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The full analytical solution of the Bloch equation when using a hyperbolic-secant driving function

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Abstract

Purpose—The frequency-swept pulse known as the hyperbolic-secant (HS) pulse is popular in NMR for achieving adiabatic spin inversion. The HS pulse has also shown utility for achieving excitation and refocusing in gradient-echo and spin-echo sequences, including new ultrashort echo-time imaging (e.g., SWIFT) and B₁ mapping techniques. To facilitate the analysis of these techniques, the complete theoretical solution of the Bloch equation, as driven by the HS pulse, was derived for an arbitrary state of initial magnetization.

Methods—The solution of the Bloch-Riccati equation for transverse and longitudinal magnetization for an arbitrary initial state was derived analytically in terms of HS pulse parameters. The analytical solution was compared to the solutions using both the Runge-Kutta method and the small-tip approximation.

Results—The analytical solution was demonstrated on different initial states at different frequency offsets with/without a combination of HS pulses. Evolution of the transverse magnetization was influenced significantly by the choice of HS pulse parameters. The deviation of the magnitude of the transverse magnetization, as obtained by comparing the small-tip approximation to the analytical solution, was < 5% for flip angles < 30°, but > 10% for the flip angles > 40°.

Conclusion—The derived analytical solution provides insights into the influence of HS pulse parameters on the magnetization evolution.

Keywords

hyperbolic secant; HS pulse; adiabatic pulse; Bloch equation; analytical solution

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Supporting Information

Appendix I – Detailed derivation of Eq. [30].

Appendix II – Proof of that Eq. [30] is the solution of Eq. [28].

INTRODUCTION

The Bloch equation for stationary spins is a system of ordinary differential equations. Analytical solutions of the Bloch equation can be obtained for some external driving functions, including a hard (square) RF pulse and the frequency-swept hyperbolic-secant (HS) pulse (1–4). Since Silver et al. first suggested that the complex form of the HS B_1 field could be used for narrow-band spin inversion in analogy to self-induced transparency in coherent optics (4), the HS pulse has been most widely used as an adiabatic pulse in NMR, providing a high degree of tolerance to B_1 inhomogeneity (i.e., adiabatic property) as well as delivering an excellent inversion profile with sharp transition regions.

At an early stage, the HS pulse was used only for spin inversion due to the non-linear phase variation created in the transverse plane. Recently, the utility of the HS pulse has been extended to include π -refocusing, as well as other flip angles ($\pi/2$) for excitation. The use of the HS pulse for π -refocusing in 2D spin-echo imaging is originally attributed to the work of Conolly et al. (5). They reported that the non-linear phase in the transverse plane can be fully compensated by using an identical pair of HS π -pulses since the non-linear phase variation produced by one HS pulse is completely cancelled out by the use of another identical HS pulse. More recently, the phase behavior of spins was theoretically analyzed when the HS pulse was used not only for refocusing but also for $\pi/2$ excitation (6,7). In particular, a *single* HS π -pulse can form a spin echo without non-linear phase provided that the $\pi/2$ -excitation is performed with another HS pulse and certain parameter relationships exist between these two HS pulses (6), e.g., the $\pi/2$ -excitation pulse length must be twice that of the π -refocusing pulse when their pulse bandwidths are equal (7).

When compared to spin inversion or refocusing, less attention has been paid to the use of the HS pulse for spin excitation ($\pi/2$) because the adiabatic condition is not satisfied in this low-flip angle region. However, it was recently proposed that the HS pulse can also be used for spin excitation in conventional 3D gradient-echo (GRE) to achieve a sharp slab profile and high signal-to-noise ratio (SNR) when receiver dynamic range is limiting (8). Also, in gradient-recalled echo-planar imaging (EPI), HS pulse excitation can recover signal drop out caused by through-plane dephasing in the brain (9).

Besides the merits of HS excitation in conventional imaging, another clever use of the HS pulse for spin excitation was suggested in the ultra-short echo-time MRI technique called SWIFT (Sweep Imaging with Fourier Transform) (10,11). The essential feature of this technique is time sharing of data acquisition with spin excitation, thereby allowing for almost zero acquisition delay, where non-linear phase contamination of signal is effectively eliminated by a correlation procedure (10). The SWIFT technique has found its use in numerous interesting applications, including dental, lung, iron oxide nanoparticles and bone imaging (12–17), and more recently, advanced versions of SWIFT have also been proposed from a technical standpoint (18–20).

