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Series Expansion for Composite Pulses in NMR

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A new finite-series representation of composite pulses is described for which the expansion parameter is the offset angle θ, $\cos\theta = \Delta\omega/\sqrt{\Delta\omega^2 + \omega_1^2}$, where $\Delta\omega$ is the offset resonance and ω_1 is the radiofrequency amplitude in frequency units. Expressed in this way, it is shown that for phase-alternating pulse sequences for spin inversion, those that perform well over a range of offsets have small contributions from higher terms in the series. Optimization is performed by first truncating the series to obtain an initial fit and then successively including higher terms. © 1992 Academic Press, Inc.

Composite pulses are used in many NMR experiments (*1*). Since it is often a good approximation to ignore interactions other than the Zeeman effect while the pulse is on, a pulse can be treated as a rotation of the spin polarizations. A composite pulse sequence is then a series of rotations usually applied at various phases in the xy plane (*2*). These rotations can be visualized very easily when the pulses are applied on resonance, but become impossible to follow for spins which are off resonance (*3*). It is these off-resonance spins, however, which are usually those that one wishes to control. Therefore the study of composite pulses is essentially the study of motions of spins which lie off resonance.

In this paper a new way of expressing composite pulses as a series is presented. This series is written as a function of increasing powers of the cosine of the offset angle,

$$\cos\theta = \frac{\Delta\omega}{\sqrt{\Delta\omega^2 + \omega_1^2}}, \qquad [1]$$

where $\Delta\omega$ is the offset of the spin resonance, ω_0, from the carrier frequency, $\Delta\omega = \omega - \omega_0$. The RF amplitude is $\omega_1 = \gamma H_1$ where H_1 is the RF field amplitude. The angle

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θ describes the effective field direction. For a finite number of pulses, the series is finite and can be written exactly. Although this way of writing the series is not unique, it is found that the coefficients can be made less sensitive to offset as powers of $\cos\theta$ increase.

By way of examples we treat phase-alternating composites applied to spin inversion over large bandwidths. Up to six pulses are treated analytically and the series can be used to test existing sequences and predict new ones. Written in this form it is clear that "good" sequences require only a few terms in the series. The higher terms become important when the series becomes "bad."

SUMMARY OF OFF-RESONANCE ANGLES FOR A SINGLE PULSE

On resonance, a pulse changes the nuclear magnetic polarization in the z direction initially given by $\phi_z(0)$ to

$$\phi_z(\beta^0) = \cos\beta^0\phi_z(0), \qquad [2]$$

where $\beta^0 = \omega_1 t$. Here t is the pulse duration. Clearly a 180° pulse takes ϕ_z to $-\phi_z$. Off resonance the result is (*4, 5*)

$$\cos\beta = \frac{1}{\Omega^2}[\Delta\omega^2 + \omega_1^2\cos\Omega t], \qquad [3]$$

where $\Omega = \sqrt{\Delta\omega^2 + \omega_1^2}$.

In general, a pulse can be expressed as a Wigner rotation matrix acting on the nuclear spin polarizations expressed as spherical tensor components, (*4, 5*),

$$\hat{\phi}_q^k(t) = \sum_{q'=-k}^{k} \mathcal{D}_{qq'}^{(k)}(\alpha + \phi, \beta, \alpha + \pi - \phi)\hat{\phi}_q^k(0), \qquad [4]$$

where k is the tensor rank and q the spherical component. The phase of the pulse is ϕ. In addition to the angle β, an azimuthal angle arises, which is given by

$$\cos\alpha = \frac{-\Delta\omega}{\Omega}\frac{\sin(\Omega t/2)}{\cos(\beta/2)} \qquad [5]$$

$$\sin\alpha = \frac{-\cos(\Omega t/2)}{\cos(\beta/2)}. \qquad [6]$$

On resonance, α is reduced to the value of $-\pi/2$. Off resonance, β and α are needed to fully describe a pulse. In this paper, only the vector magnetization is treated, $k = 1$, $q = 0, \pm 1$. A composite pulse sequence containing n pulses is then simply expressed as a product of n 3×3 rotation matrices.

