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Signal-to-Noise Ratio in Autodyne with Crossed Coils

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Abstract

The correlation functions of the amplitude of NMR signal components are calculated by means of stochastic differential equations and more accurate expression for the signal-to-noise ratio is derived. The analysis corresponds to the case without saturation in the autodyne with crossed coils.

1. Introduction

Autodyne detectors are widely used in NMR spectroscopy and applications because of simplicity, good sensitivity and reliable operation. But the ordinary autodyne possesses some drawbacks which complicate or even restrict its range of utilization.

First, the sensitivity of an autodyne essentially depends on the oscillation amplitude. Particularly it is not comfortable for saturation investigations. But this drawback is unavoidable in the ordinary autodyne since it is associated with the origin of the very oscillating system.

Secondly, the frequency response of sensitivity is also related with the oscillation amplitude. By the way, one can avoid this dependence in the autodyne with an automatic amplitude control[1] and in Robinson autodyne[2].

Thirdly, the ordinary autodyne does not permit the large oscillation amplitude because of reduction both the sensitivity and the signal-to-noise ratio. According to the experimental investigation[2, 3], the dependence of the signal-to-noise ratio on the

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oscillation amplitude has a maximum value, but for low modulation frequencies it corresponds to the small oscillation amplitude.

In a work[4] was proposed an autodyne getting rid of these drawbacks. It was achieved by formation of the radiofrequency magnetic field (r.f.m.f.) in the sample by means of two crossed coils. Independently, R.J.BLUME and D.T.EDMONDS suggested an analogous autodyne to detect the dispersion component of an NMR signal[5].

2. Autodyne with Crossed Coils

A schematic diagram of the autodyne with crossed coils is shown in Fig. 1. It consists of an ordinary autodyne (*O.A.*) with a tank coil L_R ("receiver"coil), a linear amplifier (*A.*) and a coil L_T ("transmitter" coil) orthogonal to the coil L_R. The sample under investigation is, as usual, located within the ordinary autodyne coil L_R ("receiver") and an NMR signal is detected by the ordinary autodyne. Only the r.f.m.f. in the sample is furnished by both the transmitter and the receiver coils. In order to sustain the proper polarization of an r.f.m.f., the linear amplifier (*A.*), supplying the transmitter coil, is driven by the voltage of the receiver coil. There is no direct noticeable coupling between the transmitter and the receiver coils. The right angle position of two coils permits to eliminate it. Coupling between coils occurs only at the resonance through the sample under investigation. But in the present circuit the oscillation is entirely maintained by the feedback independent of the sample, unlike the Schmelcer or "spin-coupled" oscillator, where the main feedback involves the nuclear magnetism of the sample.

In order to observe the NMR absorption component, the transmitter coil is to be supplied by the current with the phase shiht of 90° in comparison with the current in the receiver coil.

If linear polarized r.f.m. fields originated by currents of the receiver and the transmitter coils are expressed respectively $2H_x\cos\omega t$ and $-2H_y\sin\omega t$, then it is easy to see a presence of two contrarotating circularly polarized fields in the sample with corresponding amplitudes H_y+H_x and H_y-H_x. The NMR signal may be excited by the field with amplitude H_y+H_x. Evidently, this r.f.m.f. value is easily controlled by the current in the transmitter coil, while the current amplitude in the receiver coil is fixed. Therefore the oscillating conditions for the oscillator remain constant and, consequently, the sensitivity as well as the frequency response of the sensitivity of the autodyne does not depend upon the amplitude of the r.f.m.f. in the sample.

Unlike to an ordinary autodyne, the autodyne with crossed coils enables us to take into consideration the specific properties of both the very autodyne and the sample under investigation. That is, the receiver part (ordinary autodyne) can be adjusted to the maximum of the signal-to-noise ratio while the r.f.m.f. in the sample can be selected to the desirable value.

