt{2})^2}\,. \qquad [30]$$

The mean of $G_c = <e^{iX}>$ turns out to be

$$G_c(\phi) = \int_{-\phi\sqrt{2}}^{+\phi\sqrt{2}} \cos(X)\, dP(X) = J_0(\phi\sqrt{2})\,, \qquad [31]$$

where the subscript c stands for 'circular' and $J_0(x)$ is the zero-th order Bessel function (as expected, the first terms in the expansion of $G_c(\phi)$ are $1-\phi^2/2+\ldots$). Using Eq.[28] to estimate the variance ϕ^2 at time t, the post-accumulation FID weighting function G(t) becomes

$$G_c(t) = g_c(\rho) = J_0\left(\sqrt{2<\phi_f^2(t)>}\right) = J_0\left(\gamma\sigma T\sqrt{2P(\rho)}\right) \qquad [32]$$

where again $\rho=t/T$ and $P(\rho)$ is given by Eq.[29].

Two cycles of the periodic function $g_c(\rho)$ are plotted in Fig.3 against the reduced-time parameter ρ for various values of the dimensionless parameter $w = \gamma\sigma T$.

Noticeable deviations from the Gaussian approximation appear only when w exceeds about 3. In order to perceive the negative lobes of the J_0 function, the modulation would have to be unrealistically severe. The spectrum in the lower part of Fig.3. shows the resulting modulation sidebands (notice the asymmetry which makes them look as though they were improperly phased). Since the shape of the function $g_c(\rho)$ is completely determined by the parameter w, so are the relative sideband intensities and the corresponding drop of the central line height (due to the fact that the integral must remain constant).

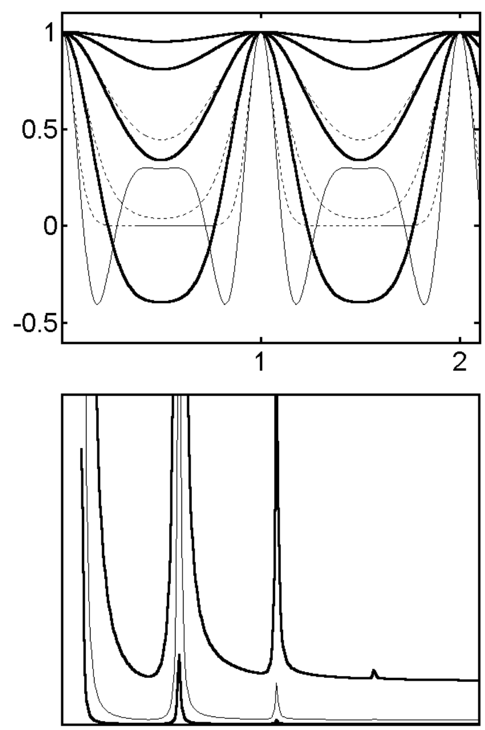

Fig.3.

Upper: The function $g_c(\rho)$ plotted against $\rho=t/T$ for $\gamma\sigma T=1$ (top), 2, 4, 8 and 16 (bottom). The dotted lines show the Gaussian approximation to Eq.[11].

Lower: FFT of an exponential decay multiplied by $g_c(\rho)$ with $\gamma\sigma T=4$. The three traces correspond to expansions of x1, x10 and x100.

A warning is needed at this point. Eq.[32] applies well to all periodic field instabilities of type A (uniform across the sample volume) but not to those of type B (non-uniform) which require an additional averaging over individual sample voxels. We can apply them directly to all cases of mains-related fluctuations (environmental pick-up, field brum, field ripple) but not to HR rotational sidebands or noisy field gradients. The additional averaging for some type-B cases shall be handled in Section IV.

IIIc. Special cases: quasi-periodic field modulation

There is an apparent qualitative discrepancy between Eq.[15] (random noise fluctuations) and Eq.[22] (purely periodic perturbation) which consists in the fact that in the first case the phase instability of the FID keeps building up without any limit, while in the periodic case it remains bounded. This makes it interesting to see what happens for periodic modulations with random frequency fluctuations.