A SERIES FOR COMPOSITE PULSES

Another way to write [3] is to use the definition of θ in [1] to obtain

$$\cos\beta = \cos[\beta^0/\sin\theta] + \cos^2\theta\{1 - \cos[\beta^0/\sin\theta]\}. \qquad [7]$$

Here the nominal flip angle β^0 in [2], is displayed in [7] even though the pulse is off resonance. On resonance, the leading term reduces to $\cos\beta^0$ and $\cos\theta$ goes to zero.

Extension of this to multiple pulses can be carried out analytically by using computer algebra, such as REDUCE, to multiply n rotation matrices together. For now we restrict the calculation to phase-alternating pulses (*3*). By computer algebra manipulations, a structure like [7] is retained and gives for n composite pulses a series of the form

$$\cos\beta_{1\ldots n} = \cos(\delta_1 - \delta_2 + \delta_3 - \cdots \pm \delta_n) + \sum_{l=1}^{n} f_{2l}(\delta_1\delta_2\cdots\delta_n)\cos^{2l}\theta \equiv \cos\delta_i + \sum_{l=1}^{n} C_{2l}. \quad [8]$$

Here $\cos\beta_{1\ldots n}$ is just the generalization of [3] from one pulse to n off-resonance pulses. The magnitude of θ is fixed for a given offset, $\Delta\omega$ (see [1]). Physically, each composite pulse causes the polarizations to rotate about the effective field at either $+\theta$ or $-\theta$ depending on the phase of the pulse being about either the positive x axis or the negative x axis. The angles δ_i are given by

$$\cos\delta_i = \cos\Omega t_i = \cos\left[\omega_1 t_i\left(\frac{\Omega}{\omega_1}\right)\right] = \cos[\beta_i^0/\sin\theta], \quad [9]$$

where β_i^0 are the nominal flip angles for the ith composite pulse.

From [7] for one pulse, only one coefficient arises, which is $C_2 = \cos^2\theta[1 - \cos(\beta^0/\sin\theta)]$. For two, three, and four pulses, the expressions for C_{2l} are given in Table 1. For five or more pulses, these expressions become too long to reproduce here. In particular the higher coefficients of $\cos\theta$ become very long and cumbersome. In the tables $\cos\theta \equiv \cos(\text{THETA})$ and for the ith pulse, $\delta_i = Z_i$. It is not necessary, however, to have an expression for each number of pulses since, as can be seen from Table 1, case n reduces to case $n - 1$ by setting the last pulse $\delta_n = 0$.

In all cases, at resonance, these expressions reduce to (cf. [8])

$$\cos\beta_{1\ldots n}^0 = \cos(\beta_1^0 - \beta_2^0 + \beta_3^0 - \cdots \pm \beta_n^0).$$

To study the effects of resonance offsets, the higher terms in series [8] are required. Here we wish to find composite pulse sequences which are insensitive to resonance offsets over a large bandwidth. Close to resonance, it is found that the higher powers of $\cos\theta$ contribute less if the nominal flip angles, β_i^0, are chosen appropriately. Series [8] is therefore a reasonable starting point for studying phase-alternating composite pulses.

Since the angles α and β can also be obtained from the 2×2 propagators of a spin $\frac{1}{2}$, the effects of n composite pulses can also be obtained by multiplying n 2×2 matrices together to give the same analytical results as [8]. The advantage of [8] is that the major off-resonance effects are organized into a series which displays a useful structure.

RESULTS

From [7] a single 180° pulse can have only $l = 1$ in [8]. Table 2 shows the results for several offsets. Inversion ($\cos\beta = -1$) is good for $|\Delta\omega/\omega_1| < 0.4$, after which it becomes bad. Here a sequence is considered good if $\cos\beta < -0.8$.

