Nonlinear Phase Adjustment of Selective Excitation Pulses

J. W. Carlson¹

Radiologic Imaging Laboratory, Toshiba America MRI, Inc., 400 Grandview Drive, South San Francisco, California 94080

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¹A continuous transformation of an RF waveform with a modified Korteweg- de Vries equation or generalization can be used to adjust the phase behavior of a selective excitation pulse while preserving the magnitude behavior of the spin response. This transformation has applications in removing or adding to the nonlinear phase properties of a selected region. © 2000 Academic Press

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INTRODUCTION

Proper design of an RF waveform for selective excitation requires consideration of both the magnitude and the phase of the spin response following application of the RF pulse. Generally, the problem of tailoring a selective excitation pulse treats both quantities simultaneously. The method presented here shows that the phase of a response can be continuously adjusted while keeping the magnitude profile of the excitation unchanged. Direct manipulation of the phase response in the selected profile through modification of the RF waveform allows the pulse designer to adjust the phase after the magnitude behavior is satisfactory. Applications in the design of RF waveforms described here include both the removal and the introduction of phase variations through a selected region. With the methods described here an odd-order polynomial phase response can be adjusted in any waveform.

This will be illustrated in two situations: the first is in flattening the phase of an excitation pulse designed with peak amplitude close to the truncation point of the waveform, and the second is an introduction in an irrelevant phase factor in an inversion pulse in order to reduce peak RF level. In the first case, the initial waveform is designed to vanish a short time after the peak amplitude. This type of pulse is advantageous for short echo time selective excitations. However, this pulse has significant phase dispersion through the selected region. A pulse designed with absolutely flat phase, on the other hand, requires a long time for the RF waveform after the peak and so is not as suitable for short echo time uses. By a careful adjustment of the phase response we can modify the initial waveform and produce a nearly flat phase with only a slight increase in the temporal extent of the RF pulse.

The calculation will be illustrated using waveforms generated

¹ Present address: Lawrence Berkeley National Laboratory, 1 Cyclotron Road, MS 64-121, Berkeley, CA 94720.

by the inverse scattering method. The inverse scattering formalism provides analytic expressions of the RF waveforms for a very broad class of selective excitation pulse profiles. Within the type of profiles with solvable waveforms is a class of profiles, the limiting case of which has a perfectly square magnitude profile (1-3). The phase response is determined by the analytic structure of the excitation profile; as such the phase of the profile is not an independent parameter. There is a limited degree of flexibility in the calculation whereby the phase of an excitation pulse can be discretely adjusted while preserving the magnitude of the profile (2); however, the method presented here is distinct and much more flexible. While the formalism is closely connected to inverse scattering theory, the method can be used on waveforms calculated by any technique.

PHASE RESPONSE FORMALISM

The time evolution of a spin- $\frac{1}{2}$ particle with only a spin degree of freedom in a magnetic field is determined by a Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\gamma\hbar}{2} \boldsymbol{\sigma} \cdot \mathbf{B}\psi,$$
 [1]

where ψ is a 2-spinor wavefunction for the spin state of the particle, γ is the gyromagnetic ratio, and σ_i are the Pauli matrices. The *z* component of the magnetic field is a constant in time while the *x* component is the time-dependent amplitude modulated applied RF field. In an imaging application, the *z* component varies linearly over space, $B_z = Gz$, while the *z* component in a spectroscopy experiment is the constant offset field seen by the nuclear spin. For most of this work the problem will be phrased using the terminology from imaging; however, every statement will have a corresponding analog in the spectroscopy viewpoint.

If we drop a constant factor of \hbar on both sides of Eq. [1] and take a second time derivative, we can rewrite Eq. [1] as a second-order differential equation,

$$-\partial_t^2 \psi = \frac{-i\gamma}{2} \partial_t (\boldsymbol{\sigma} \cdot \mathbf{B} \psi)$$
$$= \frac{-i\gamma}{2} \boldsymbol{\sigma} \cdot (\partial_t \mathbf{B}) \psi + \frac{\gamma^2}{4} (\boldsymbol{\sigma} \cdot \mathbf{B}) (\boldsymbol{\sigma} \cdot \mathbf{B}) \psi. \quad [2]$$