The simplest statistical description of such cases is by means of a normalized auto-correlation function of the type

$$c(\zeta) = e^{-|\zeta|\Delta}\cos(\omega\zeta) \qquad [33]$$

which corresponds to a Lorentzian distribution of the angular frequency ω with a half-height spread of 2Δ radians. Typically, Δ shall be expressed as a fraction of ω, i.e., $\Delta = \kappa\omega$ where κ is a positive, dimensionless factor.

We now need to evaluate Eq.[16] with $c(\zeta)$ given by the above equation. This is best achieved by verifying that, for any *complex* s, when $c(\zeta) = \mathrm{real}(e^{-s|\zeta|})$ then

$$<\phi_f^2(t)> = (\gamma\sigma)^2 t^2\, \mathrm{real}\left\{2\,\frac{1-g(st)}{st}\right\}, \qquad [34]$$

where g(x) is the function defined in Eq.[21] and real{...} is the real part of a complex quantity. Equations [20] and [28] are special cases of Eq.[34] obtained for $s = 1/T_m$ and $s = -j\omega$, respectively. The present case is covered by setting $s = \omega\eta = (2\pi/T)\eta$ with the complex quantity $\eta = \kappa\text{-}j$. Noting that $st = 2\pi\rho\eta$, one obtains the following extensions of Eqs.[28] and [29] to non-zero values of κ:

$$<\phi_f^2(t)> = (\gamma\sigma)^2\, T^2\, P(\kappa,\rho), \qquad [35]$$

where

$$P(\kappa,\rho) = 2\rho^2\, \mathrm{real}\left\{\frac{1-g(2\pi\rho\eta)}{2\pi\rho\eta}\right\}. \qquad [36]$$

The plots of $P(\kappa,\rho)$ for various values of κ are shown in Fig.4. They demonstrate that

a) the bounded behavior applies only to the idealized purely harmonic case (κ=0) and

b) in realistic cases (κ>0) the oscillations are damped and the equations derived in the last Section become rapidly inapplicable. After the first ten periods, for example, Eq.[28] is grossly in error already for κ = 0.005 (1% uncertainty in the field-modulation frequency).

The function $P(\kappa,\rho)$ can be rewritten in a less elegant but more explicit way as

$$P(\kappa,\rho) = P_d(\kappa,\rho) + P_c(\kappa,\rho)\,, \qquad [37]$$

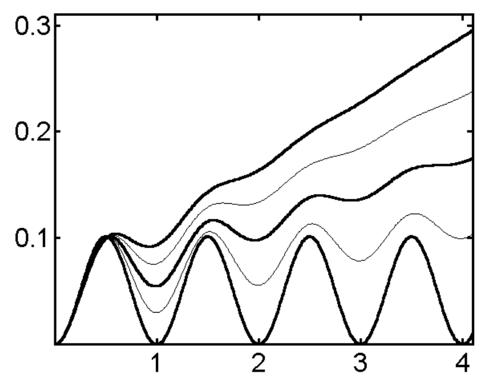

Fig.4.
Functions $P_\kappa(\rho)$ plotted against ρ=t/T for κ=0 (bottom), 0.05, 0.1, 0.15, 0.2 (top).

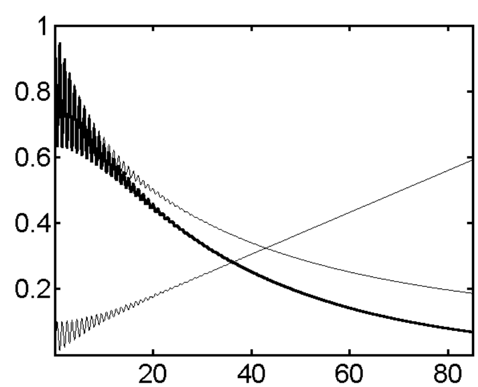

Fig.5.
Function $P(\kappa,\rho)$ for κ=0.02 and $w \equiv \gamma\sigma T$ =3 (thin) and the corresponding G(t) (thick, Eq.39). The thin decaying line shows the effect of second averaging for a field modulated by sample rotation (Eq.44).
All functions are plotted against ρ=t/T.

$$P_d(\kappa,\rho) = 2\pi\kappa N_\kappa \rho,$$
$$P_c(\kappa,\rho) = N_\kappa\{\cos\vartheta - e^{-2\pi\kappa\rho}\cos(2\pi\rho - \vartheta)\},$$
$$N\kappa = [2\pi^2(1+\kappa^2)]^{-1} \text{ and } \vartheta = \arccos[(1-\kappa^2)/(1+\kappa^2)],$$

showing that $P(\kappa,\rho)$ is a sum of two terms: $P_d(\kappa,\rho)$ which grows linearly with time (phase diffusion) and a damped-harmonic transient $P_c(\kappa,\rho)$.