TABLE 1a

Coefficients of [8] for Two Pulses

```
C2  =COS(THETA)**2*(-2.*COS(Z1-Z2)-COS(Z1+Z2)+2.*COS(Z1)
     +2.*COS(Z2)-1.)

C4  =COS(THETA)**4*(COS(Z1-Z2)+COS(Z1+Z2)-2.*COS(Z1)-
     2.*COS(Z2)+2.)
```

Note. The angles in the text are θ = THETA and $\delta_i = Z_i$.

TABLE 1b

Coefficients of [8] for Three Pulses

```
   C2  =COS(THETA)**2*(-COS(Z1-Z2-Z3)-3.*COS(Z1-Z2+Z3)+2.
.  *COS(Z1-Z2)+2.*COS(Z1-Z3)-COS(Z1+Z2-Z3)+2.*COS(Z1+Z3)
.  +2.*COS(Z2-Z3)-2.*COS(Z1)-2.*COS(Z3)+1.)

   C4  =COS(THETA)**4*(2.*COS(Z1-Z2-Z3)+3.*COS(Z1-Z2+Z3)-
.  4.*COS(Z1-Z2)-4.*COS(Z1-Z3)+2.*COS(Z1+Z2-Z3)+COS(Z1+
.  Z2+Z3)-2.*COS(Z1+Z2)-4.*COS(Z1+Z3)-4.*COS(Z2-Z3)-2.*
.  COS(Z2+Z3)+6.*COS(Z1)+4.*COS(Z2)+6.*COS(Z3)-4.)

   C6  =COS(THETA)**6*(-COS(Z1-Z2-Z3)-COS(Z1-Z2+Z3)+2.*
.  COS(Z1-Z2)+2.*COS(Z1-Z3)-COS(Z1+Z2-Z3)-COS(Z1+Z2+Z3)
.  +2.*COS(Z1+Z2)+2.*COS(Z1+Z3)+2.*COS(Z2-Z3)+2.*COS(Z2
.  +Z3)-4.*COS(Z1)-4.*COS(Z2)-4.*COS(Z3)+4.)
```

Note. The angles in the text are θ = THETA and $\delta_i = Z_i$.

For a two-pulse sequence of, for example, $90,\overline{270}$, where the bar means the phase of the second pulse is 180° from the first, Table 3 shows a substantial improvement over a single 180° pulse. At resonance the angles give $\cos(90 - 270) = -1$. As the offset increases, the C_2 and C_4 terms work to compensate off-resonance effects. C_2 is larger than C_4 for small $\Delta\omega/\omega_1$.

The above case can easily be visualized in terms of a resonance spin giving a 180° net rotation. As the number of pulses increases, this becomes impossible. Consider two sequences calculated from optimization techniques as reported by Shaka (*6*). For $n = 4$, he reports nominal flip angles of

$$34.2,\ \overline{123.0},\ 197.6,\ \overline{288.8} \qquad [10]$$

and for $n = 6$,

$$158.0,\ \overline{171.2},\ 342.8,\ \overline{145.5},\ 81.2,\ \overline{85.3}. \qquad [11]$$

For $n = 4$, the bandwidth is $|\Delta\omega/\omega_1| \sim 1$, while for $n = 6$, it is ~ 1.5. Both of these sequences have the property that

$$\cos(\beta_1^0 - \beta_2^0 + \beta_3^0 \cdots - \beta_n^0) = \cos 180°. \qquad [12]$$

