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Calculation of the Main Frequency of an NMR Signal from an Even Frequency Spectrum

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Abstract: Nuclear magnetic resonance (NMR) measurements are most often used to measure images or display the spectrum of different samples. Depending on the samples, these can be medical applications, chemistry, physics, or mineralogy. Perhaps the most beneficial use is in medicine, as it allows you to image the inside of living organs without interfering with them. When physically examining samples, the frequency spectrum of the sample is often measured, which is then converted into a map of the inhomogeneities in the layer of interest. This article addresses one of several similar problems.

Keywords: NMR signal frequency, even frequency spectrum, map of inhomogeneities, nuclear magnetic resonance, magnetic resonance imaging.

1. INTRODUCTION

The conversion of the map of inhomogeneities into a frequency spectrum using nuclear magnetic resonance (NMR) or vice versa is usually carried out today with the aid of the Fourier transform [1]-[2]. Using the NMR experiment, a signal is obtained whose frequency spectrum also contains information about the instantaneous value of the static magnetic field. Similar problems were solved in the stabilization of the magnetic field of a resistive magnet [3]. Later, many problems were repeated in the stabilization of the field of the static magnetic field standard [4]. Similar problems were described in papers [5]-[7]. Papers [8]-[9] can be considered as one of the foundations of the NMR technique. The paper [10] measures a map of inhomogeneities in the measured layer when imaging a biological sample and uses it to suppress the displacement generated by the different resonant frequencies of water and fat. The paper [11] maps the magnetic field of small coils using the NMR technique. The paper [12] deals with a hardware problem, comparing the properties of three types of RF coils and their suitability for MRI. The paper [13] describes an experiment with a special NMR technique. The authors of the paper [14] solve an almost philosophical problem. They reflect on the properties of the scientific method of measurement and its indispensability in the scientific exploration of the world around us. In the paper [4], the solution was sought by processing the complex frequency spectrum of the NMR signal. The advantage of such an approach was that a clear result was obtained, since the spectrum was an odd function of frequency. The disadvantage was that the result was not a continuous function of the input quantity. It was only partially connected. The advantage of using an even spectrum is the continuity of the output function, the disadvantage is two positive results, so one must additionally search for the correct polarity. The research described in this paper also focuses on the search for such a result. As in the paper [4], the main research method is computer simulation.

2. SUBJECT & METHODS

Imaging in NMR technology is based on the transformation of the frequency of the signal spectrum into longitudinal dimensions. The spectrum of a real analog signal is an even function of frequency. This makes it difficult to determine the correct position of the frequency line, as it is displayed twice. The problem can be solved by converting the signal into a complex signal before the spectrum is calculated [4]. The spectrum of such a signal is not an even function of frequency. Although this solves the first problem, a second problem arises: the transformation of the resulting quantity is not a continuous linear function of the input quantity. It can be said that it is linear in parts. It is therefore worth looking for algorithms with which the operation can be performed without a complex signal. One such algorithm is shown in Fig. 1: Computer simulation 1. The frequency step in both following simulations is $\frac{1}{N \times T} = 0.9313225746154784$ Hz.

Computer simulation 1

The strongest NMR signal is simulated by a real harmonic signal c with frequency $f_1 = 10000 \pm \Delta f_1$ Hz. The signal is sampled with an interval T = 0.256 µs at n = 16384 time samples. The number of samples is increased to $N = 2^{22}$ by interpolation and the spectrum of the discrete signal c is calculated using the discrete Fourier transform.

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The frequency of the frequency samples obtained is both positive and negative, so it makes sense to transform the asymmetrical unipolar frequency axis into a positive and negative symmetrical part. Fig. 1 shows that the maxima of both the negative *m1* and the positive *m2* of the frequency part are calculated. Both maxima are the same size, so there is possibility to simplify the program. However, the calculations have proven that the most accurate frequency calculation is achieved by the following procedure: The positions of both maxima on the frequency axis *pos1* and *pos2* are calculated. The positions of both maxima are positive, different and the details of the calculation can be seen in Fig. 2. At the same time, this figure shows that even in the case of a "pure harmonic" signal, the spectrum around the maximum is not linear.