To comply with such extended use of the HS pulse, here we re-visit the theoretical solution of the Bloch equation with the HS pulse as a driving function, especially to find an analytical expression of the *transverse* magnetization (M_{xy}) for an *arbitrary* initial state of

magnetization. Silver et al. first derived the theoretical solution of the Bloch equation by transforming it to the form of the Riccati equation when the HS pulse was applied as a B_1 field. However, they only provided an analytical expression of the *longitudinal* magnetization (M_z) for the initial magnetization *only* along the B_0 direction (the z axis). Later, Rosenfeld et al. derived the solution for both M_{xy} and M_z , but they were expressed in a spinor form with some general mathematical coefficients, which hinders a good grasp of the relationship between the physical parameters. In this paper, we provide an analytical expression for M_{xy} as well as M_z in the general case of having an arbitrary state of initial magnetization, e.g., in the transverse plane or along the z -axis, by solving the Bloch-Riccati equation as Silver et al. originally did. We then express M_{xy} and M_z in terms of the pulse parameters such as pulse length and bandwidth which are more convenient for analysis and characterization of the HS pulse. The analytical solutions are compared to the famous analytical expression of M_{xy} simplified by the small-tip approximation (21,22), not only for better understanding of the HS pulse behavior in a linear low flip-angle regime, but also for ascertaining the limitation of the small-tip approximation in comparison to the exact theoretical solution.

METHODS

Mathematical Expression of the HS pulse

When it was originally suggested by Silver et al. (4), the HS pulse was given in a complex form,

$$\omega_1(t) = \omega_1^{\max} \left(\text{sech}(\beta'(t - t_0)) \right)^{1+i\mu} = \omega_1^{\max} \text{sech}(\beta'(t - t_0)) e^{i\phi(t)}, \quad [1]$$

where $\omega_1^{\max}$ is the maximum pulse amplitude in rad/s, β' and μ are real constants, and $\phi(t) = \mu \cdot \ln \left(\text{sech}(\beta'(t - t_0)) \right)$. However, it is convenient to write the pulse expression in an alternative form with separation of amplitude modulation (AM) and frequency modulation (FM) (23), especially for the analysis and characterization of the HS pulse, that is

$$\omega_1(t) = AM(t) \cdot e^{i \int FM(t) dt} \quad [2a]$$

$$AM(t) = \omega_1^{\max} \text{sech} \left(\frac{2\beta}{T_p} \left(t - \frac{T_p}{2} \right) \right), \quad [2b]$$

$$FM(t) = A \tanh \left(\frac{2\beta}{T_p} \left(t - \frac{T_p}{2} \right) \right). \quad [2c]$$

Here, the pulse length (T_p) was introduced and the real coefficient β' in Eq. [1] was replaced by a new dimensionless truncation factor β which equals to $T_p\beta'/2$, so that the terms except β in the argument of the sech and tanh functions, i.e., $2/T_p(t-T_p/2)$, work as a normalized time ranging from -1 to 1 when time t varies from 0 to T_p . β is typically set such that $\text{sech}(\beta) = 0.01$ and thus $\beta = 5.2983$, implying the truncation of the pulse amplitude with 1% of $\omega_1^{\max}$ at its leading and trailing edges. The opposite frequency sweep can easily be achieved by changing the sign of β . Since FM(t) is given by $-d\phi/dt$ in clockwise spin precession, coefficient A replaces $\mu\beta'$ in Eq. [2c] and represents the amplitude of the frequency sweep in rad/s, determining the pulse bandwidth (BW), i.e., $BW = A/\pi$. On the other hand, the commonly used time-bandwidth product, $R = BW \cdot T_p = (A/\pi) \cdot T_p$, can be introduced, and its value is fixed once the pulse is generated. The real constant μ in Eq. [1] can then be expressed in terms of R and β ,

$$\mu = \frac{A}{\beta'} = \frac{A \cdot T_p}{2\beta} = \frac{R\pi}{2\beta}. \quad [3]$$

According to Eq. [3], just as μ does, β and R are expected to affect the sharpness of the transition region of the frequency-response profile and the shape of a quadratic phase of the produced M_{xy} .

The Bloch-Riccati equation and its analytical solution: $M_{xy}(t)$ and $M_z(t)$

As mentioned earlier, Silver et al. derived the analytical solution of the Bloch equation for calculating M_z only for an initial magnetization along the z axis by solving the Bloch-Riccati equation. For the purpose of completeness and as the starting point for our derivation, we first briefly describe the work by Silver et al. which includes derivation of the Bloch-Riccati equation and determination of M_z by way of finding its solution. However, the present description uses the pulse parameters introduced in the previous section.

