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Time Domain Spectroscopy of Linear Spin Wave Modes of Polarized Atomic Hydrogen Using a Linear Least Squares Technique

N. P. Bigelow, J. H. Freed and D. M. Lee

Laboratory of Atomic and Solid State Physics and
Baker Laboratory of Chemistry
Cornell University, Ithaca, NY, USA
and
B. W. Statt
Department of Physics, University of Toronto, Toronto, Ontario, Canada

The Fourier transform spectra of the free induction decays from our small tipping angle pulsed NMR experiments in spin polarized atomic hydrogen are characterized by a number of sharp resonances superimposed on an inhomogeneously broadened lineshape. The complex nature of the spectra makes quantitative analysis of the individual spin wave modes difficult, in particular hindering the extraction of damping factors and relative phases. We describe an application of a time domain fitting procedure based on a linear least squares analysis using linear prediction and singular value decomposition which yields numerical results that are compared directly to theoretical simulations.

INTRODUCTION

To date the primary technique used in the analysis of the spin wave modes in the free induction decays from our pulsed NMR experiments has been through Fourier analysis of the sampled and digitized time domain signals. A quantitative analysis of the frequency spectrum is difficult because of the overlap between the individual modes. In the past the analysis has been accomplished by fitting the experimental results to spectra generated from an analytic solution of the equations of motion which govern spin transport in the system [1]. However, the sensitivity of these fits to the adjustable parameters in the analytic solution is not sufficient to allow quantitative comparison to theoretical values for all of these parameters. In this report we describe the application of a time domain spectral decomposition technique [2,3] to aid in the analysis of the spin wave modes in our experiments.

METHOD

The method is based on a least squares fitting of the two orthogonal components of the time domain signal to a series of exponentially damped sinusoids, allowing the amplitude, frequency, damping and phase of each harmonic component to be parameters in the procedure. The fitting is linearized by use of a linear predictive (LP) method which formulates the problem as a matrix equation that is solved by a singular value decomposition (SVD). The stability of the fitting technique is enhanced by eliminating some of the singular values, an approach which assumes that the spectrum is composed of a finite number of harmonic modes that are distinguishable from the spectral content of the noise. In practice, the technique involves a geometric representation of the singular values which describe the spectral content of the signal so that a sensible cutoff can be determined for signal data as compared to noise. The final results are used to reconstruct a time domain signal which is directly compared to the actual signal. The process is then iterated with different cutoffs in order to refine the details of the fit.

The output from the fit is a table of frequencies, amplitudes, widths and phases of the individual complex Lorentzian components of the signal. The technique has a number of features which cannot easily be achieved with Fourier transformation and fitting in the frequency domain. The technique does not require the signal record to start at t=0 and continue until the signal disappears into the noise. In particular, an arbitrary 'time slice' of the signal can be taken from the free induction decay and analyzed for its spectral content without the distortions associated with frequency transformation of a truncated signal.

One of the initial assumptions in the technique is that the spectral components of the signal are Lorentzian in nature. Because this family of signals forms a complete basis set, the technique will by definition be able to fit any arbitrary signal. At first this may seem to place severe restriction on the signals which are suitable for this technique. However, unless the individual components of the signal are extremely close in frequency as compared to their widths, we find that we can reliably extract the details of the individual modes.