TABLE 1c

Coefficients of [8] for Four Pulses

```
C2=COS(THETA)**2*(-COS(Z1-Z2-Z3+Z4)+2.*COS(Z1-Z2-
. Z4)-4.*COS(Z1-Z2+Z3-Z4)-COS(Z1-Z2+Z3+Z4)+2.*COS(Z1-
. Z2+Z3)+2.*COS(Z1-Z2+Z4)-2.*COS(Z1-Z2)+2.*COS(Z1-Z3+
. Z4)-2.*COS(Z1-Z4)-COS(Z1+Z2-Z3+Z4)+2.*COS(Z1+Z3-Z4)
. -2.*COS(Z1+Z4)+2.*COS(Z2-Z3+Z4)-2.*COS(Z3-Z4)+2.*
. COS(Z1)+2.*COS(Z4)-1.)

C4=COS(THETA)**4*(COS(Z1-Z2-Z3-Z4)+3.*COS(Z1-Z2-Z3
. +Z4)-2.*COS(Z1-Z2-Z3)-6.*COS(Z1-Z2-Z4)+6.*COS(Z1-Z2
. +Z3-Z4)+3.*COS(Z1-Z2+Z3+Z4)-6.*COS(Z1-Z2+Z3)-6.*COS
. (Z1-Z2+Z4)+8.*COS(Z1-Z2)-2.*COS(Z1-Z3-Z4)-6.*COS(Z1
. -Z3+Z4)+4.*COS(Z1-Z3)+8.*COS(Z1-Z4)+COS(Z1+Z2-Z3-Z4
. )+3.*COS(Z1+Z2-Z3+Z4)-2.*COS(Z1+Z2-Z3)-2.*COS(Z1+Z2
. -Z4)+COS(Z1+Z2+Z3-Z4)-2.*COS(Z1+Z2+Z4)+2.*COS(Z1+Z2
. )-6.*COS(Z1+Z3-Z4)-2.*COS(Z1+Z3+Z4)+4.*COS(Z1+Z3)+
. 8.*COS(Z1+Z4)-2.*COS(Z2-Z3-Z4)-6.*COS(Z2-Z3+Z4)+4.*
. COS(Z2-Z3)+4.*COS(Z2-Z4)-2.*COS(Z2+Z3-Z4)+4.*COS(Z2
. +Z4)+8.*COS(Z3-Z4)+2.*COS(Z3+Z4)-10.*COS(Z1)-4.*COS
. (Z2)-4.*COS(Z3)-10.*COS(Z4)+6.)

C6=COS(THETA)**6*(-2.*COS(Z1-Z2-Z3-Z4)-3.*COS(Z1-
. Z2-Z3+Z4)+4.*COS(Z1-Z2-Z3)+6.*COS(Z1-Z2-Z4)-4.*COS(
. Z1-Z2+Z3-Z4)-3.*COS(Z1-Z2+Z3+Z4)+6.*COS(Z1-Z2+Z3)+
. 6.*COS(Z1-Z2+Z4)-10.*COS(Z1-Z2)+4.*COS(Z1-Z3-Z4)+6.*
. COS(Z1-Z3+Z4)-8.*COS(Z1-Z3)-10.*COS(Z1-Z4)-2.*COS(
. Z1+Z2-Z3-Z4)-3.*COS(Z1+Z2-Z3+Z4)+4.*COS(Z1+Z2-Z3)+
. 4.*COS(Z1+Z2-Z4)-2.*COS(Z1+Z2+Z3-Z4)-COS(Z1+Z2+Z3+Z4
. )+2.*COS(Z1+Z2+Z3)+4.*COS(Z1+Z2+Z4)-6.*COS(Z1+Z2)+
. 6.*COS(Z1+Z3-Z4)+4.*COS(Z1+Z3+Z4)-8.*COS(Z1+Z3)-10.*
. COS(Z1+Z4)+4.*COS(Z2-Z3-Z4)+6.*COS(Z2-Z3+Z4)-8.*COS
. (Z2-Z3)-8.*COS(Z2-Z4)+4.*COS(Z2+Z3-Z4)+2.*COS(Z2+Z3
. +Z4)-4.*COS(Z2+Z3)-8.*COS(Z2+Z4)-10.*COS(Z3-Z4)-6.*
. COS(Z3+Z4)+16.*COS(Z1)+12.*COS(Z2)+12.*COS(Z3)+16.*
. COS(Z4)-12.)

C8=COS(THETA)**8*(COS(Z1-Z2-Z3-Z4)+COS(Z1-Z2-Z3+Z4)
. -2.*COS(Z1-Z2-Z3)-2.*COS(Z1-Z2-Z4)+COS(Z1-Z2+Z3-Z4)
. +COS(Z1-Z2+Z3+Z4)-2.*COS(Z1-Z2+Z3)-2.*COS(Z1-Z2+Z4)
. +4.*COS(Z1-Z2)-2.*COS(Z1-Z3-Z4)-2.*COS(Z1-Z3+Z4)+4.
. *COS(Z1-Z3)+4.*COS(Z1-Z4)+COS(Z1+Z2-Z3-Z4)+COS(Z1+
. Z2-Z3+Z4)-2.*COS(Z1+Z2-Z3)-2.*COS(Z1+Z2-Z4)+COS(Z1+
. Z2+Z3-Z4)+COS(Z1+Z2+Z3+Z4)-2.*COS(Z1+Z2+Z3)-2.*COS(
. Z1+Z2+Z4)+4.*COS(Z1+Z2)-2.*COS(Z1+Z3-Z4)-2.*COS(Z1+
. Z3+Z4)+4.*COS(Z1+Z3)+4.*COS(Z1+Z4)-2.*COS(Z2-Z3-Z4)
. -2.*COS(Z2-Z3+Z4)+4.*COS(Z2-Z3)+4.*COS(Z2-Z4)-2.*
. COS(Z2+Z3-Z4)-2.*COS(Z2+Z3+Z4)+4.*COS(Z2+Z3)+4.*COS
. (Z2+Z4)+4.*COS(Z3-Z4)+4.*COS(Z3+Z4)-8.*COS(Z1)-8.*
. COS(Z2)-8.*COS(Z3)-8.*COS(Z4)+8.)
```

