# Generation of optimal excitation pulses for two energy level systems using an inverse Fourier transform method

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The response of a two energy level system to low amplitude excitation is investigated. The flip angle of magnetization or polarization is found to be linearly related to the magnitude spectrum of the excitation pulse under the approximation of low amplitude excitation. This property can be used for synthesis of optimal excitation pulses. A comprehensive algorithm for generating optimal excitation pulses is proposed based on the response theory and the stored wave form inverse Fourier transform (SWIFT) algorithm developed previously. An example of the synthesis of a notch excitation pulse is given to demonstrate the flexibility of this newly developed method.

## I. INTRODUCTION

Pulsed excitation is routinely used in rotational,[1(a)] vibrational,[1(a)] electronic,[1(b)] and magnetic resonance spectroscopy[1(c),1(d)] incorporating a broad range of research interests. Despite the obvious difference in the fields under study, they share similar principles in the basic equations of motion. The motion of such two energy level systems can be described by the Bloch equations. Further understanding of the excitation processes in these two-level systems and the ability to design flexible excitation pulses are, no doubt, very important in applications of these spectroscopic methods. A general scope in the area of pulse synthesis can be found in representative current reviews.[2]

In nuclear magnetic resonance (NMR)[3(a)] and magnetic resonance imaging (MRI),[3(b)] the complicated pulse sequences are designed to perform a wide range of experiments. In these experiments, rectangular pulse shapes are conventionally assumed since the excitation behavior of this type of pulse can be easily understood with average Hamiltonian theory. However, there are cases in which the simple combination of a series of rectangular pulses cannot achieve the desired excitation. A typical example is selective excitation for solvent suppression or imaging localization. Low energy and highly selective excitation are in great demand due to the increasing application of NMR and MRI in biological and medical sciences. Several different pulse shapes have been proposed for selective excitation,[2] e.g., sinc, modified Gaussian, Hermit, or hyperbolic secant pulses. Although these pulses are useful in many experiments, more general pulses are still in demand.

In the absence of external excitation fields, the Bloch equations reduce to linear equations and Fourier transformations can be applied for the spectral analysis. The excitation processes, on the other hand, are not linear. Therefore, it is not generally possible to directly invert the spectral analysis method to synthesize desired excitation pulses. However, the Bloch equations can be considered linear under the approximation of low level excitation or the small angle approximation.

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Tomlinson and Hill, in 1973, introduced an inverse Fourier transform excitation method for NMR solvent suppression.[4] The theoretical basis for their approach is the linear response theory. The key advantage of their method is that the desired frequency excitation profiles are provided first and the time-domain pulses are then synthesized via inverse Fourier transformation. This inverted methodology was introduced into Fourier transform mass spectrometry (FTMS) by Marshall and co-workers.[5] They also demonstrated its high selectivity and flexibility. The application of the method to FTMS is straightforward since the basic equations of motion, the Lorentz equations, are linear under reasonable approximations.[6]

In the cases of two-level systems, the inversion method requires modifications in order to apply to large angle excitation. This paper presents equations correlating the response profiles with the excitation spectra. The approach is based on the small angle approximation, and the fact that the phase is stationary when either the flip angle is near 90° or the excitation amplitude is low. For excitation with a flip angle greater than 45°, the normal linear response tretment becomes nonvalid. This work also examines the conditions in that a two-level system can still be considered as a linear one. It shows that when amplitude of excitation pulses is low the linear response of flip angles holds in some degree regardless of magnitude of the flip angles. Finally, we propose that low amplitude excitation pulses are generated by phase modulation. Since the synthesis of optimal excitation wave forms from specified frequency domain spectra has been developed in some depth,[7] we can adapt it easily to two-level systems. Due to the nonlinear nature of the Bloch equations, the resultant excitation profile is thus distorted. This distortion can be reduced using a simple optimization procedure. An example for generating a broadband notch excitation pulse is given using this newly developed method.