This expression simplifies since only the *x* component of **B** has a time dependence and $\boldsymbol{\sigma} \cdot \mathbf{B}$ squared is equal to the 2 by 2 identity matrix multiplied by B^2 . Next, define a new 2-spinor χ which is a unitary transformation of the original,

$$\chi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ -1 & 1 \end{pmatrix} \psi.$$
 [3]

We assume that there is a characteristic length scale in the problem, z_0 ; this allows us to define the dimensionless length, time, and field parameters

$$z/z_o, \quad \frac{|\gamma|Gz_o t}{2}, \quad \frac{B_x}{Gz_o}.$$
 [4]

In the χ basis, the Schrödinger equation in the dimensionless variables is diagonal and has the simpler form

$$-\frac{d^2}{dt^2}\chi + \begin{pmatrix} -B_x^2 - i\partial_t B_x & 0\\ 0 & -B_x^2 + i\partial_t B_x \end{pmatrix}\chi = k^2\chi, \quad [5]$$

with

$$k^2 = (z/z_0)^2.$$
 [6]

For sufficiently large negative and positive values of time, the applied RF field is essentially zero and the solutions to the Schrödinger equation are superpositions of the solutions of a particle in a constant magnetic field. These have a time dependence $e^{\pm ikt}$. The effect of the application of a time-dependent magnetic field in the *x* direction to a spin- $\frac{1}{2}$ particle is to rotate the spin. The superposition of states at large negative time with the superposition at large positive time are connected to one another with a unitary transformation. For the wavefunction ψ , the relation between the two forms is a multiplication of the 2-spinor by an SU(2) rotation matrix. The parameterization used here will follow Ref. (1); the SU(2) rotation matrix is

$$\begin{pmatrix} \alpha^* & \beta \\ -\beta^* & \alpha \end{pmatrix},$$
 [7]

with $|\alpha|^2 + |\beta|^2 = 1$.

Prior to the application of the RF waveform, the initial state of the spin is relaxed in the static magnetic field. The wavefunction therefore is in an up state in the original basis with a time dependence e^{ikt} . After the RF, the wavefunction in the original basis is a superposition of the an up state with a time dependence e^{ikt} and a down state with a time dependence e^{-ikt} . This implies that the upper component in the χ basis set has the limiting form

$$\chi_{1} \rightarrow \begin{cases} \frac{1}{\sqrt{2}} e^{ikt} & \text{for } t \rightarrow -\infty \\ \\ \frac{1}{\sqrt{2}} (\alpha^{*}e^{ikt} - \beta^{*}e^{-ikt}) & \text{for } t \rightarrow \infty \end{cases}$$
[8]

Since the potential in Eq. [5] is diagonal, we can consider the solutions to the upper and lower components of χ separately. Each component of χ solves a second-order differential equation which formally looks like a time-independent Schrödinger equation,

$$-\frac{d^2}{dt^2}\chi_1 + V(t)\chi_1 = k^2\chi_1.$$
 [9]

For the upper component of χ the potential in this equation is $-B_x^2 - i\partial_t B_x$ and *t* takes the place of the spatial coordinate in the Schrödinger problem. The solution for the lower component, χ_2 , is similar except that the potential is the negative of the complex conjugate of that for the upper component.

The form of this equation is referred to as a Sturm–Liouville eigenvalue problem in analysis. The basic structure is

$$Lf(t) = k^2 f(t), \qquad [10]$$

with $L = -d^2/dt^2 + V(t)$. For the NMR problem we are interested in solutions to the Schrödinger problem that are complex exponentials in time for large values of time. These are the positive energy, or scattering, solutions of the Schrödinger problem and not the normalizable, bound state negative energy solutions.

A problem associated with the study of nonlinear partial differential equations has been methods of calculating the solutions to a Sturm–Liouville eigenvalue problem after modifying the potential while keeping the eigenvalue constant. A well-established property of Sturm–Liouville problems is that we can find a one-parameter transformation of the potential which preserves the eigenvalues of the operator (4). Let *f* be any solution for an eigenvalue k^2 in a Sturm–Liouville eigenvalue problem. For a differential operator *C*, if *V* evolves in a parameter *s* according to

$$\partial_s V = [C, L] \equiv CL - LC, \qquad [11]$$

then the eigenvalues in the Eq. [10] are unchanged and the evolution of f is determined by the differential equation

$$\partial_s f = Cf(t, s).$$
[12]

(In the notation of Ref. (4), the coordinate in the Sturm–Liouville problem is labeled x and the new parameter is labeled t. This is changed here to use t as the coordinate in the Sturm–Liouville problem and s as the new variable. The op-

erator C is denoted by B in Ref. (4). The notation is changed in this paper to prevent confusion with the magnetic field.)

