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Composite Pulses without Phase Distortion

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Composite pulses for broadband spin excitation over large ranges of radiofrequency field amplitudes and resonance offsets are presented. They are derived according to a previously presented method based on the Magnus expansion in the manner of coherent averaging theory. It is shown theoretically and in simulations that these composite pulses do not introduce a strong dependence of the NMR signal phase on the rf amplitude or resonance offset, overcoming a common problem of composite pulses derived by other means. Experimental demonstrations include the use of composite π pulses for refocusing transverse magnetization in spin-echo sequences and the use of composite $\pi/2$ pulses in a simple multiple-pulse experiment. Further applications are discussed.

INTRODUCTION

Beginning with the original work of Levitt and Freeman five years ago, the development of composite pulses has been an area of active research in NMR (*1–12*) and in coherent optics (*13*). Composite pulses are sequences of phase-shifted radiofrequency pulses intended, in the case of NMR, to excite nuclear spins over a larger range of some experimental parameter than the single π or $\pi/2$ pulses that they replace. The experimental parameters considered to date are the resonance offset (*1–8*), the rf amplitude (*1–3, 6, 8–10*), and spin coupling constants (*11, 12*). Several theoretical approaches to the design of composite pulses have appeared, including simulations of magnetization trajectories (*1, 2*), geometric arguments based on rotation operators (*3, 4, 9*), approximations to adiabatic following (*7*), and iterative schemes (*10*). All of these approaches suffer from a common problem, which may be called phase distortion. The meaning and importance of phase distortion should become apparent in the following two examples and in Fig. 1.

Consider a composite $\pi/2$ pulse designed for broadband excitation with respect to the rf amplitude. The composite $\pi/2$ pulse will rotate magnetization from its equilibrium position aligned with the static magnetic field (z axis) to a position in the transverse (xy) plane over a large range of rf amplitudes. However, the specific direction in the transverse plane typically varies with the rf amplitude. If the FID signal is detected the phase of the signal will be a function of the rf amplitude. If appreciable rf amplitude inhomogeneity exists across the sample, then signals arising from different locations will partially cancel one another.

As a second example, consider a composite π pulse, again designed to cover a broad rf amplitude band. The composite π pulse will rotate magnetization from its

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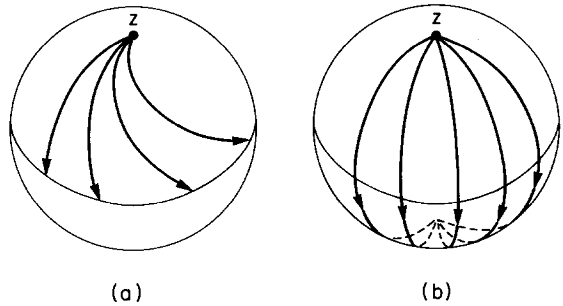

FIG. 1. Phase distortion in composite pulses. (a) As the resonance offset or the rf amplitude varies, the net rotation angle and the net rotation axis of a composite $\pi/2$ pulse change. This is indicated by magnetization trajectories on a unit sphere, corresponding to the net rotation produced by a hypothetical composite $\pi/2$ pulse for various values of the resonance offset or rf amplitude. (b) For a composite π pulse, it is the net rotation axis that changes, even though magnetization may be inverted over a range of resonance offsets or rf amplitudes.

equilibrium position parallel to the static magnetic field to a position antiparallel to the field, over a large range of rf amplitudes. For certain experiments, this broadband inversion property is all that is required. However, π pulses are also commonly used as refocussing pulses, for example in spin-echo experiments. As has been pointed out by Levitt and Freeman (*3*), the phase of the echo signal in a single echo experiment employing a composite π pulse is typically a function of the rf amplitude. If substantial rf inhomogeneity is present, significant cancellation of the echo signal may result.

Radiofrequency inhomogeneity is a particularly important factor in *in vivo* NMR studies using surface coils (*14*) and implanted coils (*15*). Surface coils may be used to achieve spatial localization of NMR signals. If a high degree of spatial localization is required, narrowband excitation may be used (*16*). However, in other applications, it is advantageous to excite signal in as large a region as possible in the neighborhood of the surface coil, for the sake of improving the signal-to-noise ratio. In such applications, broadband composite pulses would be beneficial if phase distortion could be minimized.