Fig.5 shows an example for κ = 0.02 (4% uncertainty in the modulation frequency). It is by itself sufficient, for example, to explain the empirical fact that when HR-NMR FID's are weighed by a sine-bell function (a common practice in 2D spectroscopy), mains frequency artifacts and spinning sidebands get remarkably suppressed. A sine-bell weighing in fact discriminates the starting portions of FID's (where the oscillatory phase modulation is strong) in favor of the central portions (where it is damped).

In order to assess the weight function G(t) for averaged FID's one must find out the probability distribution function for $\phi_f(t)$. This is apparently not easy since the randomness now arises simultaneously from two different sources - the random starting phase α and the random modulation frequency. The latter effect is responsible for the fact that, unlike in the preceding case, the p.d.f. of $\phi_f(t)$ has a time-dependent shape and can not be written as a starting p.d.f scaled by a non-random time-dependent factor. However, in Eqs.[37] we have already established a separation of the phenomenon into a phase-diffusion term, expected to have a normal distribution, and a purely harmonic term for which applies the circular distribution discussed in the last Section. Consequently, we expect the following formula to be applicable:

$$G(t) = \langle \exp[i\phi_f(t)] \rangle = g_n(\kappa,\rho)\, g_c(\kappa,\rho) \qquad [38]$$
$$g_n(\kappa,\rho) = \exp[-w^2 P_d(\kappa,\rho)/2],$$
$$g_c(\kappa,\rho) = J_0\left[w\sqrt{2P_c(\kappa,\rho)}\right]$$

and w = $\gamma\sigma$T. As a check, notice that i) when κ=0, $g_n(\kappa,\rho)$=1 and $g_c(\kappa,\rho)$ becomes the $g_c(\rho)$ of Eq.[32] and ii) G(t) expands again as $1-\langle\phi_f^2(t)\rangle/2+...$ When w<3, in fact, G(t) is well approximated by the much simpler expression

$$G(t) = \exp[-w^2 P(\kappa,\rho)/2]. \qquad [39]$$

There is a simple physical interpretation of the two FID weighing factors in Eq.[38]. The phase-diffusion factor $g_n(\kappa,\rho)$ is exponential with a decay rate of $\pi(\gamma\sigma)^2T\kappa N_\kappa$, corresponding to spectral convolution with a Lorentzian line of half-height width Δ = $(\gamma\sigma)^2T\kappa N_\kappa$ = $w^2(\kappa\omega)/2\pi$. This *affects indistinctly all spectral features*.

Like $g_c(\rho)$ of the previous Section, the cyclic factor $g_c(\kappa,\rho)$ gives rise to modulation sidebands in the spectra at offsets which are multiples of the field modulation frequency. Now, however, the *relative intensities of the sidebands depend on both w and κ* and, because of the exponential damping of $P_c(\kappa,\rho)$, they are *smaller* than in the case κ=0. In addition, the *damping* implies that *the sidebands are subject to an additional broadening* corresponding quantitatively to $\Delta_s=2(\kappa\omega)$.

IIId. Co-presence of several uncorrelated field modulations

According to a well-known theorem of statistics, the self-correlation function of a random function of time which is a sum of uncorrelated components is the sum of the self-correlation functions of the individual components. Considering Eq.[16] it follows that

$$\langle\phi_f^2(t)\rangle = \Sigma_r \langle\phi_{f,r}^2(t)\rangle, \qquad [40]$$

where the index r ranges over all the components and $\langle\phi_{f,r}^2(t)\rangle$ are the individual component variances. Substituted into Eq.[11] this gives

$$G(t) = \exp(-\Sigma_r \langle\phi_{f,r}^2(t)\rangle/2) = \Pi_r \exp(-\langle\phi_{f,r}^2(t)\rangle/2) = \Pi_r\, G_r(t), \qquad [41]$$

Indicating that the final effect on the averaged FID's is a multiplication by separate weighting functions, each corresponding to one of the contributing components.