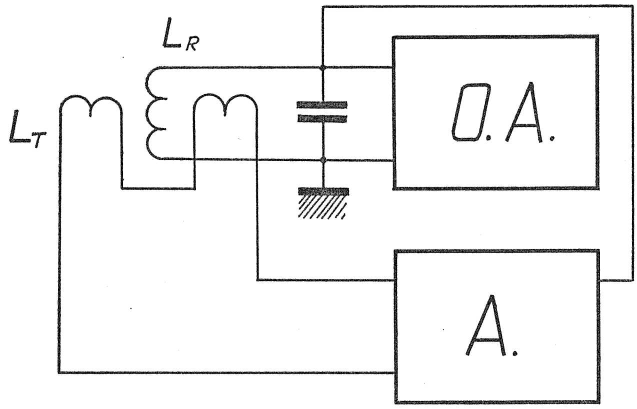

Fig. 1. Thr schematic diagram of the autodyne with crossed coils. *O. A.* is an ordinary autodyne, *A.* is a linear amplifier, L_R is a receiver coil, L_T is a transmitter coil.

The above adjustment is particularly important in case of low modulation frequencies, when the maximum signal-to-noise ratio occurs for the small oscillation amplitude. Since the signal amplitude is proportional to the value of the r.f.m.f. (in the absence of saturation)[4,6] and utilization of crossed coils enables us to enhance the signal-to-noise ratio significantly.

In the autodyne with crossed coils, any known ordinary autodyne can be employed, but the usage of an autodyne with a stable small oscillation amplitude is preferable. Therefore the autodyne with automatic amplitude control[1], Robinson autodyne[7] can be in use.

The main properties of the autodyne with crossed coils were analyzed in the reference[4] but the noise influence was not clarified satisfactorily.

3. Discussion

The actual sensitivity of the autodyne is defined as the signal-to-noise ratio. As far as noise is concerned, the fluctuations of an autodyne amplitude are usually evaluated, because the NMR signal is weak and hidden in this noise. But an NMR signal is excited by the r.f.m.f. with the fluctuating amplitude. Thus the very signal is subjected to some fluctuations. In case of an autodyne with crossed coils, these fluctuations are substantially larger. The point is to determine the effect of fluctuations to the signal amplitude. Therefore this theoretical treatment is to find out the statistical characteristics of a signal amplitude. Possession of these quantitative characteristics is to enable us to define more precise the signal-to-noise ratio. It is important in practical applications because these findings allow to determine advantages of the use of an autodyne with crossed coils in every case.

The strict and complete analysis is hardly justified in view of difficulties to construct a quite adequate mathematical model of the system and to solve the problem with enough accuracy. Therefore we are to make the next assumptions:

1. The sample under investigation is unsaturated.

2. NMR signal distortions[4,8] occured because the interaction of nuclear magnetization and an autodyne are neglected.

3. The autodyne with respect to the signal is implied to be a linear system.

4. The oscillation of an r.f.m.f. has a constant initial phase and fluctuations of the amplitude are taken as white noise[9].

These assumptions significantly simplify the calculations because we are considering the linear model and the autodyne equation is not taken into account. In the first approach such linearization is justified as far as the noise standard deviation of the fluctuations of the oscillation amplitude is small enough in comparison with the mean amplitude.

An analysis is based on the solution of the phenomenological equations of Bloch[6]. The absence of saturation allows to consider only the transverse components of a nuclear magnetization.

$$\frac{dM_x}{dt}+\frac{1}{T_2}M_x-\gamma M_yH_z+\gamma M_0H_y=0,$$
$$\frac{dM_y}{dt}+\frac{1}{T_2}M_y-\gamma M_0H_x+\gamma M_xH_z=0. \qquad (1)$$

Exciting r.f.m. fields produced by the currents in receiver and transmitter coils are respectively $H_x=2A\cos\omega t$ and $H_y=-2Ak\sin\omega t$ where k is a real coefficient, expressing the ratio of r.f.m.f. amplitudes, originated by transmitter and receiver coils. Since the amplitude of an r.f.m.f. is fluctuating, it can be represented in the following manner

$$A=A_0+\alpha(t),$$

where $A_0=\langle A\rangle$ is the mean amplitude, $\alpha(t)=A-A_0$ is the fluctuations of an amplitude. The mean of these fluctuations is $\langle\alpha(t)\rangle=0$ and the correlation function is $k(\tau)=\frac{N_0}{2}\delta(\tau)$, as white noise[9, 10], where N_0 is a constant spectral density and $\delta(\tau)$ is a delta function.