The construction of the operator, C, is given in Ref. (4). There is an infinite set of operators we can construct which are labeled by an integer index, n. The general form for the operator C_n is that it has a maximum odd-order derivative term plus a sum of lower odd-order derivative terms while the operator overall must be skew-symmetric. Up to an overall constant factor, the operator is

$$C_n = \frac{d^{2n+1}}{dt^{2n+1}} + \sum_{i=1}^n g_i(V) \frac{d^{2i-1}}{dt^{2i-1}} + \frac{d^{2i-1}}{dt^{2i-1}} g_i(V), \quad [13]$$

with the functions $g_i(V)$ determined by the requirement that $[C_n, L]$ depends only on V and its derivatives and does not contain any residual derivative operator terms. This requirement provides a set of simultaneous differential equations for the functions $g_i(V)$ which can be solved for any value of n.

The lowest order nontrivial case is a third-order operator,

$$C_{1} = 4(\partial_{t}^{3} + \frac{3}{2}V\partial_{t} + \frac{3}{4}(\partial_{t}V)).$$
[14]

The evolution of potential, *V*, generated by the differential equation [11] is the Korteweg–de Vries (KdV) equation,

$$\partial_s V + [L, C_1] = \partial_s V - \partial_t^3 V + 6V \partial_t V = 0.$$
 [15]

This can be satisfied only if the RF field satisfies a modified version of this equation,

$$\partial_s B_x + \partial_t^3 B_x + 6B_x^2 \partial_t B_x = 0.$$
 [16]

The overall constant, 4, in Eq. [14] was used to make Eq. [16] in the standard form for the modified KdV equation.

In the asymptotic regimes of large t, V approaches zero; this implies the asymptotic form for the operator C_1 is $4\partial_t^3$. This in turn implies that the arbitrary solution, f, satisfies a differential equation for large negative and positive time:

$$\partial_s f(t, s) = 4 \partial_t^3 f(t, s).$$
[17]

When we substitute our particular solution, χ_1 , into this differential equation, we can see that the solution in the χ basis set is

$$\chi_1 \rightarrow \begin{cases} \frac{1}{\sqrt{2}} e^{ikt-4ik^3s} & \text{for } t \rightarrow -\infty\\ \frac{1}{\sqrt{2}} (\alpha^* e^{ikt-4ik^3s} - \beta^* e^{-ikt+4ik^3s}) & \text{for } t \rightarrow \infty \end{cases}$$
[18]

Or, if the potential evolves according to Eq. [15], as a function

of *s* the transition amplitude for a spin up to spin up transition (the term proportional to α^*) is independent of *s* while the spin flip amplitude (the β^* term) has an *s* dependence e^{8ik^3s} . The profile of the excitation response of a waveform is proportional to the product $\alpha^*\beta$ (*I*); therefore the excitation profile will have the *s* dependence e^{-8ik^3s} .

If we were to ignore the nonlinear term in Eq. [16], then the solution to this differential equation is trivial: we could Fourier transform B_x , multiply by a phase factor e^{ik^3s} , and inverse Fourier transform. Linear response theory predicts that multiplying the slice profile by a desired phase response and inverse Fourier transforming the result gives the waveform needed for this profile. Ignoring the nonlinear effects in spin rotations is equivalent to ignoring nonlinear effects in the modified KdV equation.

NONLINEAR PHASE CORRECTION

The selective excitation desired typically in an imaging procedure and often in a spectroscopy experiment is to have a constant and uniform flip angle over a limited spatial (or frequency) range and zero response outside that range. For an RF field polarized along the *x* axis in the rotating frame, the spin flip transition amplitude, β , is $-i \sin(\theta/2)$ inside the response range and zero outside that range.

