

A new automatic phase correction method for FT NMR without using polynomial fitting

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Introduction:

Several methods (2,3,4) have been developed to automatically phase an NMR spectrum after Fourier transform of its free induction decay (FID) since Ernst (*I*) published the first automated phase correction procedure. All of these procedures use zero- and first-order phase correction as a final step, although they provide different ways to find out phase shifts at peaks by using maximization or minimization of peak areas or dispersion vs. absorption relation (DISPA). However, since they basically use phase shifts at peaks for linear fitting, first-order phase correction makes rolling baselines between peaks when the phase varies rapidly with frequency. If nonlinear (or higher-order) phase shifts which commonly occur in frequency-swept excitation are introduced into a spectrum, more complex polynomial fittings must be required. Here, a new phase correction method is proposed which corrects nonlinear phase shifts as well as linear ones without using any fitting algorithm. This method approaches phase correction by paying attention to partitioning the phase mode of a spectrum. The method is demonstrated by simulation and in phantom experiment.

Theory:

For two isochromats with offset frequencies Ω_1 and Ω_2 , the quadrature-detected NMR signal can be written as $s(t) = s_1(t) + s_2(t) = A_1 \exp(i\Omega_1 t) \exp(-\lambda_1 t) + A_2 \exp(i\Omega_2 t) \exp(-\lambda_2 t)$, where $\lambda = 1/T_2^*$, A_1 and A_2 are amplitudes of two isochromats. The spectrum of this signal is given by the sum of two Lorentzians: $S(\Omega) = S_1(\Omega) + S_2(\Omega) = A_1 / \{\lambda_1 + i(\Omega - \Omega_1)\} + A_2 / \{\lambda_2 + i(\Omega - \Omega_2)\}$. In this case, to a very good approximation, the phase of $S(\Omega)$ can be regarded as a simple combination of two phases of $S_1(\Omega)$ and $S_2(\Omega)$. Interestingly, they are partitioned by the demarcating frequency (Ω_d) which divides the phase into two regions according to the ratio of absolute values of two peaks, i.e., $\Omega_d \approx (|A_1| |\Omega_2| + |A_2| |\Omega_1|) / (|A_1| + |A_2|)$. For example, if $A_1:A_2 = 2:3$ with same λ for two peaks located at 0 and 200 Hz, Ω_d is analytically given by 79.99 Hz [Fig.1-a]. The difference in λ (or T_2^*) hardly affects Ω_d because a peak height is proportional to λ^{-1} whereas the linewidth is proportional to λ . If we perform the Fast Fourier transform (FFT) of a digitized $s(n)$, although the phase mode is a little different from that of Lorentzians due to digitization, the partition by the demarcating frequency index $k(\Omega_d)$ can also be applied [Fig.1-b]. When two peaks have their phase shifts of ϕ_1 and ϕ_2 , each phase tends to shift the phase in each partitioned region by ϕ_1 and ϕ_2 , respectively [Fig.1-c]. Therefore, the phase corrected spectrum $S_c(k) = S(k) \exp(-i\phi_1)$ in $[k(-FOV/2), k(\Omega_d)] + S(k) \exp(-i\phi_2)$ in $[k(\Omega_d), k(FOV/2)]$, where $\Omega = 2\pi k/N$ (FOV : Field of view, N : number of sampling points). The above analysis can be easily extended to the spectrum with many peaks. Lastly, phase shift at i^{th} peak is determined by calculating ϕ which maximizes the absorption Lorentzian $Ab(\Omega) = \cos\phi \operatorname{Re}(\Omega) + \sin\phi \operatorname{Im}(\Omega)$, where $\operatorname{Re}(\Omega)$ and $\operatorname{Im}(\Omega)$ are the real and imaginary parts of a spectrum.