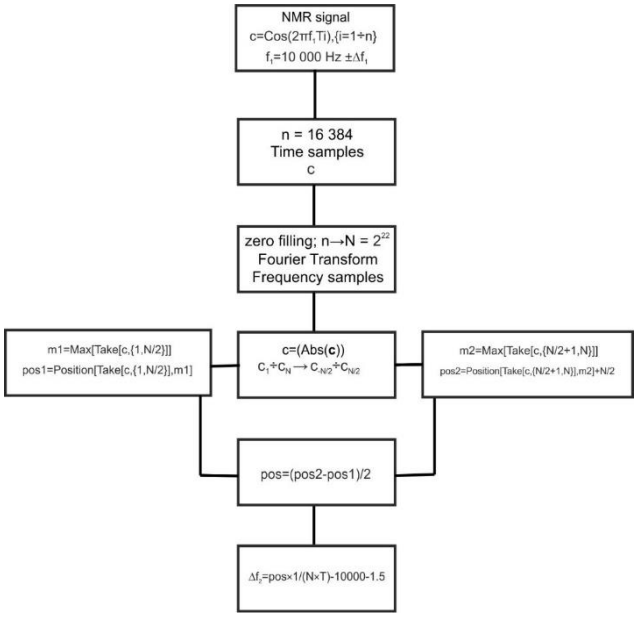


Fig. 1. An algorithm for calculating the frequency deviation of the strongest spectral line Δf_2 of an NMR signal. The algorithm is used in computer simulation 1.

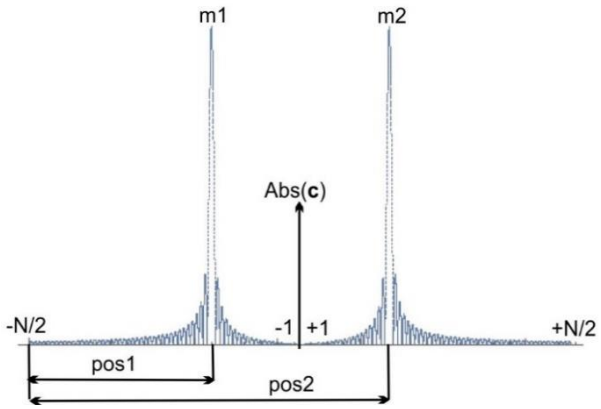


Fig. 2. The position of both maxima with the designation of important quantities.

While the main data refer to the symmetrical frequency axis, it is better to start from the original asymmetrical representation of the frequency sample numbers when calculating the position of both maxima. The partial position *pos* = (*pos2-pos1*)/2 is calculated from the maxima. The resulting value of the frequency deviation is $\Delta f_2 = pos \times \frac{1}{N \times T} - 10000 \sim 1.5$ [Hz]. The value ~1.5 is used to finely compensate for the measurement error, which can be determined by testing. In digital signal processing, individual components cannot acquire arbitrary values. When testing, it is obvious that for each value of the input quantity, the output value is distorted slightly differently. However, the maximum value of the error can be estimated, which can then be compensated for. In this case it is approximately -1.5 Hz. A more accurate calculation can be found in [4]. The error is not completely eliminated, but a correction value is found that satisfies all the useful values of the signal.

Fig. 3. shows the test of the correctness of the calculation. It is clear that the relationship between the input and the resulting value of the frequency deviation is linear as a whole. This is important to make the calculation of the resulting frequency deviation quick and easy.

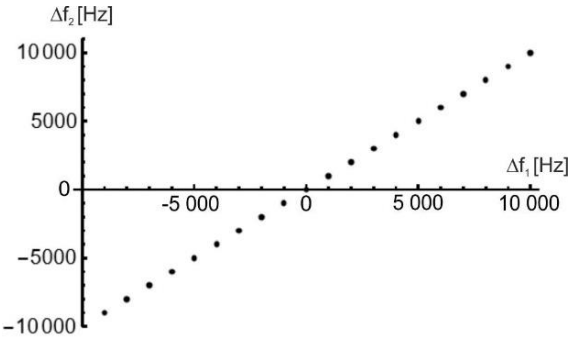


Fig. 3. The relationship between the input and output frequency deviation is linear integer. (Algorithm used in computer simulation 1: Fig. 1.)