The inverse scattering method allows one to calculate the exact RF pulse which produces a desired spin flip transition amplitude provided that the amplitude is specified as a ratio of polynomials in position (in an imaging application) or frequency (in a spectroscopy experiment). A convenient form to take is

$$\beta = \frac{-i\,\sin(\theta/2)}{1+k^{2n}},$$
[19]

where k is either position divided by the slice half-width, z/z_o , or frequency divided by the half-width of the excitation response, f/f_o . For a sufficiently large n, this describes a profile which is arbitrarily close to the ideal rectangular pulse. By examining the behavior for various values of n, we can select a pulse and profile with sufficient profile sharpness and acceptable temporal extent of the RF pulse. In general, both sharpness and temporal extent increase as n increases.

The denominator in Eq. [19] can be factored into a product of terms $k + \tau_j$, where τ_j is one of the 2*n*th root of -1, $e^{i(2j-1)\pi/2n}$. In Ref. (2) it was shown that if we were to modify the profile described in Eq. [19] by taking the product of terms in the denominator only those terms with roots that lie in the upper half plane then the RF waveform vanishes for t > 0. The basic characteristics of the profile remain the same and depend only on the number of roots used: if we select the 2*n*th roots of -1 that lie in the upper half plane (there are *n* of them), the profile is approximately the same in magnitude as if we had selected the *n*/2th order profile in Eq. [19]. In the limit of $n \rightarrow$

a

 ∞ the magnitude of this profile is a perfect rectangular selective excitation. The RF pulses generated with this form for the spin flip transition typically have most of their pulse energy concentrated shortly before time t = 0. This feature makes these pulses ideal for NMR sequences with short echo times: since every RF pulse must be truncated on both ends in order to be used in an experimental apparatus, these pulses can be truncated exactly at t = 0 with no degradation in selection profile and relatively little time for decrease in transverse magnetization due to T_2 decay. Truncation for negative times is less of a concern since as excitation pulses they generally can be extended for large negative times without any penalty in an experiment or significant truncation effects in the profile.

Computed waveform and profiles for the pulse with n = 10are shown in Fig. 1. The phase of the selected region immediately after the RF is turned off has five wraps through 2π across the selected region. In an imaging situation the slice select gradient is reversed after excitation, adjusting the linear phase across the selected region for a flat response. The phase shown in Fig. 1 is after the linear phase ramp has been removed. The phase in the center half of the selected slice is flat, but there is an apparent higher order phase twist through the slice. The result of fitting the phase in the region |k| < 1is that the phase is approximated by the odd-order polynomial

$$\phi \approx -2.592k^3 + 2.970k^5 - 3.706k^7 + \cdots$$
 [20]

We want to provide a maximum coherence of the magnetization within the selected slice; to do so requires a flatter phase to align the magnetization more completely within the selected region.

We could adjust the phase response through the discrete method described in Ref. (2). However, this requires much higher peak RF power and is not completely successful in flattening the phase in the example waveform. Alternatively we can modify the locations of the zeroes of the denominator of the spin flip transition amplitude. By moving the factors τ_i away from the prescribed locations we can achieve a higher degree of phase flatness, but this is seen to degrade the squareness of the profile of the magnitude substantially.

The computed profile shows that there is a residual cubic phase variation across the slice; this implies that we could remove it by modifying the spin flip transition to include an exponential factor

$$\beta(z, s) = \beta(z)e^{2.592ik^3}.$$
 [21]

While there is an exact solution to the waveform for a transition amplitude which is a ratio of polynomials in k, there is no such closed form solution for the waveform which includes this exponential factor. The RF waveform evolved according to the modified KdV equation has exactly the desired cubic phase dependence. It is a simple matter of solving the modified KdV



FIG. 1. (a) Amplitude modulation envelope of the RF waveform to produce a 90° excitation pulse corresponding to Eq. [17] with n = 10. The time and field are given in dimensionless units defined in Eq. [4]. (b) The resulting magnitude of the transverse magnetization (solid line, left vertical scale) and phase (dashed line, right vertical scale) immediately after the RF pulse. The phase is shown after a linear ramp has been removed. The nominal width of the selected slice extends from k = -1 to k = +1.

equation numerically to give the waveform with the cubic phase eliminated.

