

A Frequency Determination Method for Digitized NMR Signals

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Abstract. We present a high precision frequency determination method for digitized NMR FID signals. The method employs high precision numerical integration rather than simple summation as in many other techniques. With no independent knowledge of the other parameters of a NMR FID signal (phase ϕ , amplitude A , and transverse relaxation time T_2) this method can determine the signal frequency f_0 with a precision of $1/(8\pi^2 f_0^2 T_2^2)$ if the observation time $T \gg T_2$. The method is especially convenient when the detailed shape of the observed FT NMR spectrum is not well defined. When T_2 is $+\infty$ and the signal becomes pure sinusoidal, the precision of the method is $3/(2\pi^2 f_0^2 T^2)$ which is one order more precise than the ± 1 count error induced precision of a typical frequency counter. Analysis of this method shows that the integration reduces the noise by bandwidth narrowing as in a lock-in amplifier, and no extra signal filters are needed. For a pure sinusoidal signal we find from numerical simulations that the noise-induced error in this method reaches the Cramer-Rao Lower Band (CRLB) on frequency determination. For the damped sinusoidal case of most interest, the noise-induced error is found to be within a factor of 2 of CRLB when the measurement time T is 2 or 3 times larger than T_2 . We discuss possible improvements for the precision of this method.

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1 Introduction

In nuclear magnetic resonance (NMR) one often encounters a free induction decay (FID) signal $S(t)$ which takes the form of a sinusoidal function multiplied by a decaying exponential:

$$S(t) = A \cos(\omega_0 t + \phi_0) \exp\left(-\frac{t}{T_2}\right), \quad (1.1)$$

where t is time, A is the signal amplitude, $\omega_0 = 2\pi f_0$ is the resonance frequency, ϕ_0 is the signal phase, and T_2 is the transverse spin relaxation time. In practice, limited by experimental conditions, parameters, like f_0 , ϕ_0 , etc., usually cannot be determined without error, on one hand, $S(t)$ is disturbed by various noises, on the other hand, $S(t)$ can neither be digitized with infinitesimal time intervals nor observed for an infinitely long time. It is of a general interest to determine these parameters using various types of analysis. In particular, the determination of the resonance frequency precisely for a digitized FID signal $S(t)$ observed over a finite time is crucial for recent experiments [1–3] searching for possible new spin dependent interactions which, if present, would cause a tiny shift of the resonance frequency.

When $T_2 \rightarrow +\infty$, Eq. (1.1) can be simplified to:

$$S(t) = A \cos(2\pi f_0 t + \phi_0). \quad (1.2)$$

In this case, many different algorithms using Fast Fourier transform (FFT) or Digital Fourier transform (DFT) [4, 5] were developed for frequency and spectra estimation in power systems. For sinusoidal signals, by using $\ddot{S}(t) = -\omega_0^2 S(t)$, one can obtain ω_0 [6] from a linear fit of $\ddot{S}(t)$ to $S(t)$, where $\ddot{S}(t)$ is derived by finite differentiation of the digitized signal $S(t)$, but extra noise filtering is needed since the second derivative is susceptible to high frequency noise.

To determine the frequency precisely and to reduce the noise without filtering, we propose a different approach in this paper based on integration. We argue that our approach is especially valuable in situations when the shape of the signal in frequency space possesses bias. The structure of this paper is as follows. We first describe the basic principle of the method with an example. We then thoroughly analyze the method and derive its precision. The effect of noise is discussed in the following section. Possible improvements are discussed in the conclusion.

2 The basic principle

Consider a pure sinusoidal signal $S(t) = A \cos \omega_0 t$ observed for a finite time T . By multiplying $S(t)$ by another sinusoidal function of frequency ω and integrating over a time interval of length T , a function \mathcal{L} of ω can be defined as:

$$\mathcal{L}(\omega) = \frac{1}{T} \int_0^T A \cos(\omega_0 t) \cos(\omega t) dt. \quad (2.1)$$