## II. RESPONSE OF A TWO-LEVEL SYSTEM TO LOW AMPLITUDE EXCITATION

We first consider an arbitrary excitation pulse

$$\Omega(t) = \Omega_x(t)\cos(\omega t)\mathbf{i} + \Omega_y(t)\sin(\omega t)\mathbf{j}, \quad (1)$$

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where **i** and **j** are the unit vectors along $x$ and $y$ directions, respectively. This form for the field implies that the pulse is applied with a carrier frequency $\omega$ and that in real laser or NMR experiments the bandwidth of interest is much less than the carrier frequency. The carrier is usually chosen to be close to the resonance frequencies. This does not set any limitation of generality to both the pulse amplitude and phase since both $\Omega_x$ and $\Omega_y$ can be varied independently.

The relation of $\Omega(t)$ to the excitation magnetic $B(t)$ or electric $E(t)$ field can be expressed as

$$\Omega(t) = (\gamma\mu_0/\hbar)B(t) \quad (2)$$

or

$$\Omega(t) = \boldsymbol{\mu}\cdot\mathbf{E}(t)/\hbar. \quad (3)$$

The Bloch equations for a two energy level system with negligible relaxation processes can be written in the rotating frame as

$$\frac{d\sigma_x(\Delta\omega;t)}{dt} = -\sigma_z(\Delta\omega;t)\Omega_y(t) + \Delta\omega\sigma_y(\Delta\omega;t), \quad (4)$$

$$\frac{d\sigma_y(\Delta\omega;t)}{dt} = \sigma_z(\Delta\omega;t)\Omega_x(t) - \Delta\omega\sigma_x(\Delta\omega;t), \quad (5)$$

$$\frac{d\sigma_z(\Delta\omega;t)}{dt} = \sigma_x(\Delta\omega;t)\Omega_y(t) - \sigma_y(\Delta\omega;t)\Omega_x(t), \quad (6)$$

where $\Delta\omega$ $(\omega - \omega_0)$ is the difference between the carrier frequency $(\omega)$ and the resonance frequency $(\omega_0)$. Neglecting the relaxation processes is a reasonable approximation when the pulse duration is much shorter than the relaxation times $T_1$ and $T_2$. By introducing a transverse magnetization or polarization

$$\sigma(\Delta\omega;t) = \sigma_x(\Delta\omega;t) + i\sigma_y(\Delta\omega;t), \quad (7)$$

Eqs. (4) and (5) can be combined into

$$\frac{d\sigma(\Delta\omega;t)}{dt} = -i\Delta\omega\sigma(\Delta\omega;t) + i\sigma_z(\Delta\omega;t)\Omega(t). \quad (8)$$

Here

$$\Omega(t) = \Omega_x(t) + i\Omega_y(t). \quad (9)$$

The normalized magnetizations or polarizations $\sigma_x$, $\sigma_y$, and $\sigma_z$ can be expressed in spherical coordinates as

$$\sigma_x = \cos\phi \sin\theta, \quad (10)$$

$$\sigma_y = \sin\phi \sin\theta, \quad (11)$$

$$\sigma_z = \cos\theta, \quad (12)$$

where $\theta$ is the flip angle and $\varphi$ is the phase of projection of magnetization or polarization on the $x$–$y$ plane. By converting Eq. (8) to spherical coordinates, the following equation can be easily obtained:

$$\left[\frac{d\theta}{dt}\cos\theta + i\sin\theta\left(\frac{d\phi}{dt} - \Delta\omega\right)\right]e^{i\phi} = i\cos\theta\Omega(t). \quad (13)$$

### A. Small angle approximation

We first consider the case when the flip angle $(\theta)$ is small $(\theta \approx 0)$. Therefore, $\tan\theta \approx \theta$ and Eq. (13) becomes

$$\left[\frac{d\theta}{dt} + i\theta\left(\frac{d\phi}{dt} - \Delta\omega\right)\right]e^{i\phi} = i\Omega(t) \quad (14)$$

or equivalently,

$$d\left[\theta e^{i(\phi - \Delta\omega t)}\right] = i\Omega(t)e^{-i\Delta\omega t}\,dt. \quad (15)$$

The well-known linear response theorem can be easily obtained by direct integration of the above equation

$$\theta(t) = ie^{-i(\phi - \Delta\omega t)}\int \Omega(\tau)e^{-i\Delta\omega\tau}\,d\tau. \quad (16)$$