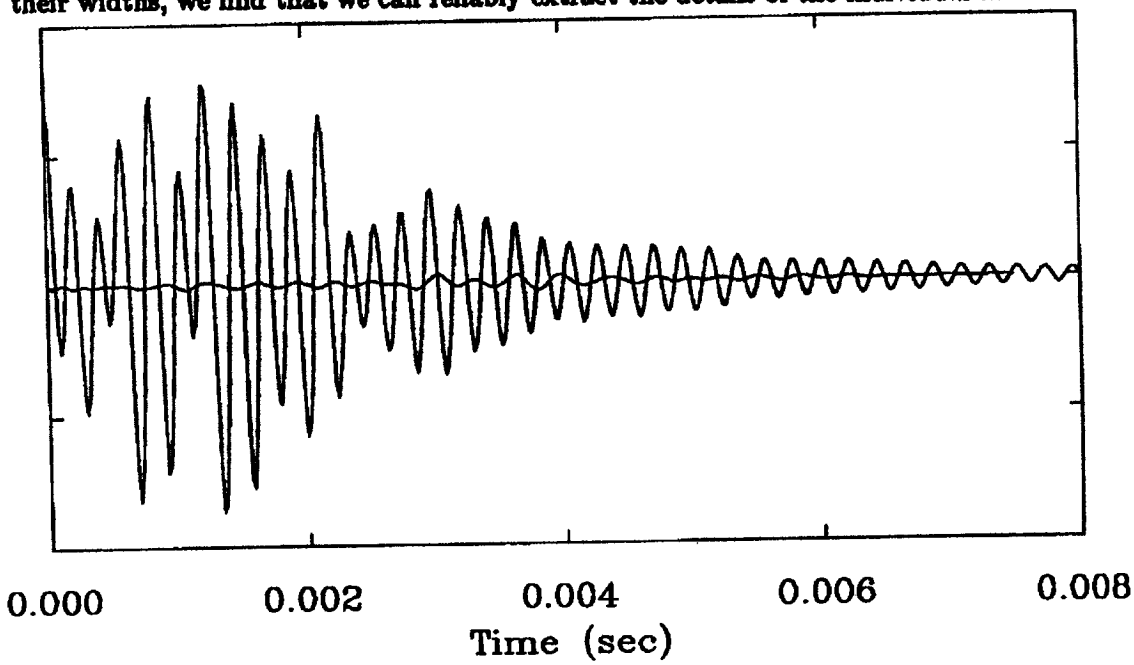

Figure 1. The free induction decay for pulsed NMR experiment in polarized atomic hydrogen. Superimposed on the signal is the signal reconstructed from the LPSVD fit to the data as well as the residual signal formed by subtracting the fit from the initial data. The residual signal has been scaled up in amplitude by 4 to enhance detail.

APPLICATION EXAMPLE

In order to assess the usefulness and accuracy of this method in the analysis of our NMR data we have started by fitting the free induction decays generated by a modeling program. The program is based on the analytic solution of the linearized equations of motion for our system. The results of the program have been compared to experimental results and shown to accurately represent the data [1]. The computer results were chosen

because the parameters which describe the individual modes in the spectra are accurately known and can be directly compared with the results of the LPSVD fit.

Figure 1 shows a comparison between a free induction decay of a typical first iteration fit and the starting signal; Figure 2 shows a comparison of the Fourier spectra for the same run. The numerical results of the first 7 spectral components are shown in Table 1 and are compared to the known values for the input signal. In this example the point spacing in the initial signal is 2 μsec and the fit was performed using only the first 250 points. As a starting point the routine was allowed to use up to 80 spectral components in fitting, only 15 of which were allowed to be considered significant (i.e. the remaining terms were to be attributed to spectral content of the noise). The comparison of the frequency spectra shows a striking agreement between the starting signal and the fit, an agreement which is confirmed in the residual signal formed by a subtraction of the starting time domain signal from the signal reconstructed from the fitting results.

