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Discrete Fourier Transformation of NMR Signals. The Relationship between Sampling Delay Time and Spectral Baseline

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Fourier transformation is the most commonly used method for converting time-domain NMR signals into frequency-domain data. It is well known that a delay in sampling the first data point of the FID can result in distortion of the baseline (offset and curvature) of the frequency-domain spectrum. Early analyses (1, 2) of this problem led to the conclusion that spectral distortions are minimized if the free-induction decay signal is sampled without delay, i.e., the first time-domain data point is acquired when all time-domain signal components are in phase. However, this conclusion is based on the theory of continuous Fourier transformation. As pointed out by Otting *et al.* (3), when the NMR signal is processed using a discrete Fourier transform (DFT) and the FID is sampled without delay, the first time-domain data point must be multiplied by 0.5 prior to DFT in order to minimize baseline offset. Recently, it has been shown experimentally and by calculated examples (4) that baseline offset and curvature are minimized if sampling of the FID is delayed by half a dwell time. Below we demonstrate that this result follows directly from the mathematics of the DFT. We further show that all sampling delays other than zero, one-half, or one full dwell time lead to significant baseline curvature.

The DFT is defined as

$$F\left(\frac{l}{N\Delta t}\right) = \sum_{k=0}^{N-1} S(k\Delta t)\exp(-i2\pi lk/N), \quad [1]$$

where S is the FID composed of N data points, Δt is the sampling interval or dwell time, and the variables l and k refer to the lth and kth data point in the frequency and time domains, respectively. The DFT yields data only at frequencies $\nu = l/N\Delta t$. To simplify the discussion $S(t)$ is assumed to consist of P exponentially damped sinusoids and, as DFT is a linear operation, a single such frequency component can be considered without loss of generality, and the FID is given by

$$S_k = S(k\Delta t) = a\exp[(i2\pi\nu_0 - R_2)(k\Delta t + T_d) + i\psi], \quad k = 0, 1, 2, \ldots, N-1, \quad [2]$$

where Δt is the dwell time, ψ, a, R_2, and ν_0 are the initial phase, amplitude, transverse relaxation rate, and frequency of the resonance considered, respectively, and T_d is the sampling delay time between the RF pulse and the first data point of the FID. For complex data, the initial phase ψ can be removed by multiplication of the FID by $\exp(-i\psi)$, and this term may therefore be ignored. The frequency-domain spectrum is obtained by substituting Eq. [2] into Eq. [1] and carrying out the summation (5, 6)

$$F(\nu) = \sum_{k=0}^{N-1} A\exp\{k[(i2\pi(\nu_0 - \nu) - R_2)\Delta t]\}$$

$$= A\frac{1 - \exp\{[i2\pi(\nu_0 - \nu) - R_2]T_{acq}\}}{1 - \exp\{[i2\pi(\nu_0 - \nu) - R_2]/\mathrm{SW}\}}, \quad [3]$$

where the spectral width, SW, equals $1/\Delta t$, the total acquisition time, T_{acq}, equals $N\Delta t$, and $A = a\exp[(i2\pi\nu_0 - R_2)T_d]$. The right-hand side of Eq. [3] reduces to a Lorentzian in the limits $\Delta t \to 0$ ($\mathrm{SW} \to \infty$) and $T_{acq} \to \infty$.

As A in Eq. [3] contains a linear frequency-dependent phase term, $\exp(i2\pi\nu_0 T_d)$, a linear phase correction is generally used to make all signals absorptive. If the spectrum is arranged such that the frequency ν_0 is within the range $[-\mathrm{SW}/2, \mathrm{SW}/2]$, the linear phase correction involves multiplication of the nth data point by $\exp[i(\phi_0 + \phi_1 n/N)]$, where ϕ_0 and ϕ_1 are the zeroth- and first-order phase corrections and N is the total number of complex data points of the FID (including zero filling). As no phase correction is ever needed for a resonance at $\nu_0 = 0$, it immediately follows that $\phi_0 = -\phi_1/2$ and $\phi_1 = 2\pi T_d/\Delta t$. For example, when T_d is half a dwell time, $\phi_0 = -90°$ and $\phi_1 = 180°$.