Note. The angles in the text are θ = THETA and $\delta_i = Z_i$.

TABLE 2

A Single 180° Pulse as a Function of Offset

$\Delta\omega/\omega_1$	$\cos\beta$	=	$\cos\beta_i$	+	C_2
0	−1		−1		0
0.2	−0.921		−0.998		+0.077
0.4	−0.699		−0.971		+0.272
0.6	−0.373		−0.867		+0.494
0.8	+0.0249		−0.636		+0.638

Table 4 shows that the higher terms in the series representation of [10] are less important than the lower terms. Only when the sequence fails do the higher terms contribute significantly. Similar results also occur for the $n = 6$ example [11].

From other numerical studies it is generally found that although the higher terms C_{2l} in [8] are important, they are small for small offsets. This suggests that an appropriate scheme for finding new sequences which have desired characteristics is to neglect the higher terms and optimize using only the first few terms in the series. Since the analytical forms of the higher terms C_{2l} become longer (see Tables 1), the truncation simplifies the function to be optimized. The angles so found can be used as initial guesses for when the higher terms are included. Moreover, having algebraic expressions for [8] makes it possible to find derivatives of the function to be optimized, a requirement of some better computer optimization routines.

Using such a scheme, a three-pulse sequence which is good to $|\Delta\omega/\omega_1|$ of about 1.1 is

$$86.8, \overline{205.5}, 304.5. \qquad [13]$$

This performs better than the four-pulse sequence [10]. A four-pulse sequence which is valid to $|\Delta\omega/\omega_1| \sim 1.5$ is

$$38.2, \overline{110.7}, 159.3, \overline{249.5}. \qquad [14]$$

This performs as well as the six-pulse sequence of [11]. For six pulses, a new sequence is found,

TABLE 3

Two Phase-Alternated Composite Pulses of $90\overline{270}$ as a Function of Offset

$\Delta\omega/\omega_1$	$\cos\beta_{12}$	=	$\cos\beta_i$	+	C_2	+	C_4
0	−1		−1		0		0
0.2	−0.990		−0.998		+0.00492		+0.00274
0.4	−0.871		−0.971		+0.0725		+0.02750
0.6	−0.517		−0.867		+0.298		+0.05192
0.8	−0.0183		−0.634		+0.604		+0.01334