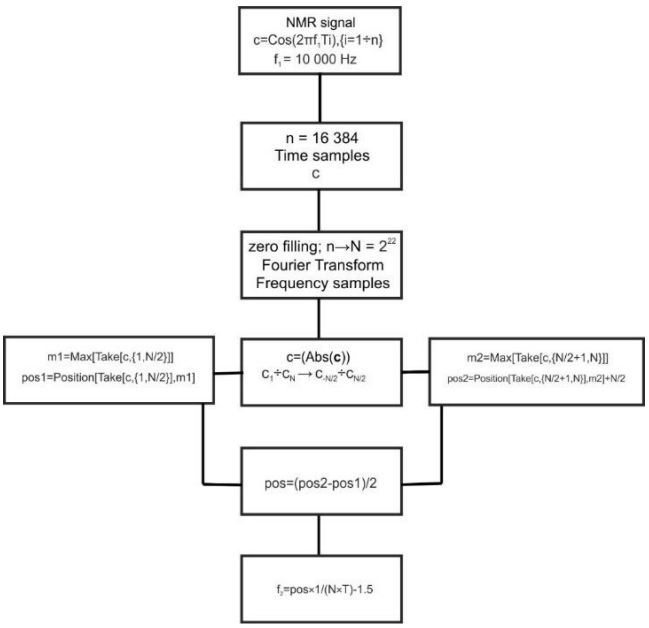


Fig. 4. An algorithm for calculating the frequency of the strongest spectral line of an NMR signal. The algorithm is used in computer simulation 2.

Computer simulation 2:

The simulated input signal contains a harmonic component with frequency Δf_1, this is the frequency of the NMR signal we are interested in, and f_1 is an auxiliary frequency (Fig. 4). In fact, we do not know at least one of these frequencies at the beginning of the calculation and we do not even know what the function looks like. In practice, it may not be advantageous to determine f_1 and especially Δf_1 separately. In this case, the sum of f_1 and Δf_1 is considered as one frequency and at the end of the calculation we do not subtract 10000 Hz from the value marked Δf_2. The input frequency can therefore vary from 0 to a theoretically arbitrary positive value (Fig. 4). The absence of a negative frequency does not usually matter, because the frequencies that we measure in nature (or in an experiment) are not negative either. The existence of negative frequencies is only advantageous for calculations. The relationship between the input and output frequencies is again linear, as can be seen in Fig. 5

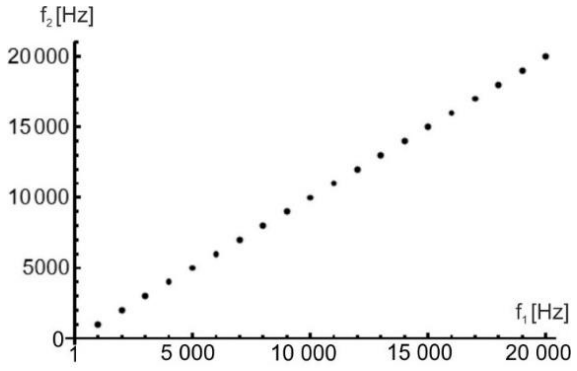


Fig. 5. The relationship between the input and output frequencies is also linear in its entirety. (Algorithm used in computer simulation 2: Fig. 4.)

3. RESULTS

The question is whether both methods of calculating the output frequency are equivalent. At first glance, it seems as if yes, as if we only make decisions based on the overall context of the calculation. Calculations and experience from older experiments [3] as well as from current simulations prove that significant errors occur when calculating frequencies close to 0 Hz according to Fig. 4 (or -10000 Hz according to Fig. 1). In such cases, it is advantageous to adjust the calculation so that the method shown in Fig. 1 can be used. In this case, the zero coordinate is only virtual and the error has no reason to occur. The reason for this phenomenon can be found in Fig. 2 and in the fact that a digital signal cannot acquire an arbitrary value (the frequency only changes with a step, or a larger multiple thereof). The spectrum is not linear even in the case of a purely harmonic signal, let alone in the case of a real NMR signal, where the harmonic signal is only one of the components of the measured signal. It has already been mentioned that the error consists of a "calculated error" [4] and a "measured error" that has been taken into account in these simulations. Both errors should be controlled and sufficiently low to comply with the permissible inaccuracy of the frequency determination.