IV. Second averaging for type-B instabilities

We have already anticipated that in those cases where the field fluctuations are not the same for all voxels (type B noise/modulations), one has to average the results for over all the voxels.

We know, of course, that the NMR signals from individual voxels sum up linearly. Since this is only true about the complex signal vector and its projections (not about the phase and/or modulus), the averaging over the sample volume shall be applicable only to the weighing functions G(t) of Eqs.[22, 32, and 38]. Even so, there is no *a-priori* guarantee that such an averaging shall preserve the simple picture in which the final effect on averaged FID's is their multiplication by a well-defined time function. Since, in principle, each voxel is weighed differently, the factorization of the averaged signal into an 'undisturbed' FID and a 'global' multiplier function might be impossible. We shall therefore concentrate first on showing that there is a wide class of situations in which such a factorization is still valid.

In general, the G(t) of a single voxel is function of time t, of the *time-independent parameters* p_i characterizing the field perturbations (such as their mean-square-amplitudes, characteristic times, etc.) and of other time-independent quantities (such as transmitter/receiver efficiency, density of nuclei, etc):

$$G(t) \equiv G(t;\, p_1,p_2,p_3,\ldots). \qquad [41]$$

Assume that one of the parameters, say $p \equiv p_1$, has a non-trivial distribution over the sample voxels. It is then possible to find a distribution function for p in terms of the fraction v(p) of voxels in which its value lies between p and p+dp. Once v(p) is known, G(t) can be averaged over the whole sample volume using the simple integral formula

$$< G(t) >_V \;= \int_V G(t;p,p_2,p_3,\ldots)\, v(p)\, dp = G_v(t;p_2,p_3,\ldots) \equiv G_v(t). \qquad [42]$$

As anticipated, the result is again a simple weighing function $G_v(t)$. The approach can be easily extended to situations with a number of voxel-dependent parameters but we shall refrain from doing so in this Note.

Let us consider two practical special cases:

a) Periodic field modulation due to sample rotation (HRNMR).

In this case the voxels located along the rotation axis do not perceive any modulation, while those located on the edge of the cylindrical sample are influenced most. Assuming the presence of a small residual *linear* field gradient[9] perpendicular to the rotation axis, the modulation amplitude b is proportional to the distance of the voxel from the axis, while all other characteristics of the modulation (the period T and the instability factor) are constant across the sample.

It is elementary to show that in this case $\sigma^2=b^2/2$ has a uniform distribution, i.e., $v(\sigma^2) = 1/\sigma^2_{max}$ for σ^2 comprised between 0 (rotation axis) and some σ^2_{max} (sample edge). Evidently, $v(\sigma^2)$ vanishes outside this interval. Since all the G(t) functions for individual-voxel are given by Eq.[38], we have

$$G_v(t) = (1/\sigma^2_{max}) \int_0^{\sigma^2_{max}} g_n(\kappa,\rho)\, g_c(\kappa,\rho)\, d\sigma^2 \quad . \qquad [43]$$

The evaluation of the integral, though not difficult, requires numeric methods. However, in normal HRNMR practice we have always $w_{max} \equiv \gamma\sigma_{max}T << 3$ (the sample-spinning modulation of FID's is never *severe*) so that the approximation of Eq.[39] is applicable and we obtain

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[9] This is doubtless a simplistic approximation. The very fact that most HR-NMR instruments mount 8 or more 'non-spinning' shims indicates that the residual field inhomogeneity may be much more complex. However, higher spherical components simply generate rotational artifacts at multiples of the sample-rotation frequency and, due to their different symmetries, the various modulation orders are practically uncorrelated so that their separate effects are additive.