### B. Stationary phase

Equation (16) is valid only when the flip angle $(\theta)$ is small. When the flip angle is near $\pi/2$, a different approach is required for the integration. When $\theta = \pi/2$, Eq. (13) clearly implies

$$\frac{d\phi}{dt} - \Delta\omega = 0 \quad (17)$$

or

$$\phi - \Delta\omega t = \phi_0, \quad (18)$$

where $\varphi_0$ is a constant. This equation, we refer to as the stationary phase condition, must be satisfied when $\theta = \pi/2$, regardless of the frequency and the phase angle. If $\Omega(t)$ is chosen so that

$$\tan\theta\left(\frac{d\phi}{dt} - \Delta\omega\right) \approx 0, \quad (19)$$

Eq. (13) becomes

$$\frac{d\theta}{dt} = i\Omega(t)e^{-i\phi} = ie^{-i\phi_0}\Omega(t)e^{-\Delta\omega t}. \quad (20)$$

Integrating Eq. (20) near $\theta \approx \pi/2$ with respect to Eq. (18) gives

$$\theta = ie^{-(\phi - \Delta\omega t)}\int \Omega(\tau)e^{-i\Delta\omega\tau}\,d\tau. \quad (21)$$

It is obvious that Eq. (21) has the same structure as Eq. (16), which was derived on the basis of the small angle approximation. However, we must remember that Eqs. (16)and (21) are not exact solutions of the Bloch equations. Deviation is expected when the flip angle is far away from the "poles" $(\theta = 0$ or $\pi)$ and the "equator" $(\theta = \pi/2)$. For example, when $\theta = \pi/4$, the solution underestimates the contribution of the "phase acceleration" $(d\varphi/dt - \Delta\omega)$ by a factor of $\pi/4$ $(\theta/\tan\theta$ for $\theta = \pi/4)$. To minimize the deviation, the phase acceleration itself should be kept minimal. In order to expand Eqs. (16) and (21) throughout the whole excitation process, the following criterion must be satisfied for any value of $\theta$:

$$\tan\theta\left(\frac{d\phi}{dt} - \Delta\omega\right) \approx 0. \quad (22)$$

Now we seek a sufficient condition in which the low amplitude or phase acceleration criterion, Eq. (22), is satisfied for any value of $\theta$. The imaginary part of Eq. (13) can be written as

$$\tan\theta\left(\frac{d\phi}{dt}-\Delta\omega\right)=\frac{1}{2i}[\Omega(t)e^{-i\phi}-\Omega^*(t)e^{i\phi}]$$
$$=|\Omega(t)|\sin(\eta-\phi), \quad (23)$$

where $\Omega^*=\Omega_x-i\Omega_y$ and $\eta$ is the phase of the excitation pulse. If the magnetization or polarization phase ($\varphi$) follows the excitation phase ($\varphi\approx\eta$), according to Eq. (23), then Eqs. (16) or (21) are good approximate solutuions of the Bloch equations. Since we are interested in broadband excitation and do not intend to discriminate excitation over the frequency range of interest, it is difficult to keep the condition of equal phases ($\varphi\approx\eta$). A sufficient condition for the criterion of Eq. (22) is therefore that of the low pulse amplitude $|\Omega(t)|\approx 0$.

The results derived here do not impose a limitation on the flip angle. Rather they can be used to analyze large flip angle excitation provided that the excitation periods are sufficiently long. Equations (16) or (21) should be useful for predicting the response of the magnetization or polarization to low amplitude excitation signals. For example, the flip angle under excitation of a low amplitude linear frequency sweeping signal can be described by the Fresno integral.[8] In the following sections, the focus will be on the synthesis of excitation pulses with the desired flip angle response profiles.

## III. ALGORITHM FOR GENERATING INVERSE FOURIER TRANSFORM EXCITATION PULSES

First, the problem of synthesis of excitation pulses needs to be defined. For simplicity, all the magnetization or polarizations are considered initially to be in the equilibrium states, i.e., $\theta_i(\Delta\omega)=0$ for all $\Delta\omega$. The question is how to synthesize an excitation pulse which brings the magnetizations or polarizations to the *desired* final states $\theta_f(\Delta\omega)$ and $\varphi_f(\Delta\omega)$. If the initial time is at $t=-T$ and the final states are observed at $t=0$, Eqs. (16) or (21) become

$$\theta_f(\Delta\omega;t=0)e^{i\phi_f(\Delta\omega;t=0)}=i\int_{-T}^{0}\Omega(\tau)e^{-i\Delta\omega\tau}\,dt. \quad (24)$$

