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# NOTES

## Composite Inversion Pulses of Short Total Duration*

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Composite pulse sequences have been extensively studied (*1*) and found to be useful in a number of applications since their introduction in 1979 by Levitt (*2*). Examples of the use of composite pulses are: offset-insensitive inversion ($\pi$) pulses (*1*) (i.e., $M_z \rightarrow -M_z$), offset-insensitive $\pi/2$ pulses (e.g., $M_z \rightarrow M_x$) with small phase distortions (*3, 4*), and $\pi$ pulses insensitive to offsets and also insensitive to phase distortion (e.g., $M_x \rightarrow -M_x$).

Regarding inversion pulses, numerous early studies, both theoretical and experimental (*2, 5–7*), have been undertaken and numerous composite pulse sequences have been suggested. Some of these contain many pulses obtained by an unconstrained minimization approach (*8*). Despite these investigations, the simple three-pulse sequence $90^\circ_{0^\circ}$ $180^\circ_{90^\circ}$ $90^\circ_{0^\circ}$ is used for inversion on the majority of spectrometers because the longer and more elaborate the composite pulse sequences, the less likely they are to be used by the spectroscopist. In this paper we report two- and three-pulse composite sequences which perform better than the $90^\circ_{0^\circ}$ $180^\circ_{90^\circ}$ $90^\circ_{0^\circ}$ sequence. We restrict the number to a maximum of three, not only because of computer memory limitations, but also so that these might be short enough to remain hard and to serve as alternatives to the $90^\circ_{0^\circ}$ $180^\circ_{90^\circ}$ $90^\circ_{0^\circ}$ sequence.

Our approach to the problem of obtaining offset-insensitive composite pulse sequences is to start with the well-known fact that a product of rotations is itself a rotation. Since a hard pulse is described by a rotation, composite pulses can be studied from the properties of Wigner rotation matrices (*9–11*),

$$\mathbf{D}(\Omega) = \prod_{i=1}^{n} \mathbf{D}(\Omega_i). \qquad [1]$$

The time- and offset-dependence Euler angles $\Omega_i$ are well known (*10, 11*) and are needed to describe the resonance offset $\Delta\omega = \omega - \omega_0$, where $\omega$ is the carrier frequency and $\omega_0$ the Larmor frequency. Our first work on this topic (*10*) used the properties of the rotation matrices (*9*) to understand some existing pulse sequences. Later (*11*), general formulas were given without approximations which describe the resultant angles in terms of the composite angles for any number of pulses. Therefore, to study composite pulses of practical number, approximate methods, such as average Hamiltonian theory (*3*), are not needed. The approach of (*11*) was put to use (*12*) to find three phase-alternating composite pulse sequences composed of three-, four-, and six-component pulses. These performed well to offsets ($|\Delta\omega/\omega_1|$, where $\omega_1$ is the RF amplitude) of respectively 1, 1.5, and 1.8. These composite pulse sequences were found by using the exact relations in (*11*) to obtain analytical expressions for $\cos(\beta_{1\ldots n})$, where $\beta_{1\ldots n}$ is the net result of $n$ composite pulses. This expression, along with the analytical expressions for the derivatives, can be used in minimization routines to constrain $\cos(\beta_{1\ldots n})$ to equal $-1$ as a function of $\Delta\omega/\omega_1$. As $n$ increases, however, the size of the algebraic expressions increases by about the power $n$.

In this paper, we extend the methods of (*11*) and (*12*) from phase-alternating to arbitrary-phase composite pulses and seek nominal flip angles $\beta_i^0$ and phases $\phi_i$ such that

$$(\beta_1^0)_0 \, (\beta_2^0)_{\phi_2} \, (\beta_3^0)_{\phi_3} \qquad [2]$$

is as insensitive as possible to offsets $\Delta\omega/\omega_1$. Using the algebraic computer language REDUCE, the result of multiplying two and three rotation matrices is calculated for use in a minimization routine. By this method, the flattest two-pulse composite sequence is