Analogous phase distortion problems occur with composite pulses designed for broadband excitation with respect to resonance offsets. Resonance offsets due to chemical shifts can be a significant factor in high-field NMR spectrometers unless high-power rf transmitters and probes are used. In NMR imaging systems, resonance offsets on the order of 10 kHz are imposed by static field gradients. The very high rf powers that would be required to make such offsets insignificant in a large-scale imaging system are impractical. Thus, composite pulses with minimal phase distortion should be of general use in imaging techniques that require broadband excitation in the presence of field gradients (*17*).

Phase distortion arises from two characteristics of the theoretical approaches used to design composite pulses. The first is that attention is directed toward a particular initial condition of the spin system, namely thermal equilibrium. The fact that the effect of a pulse sequence on a particular initial condition is independent of some experimental parameter does not ensure that the effect on an arbitrary initial condition will be independent of that parameter. The second characteristic is that generalized performance criteria are used. In particular, a composite $\pi/2$ pulse is taken to be any sequence that rotates magnetization from the z axis into the xy plane, without regard for the direction in that plane. Mathematically, the source of phase distortion can be seen by examining the general form of rotation operators that correspond to composite pulses. Acting on an isolated spin, any pulse sequence has the net effect of a rotation operator R of the form

$$R = \exp(-i\boldsymbol{\alpha}\cdot\mathbf{I}) \qquad [1]$$

where the direction of $\boldsymbol{\alpha}$ is the net rotation axis and the magnitude of $\boldsymbol{\alpha}$ is the net rotation angle. $\mathbf{I}$ is the spin angular momentum vector operator. For the special case of a composite π pulse, R can be written

$$R \approx \exp(-iI_z\beta_1)\exp(-iI_x\pi)\exp(iI_z\beta_1). \qquad [2]$$

For a composite $\pi/2$ pulse

$$R \approx \exp(-iI_z\beta_2)\exp(-iI_x\pi/2)\exp(-iI_z\beta_3) \qquad [3]$$

The equalities in Eqs. [2] and [3] hold approximately over the range of rf amplitude or resonance offset for which the composite pulse is effective. However, within that range, β_1 or β_2 and β_3 are typically not constant. Thus, $\boldsymbol{\alpha}$ in Eq. [1] is a function of the rf amplitude or resonance offset. Phase distortion in composite π pulses results from a varying net rotation axis; phase distortion in composite $\pi/2$ pulses results from variations in both the net rotation axis and the net rotation angle. Illustrations of these effects appear in Fig. 1.

We have introduced a method for constructing composite pulses that are equivalent to constant net rotations (*6, 12*). The method is based on the Magnus expansion in the manner of coherent averaging theory (*18, 20*). It differs from other methods in that it treats the overall transformation brought about by a composite pulse, rather than treating only a single initial condition. We have already demonstrated its usefulness in constructing composite π pulses for liquid (*6*) and solid state (*12*) NMR. In this paper, we present additional composite π and composite $\pi/2$ pulses that compensate for rf inhomogeneity and for resonance offset effects. Specifically, we demonstrate that these composite pulses are free from serious phase distortion problems.

THEORY

The theory has been presented in detail elsewhere (*6, 12*). We begin with the rotating frame Hamiltonian during an arbitrary pulse sequence

$$\mathcal{H} = \mathcal{H}_{\mathrm{rf}}(t) + V \qquad [4]$$

$$\mathcal{H}_{\mathrm{rf}}(t) = \omega_1^0[I_x\cos\phi(t) + I_y\sin\phi(t)] \qquad [5]$$

where ω_1^0 is the nominal rf amplitude, and $\phi(t)$ is the rf phase. For the rf inhomogeneity case

$$V = \delta\omega_1[I_x\cos\phi(t) + I_y\sin\phi(t)] \qquad [6a]$$

where $\delta\omega_1$ is the deviation of the rf amplitude from its nominal value. For the resonance offset case

$$V = \Delta\omega I_z \qquad [6b]$$

where $\Delta\omega$ is the resonance offset.