In order to simplify the subsequent discussion, four symbols are defined as follows: $\omega_0 = 2\pi(\nu_0 - \nu)$, $h = \mathrm{SW}/R_2$, $b = (R_2 - i\omega_0)/\mathrm{SW}$, and $x = 2T_d\mathrm{SW}$. Applying a linear phase correction by multiplying Eq. [3] with $\exp(-i2\pi\nu T_d)$ results in

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$$F(\nu) = (1/2)a[1 - \exp(-Nb)] \times \exp[(1-x)(b/2)]\mathrm{csch}(b/2). \quad [4]$$

With the assumption that $\exp(-Nb) \rightarrow 0$ (i.e., no truncation) and use of the series expansions

$$\exp[(1-x)(b/2)] = 1 + (b/2)(1-x) + (b^2/8)(1-x)^2 + (b^3/48)(1-x)^3 + \cdots,$$

and

$$\mathrm{csch}(b/2) = (2/b) - (b/12) + (7b^3/2880) + \cdots,$$

the real part of Eq. [4] yields a "phased" spectrum of the form

$$\mathrm{Re}[F(\nu)] = a[L(\omega_0) + f_0(x) + f_1(\omega_m, x) + \cdots] \quad [5]$$

with

$$L(\omega_0) = \frac{h}{1 + (\omega_0/R_2)^2},$$

$$f_0(x) = \left\{\frac{(1-x)}{2} - \frac{[(1/3) - (1-x)^2]}{8h} - \frac{[x(1-x)(2-x)]}{48h^2} + \frac{[7 - 30(1-x)^2 + 15(1-x)^4]}{5760h^3}\right\} + \cdots,$$

and

$$f_1(\omega_0, x) = \frac{(\omega_0/\mathrm{SW})^2[x(1-x)(2-x)]}{48} - \frac{(\omega_0/\mathrm{SW})^2[7 - 30(1-x)^2 + 15(1-x)^4]}{1920h} + \cdots.$$

Equation [5] expresses the relationship between x ($=2T_d/\Delta t$) and the baseline. The first term, $L(\omega_0)$, gives rise to a Lorentzian-type peak. The function $f_0(x)$ represents a constant spectral baseline offset whereas $f_1(\omega_0, x)$ represents baseline curvature. When the spectral width is much larger than the linewidth ($h \gg 1$), one obtains $f(x) = (1-x)/2$ and $f_1(\omega_0, x) = (\omega_0/\mathrm{SW})^2 x(1-x)(2-x)/48$. The curvature term, $f_1(\omega_0, x)$, equals 0 only when x equals 0, 1, or 2, i.e., when T_d is zero, one-half, or one full dwell time.

If the spectral width is much larger than the linewidth, Eq. [5] shows that the constant baseline offset equals $a(0.5 - T_d/\Delta t)$. To a first approximation, this baseline offset is therefore equal to the first data point of the time-domain signal, scaled by $(0.5 - T_d/\Delta t)$. Consequently, the baseline offset can largely be removed by subtracting the scaled first data point from every $F(\nu)$. If the initial phase of the time-domain signal (ψ in Eq. [2]) is not zero at time zero but has been corrected to obtain a phased spectrum, the same phase correction [multiplication by $\exp(-i\psi)$] must be applied to the first data point of the FID prior to scaling and subtraction from the phased spectrum.

The subtraction procedure mentioned above is similar but not identical to the scaling of the first time-domain data point prior to DFT and phase correction (*3*). In the latter procedure, the first time-domain data point is multiplied by $(0.5 + T_d/\Delta t)$, which is equivalent to subtracting a fraction $(0.5 - T_d/\Delta t)$. Although Fourier transformation of this "subtracted fraction" of the first time-domain data point yields the same baseline offset as the procedure described above, the subsequent linearly frequency-dependent phase correction is automatically applied to this baseline offset term, adding to the baseline curvature and changing the average baseline offset.