$$198.5^\circ_{0^\circ} \; 382.3^\circ_{204^\circ}. \qquad [3]$$

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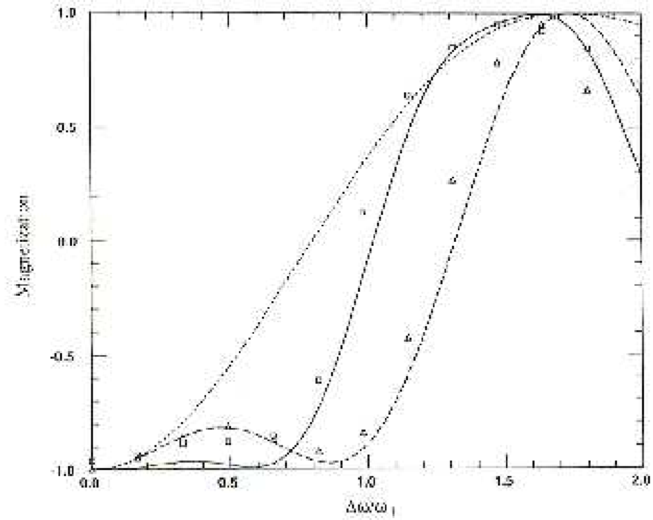


FIG. 1. Comparison of a simple 180° inversion pulse (---) the $90^\circ_{0^\circ}$ $180^\circ_{90^\circ}$ $90^\circ_{0^\circ}$ composite pulses (– – –, △), and $198^\circ_{0^\circ}$ $382^\circ_{84^\circ}$ composite pulses (—, □). The lines are theoretical and the points are experimental.

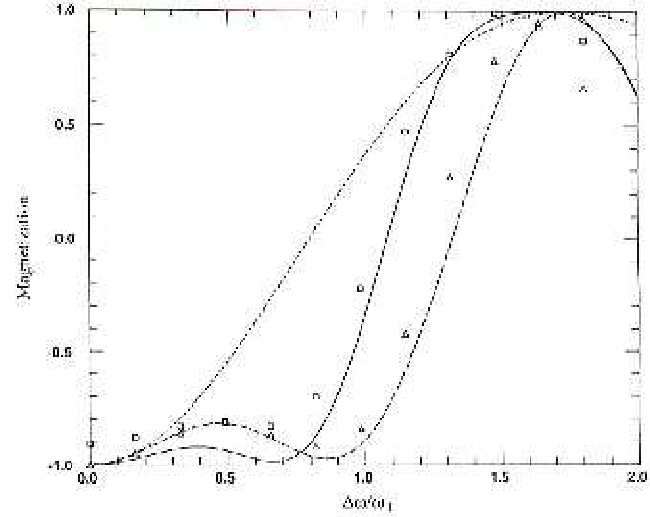


FIG. 2. Comparison of a simple 180° inversion pulse (---), the $90^\circ_{0^\circ}$ $180^\circ_{90^\circ}$ $90^\circ_{0^\circ}$ composite pulses (– – –, △), and the $183^\circ_{0^\circ}$ $370^\circ_{210^\circ}$ composite pulses (—, □). The lines are theoretical and the points are experimental.

This is plotted in Fig. 1 and compared to a simple 180° pulse and a $90^\circ_{0^\circ}$ $180^\circ_{90^\circ}$ $90^\circ_{0^\circ}$ sequence. Although [3] does not extend out as far as the $90^\circ_{0^\circ}$ $180^\circ_{90^\circ}$ $90^\circ_{0^\circ}$ sequence, it is much flatter and inverts spins by about 80% out to an offset $|\Delta\omega/\omega_1|$ of 0.8. The sequence $183^\circ_{0^\circ}$ $370^\circ_{210^\circ}$ is shown in Fig. 2 and, although not as flat as [3], extends out to slightly higher offsets.