If the pulse possesses nonzero amplitude only in $[-T,0]$, the above integration can be expanded to infinity in both directions

$$\theta_f(\Delta\omega)e^{-i\phi_f(\Delta\omega)}=i\int_{-\infty}^{\infty}\Omega(\tau)e^{-i\Delta\omega\tau}\,d\tau=iF(\Delta\omega). \quad (25)$$

Here $F(\Delta\omega)$, the excitation spectrum, is the Fourier transform of $\Omega(t)$. The flip angle and the phase are related to the excitation spectrum by

$$\theta_f(\Delta\omega)=M(\Delta\omega) \quad (26)$$

and

$$\phi_f(\Delta\omega)=P(\Delta\omega)+\pi/2, \quad (27)$$

where $M(\Delta\omega)$ is the magntidue spectrum of $\Omega(t)$ and $P(\Delta\omega)$ is its phase spectrum

$$F(\Delta\omega)=\int_{-\infty}^{\infty}\Omega(\tau)e^{-i\Delta\omega\tau}\,d\tau=M(\Delta\omega)e^{iP(\Delta\omega)}. \quad (28)$$

Equation (26) can be considered as an expansion of the well-known area theorem to broadband cases. These results suggest that the excitation pulse can be synthesized using the inverse Fourier transform method. A pulse with an arbitrary magnitude spectrum $[M(\Delta\omega)]$ or flip angle response profile $[\theta_f(\Delta\omega)]$ can be specified. On the other hand, the corresponding phase spectrum $[P(\Delta\omega)$ or $\varphi_f(\Delta\omega)]$ must be chosen so that the amplitude of the pulse is small enough to satisfy the low amplitude criterion [Eq. (22)].

In previous work, an algorithm to generate low peak power excitation signals from given magnitude spectra has been developed.[7] The basic idea of the algorithm is to distribute excitation power uniformly in a time interval using phase shifting.[9] The pulse power and therefore the amplitude of the pulse in the so-called power distributing period is nearly constant. The average amplitude in the power distributing period is inversely proportional to the square root of the time length of the period (see the Appendix). The power leakage outside the distributing period can be reduced by smoothing the magnitude spectrum.[6] Since the flip angle and phase response can be easily correlated with the excitation spectra [Eqs. (26) and (27)], this algorithm can be directly adapted to two-level systems.

In the following, an algorithm for producing an optimal excitation signal with an arbitrary flip angle response spectrum is proposed. First, the desired flip angle response $[\theta_f(\Delta\omega)$ or $M(\Delta\omega)]$ spectrum is specified. The pulse duration and the power distributing period can be estimated from the resolution and amplitude requirements. The phase spectrum is then calculated using Eq. (3) of Ref. 7. The excitation signal is obtained by inverse Fourier transformation of the phase and magnitude spectra. Equations (26) and (27) are derived from the approximate solutions of the Bloch equations. The deviation of the true response of the synthesized pulse from the desired (specified) response is expected. This deviation can be minimized using a simple optimization procedure described below. The true response $[\theta_{t1}(\Delta\omega)]$ of the first synthesized pulse from $\theta_f$ can be obtained by solving the Bloch equations numerically. A corrected response $[\theta_{c1}(\Delta\omega)]$ is calculated by subtracting the desired response $[\theta_f(\Delta\omega)]$ from the difference between the true response $\theta_{t1}$ and the desired response $\theta_f$.

$$\theta_{c1}=\theta_f-(\theta_{t1}-\theta_f)=2\theta_f-\theta_{t1} \quad (29)$$

the corrected response $\theta_{c1}$ can be used to produce the optimized pulse. The true response of the optimized pulse should deviate less from the desired one. The procedure can be repeated many times to obtain an excitation pulse with a high degree of agreement between the true response and the desired excitation profile.

The algorithm proposed above focuses on the improvement of the flip angle response. The phase response can also be optimized independently using the same procedure since the phase response $[\varphi(\Delta\omega)]$ is also linearly related to the phase spectrum $[P(\Delta\omega)]$ of the excitation pulse [Eq. (27)].