Solving the modified KdV equation numerically is a straightforward boundary value problem which can be done

using the implicit spectral technique (5). Given an initial condition $B_x(t, s)$ for some value of s, the solution at s + ds is approximated by

$$B_{x}(t, s + ds) - B_{x}(t, s)$$

$$\approx -\frac{ds}{2} \left(\partial_{t}^{3}B_{x}(t, s + ds) + \partial_{t}^{3}B_{x}(t, s) + 2\partial_{t}(B_{x}^{3}(t, s + ds) + B_{x}^{3}(t, s))\right).$$
[22]

Let $\hat{B}_x(\omega, s)$ be the Fourier transform in *t* of B_x and $\hat{B}_x^3(\omega, s)$ be the Fourier transform of B_x^3 . This allows us to reduce Eq. [22] to

$$\hat{B}_x(\omega, s+ds) = \frac{1-i\omega^3 ds/2}{1+i\omega^3 ds/2} \hat{B}_x(\omega, s) + \frac{i\omega ds}{1+i\omega^3 ds/2} \times (\hat{B}_x^3(\omega, s) + \hat{B}_x^3(\omega, s+ds)).$$
[23]

The right-hand side of Eq. [23] contains the Fourier transform of B_x^3 at both *s* and s + ds. We can solve this iteratively by initially replacing $\hat{B}_x^3(\omega, s + ds)$ on the right-hand side with the value at *s*. After a Fourier transform, the left-hand side gives a first estimate for $B_x(t, s + ds)$. Cube this in the time domain, Fourier transform, and then use this as the estimate for $\hat{B}_x^3(\omega, s + ds)$ on the right-hand side in the first iteration. This process can be repeated until it converges in usually a few iterations.

An example of the evolved solution for the waveform at s = -0.324 and the computed profile are shown in Fig. 2. Again, the phase is displayed after the linear phase ramp has been removed. The overall flatness of the phase of the response is apparent. Improvements in the coherence result in 43% more signal within the nominal selected slice, |k| < 1. The cubic component to the phase variation across the slice is removed, but the fifth- and higher-order contributions are unchanged.

The remaining phase variation is fifth and higher order. Higher order generalizations of the method of Ref. (4) can be used to generate higher-order versions of the KdV equation. For any value of n, we can generate an operator C_n so that in the asymptotic regime the scattering states satisfy

$$\partial_s f(t, s) = c_n \partial_t^{2n+1} f(t, s).$$
[24]

Evolution of the RF waveform with Eq. [11] will result in modified (2n + 1)th-order phase without changing other contributions.

The fifth-order phase can be removed through evolution by the partial differential equation derived using the same methods as the third-order correction. The proper equation is



FIG. 2. (a) RF waveform with the cubic phase contributions removed. The temporal extent and peak amplitude of the waveform have increased slightly. (b) The calculated magnitude and phase of the RF pulse with the cubic phase contribution removed.

$$\partial_{s}B_{x} + \partial_{t}^{5}B_{x} + \partial_{t}(6B_{x}^{5} + 10B_{x}(\partial_{t}B_{x})^{2} + 10B_{x}^{2}\partial_{t}^{2}B_{x}) = 0.$$
[25]

The asymptotic form of the evolution equation for the scattering solutions is

$$\partial_s f(t, s) = 16 \partial_t^5 f(t, s).$$
[26]

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FIG. 3. RF waveforms with additional corrections for fifth- and seventh-order phase errors (left) and resulting transverse magnetization graphs (right). The waveform with third- and fifth-order correction (upper two graphs) is only a minor modification of the previous case, while the addition of the seventh-order correction drastically expands the temporal extent of the waveform and makes it more nearly symmetric. The waveform with the third- and fifth-order correction has less coherent magnetization than the third-order correction alone; this is due to a partial cancellation of the fifth- and seventh-order effects.

The spin flip transition amplitude has a phase dependence e^{32iks^5} . The seventh-order correction is determined by the evolution equation for the RF field,

$$\partial_{s}B_{x} + \partial_{t}^{7}B_{x} + \partial_{t}(20B_{x}^{7} + 140B_{x}^{3}(\partial_{t}B_{x})^{2} + 70B_{x}^{4}\partial_{t}^{2}B_{x} + 70(\partial_{t}B_{x})^{2}\partial_{t}^{2}B_{x} + 42B_{x}(\partial_{t}^{2}B_{x})^{2} + 56B_{x}\partial_{t}B_{x}\partial_{t}^{3}B_{x} + 14B_{x}^{2}\partial_{t}^{4}B_{x}) = 0, \qquad [27]$$

and the asymptotic form of the equation for the scattering solutions,

$$\partial_s f(t, s) = 64 \partial_t^7 f(t, s), \qquad [28]$$

with an associated phase dependence of the transition amplitude $e^{-128iks^7}$.