The best three-pulse composite sequence is

$$247.6^\circ_{0^\circ}\ 120^\circ_{227.9^\circ}\ 81.8^\circ_{80.3^\circ}, \qquad [4]$$

which performs much better than the $90^\circ_{0^\circ}$ $180^\circ_{90^\circ}$ $90^\circ_{0^\circ}$ sequence and works out to $|\Delta\omega/\omega_1| \cong 1.4$ (Fig. 3). Other good three-pulse composites are

$$78^\circ_{0^\circ}\ 195^\circ_{182^\circ}\ 318^\circ_{12^\circ}, \qquad [5]$$

which is very flat out to $|\Delta\omega/\omega_1| \cong 1$ (see Fig. 4), while

$$86^\circ_{0^\circ}\ 160^\circ_{180^\circ}\ 260^\circ_{0^\circ} \qquad [6]$$

is less flat but is good to about $|\Delta\omega/\omega_1| \cong 1.25$ (see Fig. 5). Finally, Fig. 6 shows a sequence obtained by minimization which is almost the reverse of [6] being $260^\circ_{0^\circ}$ $161^\circ_{190^\circ}$ $85^\circ_{1^\circ}$.

The two-pulse composite sequences, by varying the two flip angles and one phase angle, form a three-dimensional parameter space, while the three-pulse composite sequences form a five-dimensional parameter space. Since the minimization routines are nonlinear, the starting guesses are critical. We have tried numerous starting guesses and, for the two-pulse composites that converge, all end up close to [3], while for the three-pulse sequences, all converging starting guesses end up close to either [4] or [5]. We conclude that we have located the absolute minimums of these parameter spaces.

Extension to higher numbers of pulse components will be possible for four, but, with the present computer memory limitations, no higher. The seven-dimensional parameter space for $n = 4$ is described by a function of the type shown in (*12*, Table 1), but it has about 10,000 lines of FORTRAN code. To go beyond $n = 4$, numerical functions and derivatives will be needed, although a four-pulse composite sequence might be sufficient while still being not too cumbersome for practical experimental use.

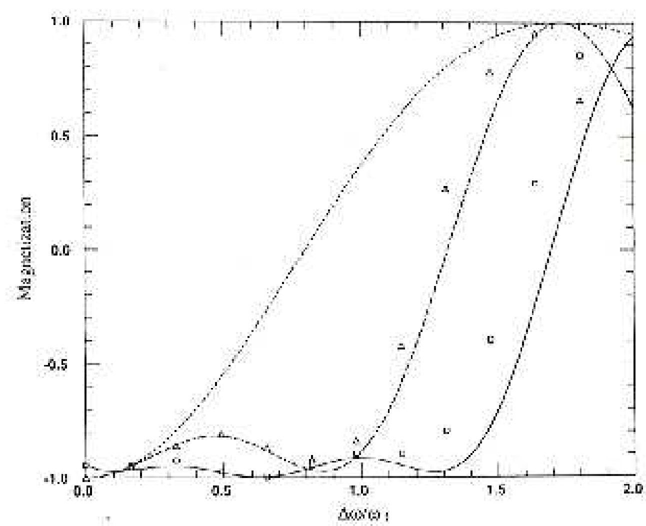


FIG. 3. Comparison of a simple 180° inversion pulse (---), the $90^\circ_{0^\circ}$ $180^\circ_{90^\circ}$ $90^\circ_{0^\circ}$ composite pulses (– – –, △), and the $248^\circ_{0^\circ}$ $120^\circ_{228^\circ}$ $82^\circ_{80^\circ}$ composite pulses (—, □). The lines are theoretical and the points are experimental.

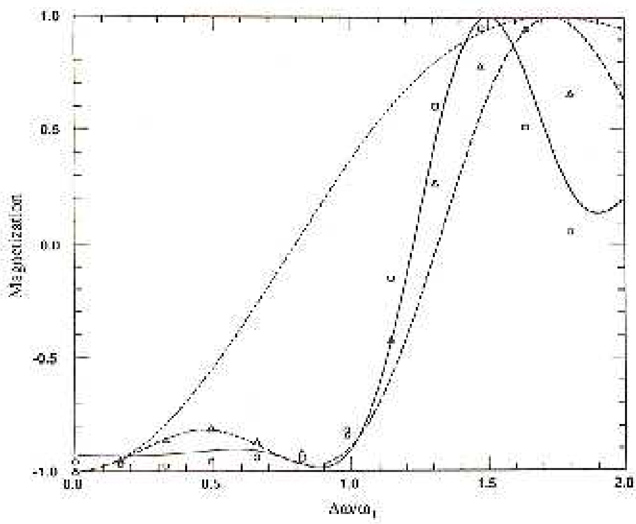


FIG. 4. Comparison of a simple 180° inversion pulse (---), the $90^\circ_0$ $180^\circ_{90}$ $90^\circ_0$ composite pulses (– – –, △), and the $78^\circ_0$ $195^\circ_{132}$ $318^\circ_2$ composite pulses (—, □). The lines are theoretical and the points are experimental.