4. DISCUSSION & CONCLUSIONS

The calculations according to both algorithms are indeed very similar, but the differences in the accuracy of the results are considerable. Especially in the area close to zero frequency. The components of the positive and negative maximum are partially mixed, distortions occur and the determination of the maximum frequency component is more difficult, the error can occur more easily. This applies to the measurement with the frequencies of both polarities of the spectrum, but also to the measurement with only one polarity. In the calculation according to simulation 2, an error greater than the expected 1.5 Hz occurs near the zero result value. The Mathematica 12.3. program package (Wolfram Research Inc., Champain IL) was used for the simulations. The solution of all problems was based on the use of this package and the instructions contained therein. With a different programming language or with different programming experience, many details can be solved differently than described. The situation when determining a result close to zero is shown in Fig. 6 (computer simulation 2). The image was created for illustration purposes only, it does not correspond exactly to Fig. 5. You can also use the figure to estimate the value of the result from which it can be considered accurate. Obviously, the size of the error has a certain correlation with the width of the spectrum (Fig. 2). Theoretically, the magnitude of the frequency determination error close to zero frequency should therefore be calculable, but it would be necessary to know the spectrum width around the signals *pos1* and *pos2* and this varies with the input signal. Fig. 7 shows a similar situation in the calculation according to computer simulation 1. Fig. 7(b) the images were artificially created to illustrate the emerging situation. They are similar to the data from the simulations in Fig. 7(a), but they do not correspond exactly. However, another additional error can occur with such a procedure: the accuracy of the zero point may be slightly different from the actual zero (due to the discrete nature of the frequency). The error can be easily detected by examining the situation around the zero point. It is similar to Fig. 7, but it is not necessary to make a picture, it is enough to calculate the position of the zero frequency sample. From this, the value of the sample frequency can be easily determined.

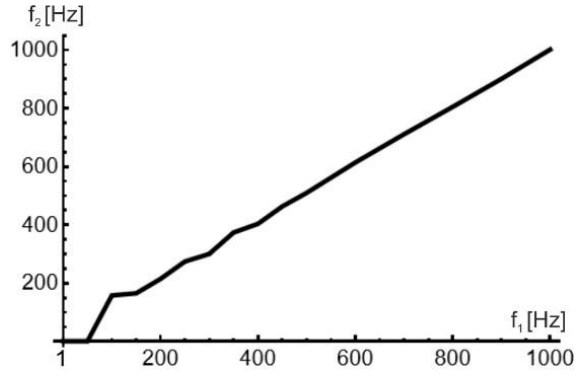
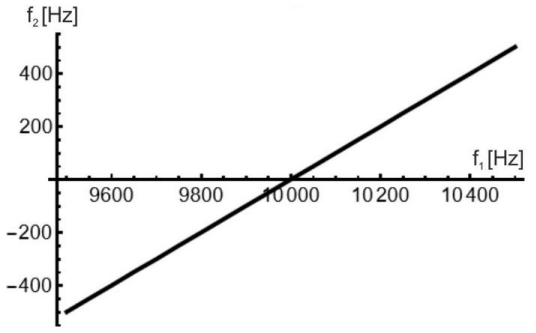
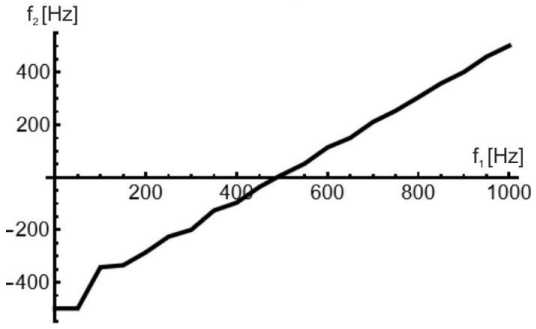


Fig. 6. The error occurs close to zero frequency. It can be overridden by generating a virtual zero at a higher frequency value. (Algorithm used in computer simulation 2: Fig. 4.)



(a)



(b)

Fig. 7. Error occurring near zero frequency suppressed by virtual zero (at 10000 or 500 Hz). (Algorithm used in computer simulation 1: Fig. 1.)

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