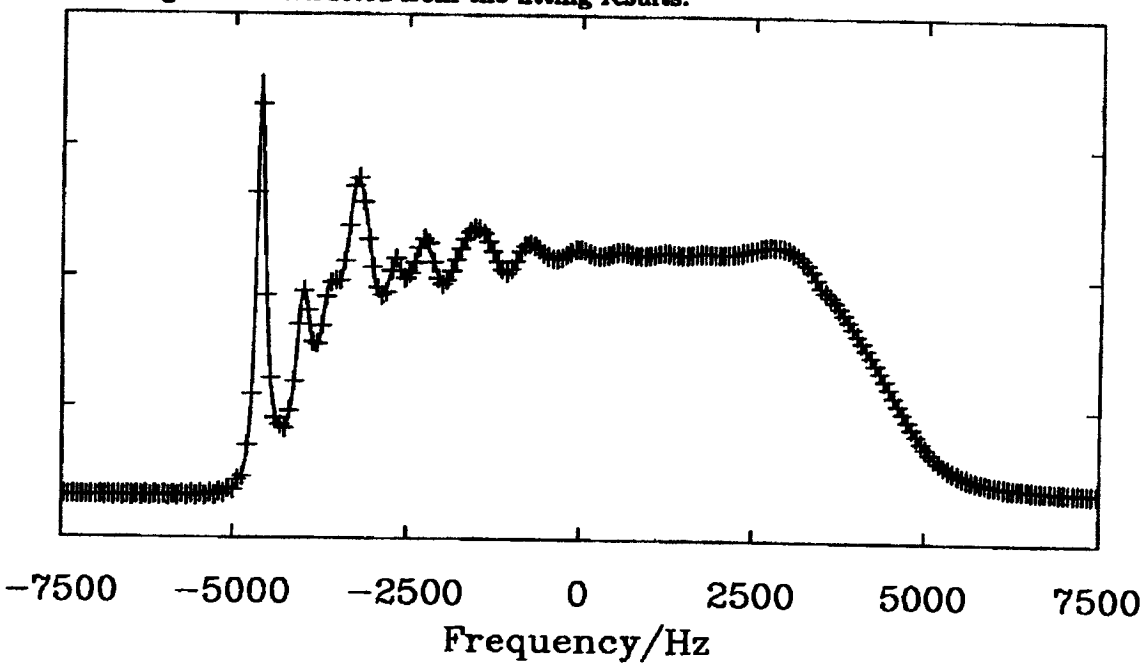

Figure 2. The fourier spectra for the example shown in Figure 1, as described in text. The continuous line is the spectra of the initial signal and the crosses are results of the LPSVD fit.

The results shown in Table 1 characterize a number of features of the application of LPSVD to the spin wave problem. The fit to the first and most prominent peaks is very good for all parameters of each component. The first major discrepancy is seen in the phase of the third mode, the mode which corresponds to the shoulder on the third clearly resolved peak in the frequency spectrum. In general, the first indication of a resolution problem in the fit of a particular mode is consistently reflected in the phase and width. The amplitudes of the components in the fit deviate more from the known values for the higher order modes. This effect is due to the increasing overlap of the higher modes with

their neighbors and the background lineshape. The fit also produces results not shown in Table 1 which correspond to the broad relatively flat portion on the right side of the spectrum. The fitting parameters for this portion of the spectrum bear little resemblence to the known components in the initial signal. The character of these components in the fit reflects an attempt to fit the broad flat region with a minimum number of broad flat Lorentzians and therefore neglects the underlying structure of many closely spaced modes.

Frequency (kH_z)		Inverse Linewidth $T_2(msec)$		Amplitude		Phase (degrees)	
lpsvd fit	initial signal	lpsvd fit	initial signal	lpsvd fit	initial signal	lpsvd fit	initial signal
4.626	4.627	2.148	2.152	4.399	4.391	9.46	9.58
4.009	4.017	1.184	1.198	3.198	3.054	6.73	11.2
3.653	3.644	0.77	1.02	4.02	2.50	27.3	6
	3.460		.86		1.33		7.31
3.246	3.264	0.79	.97	6.2	3.7	9.73	9.6
	3.11		.87		2.8		0.6
2.690	2.698	1.51	0.81	0.89	1.6	11.2	-20.1
	2.655		0.72		0.26		11.2
	2.30		0.70		0.27		9.6
2.19	2.28	0.77	0.65	0.31	0.21	-48	6.1
	2.10		0.58		0.12		7.3
1.509	1.483	0.205	0.280	0.31	0.26	6.2	9.6

Table. Comparison between spectral content of initial signal and results of LPSVD fit for an NMR free induction decay in spin polarized atomic hydrogen. Only the first seven dominant modes are shown.