Substitution of H_x and H_y to Eq. (1) in rotating frame[6] yields

$$\frac{dv}{dt}=-\Delta u-\frac{1}{T_2}v+\gamma M_0A(1+k),$$
$$\frac{du}{dt}=\Delta v-\frac{1}{T_2}u, \qquad (2)$$

where v and u are the absorption and the dispersion components of an NMR signal respectively, $\Delta=\gamma H_z-\omega$ is detuning with respect to the resonance frequency. Averaging of Eq.(2) gives the mean values for the components of an NMR signal. In order to get an undistorted signal, the slow passage through the resonance area is in use.

Therefore $\Delta\approx$ const and subsequently $\frac{d<v>}{dt}\to 0$ and $\frac{d<u>}{dt}\to 0$. Then, mean values for the absorption and the dispersion components are found as

$$<v>=\frac{1}{1+\Delta^2T_2^2}\gamma M_0T_2(1+k)A_0, \qquad <u>=\frac{\Delta T_2}{1+\Delta^2T_2^2}\gamma M_0T_2(1+k)A_0. \quad (3)$$

Fluctuations of these components can be represented as follows: $x=v-<v>$, $y=u-<u>$.

Owing to the linearity of Eq.(2) these fluctuations obey the next equations

$$\frac{dx}{dt}=-\Delta y-\frac{1}{T_2}x+\gamma M_0\ (1+k)\alpha(t),$$
$$\frac{dy}{dt}=\Delta x-\frac{1}{T_2}y. \quad (4)$$

Now, let us consider the statistical characteristics of these fluctuations. Since equations are linear, we can easily replace this system by the equations with separated variables,

$$\frac{d^2x}{dt^2}+\frac{2}{T_2}\frac{dx}{dt}+\left(\frac{1}{T_2^2}+\Delta^2\right)x=\gamma M_0(1+k)\left[\alpha'(t)+\frac{1}{T_2}\alpha(t)\right], \quad (5)$$

$$\frac{d^2y}{dt^2}+\frac{2}{T_2}\frac{dy}{dt}+\left(\frac{1}{T_2^2}+\Delta^2\right)y=\Delta\gamma M_0(1+k)\alpha(t). \quad (6)$$

In the assumption of a slow passage through the resonance, one can consider $\Delta\approx$ const and solutions of Eqs. (5) and (6) yield the following stationary processes

$$x=\frac{1}{\Delta}\gamma M_0(1+k)\int_{-\infty}^{z}\left[\alpha'(t)+\frac{1}{T_2}\alpha(t)\right]\sin\Delta(z-t)\exp\left[\frac{1}{T_2}(t-z)\right]dt, \quad (7)$$

$$y=\gamma M_0(1+k)\int_{-\infty}^{z}\alpha(t)\sin\Delta(z-t)\exp\left[\frac{1}{T_2}(t-z)\right]dt. \quad (8)$$

Obviously, the means are $<x>=<y>=0$ and the correlation functions of the fluctuations of absorption and dispersion components are the next[10] respectively

$$k_a(\tau)=\frac{1}{\Delta^2}\gamma^2M_0^2(1+k)^2\exp\left[-\frac{2z+\tau}{T_2}\right]\int_{-\infty}^{z}\int_{-\infty}^{z+\tau}<\left[\alpha'(p)+\frac{1}{T_2}\alpha(p)\right]\left[\alpha'(q)+\frac{1}{T_2}\alpha(q)\right]>\times$$
$$\times\sin\Delta(z-p)\sin\Delta(z-q+\tau)\exp\frac{p+q}{T_2}dp\,dq, \quad (9)$$

$$k_d(\tau)=\gamma^2M_0^2(1+k)^2\exp\left[-\frac{2z+\tau}{T_2}\right]\int_{-\infty}^{z}\int_{-\infty}^{z+\tau}<\alpha(p)\alpha(q)>\times$$
$$\times\sin\Delta(z-p)\sin\Delta(z-q+\tau)\exp\frac{p+q}{T_2}dpdq. \quad (10)$$