## IV. AN EXAMPLE

In this section, an example is presented to demonstrate the capability and flexibility of the method. The task is to synthesize an excitation pulse which produces a $\pi/2$ notch flip angle profile $[\theta_f(\Delta\omega)]$ as shown in Fig. 1(a). Several factors must be considered before the phase spectrum can be calculated. First, the length $(T_d)$ of the power distributing period should be sufficiently long to reduce the pulse amplitude. Since the transitions near $\Delta\omega = 0$ are quite sharp, some time length $(T_1)$ is needed for accomodating the "power leakage," while a short time duration $(T_2)$ is required for the slower transitions near $\pm\Delta\omega_0$. The magnitude spectrum specified is symmetrical. If the phase spectrum is chosen to be antisymmetrical, the resultant pulse will be real. A real excitation pulse implies that the excitation is only applied in the $x$ direction, and it can be decomposed into two counter-rotating fields. The phase spectrum [Fig. 1(b)] can then be calculated using Eq. (3) in Ref. 7(a).

The pulse shown in Fig. 1(c) is synthesized using inverse Fourier transformation from the magnitude [Fig. 1(a)] and phase [Fig. 1(b)] spectra. The true response of the pulse is obtained by solving the Bloch equations numerically using the Runge–Kutta method. The simulated response for the flip angle and phase is shown in Figs. 1(d) and 1(e), respectively. Although the flip angle response [Fig. 1(d)] basically agrees with the desired response [Fig. 1(a)], there are deviations near the transitions. A corrected magnitude spectrum [Fig. 2(a)] is constructed using Eq.

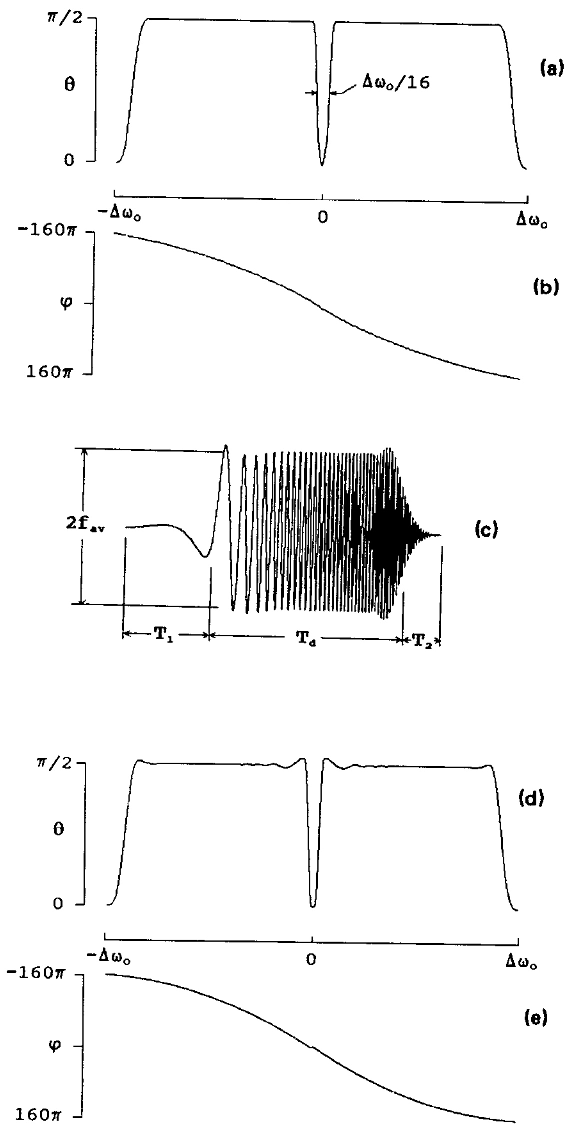


FIG. 1. Generation of a $\pi/2$ notch excitation pulse. (a) The specified flip angle response spectrum. The "well" width is about $\Delta\omega_0/16$. Since it is not important for the transitions at $\Delta\omega = \pm\Delta\omega_0$, the spectral edges have been heavily smoothed (see Ref. 7). (b) The phase response spectrum. It is essentially a quadratic function in $[0,\Delta\omega_0]$ or $[-\Delta\omega_0,0]$ and is chosen to be antisymmetrical so that the pulse becomes real. (c) The synthesized pulse. The total pulse length is equal to the summation of the power distributing period $T_d$, the accomodation periods ($T_1$ and $T_2$) for the power leakage. The sharp transitions near $\Delta\omega = 0$ in (a) requires a longer time duration $(T_1)$. Much shorter time $(T_2)$ is needed for slower transition near $\pm\Delta\omega$. Shown in (d) and (e) are the true flip angle and phase response, respectively. They are obtained by solving the Bloch equations numerically.