$$G_v(t) = (1/\sigma^2_{max}) \int_0^{\sigma^2_{max}} \exp\left[-\sigma^2\gamma^2 T^2 P(\kappa,\rho)/2\right] d\sigma^2 = \frac{1-\exp[-w^2_{max}\, P(\kappa,\rho)/2]}{w^2_{max}\, P(\kappa,\rho)/2}\,. \qquad [44]$$

This explicit formula is easy to evaluate (see Fig.5 for an example). When compared with Eq.[39] it shows an initial decay rate which is the same for both formulae provided w^2 in Eq.[39] is replaced with the 'average' value of $w_{max}^2/2$. However, while the initial behavior can be matched, the asymptotic behavior ($\rho\rightarrow\infty$) is qualitatively different. Due to the term $P_d(\kappa,\rho)$ in $P(\kappa,\rho)$, the latter tends to grow linearly when ρ is large. The consequence is an asymptotic exponential decay in Eq.[39] and a much slower decay of the $1/\rho$ type in Eq.[44].

In the frequency domain this leads, apart from the appearance of rotational sidebands, to relatively modest broadening of the tops of spectral peaks combined with a heavier broadening of their feet's. The fact that *unstable spinning*, combined with incorrect settings of non-spinning shims can broaden the feet of spectral lines has long been suspected and even used in an improper way (installation and service engineers are quite prone to blame spinners rather than magnets for bad resolution). Eqs.[37] and [44] endow this feeling with quantitative rigor.

b) Field-gradients noise (MRI)

Most MRI techniques acquire FID's in the presence of externally imposed field gradients. Since the gradient-generating circuitry can't be completely noiseless, it gives rise to spatially correlated fluctuations of the generated linear gradients. Due to the gradient coils construction, the gradient field (or, more exactly its z-component) generated in the central plane perpendicular to the gradient axis is null, but it grows linearly with the distance of a voxel from the said plane (positive on one side and negative on the other). Consequently, there again exists a distribution $v(\sigma^2)\sigma^2$ of signal contributions arising from those voxels in which the gradient noise has variance σ^2.

The exact form of the $v(\sigma^2)$ distribution is rather complex and closely interwoven with the image itself, indicating that it leads to patterned image artifacts rather than to a simple, uniform loss of resolution. A complete analysis of such artifacts is decidedly beyond the scope of this paper but the approach appears to be both sound and viable.

V. Conclusions

We have shown how the phase noise due to magnetic field instabilities (or, alternatively but less likely, the phase noise of the reference frequency) propagate into NMR data such as FID’s and their Fourier transforms. We have also delimited several typical types of magnetic field noise (random, periodic, and mixed) and derived a number of novel specific formulae covering the individual cases.

However, there is much which still needs to be done. So far discussed only the artifacts due to the statistical bias of signal phase projections which can be appreciated in averaged FID's. We should also try and establish some of the statistical characteristics of single-scan FID's and spectra or, more generally, those which pertain to the averages obtained after a limited number of scans.

This means asking questions like: having acquired N scans,

a) what is the expected error in the FID signal intensity at time t,
b) what are the probability distribution functions for spectral *peak heights*,
c) how much do spectral line *shapes* fluctuate between individual scans,
d) what are the probability distribution functions for artifacts such as modulation sidebands.

According to Eq.[3], question (a) boils down to the probability distribution of $\exp[j\phi_f(t)]$ which is relatively easy to handle. The other questions, however, may be a bit more difficult to tackle.

Another unfinished chapter regards the practical consequences of the theory presented in this paper and the ways it can be used to remove or suppress field-noise artifacts. There are several avenues how this task can be tackled using alternative accumulation strategies (modulus & phase accumulation) or temporarily storing all individual scans and applying evaluation algorithms other than plain averaging at the end of the acquisition period. The latter approach has now become feasible thanks to continuing rapid advances of electronics, particularly in terms of memory capacity and mass-data evaluation speeds.

Clearly, there is much more work to be done. The promise is a significant increase in spectral resolution and a corresponding increase in spectral sensitivity (ratio of peak height to noise amplitude), removal of rotational sidebands, and correction of a number of other artifacts linked to random magnetic field variations.

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There are surprisingly few articles in the literature dealing with the important topic of field-noise effects in NMR. The only ones I have found are:

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