CONCLUSIONS

The use of the LPSVD technique in the analysis of spin wave spectra in spin polarized atomic hydrogen will play an important role in a number of aspects of the experimental work. In the linear regime, the technique can be used to achieve a detailed fit to the individual modes. The results can then be compared to analytic solutions of the equations of motion as well as being used as initial conditions for a nonlinear least squares fit of the frequency spectra. In spin wave experiments in the nonlinear regime there have been a number of recent observations which indicate that the assessment of the relative phase of

individual components will play an important role in isolation of the nonlinear modes of the system. Figure 3 shows an example of a fit to one of the nonlinear Fourier spectra discussed in reference 4, this volume. Although there is good reason to expect that the nonlinear modes may be extremely non-Lorentzian in nature, this technique can be used to provide an measure of phase variation in the spectral content as well as providing a means of extracting the phases of any linear modes that may be present.

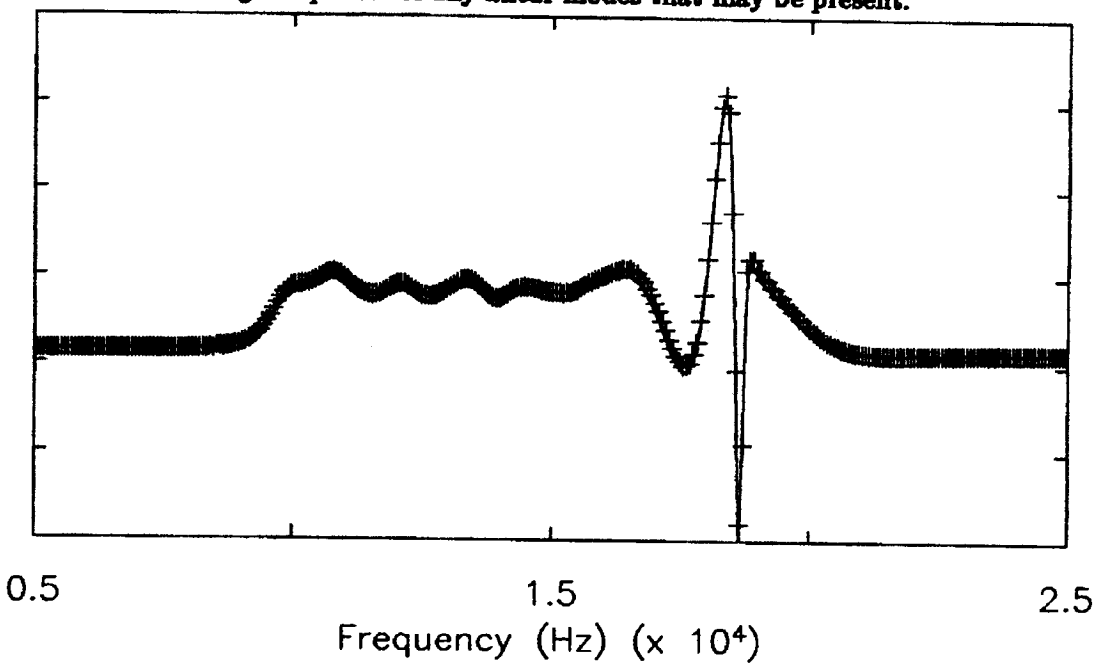

Figure 3. Fourier spectrum for large tipping angle pulsed NMR experiment which examines nonlinear effects on spin wave modes in spin polarized atomic hydrogen. The continuous line is the transform of the initial signal and the crosses are results from LPSVD fit.

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