Since spin relaxation times are usually much longer than the pulse length, the Bloch equation can be expressed in a simple vector form as

$$\frac{\partial \mathbf{M}_{rot}}{\partial t} = \gamma \mathbf{M}_{rot} \times \mathbf{B}_{eff}, \quad [4]$$

where $\mathbf{M}_{rot}$ represents the magnetization vector in the rotating frame and $\mathbf{B}_{eff}$ is the effective magnetic field defined as a vector sum of the B_1 field and the resonance-offset field. Using a complex notation of $M_{xy} = M_x + iM_y$ in Eq. [4], two first-order differential equations can be obtained in terms of M_{xy} and M_z :

$$\begin{cases} \frac{dM_{xy}}{dt} + i\Omega M_{xy} - i\omega_1(t)M_z = 0 \\ \frac{dM_z}{dt} - \frac{i}{2} [\omega_1^*(t)M_{xy} - \omega_1(t)M_{xy}^*] = 0, \end{cases} \quad [5a][5b]$$

where $\omega_1(t) = \gamma B_1(t)$ and the asterisk $*$ denotes a complex conjugate. In this case, introducing a new variable f defined as

$$f = \frac{M_{xy}}{M_0 + M_z}, \quad [6]$$

where M_0 is an initial equilibrium magnetization, equations [5a] and [5b] can be reduced to a single equation

$$\frac{df}{dt} + i\Omega f + \frac{i}{2}\omega_1^*(t)f^2 - \frac{i}{2}\omega_1(t) = 0. \quad [7]$$

Equation [7] has the form of the Riccati equation in terms of f and is dubbed the Bloch-Riccati equation (4).

With the driving function of Eq. [2] and by using the identity of hypertrigonometric functions and introducing two new variables p and q defined as

$$p(t) = \frac{1}{2} \left(1 + \tanh \left(\frac{2\beta}{T_p} \left(t - \frac{T_p}{2} \right) \right) \right), \quad [8]$$

$$q(t) = \exp \left[\frac{i}{2} \int_0^t \omega_1^*(t') f dt' \right], \quad [9]$$

respectively, Eq. [7] can be transformed to the hypergeometric equation

$$p(1-p) \frac{d^2 q}{dp^2} + \left[-\left(1 + i \frac{R\pi}{2\beta}\right)p + \frac{1}{2} + i \frac{1}{4\beta} (\Omega T_p + R\pi) \right] \frac{dq}{dp} + \left(\frac{\omega_1^{\max} T_p}{4\beta} \right)^2 q = 0, \quad [10]$$

where $R = (A/\pi) \cdot T_p$. With reference to the canonical form of the hypergeometric equation, the general solution of Eq. [10] can be written in terms of the hypergeometric functions, yielding,

$$q(p) = C_A F(a, b, c; p) + C_B p^{1-c} F(a - c + 1, b - c + 1, 2 - c; p), \quad [11]$$

where $F(a, b, c; p)$ represents the Gauss hypergeometric series, ${}_2F_1(a, b, c; p)$; C_A and C_B are arbitrary constants; a , b , and c are expressed as

$$\begin{cases} a = \frac{R\pi}{4\beta} \left(i + \sqrt{\left(\frac{\omega_1^{\max}}{A}\right)^2 - 1} \right) \\ b = \frac{R\pi}{4\beta} \left(i - \sqrt{\left(\frac{\omega_1^{\max}}{A}\right)^2 - 1} \right) \\ c = \frac{1}{2} + i \frac{R\pi}{4\beta} \left(\frac{\Omega}{A} + 1 \right) \end{cases} \quad [12]$$

Then, the solution of the Bloch-Riccati equation [7], f , is attained from dq/dp (Eqs. [9] and [11]) in terms of hypergeometric functions and pulse parameters as

$$f = \frac{2\beta\omega_1(t)}{iT_p(\omega_1^{\max})^2} \left[C_A \frac{ab}{c} \frac{F(a+1, b+1, c+1; p)}{q} + C_B \frac{(1-c)p^{-c} F(a-c+1, b-c+1, 2-c; p)}{q} + C_B \frac{(a-c+1)(b-c+1)}{2-c} \frac{p^{1-c} F(a-c, b-c, 1-c; p)}{q} \right] \quad [13]$$

In the work by Silver et al., only a simplified version of $|f|$ was provided assuming an initial magnetization along the z axis ($M_{xy0} = 0$ and $M_{z0} = 1$). Once a complete version of f is obtained, the full solution of the Bloch equation, M_{xy} and M_z , can easily be derived from the definition of f in Eq. [6]:

$$\frac{M_{xy}}{M_0} = \frac{2f}{1+|f|^2}, \quad \frac{M_z}{M_0} = \frac{1-|f|^2}{1+|f|^2} \quad [14]$$