Since $\alpha(t)$ is white noise, thus the integrand correlation functions are to be found as follows[10]

$$<\alpha(p)\alpha(q)>=\frac{N_0}{2}\delta(p-q),$$

$$<[\alpha'(p)+\frac{1}{T_2}\alpha(p)][\alpha'(q)+\frac{1}{T_2}\alpha(q)]>$$

$$=<\alpha'(p)\alpha'(q)>+\frac{1}{T_2}<\alpha'(p)\alpha(q)>+\frac{1}{T_2}<\alpha(p)\alpha'(q)>+\frac{1}{T_2^2}<\alpha(p)\alpha(q)>$$

$$\approx-\frac{N_0}{2}\delta''(p-q)+\frac{1}{T_2}\frac{N_0}{2}\delta'(p-q)-\frac{1}{T_2}\frac{N_0}{2}\delta'(p-q)+\frac{1}{T_2^2}\frac{N_0}{2}\delta(p-q)$$

$$=\frac{1}{T_2^2}\frac{N_0}{2}\delta(p-q)-\frac{N_0}{2}\delta''(p-q).$$

By substituting these to Eqs. (9), (10) and integrating, the next correlation functions of fluctuations of both the absorption and the dispersion components are obtained

$$k_a(\tau)=\frac{N_0}{8}\frac{\gamma^2M_0^2(1+k)^2T_2}{1+\Delta^2T_2^2}[(2+\Delta^2T_2^2)\cos\Delta\tau-\Delta T_2\sin\Delta\tau]\exp\left(-\frac{|\tau|}{T_2}\right), \quad (11)$$

$$k_d(\tau)=\frac{N_0}{8}\frac{\gamma^2M_0^2(1+k)^2\Delta T_2^2}{1+\Delta^2T_2^2}[\Delta T_2\cos\Delta\tau+\sin\Delta\tau]\exp\left(-\frac{|\tau|}{T_2}\right). \quad (12)$$

Evidently these correlation functions correspond to narrow band gaussian random processes[9, 10].

Variances are given by

$$\sigma_a^2=k_a(0)=\frac{N_0}{8}\gamma^2M_0^2T_2(1+k)^2\frac{2+\Delta^2T_2^2}{1+\Delta^2T_2^2}\approx\frac{N_0}{8A_0^2}\frac{(\sqrt{2}+\Delta^2T_2^2)^2}{T_2}<v>^2, \quad (13)$$

$$\sigma_d^2=k_d(0)=\frac{N_0}{8}\gamma^2M_0^2(1+k)^2\frac{\Delta^2T_2^3}{1+\Delta^2T_2^2}=\frac{N_0}{8A_0^2}\frac{1+\Delta^2T_2^2}{T_2}<u>^2. \quad (14)$$

The effective noise pass-band[10] for the absorption component is π/T_2. Therefore the power through this pass-band is $N_0\,(1+k)^2\,\pi/T_2$. The amplitude of a rotating r.f.m.f. is $(1+k)A_0$ and a power is $(1+k)^2A_0^2$. If the ratio of these powers is denoted as

$$\chi^2=\frac{N_0(1+k)^2\pi/T_2}{(1+k)^2A_0^2},$$

then variances can be rewritten in more convenient manner

$$\sigma_a^2=\frac{1}{8\pi}\chi^2(\sqrt{2}+\Delta^2T_2^2)^2<v>^2, \quad (15)$$

$$\sigma_d^2=\frac{1}{8\pi}\chi^2(1+\Delta^2T_2^2)<u>^2. \quad (16)$$

Standard deviations or r.m.s. values

$$\sigma_a = \frac{\chi}{2\sqrt{2\pi}}(\sqrt{2} + \Delta^2 T_2^2)\langle v \rangle, \tag{17}$$

$$\sigma_d = \frac{\chi}{2\sqrt{2\pi}}\sqrt{1+\Delta^2 T_2^2}\langle u \rangle, \tag{18}$$

are directly proportional to the corresponding component and also depend on the tuning Δ. Therefore the larger signal obtained is accompanied by intense fluctuations.