Figure 1 illustrates the baseline curvature and offset of a simulated spectrum for a T_d value of $0.25\Delta t$, for a time-domain signal containing two exponentially decaying signals of equal amplitude at frequencies of 0 and 0.4SW and linewidths at half-height of 0.005SW. Empirical functions for the baseline offset and curvature are defined by considering only that fraction of the baseline which is distant by more

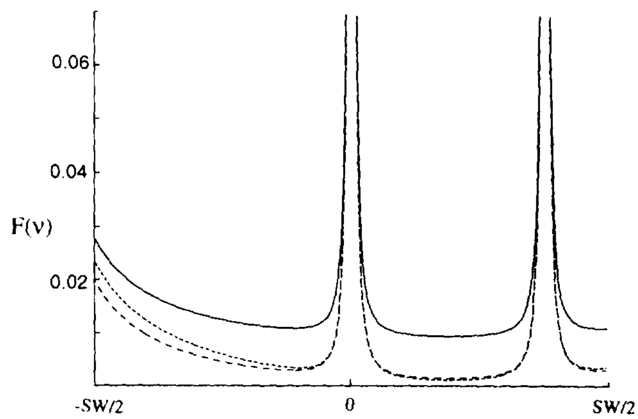

FIG. 1. Baseline region of a simulated spectrum, obtained from Fourier transformation of a time-domain signal, containing two frequency components, one at $\nu = 0$ and one at $\nu = 0.4$SW. The linewidth at half-height for each of the components is set to SW/200. This time-domain signal is described by $S_k = \exp[-(k + 0.25)(\pi\mathrm{SW}/200)] + \exp[-(k + 0.25)(\pi\mathrm{SW}/200 + 0.4i)]$, with $k = 0, \ldots, 1023$, i.e., with sampling of the first data point delayed by one-quarter dwell time. The solid line corresponds to the phase-corrected Fourier transform; short dashes correspond to the case where the first data point has been scaled by 0.75 prior to Fourier transformation and phase correction. Long dashes correspond to the spectrum obtained by subtracting the Fourier transform of $0.25S_0$ from the phase-corrected Fourier transform. The spectral amplitude has been scaled such that the resonance at zero frequency has unit intensity.

than 20 times the linewidth from the center of either resonance. Thus, the baseline extends from −0.5SW to −0.1SW and from 0.1SW to 0.3SW. The offset function, $O(T_d)$, is simply defined as the average deviation from zero of all B baseline points in the region defined above. The curvature, $C(T_d)$, is defined as the root-mean-square deviation (rmsd) of the spectral baseline from $O(T_d)$:

$$C(T_d) = \left(\sum [F(n/N\Delta t) - O(T_d)]^2/B \right)^{1/2}, \quad [6]$$

where the summation extends over all B data points in the baseline region defined above. The short dashes in Fig. 2 show the baseline offset and curvature of the spectrum, after application of the linearly frequency-dependent phase correction, as a function of the delay time T_d, with and without scaling of the first data point. Although multiplication of the first time-domain data point by $(0.5 + T_d/\Delta t)$ reduces the baseline offset (Fig. 2A), this scaling procedure *increases* baseline curvature (Fig. 2B) for all values of $T_d/\Delta t$. In contrast, if $(0.5 - T_d/\Delta t)S_0$ is subtracted from the unscaled spectrum of Eq. [5], the baseline offset is reduced more than with simple scaling alone and additionally the curvature is not increased (long dashes in Fig. 2). However, it is clear that for neither of the two correction procedures are adequate baselines obtained unless $T_d = 0$ or $T_d = \Delta t/2$. For $T_d = 1$, the curvature is at a minimum, but baseline offset is large.

The above discussion has focused on Fourier transformation of complex data. A real time-domain signal, $S_k = a \cos[(2\pi\nu_0)(k\Delta t + T_d) + \psi]\exp[-kR_2(k\Delta t + T_d)]$, can be written as the sum of two complex signals with opposite frequency and phase by substituting zeroes for the imaginary component:

$$S_k = (1/2)\{a \exp[(i2\pi\nu_0 - R_2)(k\Delta t + T_d) + i\psi] + a \exp[(-i2\pi\nu_0 - R_2)(k\Delta t + T_d) - i\psi]\}. \quad [7]$$