The effect of a pulse sequence of length τ on a spin system is given by the propagator $U(\tau)$, which can be written

$$U(\tau) = U_{rf}(\tau)U_{v}(\tau) \qquad [7]$$

$U_{rf}(\tau)$ is the propagator for the rf interaction alone, i.e. the case $V = 0$. It is purely a rotation operator. $U_v(\tau)$ is the propagator arising from V in an interaction representation with respect to $\mathcal{H}_{rf}(t)$. We make a Magnus expansion (*18–20*) of $U_v(\tau)$:

$$U_v(\tau) = \exp[-i(V^{(0)} + V^{(1)} + \cdots)\tau] \qquad [8]$$

$$V^{(0)} = \frac{1}{\tau}\int_0^\tau dt\, \tilde{V}(t)$$

$$V^{(1)} = \frac{-i}{2\tau}\int_0^\tau dt_1 \int_0^{t_1} dt_2[\tilde{V}(t_1), \tilde{V}(t_2)]$$

$$\tilde{V}(t) = U_{rf}(t)^{-1}VU_{rf}(t). \qquad [9]$$

The exponent in Eq. [8] is a power series in $\Delta\omega$ or $\delta\omega_1$. If a pulse sequence can be found for which the low-order terms in the series are zero, $U_v(\tau)$ will be approximately the unit operator for some range of $\Delta\omega$ or $\delta\omega_1$. Then, from Eq. [7], the overall propagator will be a constant rotation, namely $U_{rf}(\tau)$. This is why the Magnus expansion approach leads to composite pulses without phase distortion.

Composite π pulses must satisfy the equation

$$U_{rf}(\tau)I_zU_{rf}(\tau)^{-1} = -I_z. \qquad [10a]$$

Composite $\pi/2$ pulses must satisfy the equation

$$\mathrm{Tr}[I_zU_{rf}(\tau)I_zU_{rf}(\tau)^{-1}] = 0. \qquad [10b]$$

Consider a general sequence of N pulses. $V^{(n)}$ in Eq. [8] is a function of the N phases and N pulse lengths in that sequence. We wish to set $V^{(n)} = 0$ for $0 \leqslant n \leqslant M$. In addition, we wish to satisfy Eq. [10a] or [10b]. We therefore have a system of simultaneous (nonlinear) equations, with the variables being the pulse lengths and phases. Note that $V^{(n)} = 0$ consists of three component equations, corresponding to I_x, I_y, and I_z. We choose N to be large enough that a solution to the required equations exists.

For short sequences, expressions for $V^{(0)}$ and $V^{(1)}$ as functions of the pulse lengths and phases are easily derived. If the expressions are simple, composite pulses may be found by hand. In general, it is easier to write a computer program that evaluates the desired $V^{(n)}$ for any N-pulse sequence and conducts a search through possible pulse lengths and phases to find the best solution to the simultaneous equations. The resulting sequences, or composite pulses, are then not always exact solutions to the equations, but can be made very close. In this paper, we present composite pulses, with $V^{(0)} = 0$ (zeroth order) and with both $V^{(0)} = 0$ and $V^{(1)} = 0$ (first order). Throughout the paper, composite pulses are described by the standard notation, $(\theta_1)_{\phi_2}(\theta_2)_{\phi_2} \cdots (\theta_N)_{\phi_2}$, where θ_i and ϕ_i are the flip angle and phase of the i^{th} pulse in degrees. Although we treat rf inhomogeneity and resonance offsets separately below, it is possible to derive composite pulses for broadband excitation with respect to both $\delta\omega_1$ and $\Delta\omega$ simultaneously by taking V to be the sum of the right sides of Eqs. [6a] and [6b].

COMPENSATION FOR RADIOFREQUENCY INHOMOGENEITY

Composite π Pulses

We have already suggested the sequence $180_0 180_{120} 180_0$ for broadband inversion with respect to the rf amplitude (*6*). For this sequence, $V^{(0)} = 0$, exactly. Levitt has suggested the sequence $90_0 360_{120} 90_0$, among others (*9*). For $90_0 360_{120} 90_0$, $V^{(0)} = -\delta\omega_1 I_z/\sqrt{3}$. Surprisingly, the two composite π pulses give identical spin population inversion as a function of the rf amplitude. In both cases, the inversion is given by the expression $-\cos^3\theta + 3\sin^2\theta(1 - \cos\theta)/4$, where $\theta = \pi(\omega_1^0 + \delta\omega_1)/\omega_1^0$. As usual, inversion is defined to be the negative of the final z component of magnetization, assuming an initial unit magnetization aligned with the positive z axis.