Methods:

The program for the proposed method was developed using MATLAB 6.1. Three simulations of a FID signal were generated to test its performance. In all simulations, acquisition time was 1s. In the simulation for Fig.1, $A_1 = 4$ and $A_2 = 6$ with same T_2^* of 0.1s were used for two isochromats at 0 and 0.2 kHz. And, for Fig.1-c, two peaks were assumed to have phase shifts of $(3/4)\pi$ and $\pi/2$. N was 1,024. In another simulation for Fig.2, a spectrum with four peaks at -0.5, 0.2, 0.5, and 1 kHz was generated with strong linear phase shifts. All peaks have same A and T_2^* of 6 and 50ms. N was 4,096. The third simulation for Fig.3 was generated with strong quadratic phase shifts. Six isochromats of -1, -0.5, 0.1, 0.5, 1 and 1.5 kHz were assumed with same A of 6 with T_2^* of 50, 40, 25, 35, 45 and 60 ms, respectively. N was 4,096. For experimental data, a phantom experiment for NAA spectrum was performed in 9.4T with STEAM sequence. TR/TE was 6s/0.02s. Acquisition time was 2.0032s. N was 20,032.

Results: Fig.1 shows that a spectrum with two isochromats can be partitioned into two regions by the demarcating frequency weighted by absolute values of two peaks. And, when phase shifts were given in two peaks, each region partitioned by Ω_d (≈ 80 Hz) approximately is shifted by $(3/4)\pi$ ($=2.37$ rad) and $\pi/2$ ($=1.57$ rad), respectively [Fig. 1-c]. In Fig.2, in case of strong frequency-dependent phase shifts, the new method provides better phase-corrected spectrum than first-order phase correction with less rolling baselines. Fig.3 shows that the new method also corrects nonlinear phase errors well (here, quadratic phases). As compared to quadratic polynomial fitting, it works better especially when strong nonlinear phase shifts exist. Finally, as illustrated in Fig.4, it also works well on an experimental spectrum with spectral multiplets as well as a single peak.

Conclusion: The new method proposed here partitions a spectrum by the demarcating frequency which divides its phase into subregions and corrects phase shift in each subregion without using polynomial fitting. It works well on both linear and nonlinear phase shifts. It has big advantage over first- and higher order phase corrections, especially when strong phase shifts exist, in that there is less rolling baselines and it doesn't need phase-unwrapping which is required for fitting. This new phase correction method is simple, easy to implement, and not time consuming as well.

References: (1) R.Ernst, *JMR* 1, 7-26 (1969) (2) E.Craig & A.Marshall, *JMR* 76, 458-475 (1988) (3) E.Wachter *et al*, *JMR* 82, 352-359 (1989) (4) F.Montigny *et al*, *Anal. Chem.* 62, 864-867 (1990)

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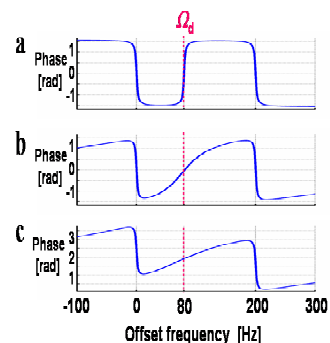


Fig.1 The phase modes of (a) Lorentzians (b) Spectrum after FFT (c) Phase-shifted spectrum after FFT

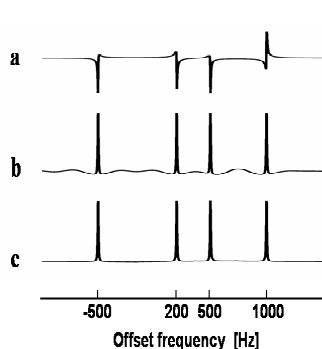


Fig.2 Simulation (a) Linear phases (b) First-order phase correction (c) New phase correction

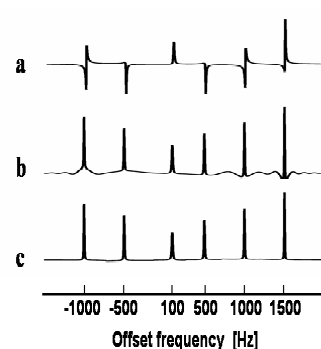


Fig.3 Simulation (a) Quadratic phases (b) Second-order phase correction (c) New phase correction

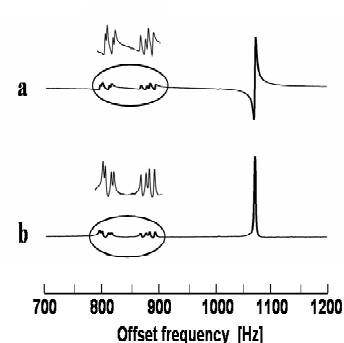


Fig.4 Experimental spectrum (NAA spectrum) (a) Before phase correction (b) New phase correction