TABLE 4

Four-Pulse Sequence of [10] as a Function of Offset

$\Delta\omega/\omega_1$	$\cos\beta_{123}$	$= \cos\beta_i$	$+ C_2$	$+ C_4$	$+ C_6$	$+ C_8$
0.0	−1	−1	0	0	0	0
0.2	−0.986	−0.997	+0.0132	−0.00223	+0.00004	−0.00001
0.4	−0.983	−0.966	−0.00865	−0.0114	+0.00254	−0.0006
0.6	−0.992	−0.856	−0.187	+0.0139	+0.0358	−0.00213
0.8	−0.993	−0.6185	−0.537	−0.0203	+0.181	+0.0020
1.0	−0.966	−0.242	−0.830	−0.321	+0.332	+0.0958
1.2	−0.463	+0.220	−0.735	−0.373	+0.119	+0.305
1.4	+0.594	+0.661	−0.263	+0.186	−0.147	+0.156

$$140, \overline{149.3}, 315.3, \overline{115.2}, 70.3, \overline{83.5}, \qquad [15]$$

which extends the offset range out to just over 2, an improvement of 25% over [11]. Table 5 lists the series decomposition for this last case, which is typical. Note that the three new pulse sequences [13]–[15] do not satisfy [12]. The resulting small error at resonance is one consequence of obtaining the extended range of offset insensitivity.

The new sequences presented here for $n = 3$, 4, and 6 significantly improve the range of bandwidth insensitivity. It is unlikely that these bandwidths can be further improved using phase-alternating sequences without including more pulses. These series appear to be unique since the initial guesses are dictated by optimization of a truncated series at small offsets. To compare with Shaka's work, 11 pulses were needed in his work to extend out to $|\Delta\omega/\omega_1|$ of 2, whereas here the same limits are reached with only 6 pulses.

The restriction to phase-alternating pulses can be dropped to allow pulses of arbitrary phase. This introduces considerably more flexibility and it might be expected that a

TABLE 5

Six-Pulse Sequence of [15] as a Function of Offset

$\Delta\omega/\omega_1$	$\cos\beta_{123456}$	$= \cos\beta_i$	$+ C_2$	$+ C_4$	$+ C_6$	$+ C_8$	$+ C_{10}$	$+ C_{12}$
0	−0.999	−0.999	0	0	0	0	0	0
0.2	−0.987	−1.000	+0.007	+0.008	−0.002	0	0	0
0.4	−0.968	−0.980	+0.026	−0.008	−0.009	+0.004	+0.001	0
0.6	−0.992	−0.889	−0.392	+0.596	−0.436	+0.145	+0.017	+0.001
0.8	−0.960	−0.675	−2.887	+9.947	−14.241	+9.347	−2.746	+0.296
1.0	−0.993	−0.321	−9.56	+47.78	−93.9	+85.24	−35.79	+5.62
1.2	−0.916	+0.131	−19.9	+117.5	−270.9	+291.1	−147.3	+28.5
1.4	−0.998	+0.583	−28.6	−174.3	−415.7	+467.6	−251.6	+52.4
1.6	−0.902	+0.908	−28.8	+160.8	−355.4	+369.5	−183.3	+35.4
1.8	−0.988	+0.995	−18.88	+85.2	−157.1	+129.8	−47.5	+6.4
2.0	−0.711	+0.796	−5.00	+13.04	−20.8	+12.66	−1.40	+0.043
2.2	−0.532	+0.353	+4.34	−14.53	+8.57	+0.665	+0.012	0

few pulses will be insensitive to offsets over much wider ranges than phase-alternating sequences.

During the optimization procedures, it was also discovered that phase-alternating composite pulses could be found very easily which would invert at a selected specific offset. Moreover such sequences were not unique, with several giving inversion at the same value of $\Delta\omega/\omega_1$, depending upon the initial guesses in the optimization.

This paper has addressed only inversion pulses. Exactly the same criteria have been found for any total angle. An added complication, however, is that the azimuthal angle, [5] and [6], must also be controlled. For example, a 90° pulse may be made insensitive to offset over a wide range, but the azimuthal phase also needs to be compensated; otherwise, the 90° pulse comes down to the *xy* plane incoherently, like an umbrella. Further work is needed to address these and other aspects of predicting composite pulse sequences.

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Note added in proof. Recent experiments show that the new pulse sequences [13]–[15] perform as expected (*7*).

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