Although their inversion properties are the same, the results of using the two composite π pulses as composite refocussing pulses in a $\pi/2$–τ–π–τ spin-echo experiment are quite different. If the rf amplitude of the composite refocussing pulse is varied between 0.6 and 1.4 times its nominal value, or equivalently if the pulse lengths are misset between 0.6 and 1.4 times their nominal lengths, the magnitude of the echo will be practically constant. However, the phase of the echo varies over a range of 224° with the $90_0 360_{120} 90_0$ sequence. With the $180_0 180_{120} 180_0$ sequence, the phase varies by only 31°. This result is demonstrated in Fig. 2.

A somewhat better composite π pulse is the sequence $180_0 180_{105} 180_{210} 360_{59}$, for which $V^{(0)} = \delta\omega_1(-0.0016 I_x + 0.0007 I_y)$ and $V^{(1)} = (\delta\omega_1)^2(0.0004 I_z)/\omega_1^0$. In Fig. 3, we show plots of inversion as a function of the rf amplitude for $180_0 180_{120} 180_0$ and $180_0 180_{105} 180_{210} 360_{59}$. As anticipated, the inversion bandwidth increases in going from a zeroth-order to a first-order composite pulse. When the first order composite pulse is used as a composite refocussing pulse, the phase of the echo varies over a range of only 16° when the rf amplitude varies from 0.6 to 1.4 times its nominal value. Thus, either $180_0 180_{120} 180_0$ or $180_0 180_{105} 180_{210} 360_{59}$ may be used as a composite refocussing pulse in the presence of substantial rf inhomogeneity without serious phase distortion problems. In the notation of Eq. [2], $\beta_1 = 240°$ for $180_0 180_{120} 180_0$; $\beta_1 = 105°$ for $180_0 180_{105} 180_{210} 360_{59}$.

Composite $\pi/2$ Pulses

In Figs. 4a and 5a, we show plots of the signal magnitude following excitation by composite $\pi/2$ pulses as a function of the rf amplitude. Results for two composite $\pi/2$ pulses are shown. The first, $90_0 180_{105} 180_{315}$, has $V^{(0)} = -\delta\omega_1(0.0071 I_x)$. The second, $270_0 360_{169} 180_{33} 180_{178}$, has $V^{(0)} = \delta\omega_1(0.0001 I_x - 0.0002 I_z)$ and

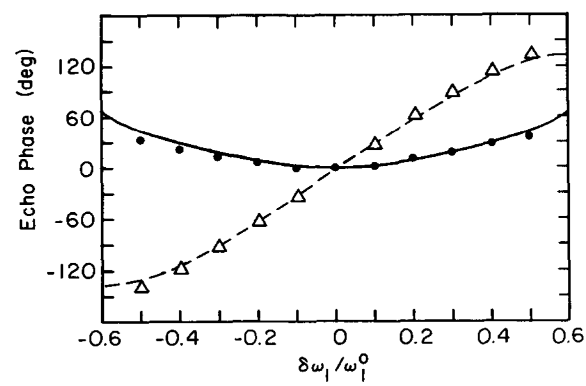

FIG. 2. The phase of the echo signal in a spin-echo experiment using a composite π refocusing pulse, as a function of the ratio of the miscalibration of the rf amplitude ($\delta\omega_1$) to the nominal rf amplitude (ω_1^0). Results are shown for two composite π pulses: $180_0180_{120}180_0$, with experimental data in dots and simulations in the solid line, and $90_0360_{120}90_0$, with experimental data in triangles and simulations in the dashed line. Although the two composite pulses invert longitudinal magnetization equally well, their performance in refocussing transverse magnetization is markedly different. The experiments were performed on a small $H_2O_{(l)}$ sample by missetting pulse lengths to mimic the miscalibrations of the rf amplitude.

$V^{(1)} = -(\delta\omega_1)^2(0.0003I_y)/\omega_1^0$. Again, the excitation bandwidth increases in going from a single $\pi/2$ pulse to a zeroth-order composite $\pi/2$ pulse to a first-order composite $\pi/2$ pulse.

