Joint time-frequency analysis in NMR spectroscopy

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I. Theoretical background

1. Signal analysis and synthesis

From the mathematical analysis it is known, that for any time function x(t), which is capable of being integrated and of integrable square modulus over the time interval [0, T], there exist integrals:

$$c_n = \int_0^T x(t) S_n(t) dt \qquad (1)$$

where $S_n(t)$ (n = 0, 1, 2, . . .) represents a function series similar to x(t). If the series $S_n(t)$ is orthogonal over interval [0,T], what means

$$\int_0^T S_n(t) S_m(t) dt = \begin{cases} K \neq 0 & \text{if} \quad n=m \\ 0 & \text{otherwise} \end{cases} \qquad (2)$$

the waveform x(t) can then be represented as a weighted sum of basis functions:

$$x(t) \propto \sum_{n=0}^{\infty} c_n S_n(t) \qquad (3)$$

with mean-square approximation error:

$$MSE = \int_0^T [x(t) - \sum_{n=0}^{N-1} c_n S_n(t)]^2 dt \qquad (4)$$

If this error monotically decreases to zero as N becomes very large, this is the case for a complete orthogonal series, what can be expressed by Parseval's equation:

$$\sum_{n=0}^{N-1} c_n^2 = \int_0^T x^2(t) dt \qquad (5)$$

The physical meaning of Eq.(5) is to state that the energy contained within the series will be the same whether in the time or transformed domain.

2. Frequency and time domain analysis

The MSE depends on the type of functions $S_n(t)$ chosen for the linear approximation to waveform x(t). If the shape of this waveform is similar to that of function used, then the MSE will be also small. In many practical cases the waveform x(t) has sinusoidal components. The circular functions with their orthogonal property are the most wide used to spectral decomposition. The integral (1) now has a form:

$$c_n = \frac{1}{T}\int_0^T x(t)\exp(-in\omega_0 t)dt \tag{6}$$

This is the case of Fourier transform.

The base function S(t), so-called orthogonal analysis window function, can be selected with a large degree of freedom. For instance, if S(t) is a Dirac's function:

$$\delta(t) = \begin{cases} 0 & \text{if} \quad t \neq 0 \\ 1 & \text{if} \quad t=0 \end{cases} \tag{7}$$

where $\int_{-\infty}^{\infty}\delta(t)dt = 1$, the coefficients in Eq.(1)

$$c_m = \frac{1}{T}\int_0^T x(t)\delta(t - m\Delta t)dt \tag{8}$$

where $T = M \cdot \Delta t$, represent sampled waveform x(t) with interval Δt. Now the coefficients c_n are from time domain.

In summary, the result of analysis depends on a selected analysis window function. In case of Fourier transform, is used a combination of sinusoids to represent a time waveform. The energy of the sine function is uniformly distributed along the time axis and concentrated at one frequency. The sinusoids used as a analysis window functions are localized in the frequency domain and therefore, the result of the analysis is in frequency domain. For comparison, the energy of the Dirac's function is concentrated in a very narrow time interval and uniformly distributed between all frequencies, The narrow pulses are well localized in time domain. In consequence, analyzed waveform is "copied" to its discrete representation in time domain [1,2].

3. Joint time-frequency analysis (JTFA)

The theorem expressed by Eq.(1) extended on a time and frequency domains, can be written in a form:

$$c_{m,n}=\frac{1}{T}\int_0^T x(t)\gamma_{m,n}(t)dt \tag{9}$$

where γ_{mn} represents orthogonal function series. In this case othogonality means

$$\int_0^T \gamma_{mn}(t)\cdot\gamma_{m'n'}(t)dt=\begin{cases}K>0 & \text{if} \quad m=m' \text{ and } n=n' \\ 0 & \text{if otherwise}\end{cases} \tag{10}$$

One example of orthogonal series is set pulses obtained from pure sine-cosine waveform modulated by Gaussian function [3]. The condition of orthogonality (10) in terms m of time obtains here since only one of the signals is allowed to differ from zero at any one time. The orthogonality of sine-cosine function in terms n of frequency has been shown before. This analysis window function is localized in time and frequency domain simultaneously:

$$\gamma_{m,n}(t)=\varphi_m(t)\exp(-in\omega_0 t) \tag{11}$$

where $$\varphi_m(t)=\frac{1}{\sigma\sqrt{2\Pi}}\exp[-\frac{(t-m\Delta t)^2}{2\sigma^2}]$$

The coefficients (9) represent now so-called short time Fourier transform (STFT), which discretizes the signal to the time-frequency plane [4].

II. Application

The above summary from the signal theory illustrates the principle of the operation of the developed software and hardware

1. Software

The STFT algorithm have been applied to the analysis of the NMR pulse signal. The obtained result shows not only how did the signal involve in time but also make visibly fine structure. The improving a resolution is achieved by optimalization the bandwidth of the Gaussian function [5].

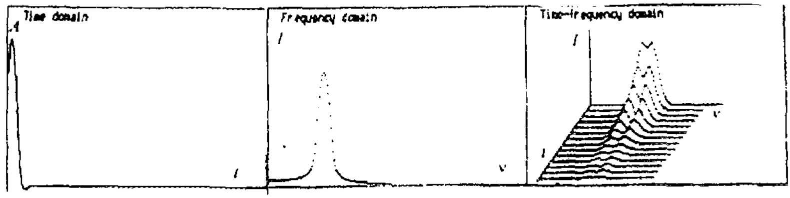

Fig. 1. The STFT algorithm simplify the analysis process. The FT appears only slight distortion of the line shape. Then complex procedures must be use to approximate data to known functions.

2. *Hardware*

In the recent years, aided by the power and capability of digital signal processing, in our laboratory is continuously developing a digital lock-in detection technique [6]. Based on STFT, the last model has many outstanding features in comparison with the best commercially available analog lock-in amplifiers [7].

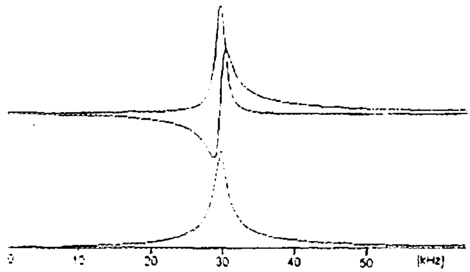

Fig.2.
One of the feature of the digital lock-ins, which operate on STFT is the frequency characteristic without side bands with high rejection of harmonic or subharmonic of the reference frequency. On the figure result of one self-test obtained by tuning the excitation generator versus reference.

References

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