The coefficients C_A and C_B in Eq. [13] can be determined from the boundary conditions of q and dq/dp . While $p(0) = p_0 = 1/2(1 - \tanh\beta)$ approximately equals 0 as t goes to 0 in Eq. [8], $q(0) = 1$ from Eq. [9]. These conditions can be applied to $q(t)$ in Eq. [11],

$$\lim_{t \rightarrow 0} q(t) = \lim_{p \rightarrow 0} [C_A F(a, b, c; p) + C_B p^{1-c} F(a-c+1, b-c+1, 2-c; p)] = 1, \quad [15]$$

and the coefficient C_A is thus given by

$$C_A = \frac{1 - C_B p_0^{1-c} F(a-c+1, b-c+1, 2-c; p_0)}{F(a, b, c; p_0)} \approx 1. \quad [16]$$

The coefficient C_B can be determined by comparing two different expressions of dq/dp . One expression is obtained from Eq. [9] using the chain rule:

$$\begin{aligned} \lim_{t \rightarrow 0} \frac{dq}{dp} &= \lim_{t \rightarrow 0} \frac{dq}{dt} \frac{dt}{dp} = \lim_{t \rightarrow 0} \frac{\frac{i}{2} \omega_1^*(t) f q}{\frac{dp}{dt}} \\ &= \lim_{t \rightarrow 0} \frac{i T_p \omega_1^{\max} 2^{1-i \frac{R\pi}{2\beta}} [p(1-p)]^{-\frac{1}{2}-i \frac{R\pi}{4\beta}} f q}{8\beta}. \end{aligned} \quad [17]$$

Another expression of dq/dp is obtained from Eq. [11] which can be approximated to a simpler form as t goes to 0:

$$\begin{aligned} \lim_{t \rightarrow 0} \frac{dq}{dp} &= \lim_{t \rightarrow 0} C_A \frac{ab}{c} F(a+1, b+1, c+1; p_0) \\ &\quad + C_B (1-c) p_0^{-c} F(a-c+1, b-c+1, 2-c; p_0) \\ &\quad + C_B p_0^{1-c} \frac{(a-c+1)(b-c+1)}{2-c} F(a-c+2, b-c+2, 3-c; p_0) \\ &\approx \lim_{t \rightarrow 0} C_A \frac{ab}{c} + C_B (1-c) p_0^{-c} \end{aligned} \quad [18]$$

In Eq. [18], the third term of the derivative can be neglected since p_0^{1-c} is very small ($p_0 \approx 0$). By comparing Eq. [17] with Eq. [18], C_B can be obtained as

$$\begin{aligned} C_B &= \frac{i \omega_1^{\max} T_p}{2^{2+i \frac{R\pi}{2\beta}} (1-c)\beta} f_0 \lim_{t \rightarrow 0} p^{i \frac{\Omega T_p}{4\beta}} = \frac{i \omega_1^{\max} T_p}{2^{2+i \frac{R\pi}{2\beta}} (1-c)\beta} f_0 p_0^{i \frac{\Omega T_p}{4\beta}} \\ &= \frac{i \omega_1^{\max} T_p}{2^{2+i \frac{R\pi}{2\beta}} (1-c)\beta} f_0 e^{i \phi_0} \end{aligned} \quad [19]$$

where

$$\phi_0 \equiv \frac{\Omega T_p}{4\beta} \ln p_0 = \frac{\Omega T_p}{4\beta} \ln \frac{1}{2} (1 - \tanh \beta) \quad [20]$$

and for an arbitrary initial magnetization, e.g. in the transverse plane ($M_{xy0}=1, M_{z0}=0$) or along the z axis ($M_{xy0}=0, M_{z0}=1$), or any magnetization state between them, f_0 can be calculated from Eq. [14], whereby

$$\begin{cases} f_0 = \lim_{t \rightarrow 0} f(t) = \left(\frac{1}{|M_{xy0}|} - \sqrt{\frac{1}{|M_{xy0}|^2} - 1} \right) e^{i \phi_{M_{xy0}}}, & \text{if } M_{xy0} \neq 0 \\ f_0 = \lim_{t \rightarrow 0} f(t) = 0, & \text{if } M_{xy0} = 0 \end{cases} \quad [21]$$