Plots of the signal phase as a function of the rf amplitude for the two sequences are given in Figs. 4b and 5b. The sequence $270_0360_{169}180_{33}180_{178}$ is particularly free of phase distortions, with the signal phase remaining within a range of 15° for

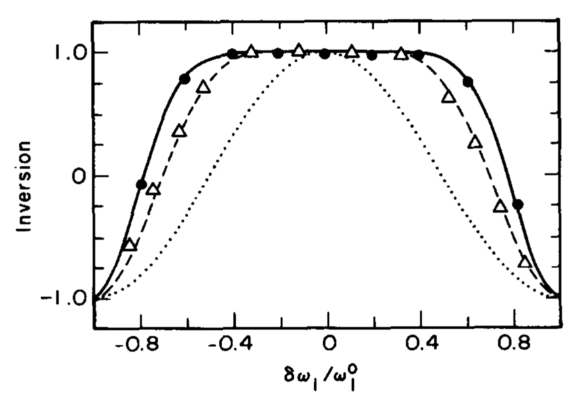

FIG. 3. The extent of the inversion of magnetization, or of spin populations, as a function of the relative miscalibration of the rf amplitude for a single π pulse (simulations in the dotted line), the zeroth order composite π pulse $180_0180_{120}180_0$ (experimental data in triangles, simulations in the dashed line), and the first-order composite π pulse $180_0180_{105}180_{210}360_{59}$ (experimental data in heavy dots, simulations in the solid line). The inversion bandwidth increases with the order to which rf amplitude miscalibration effects are canceled in the theory.

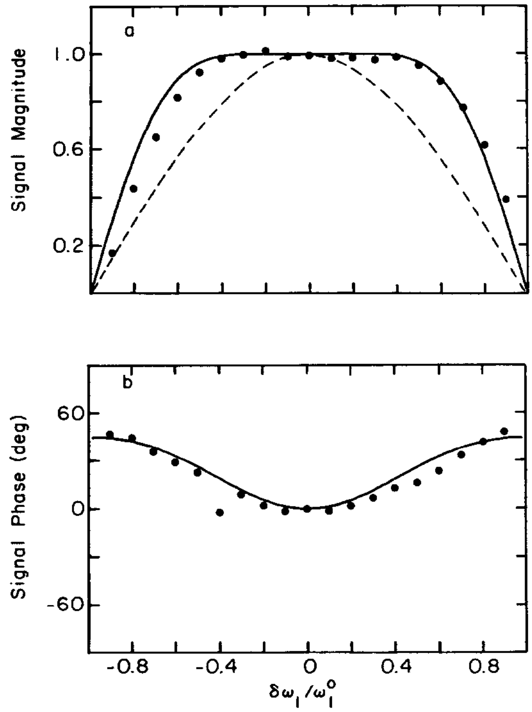

FIG. 4. The signal magnitude (a) and phase (b) following spin excitation by the zeroth-order composite $\pi/2$ pulse $90_0180_{105}180_{315}$, as a function of the relative rf amplitude miscalibration. Experimental data appears in dots and simulations in the solid lines. For comparison, the signal magnitude following a single $\pi/2$ pulse is shown in the dashed line.

rf amplitudes between 0 and 2 times the nominal value. For $90_0180_{105}180_{315}$, $\beta_2 = 60°$ and $\beta_3 = 0°$ in the notation of Eq. [3]; for $270_0360_{169}180_{33}180_{178}$, $\beta_2 = 110°$ and $\beta_3 = 180°$.

Composite $\pi/2$ pulses with larger excitation bandwidths may be constructed by other means, in particular the recursive expansion procedure of Levitt and Ernst (*10*). For example, they suggest the sequence $90_090_{270}90_090_{90}90_{180}90_{90}90_090_{90}$. That sequence gives better than 0.99 times the maximum signal magnitude for rf amplitudes between 0.5 and 1.5 times the nominal value. However, over the same range, the signal phase varies by 71°.