Signal-to-Noise Ratio

The signal-to-noise ratio is usually defined as

$$\eta = \frac{\text{signal maximum amplitude}}{\text{noise standard deviation.}}.$$

Let us analyze the absorption component. The signal amplitude is expressed by Eq. (3), and can be rewritten as $\langle v \rangle = (1+k)\langle v^* \rangle$, where $\langle v^* \rangle$ is the signal value originated merely by the r.f.m.f. of the receiver coil.

The noise standard deviation is a sum of the receiver coil and the standard deviation of signal amplitude fluctuations. Summation has to be performed algebraically because of the correlation of these two random processes.

In every spectrometer, the narrow band amplification is in use. It permits to suppress the noise power at the output without affecting the signal amplitude and, therefore, to gain the sufficient signal-to-noise ratio.

Now we can evaluate the noise standard deviation. Let the pass-band of a spectrometer be δF. Then the noise standard deviation is expressed in the next way[9]

$$\sigma = \sqrt{\int_{\delta F} S(\Omega)\, df},$$

where $S(\Omega)$ is the noise spectral density.

The width of the signal spectrum is small owing to the slow passage rate through the resonance area. Therefore the pass-band δF of the spectrometer is usually made narrow in comparison with the noise spectral density. Consequently, it is admissible to consider this density constant within pass-band δF. So

$$\sigma \approx \sqrt{S(\Omega_{\delta F})\ \delta F}.$$

Thus the total noise standard deviation at the output is considered to be proportional to

$$\sigma_\Sigma = \sqrt{N_0\, \delta F} + \sqrt{S_s(\Omega_{\delta F})\delta F}, \tag{19}$$

where N_0 is the spectral density of r.f.m.f. amplitude fluctuations of the receiver coil, $S_s(\Omega)$ is the spectral density of the absorption component fluctuations. The last spectral density is easily obtained by the Fourier transform of the correlation function Eq. (13),

$$S_s(\Omega)\approx\frac{1}{4}\cdot\frac{N_0\gamma^2M_0^2T_2^2(1+k)^2}{1+(\Omega^2+\Delta^2)T_2^2}(1+\frac{1}{1+\Delta^2T_2^2}). \tag{20}$$

Within our assumptions, the maximum signal and density $S_s(\Omega_{\delta F})$ correspond to the case $\Delta=\Omega=0$, thus

$$S_s(\Omega_{\delta F})=\frac{N_0}{2}\gamma^2T_2^2M_0^2(1+k)^2=\frac{N_0}{2A_0^2}(1+k)^2<v^*>^2_{max}. \tag{21}$$

Substitution of Eq.(21) to Eq.(19) and use of Eq.(3) yield the next signal-to-noise ratio

$$\eta=\frac{<v^*>_{max}}{\sqrt{N_0\delta F}}\cdot\frac{1+k}{1+\sqrt{2}(1+k)\frac{<v^*>_{max}}{2A_0}}. \tag{22}$$

Here we can select expressions with the individual meaning, namely:

$\frac{<v^*>_{max}}{\sqrt{N_0\delta F}}=\eta^*$: the signal-to-noise ratio in the absence of an r.f.m.f. of the transmitter coil; it represents the case of the ordinary autodyne.

$\frac{<v^*>_{max}}{2A_0}=\zeta^*$: the ratio of the maximum signal to the r.f.m.f. full amplitude of the receiver coil, i.e. a modulation index.

On the base of these marks, we obtain the final expression

$$\eta=\eta^*\frac{1+k}{1+\sqrt{2}(1+k)\zeta^*}. \tag{23}$$

For weak signals, ζ^* is to be very small and product $\sqrt{2}(1+k)\zeta^*$ can be neglected, since k is restricted by the saturation of the sample. Thus the signal-to-noise ratio becomes

$$\eta=\eta^*(1+k). \tag{24}$$

In case of saturation investigations, k can be larger, but the signal-to-noise ratio η is likely to decrease because of the reduction of the signal amplitude.

Therefore, on the basis of the present treatment and the experimental investigations of the noise and sensitivity characteristics of autodynes[2,3] one can conclude that utiltzation of the autodyne with crossed coils in case of weak signals does not reduce the signal-to-noise ratio in favor of more extensive possibilities of this autodyne.

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