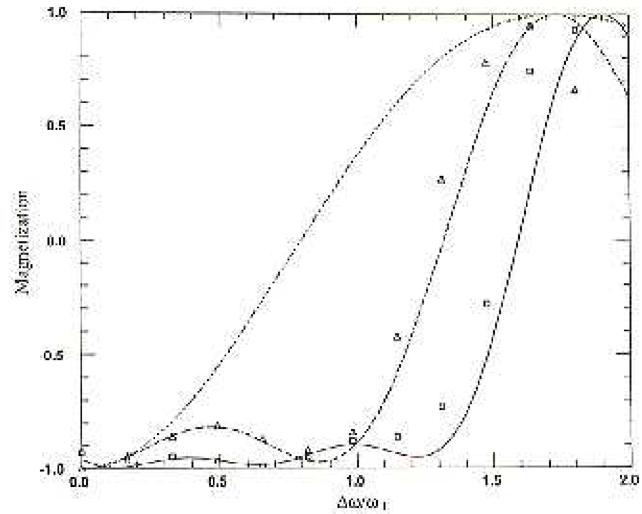


FIG. 6. Comparison of a simple 180° inversion pulse (---), the $90^\circ_0$ $180^\circ_{90}$ $90^\circ_0$ composite pulses (– – –, △), and the $260^\circ_0$ $161^\circ_{90}$ $85^\circ_0$ composite pulses (—, □). The lines are theoretical and the points are experimental.

The experimental points in Figs. 1–6 are for a 2% $H_2O$ sample in $D_2O$ lightly doped with $Cr(AcAc)_3$. All data were collected at 500 MHz on a Varian VXR 500S NMR spectrometer at a radiofrequency field strength of 1.22 kHz for line inversion. The agreement between theory and experiment is convincing. Furthermore, the sequences are robust to about 1° of the theoretically predicted sequences. Most modern research-grade spectrometers can now accurately perform small-angle phase shifts, so there should be no reason to limit ourselves to 90° phase shifts as was the case when the $90^\circ_0$ $180^\circ_{90}$ $90^\circ_0$ sequence was first proposed.

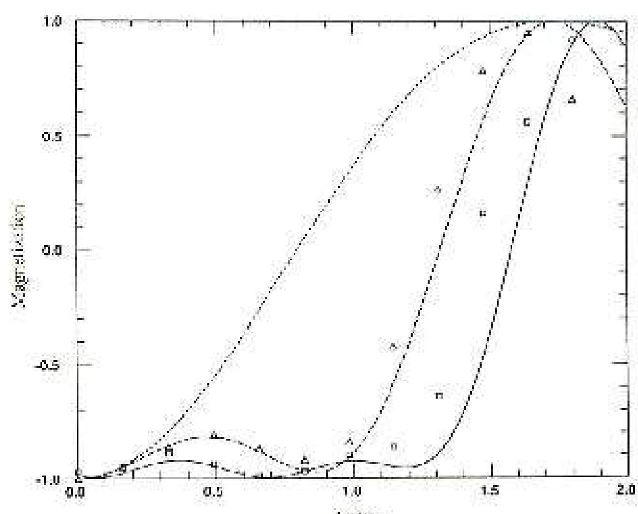


FIG. 5. Comparison of a simple 180° inversion pulse (---), the $90^\circ_0$ $180^\circ_{90}$ $90^\circ_0$ composite pulses (– – –, △), and the $86^\circ_0$ $160^\circ_{180}$ $260^\circ_0$ composite pulses (—, □). The lines are theoretical and the points are experimental.

## ACKNOWLEDGMENTS

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