COMPENSATION FOR RESONANCE OFFSET

Composite $\pi/2$ Pulse

Freeman and Hill have shown that a single $\pi/2$ pulse already compensates for resonance offset effects to a large extent, at least for the purpose of rotating longitudinal magnetization into the transverse plane (*21*). The amplitude of the FID signal following a single $\pi/2$ pulse remains within 0.99 times its maximum for resonance offsets between $0.9\omega_1^0$ and $-0.9\omega_1^0$. There is a phase distortion of 80° over

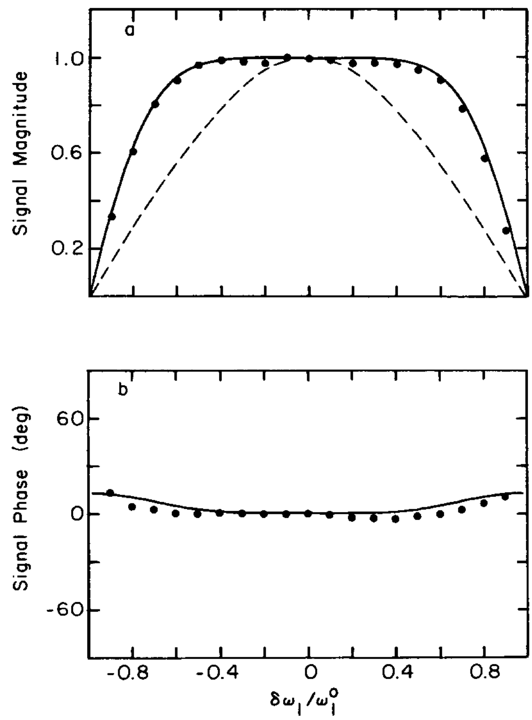

FIG. 5. Same as Fig. 4, but for the first-order composite $\pi/2$ pulse $270_0 360_{169} 180_{33} 180_{178}$. The amount of phase distortion decreases significantly as the theoretical order increases.

that range, but the phase is very nearly a linear function of $\Delta\omega$ and is therefore easily corrected in the spectrum resulting from a single pulse. However, there are applications in which $\pi/2$ pulses are required to do more than rotate longitudinal magnetization into the transverse plane. Examples include multiple-pulse line narrowing (*20, 22, 23*) and time reversal (*24, 25*) experiments. In such experiments, rf pulses act on spins far from thermal equilibrium. More commonly, the pulses are thought of as rotations acting on the internal spin Hamiltonian, making it time dependent in the manner of Eq. [9]. If the net rotation of a composite $\pi/2$ pulse varies with the offset, there is no general way to incorporate it into multiple-pulse techniques. However, small errors in single pulses due to the offset accumulate over long trains of pulses. Thus, if a line narrowing or time reversal sequence is performed in an inhomogeneous static field, as in a solid state NMR imaging experiment (*26*), it may be desirable to use composite $\pi/2$ pulses that are equivalent to constant rotations over a range of resonance offsets.

One composite $\pi/2$ pulse with that property is the sequence $385_0 320_{180} 25_0$, for which $\bar{V}^{(0)} = \Delta\omega(0.0026I_y + 0.0026I_z)$ and $\bar{V}^{(1)} = -(\Delta\omega)^2(0.0026I_x)/\omega_1^0$. A simple example of its performance in a multiple-pulse experiment is shown in Fig. 6. The experiment consists of applying a train of $\pi/2$ pulses separated by delays, with the signal being sampled once in the center of each delay. This is a commonly used technique for calibrating and adjusting rf amplitudes (*27*). When the pulses are

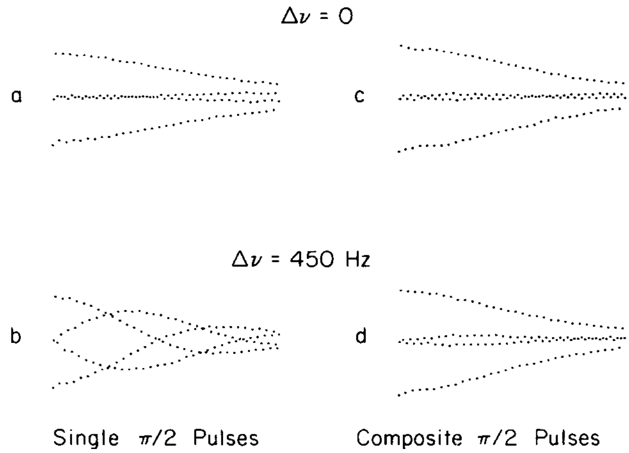

FIG. 6. Signal traces generated by applying a train of closely spaced $\pi/2$ (a, b) and composite $\pi/2$ (c, d) pulses to a small bulb of $H_2O_{(l)}$, with the signal sampled once after each $\pi/2$ pulse. The composite $\pi/2$ pulse is $385_0 320_{180} 25_0$, designed to be free of resonance offset effects to first order in the theory. In a and c, the pulses are applied on resonance with an rf amplitude of 3 kHz. In b and d, the pulses are off resonance by 450 Hz. The signal trace in b exhibits an obvious offset dependence; the trace in d is largely unaffected by the offset, due to the absence of appreciable phase distortion in the composite $\pi/2$ pulse.