The final adjusted waveforms (using the values s = -0.0928 for the fifth-order evolution and s = -0.0290 for the seventh-order) and profiles are shown in Fig. 3. In the original profile there was a partial cancellation of the effects of the fifth- and seventh-order phase variation across the selected

region. This manifests itself as an apparent degradation of the phase behavior after only the fifth-order correction is applied. The integrated magnetization within the selected slice is 23% below the profile with only the third-order correction. The basic property of the pulse is preserved in the third- and fifth-order correction: the pulse is largely confined to t < 0with only a minor change in the peak amplitude. With the seventh-order correction, the pulse substantially extends through 0 and becomes much more nearly time symmetric. Elimination of the seventh-order phase adds only more than 1% to the total magnetization within the selected slice compared to the third-order corrected pulse-it is only 0.3% below the magnetization of a perfect pulse-however, it comes at the cost of greatly extending the time of the pulse. In an experiment in which we wish to truncate the RF pulse soon after the peak RF, we would expect that the waveform in the last example would have a much larger truncation artifact in the profile; this result is confirmed in calculations. However, the pulse with only the third-order phase correction applied has very nearly the same integrated signal but still allows truncation of the pulse close to the peak. As an excitation pulse with

FIG. 4. Shown are 180° inversion pulses corresponding to s = 0 (solid line), s = 0.5 (dashed line), and s = 1.0 (dot-dashed line). All three waveforms give precisely the same inversion profile.

short echo times, the waveform with only the third-order correction is preferable to either with higher-order corrections.

INVERSION PULSES WITH DECREASED AMPLITUDE

As is apparent from the preceding results, achieving a higher degree of phase flatness produces RF waveforms with higher peak RF power. As an alternative to using cubic phase adjustment to flatten the phase response, we can purposely distort the phase response in situations where it is not important if we can achieve lower peak RF waveforms as a result. For example, for inversion pulses the phases of the transition amplitudes are unimportant. Any waveform which evolves according to a modified KdV equation produces identical inversion profiles.

The 180° pulses with the profile described by Eq. [19] show a large peak amplitude for flip angles close to 180° at high order (6). This behavior can be largely ignored if we purposely produce waveforms at angles a few degrees away from 180° ; the difference in the magnetization response is negligible.

Evolution of the waveform with a generalized modified KdV equation will generate an odd-order phase variation which does not enter in the behavior of the inversion profile. An example behavior showing a n = 10 waveform with θ set to 179° is shown in Fig. 4. The solid line shows the time-symmetric waveform calculated with the inverse scattering formalism. The peak RF strength is approximately three times the value

given by a sinc waveform at the same nominal slice thickness. After evolution with the modified KdV equation to s = 0.5 (dashed line) or s = 1 (dashed–dotted line) the pulse loses the time symmetry and reduces the peak RF by almost a factor of 3, yet maintains precisely the same inversion profile.

The additional phase twists would make this pulse unsuited to a refocusing pulse unless the excitation pulse was designed to have a matching nonlinear phase behavior.

CONCLUSIONS

Two cases which have been exactly solved in the past have been time-symmetric excitation pulses and time truncated pulses, those which vanish beyond t = 0. While the former pulse has perfectly flat phase, the temporal extent of the waveform makes them difficult to achieve short echo times in selective excitation experiments. The latter pulses, however, have significant signal degradation because of incomplete phase coherence in the selected region.

Subtle changes in the phase response of selective excitation profiles can have a large impact on the waveforms used to generate them. Waveforms which normally produce an unacceptable amount of phase variations through a selected slice can be adjusted to a much higher degree of flatness with only a minor modification of the pulse. However, in other cases demanding absolute flatness can result in large modifications to the pulse. In cases examined here, the additional phase flatness in an excitation pulse produced by removing fifth- and seventhorder phase variation greatly extends the pulse and produces no significant change in the magnetization within the slice. By only correcting for a third-order phase variation, we achieve nearly all possible phase coherence and still largely maintain the ability to truncate the pulse after its peak.

For the inversion pulse, phase is irrelevant. Producing a pulse with flat phase normally results in high peak RF power; relaxing this phase constraint produces pulses with much lower peak RF power.

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