Although signals acquired using the Redfield (*7*) or TPPI (*8*) protocol are acquired as real data, an additional complication arises in this case from the fact that the carrier frequency is located in the center of the real Fourier transform and not at its left-hand side. At the time that the first data point (S_0) is sampled, the phase of the signal therefore equals $2\pi(\nu_0 - SW/4)T_d + \psi$, where SW refers to the spectral width ($1/\Delta t$) after the data have been converted to the complex format. Equation [7] then must be rewritten as

$$S_k = (1/2)\{a \exp[i2\pi\nu_0 - R_2)(k\Delta t + T_d) + i(\psi - \pi T_d/2\Delta t)] + a \exp[(-i2\pi\nu_0 - R_2)(k\Delta t + T_d) - i(\psi - \pi T_d/2\Delta t)]\}. \quad [8]$$

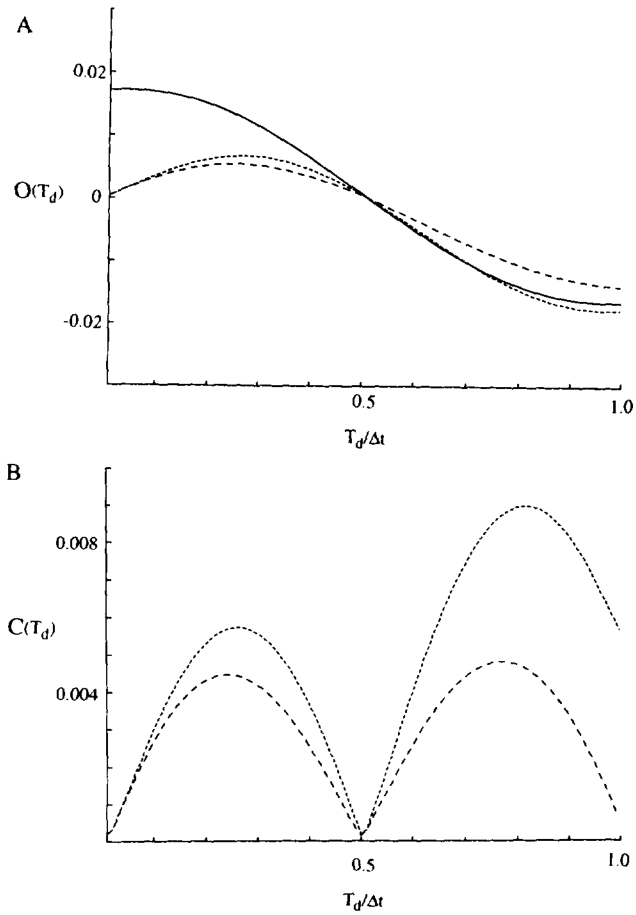

FIG. 2. The baseline offset, $O(T_d)$, and curvature, $C(T_d)$, as defined in the text for the regular phase-corrected Fourier transform (solid line), for the phase-corrected Fourier transform after scaling of the first data point by $[0.5 + (T_d/\Delta t)]$ (short dashes), and for unscaled phase-corrected Fourier transform after subtracting $[0.5 - (T_d/\Delta t)]S_0$ (long dashes). For the curvature function, the solid line coincides with long dashes, and therefore only the latter are shown.

The requirement for minimal baseline curvature caused by frequency-dependent phase correction remains that T_d is zero, one-half, or one full dwell time. However, as the frequency-independent phase error, $\psi - \pi T_d/2\Delta t$, is of opposite sign for the true signal component and its mirror image, an additional baseline distortion results if the true resonance and its mirror image cannot be phase-corrected simultaneously (*9*). Therefore, in the case of TPPI, an additional requirement is given by

$$\psi - \pi T_d/2\Delta t = n\pi/2 \quad (n = 0, 1, 2, 3), \quad [9]$$

which means that if $T_d = 0$, ψ should be $n\pi/2$ (*9*). If $T_d = \Delta t/2$, ψ must be $\pi/4 + n\pi/2$, and if $T_d = \Delta t$, ψ must be equal to $n\pi/2$ (*10*). The baseline offset terms, $f_0(x)$ in Eq. [5], associated with the true resonance and with its mirror image are of opposite sign if n in Eq. [9] is 1 or 3, resulting in minimal baseline offset. Thus, if $T_d = 0$, ψ should be $\pi/2$ or $3\pi/2$, corresponding to sinusoidal modulation (*3*); if $T_d = \Delta t/2$, ψ should be $\pi/4$ or $5\pi/4$, and when $T_d = \Delta t$, ψ should be 0 or π, corresponding to cosinusoidal modulation (*10*).

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