applied on resonance, a characteristic signal pattern of three lines results. In Figs. 6a and b, it is apparent that the signal pattern deteriorates considerably at resonance offsets of $0.15\omega_1^0$ when single $\pi/2$ pulses are used. This is primarily due to phase distortion in the $\pi/2$ pulses rather than free precession during the delays, since long $\pi/2$ pulses (84 μs) and short delays (20 μs) were used. When composite $\pi/2$ pulses are substituted for the single $\pi/2$ pulses, the signal pattern is much less sensitive to resonance offsets, as shown in Figs. 6c and d. Again, 20 μs delays were used, but the length of each composite $\pi/2$ pulse was 688 μs so that the signal patterns in Figs. 6c and d actually represent a longer time than those in Figs. 6a and b.

Composite π Pulses

Composite π pulses that compensate for resonance offset effects have already been described (*6*). A zeroth-order sequence is $90_0 270_{90} 90_0$, with $V^{(0)} = 0$ exactly. This sequence was derived earlier by Levitt and Freeman (*3*), using a different theoretical approach. We note that $V^{(0)} = 0$ for any inverting sequence of the form $\theta_0 \theta'_\phi \theta_0$ satisfying $\theta' = 2n\pi - \theta$ and $\cos\phi = \cos\theta/(\cos\theta - 1)$. A first-order sequence is $336_0 246_{180} 10_{90} 74_{270} 10_{90} 246_{180} 336_0$, with $V^{(0)} = \Delta\omega(0.0005 I_x + 0.0010 I_y)$ and $V^{(1)} = (\Delta\omega)^2(0.0002 I_x - 0.0001 I_y + 0.0001 I_z)/\omega_1^0$. These composite π pulses may be used as refocussing pulses without introducing large, offset-dependent phase distortions. In an echo experiment, the first-order sequence contributes less than 1° to the variation in the phase of the echo for resonance offsets between $-0.6\omega_1^0$ and $0.6\omega_1^0$. As defined in Eq. [2], $\beta_1 = 135°$ for $90_0 270_{90} 90_0$; $\beta_1 = -27°$ for $336_0 246_{180} 10_{90} 74_{270} 10_{90} 246_{180} 336_0$.

DISCUSSION

As we have emphasized above, the novel feature of the composite pulses presented in this paper is their lack of large phase distortions. The impact of phase distortions varies from experiment to experiment, so that the decision of whether to use these composite pulses or composite pulses derived by other means must be made after a careful analysis of the experiment to be performed. In some cases, phase distortion is inconsequential, for example in the use of composite π pulses for inversion–recovery measurements of spin–lattice relaxation times (*1, 2*), for heteronuclear decoupling (*5, 28*), and in certain two-dimensional heteronuclear chemical-shift correlation experiments (*29*). In those cases, the phase of the signal that is eventually detected is independent of the phase of the π pulse. In other NMR techniques, distortions inherent in individual composite pulses can be made to cancel if multiple-composite pulses are used. This approach has been demonstrated in composite pulse versions of Carr–Purcell sequences (*3*) and quadrupole-echo experiments (*11*). Levitt and Ernst have given a detailed treatment of the incorporation of multiple-composite pulses into INADEQUATE experiments in such a way that most of the phase distortions in the individual composite pulses approximately cancel (*30*). In addition, they give general suggestions for designing composite pulse versions of similar experiments. Composite pulses can not be blindly substituted for single pulses; rather, they must be cleverly chosen and matched. Even so, phase distortions do not entirely disappear. Although they prevent phase distortion effects from accumulating over several composite pulses, Levitt and Ernst's prescriptions typically leave behind the distortion of the final composite pulse. Thus, particularly in situations of rf inhomogeneity where signal cancellation can occur, the problems arising from phase distortion are not eliminated.