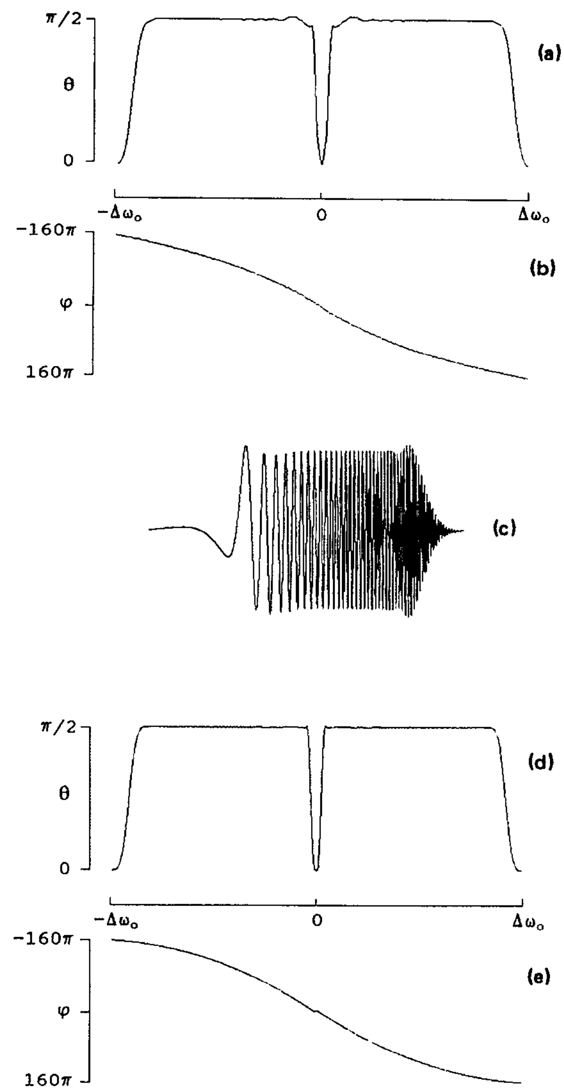


FIG. 2. Illustration of a simple optimizing procedure for improving the flip angle response. (a) The corrected flip angle response spectrum. (b) The corresponding phase spectrum. (c) The optimized pulse obtained by inverse Fourier transformation from (a) and (b). (d) and (e) are the true response of the pulse. The flip angle response spectrum (d) is now essentially the same as specified [Fig. 1(a)].

(29) in order to reduce the deviations. The corresponding phase is calculated [Fig. 2(b)] and the corrected pulse [Fig. 2(c)] is thus synthesized. The true response [Fig. 2(d)] of the flip angles of the corrected pulse is almost identical to what was originally specified [Fig. 1(a)].

It is interesting to examine the time evoluation of the magnetization or polarization under excitation of the synthesized pulse [Fig. 1(c)]. Figure 3 shows the simulated trajectories of both the flip angle and phase with a resonance frequency of $\Delta\omega_1$ ($=\Delta\omega_0/3$). The synthesized pulse behaves basically as a linear frequency sweeping signal in the power distributing period [$T_d$ in Fig. 1(c)]. As predicted from Eqs. (16) or (21), the flip angle basically follows a Fresno integral. For large flip angles, the phase approaches to a straight line with a slope of the resonance frequency $\Delta\omega_1$.

It should be pointed out that frequency sweep or chirp excitation is closely related to adiabatic rapid passes (ARP)[10] that can generate complete population inversion ($\theta=\pi$). This requires that the frequency sweeping rate is sufficiently low. A current experiment using frequency sweep modulated picosecond laser pulses for population inversion of electronic states has demonstrated that the frequency sweep pulses achieve population inversion more effectively than unmodulated pulses.[11] The pulse synthesized in this section is essentially a frequency sweep signal in the so-called power distribution period. Unlike normal frequency sweep pulses, the pulse has amplitude that gradually decreases outside of the power distribution period. This is partially responsible for the frequency selectivity of the pulse. Through the optimization procedure, the flip angle frequency response of the pulse is also improved.