Phase distortions may be inconsequential if composite pulses are used to overcome a miscalibration of the rf amplitude or a single resonance offset value, rather than true rf or static field inhomogeneity or a range of chemical shifts (*31*). In such a situation, the rotation produced by the composite pulse will be constant throughout the sample, since the rf amplitude or resonance offset does not vary.

With the above exceptions in mind, phase distortions do have important consequences in some of the simplest NMR experiments when a range of rf amplitudes or resonance offsets exists. The simplest experiment involving composite pulses is to give a single composite $\pi/2$ pulse and collect the ensuing FID. If rf inhomogeneity is significant, as is the case in *in vivo* experiments using surface coils, and if the goal is to generate the largest possible signal from the largest possible spatial region, then minimal phase distortion is essential. Only slightly more complicated than a single pulse experiment is a $\pi/2$–τ–π–τ echo experiment. It is conceivable that a composite $\pi/2$ pulse and composite π pulse pair with mutually canceling phase distortions can be found. However, no such pair has yet been proposed. Thus, if composite pulses are to be substituted for both the $\pi/2$ and the π pulse in an echo experiment, as would be likely in the presence of rf inhomogeneity, they should both have minimal phase distortion. If compensation for resonance offset effects is required, it may be best to use a single $\pi/2$ pulse and a composite π pulse. Assuming that the composite π pulse contributes negligible phase distortion, the remaining distortion in the echo arises only from the $\pi/2$ pulse. The usual linear phase correction in the spectrum is then sufficient.

Identical considerations apply to 2D echo experiments, i.e., 2D *J*-resolved spectroscopy (*32, 33*), and to other techniques in which echo sequences appear, such as DEPT (*34*). If DEPT is used to transfer polarization from proton spins to a carbon-13 spin, phase distortion effects due to composite pulses applied to the protons can be removed by the method of Levitt and Ernst (*30*). The detected carbon-13 signal will still be susceptible to phase distortion if composite pulses are applied to the carbon-13 spin, however. The same remarks apply to polarization transfer by INEPT (*35*). In general, other 2D techniques are open to phase distortion problems as well. These techniques include homonuclear and heteronuclear chemical-shift correlation spectroscopy (*33*) and 2D cross relaxation spectroscopy (*36*). Phase distortion in composite pulses would also affect signals detected in multiple-quantum NMR experiments (*37*).

The composite pulses derived from the Magnus expansion approach often involve unusual rf phase shifts; that is, phase shifts other than the common multiples of 90°. In our experiments, the phase shifts were usually accomplished with a digitally controlled phase shifter based on a commercial Daico unit, capable of 360°/256 phase increments. Alternatively, the rf phases can be set by inserting delay lines of the appropriate length into a quadrature generation circuit. Simulations indicate that the composite pulses can typically tolerate 5 or 10° deviations from the quoted phase shifts without a serious degradation of performance. Thus, a phase shifter that produces rf phases in 15° increments would be sufficient. Similar phase shifting capabilities are necessary for other NMR techniques, notably multiple-quantum spectroscopy (*37*).

It is possible that composite pulses that produce constant net rotations may be found by other means. For example, such composite pulses could be found by a computer search through all possible *N*-pulse sequences. For each possible sequence, it would be necessary to compute the transformation produced by the sequence acting on a complete set of independent initial conditions. In the case of compensation for rf inhomogeneity or resonance offsets, this means that the effect of the pulse sequence on initial density operators of both I_z and I_x would be calculated. Additionally, the calculations would have to be repeated for many values of rf amplitude or resonance offset to determine whether the transformation was independent of that parameter. On the other hand, with our approach it is only necessary to check Eq. [10] and evaluate $V^{(0)}$ and $V^{(1)}$. Thus, from a practical standpoint, our approach is computationally more efficient. It should also be realized that the low-order terms in the Magnus expansion in Eq. [8] must be nearly zero for any pulse sequence that corresponds to a constant net rotation, regardless of how that pulse sequence is discovered.

To conclude, we have demonstrated a unique property of composite pulses derived with the Magnus expansion, namely their lack of phase distortion. New composite π and $\pi/2$ pulses with compensation for rf inhomogeneity or resonance offset effects have been introduced. We have pointed out the need for composite pulses without phase distortion in several NMR techniques, including some of the simplest and most widely used. With the minimization of phase distortions, composite pulses are likely to have a greater impact on *in vivo* and NMR imaging studies as well as the more traditional liquid and solid state experiments.

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