If the magnitude spectrum is chosen to spin from $-3200$ to 3200 Hz ($\Delta\omega_0=3200$ Hz), the length of the time-domain pulse synthesized is 40 ms. The synthesized pulse should be found useful for solvent-suppression excitation in NMR experiments and for imaging localization in MRI. The pulse length can be reduced (e.g., to 10 ms) by shortening the power distributing period. The trade off will be the larger deviation of the flip angle response.

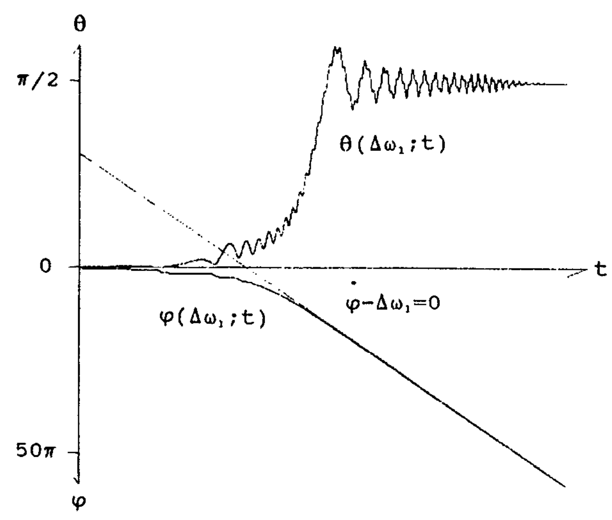


FIG. 3. Time evolution of flip angle and phase for the magnetization or polarization at $\Delta\omega_1=\Delta\omega_0/3$ during excitation of the synthesized pulse [Fig. 1(c)]. As predicted, the flip angle is basically a Fresno integral and the phase stationary condition is achieved at a low flip angle level.

## V. CONCLUSION

The response of a two-level system to low amplitude excitation has been studied. Under the assumption of low amplitude excitation, the flip angle is linearly related to the spectrum of the excitation pulse. The significance of the results is that it allows one to predict the response to low amplitude excitation without having to solve the Bloch equation directly. It also permits one to synthesize the excitation signals to achieve the desired responses. The basic limitation of the method is that it requires long time periods to produce broadband and large flip angle excitations.

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## APPENDIX

Estimation of the average amplitude using the Parseval's equation was first proposed by Goodman.[12] Here we derive an equation to correlate the length of the time period for distributing excitation power and the average amplitude of the pulse in the power distributing period using the Parseval's formula,

$$\int_{-\infty}^{\infty}|f(t)|^2\,dt=\frac{1}{2\pi}\int_{-\infty}^{\infty}|F(\omega)|^2\,d\omega. \quad \text{(A1)}$$

Here $f(t)$ is the time domain wave form and $F(\omega)$ is its spectrum. Since the excitation power is uniformly distributed over a time period that we denote as $T$ or $(t_1-t_0)$; amplitude of the time domain wave form does not vary significantly in the region of $T$. Let $f_0$ be the average value of the amplitude of $f(t)$ in $T$. Since most of the power of the wave form is confined in the region $T$ and the wave form behaves essentially like a constant amplitude and phase modulated signal $[f_0e^{i\varphi(t)}]$, we have

$$\int_{-\infty}^{\infty}|f(t)|^2\,dt\approx\int_{t_0}^{t_1}|f_0e^{i\phi(t)}|^2\,dt\approx f_0^2(t_1-t_0), \quad \text{(A2)}$$

where $f_0$ is evaluated as a base-to-peak value. If the spectrum $F(\omega)$ and the power distribution length ($T=t_1-t_0$) are predetermined, the average amplitude of the wave form can be estimated easily by

$$f_0\approx\left\{\frac{1}{2\pi T}\int_{-\infty}^{\infty}|F(\omega)|^2\,d\omega\right\}^{1/2}. \quad \text{(A3)}$$

If the power distribution period is sufficiently long, the accuracy of the estimation can be expected to be high. The average amplitude ($f_0$) is therefore approximately inversely proportional to square root of the power distributing period ($T$).

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