Because C_A and C_B are now determined, leading to the solution of f (Eq. [13]), equation [14] provides a *complete* set of solutions (i.e., for M_{xy} and M_z) for any initial state of magnetization when the HS pulse is used for spin excitation. In the case of initial state $M_{xy0} = 0$ and $M_{z0} = 1$, C_B is equal to 0 and Eq. [13] can be simplified to

$$f = \frac{iT_p\omega_1(t)}{8\beta c} \frac{F(a+1, b+1, c+1; p)}{F(a, b, c; p)} \quad [22]$$

If we focus on the final state of the magnetization at the end of the HS pulse duration ($t \rightarrow T_p$), the magnitude of f in Eq. [22] can be further reduced to (4)

$$|f|_{p \rightarrow 1} = \left(\frac{\cosh^2\left(\frac{R\pi^2}{4\beta}\right) - \cosh^2\left(\frac{R\pi^2}{4\beta}\sqrt{1 - (\omega_1^{\max}/A)^2}\right)}{\cosh^2\left(\frac{R\pi^2\Omega}{4\beta A}\right) + \sinh^2\left(\frac{R\pi^2}{4\beta}\sqrt{1 - (\omega_1^{\max}/A)^2}\right)} \right)^{\frac{1}{2}} \quad [23]$$

In this case, for an on-resonance isochromat ($\Omega = 0$), M_z at the end of pulse duration is simply obtained by substituting Eq. [23] into [14] as

$$\frac{M_z}{M_0}|_{p \rightarrow 1} = \frac{1 + \cosh\left(\frac{R\pi^2}{2\beta}\sqrt{1 - (\omega_1^{\max}/A)^2}\right)}{\cosh^2\left(\frac{R\pi^2}{4\beta}\right)} - 1 \quad [24]$$

By using $M_z/M_0 = \cos\theta$, where θ is the flip angle, Eq. [24] leads to an equation for the peak RF amplitude $\omega_1^{\max}$ needed to produce a given θ value (9),

$$\omega_1^{\max} = A \sqrt{\left\{ \frac{2\beta}{R\pi^2} \cos^{-1} \left[\cos\theta \cosh^2\left(\frac{R\pi^2}{4\beta}\right) + \sinh^2\left(\frac{R\pi^2}{4\beta}\right) \right] \right\}^2 + 1}. \quad [25]$$

In a low RF power regime where $\omega_1^{\max}/A \ll 1$, $\omega_1^{\max}$ can be expressed in a much simpler form because, interestingly, Eq. [24] is equal to a cosine function if we neglect the higher-order terms including the third term in the Taylor expansion, leading to

$$\begin{aligned} \frac{M_z}{M_0}|_{p \rightarrow 1} = \cos\theta &\cong 1 - \frac{1}{2} \frac{R\pi^2}{\beta} \left(\frac{\omega_1^{\max}}{A}\right)^2 + \frac{1}{16} \left(\frac{R\pi^2}{\beta}\right)^2 \left(\frac{\omega_1^{\max}}{A}\right)^4 \dots \\ &\approx \cos\left(\frac{\omega_1^{\max}}{A} \sqrt{\frac{R\pi^2}{\beta}}\right) = \cos\left(\omega_1^{\max} \sqrt{\frac{T_p}{\beta \cdot BW}}\right) \end{aligned} \quad [26]$$

It is apparent here that the argument of the resulting cosine function is the flip angle, which is in agreement with the work in Ref. (24). Accordingly, at low flip angles, Eq. [25] can be approximated by the simple expression,

$$\omega_1^{\max} \approx A\theta \sqrt{\frac{\beta}{R\pi^2}}. \quad [27]$$

Comparison with the solution based on the small-tip approximation

A simplified version of the analytic Bloch solution has previously been proposed for an initial magnetization along the z axis with an arbitrary driving function using the famous small-tip approximation (21,22). The small-tip approximation ($M_z \approx M_0$) simplifies the Bloch equation with respect to M_{xy} as

$$\frac{dM_{xy}(t)}{dt} + i\Omega M_{xy}(t) - i\omega_1(t) M_0 = 0 \quad [28]$$

The analytic solution of a first-order linear differential equation is well known, and with an initial condition of $M_{xy0} = 0$ and $M_{z0} = 1$, the solution of Eq. [28] is given by

$$\frac{M_{xy}(t, \Omega)}{M_0} = i\gamma \int_0^t \omega_1(\tau) e^{-i\gamma\Omega(t-\tau)} d\tau. \quad [29]$$

Since Eq. [29] is based on the small-tip approximation, it is interesting to explore the effective working range of Eq. [29] from the viewpoint of the complete analytical solution

derived in the previous section. Provided that $\sqrt{\frac{R\pi}{\beta}} \frac{\omega_1^{\max}}{A} \ll 1$, by keeping only the leading-

order term in Eq. [12] neglecting the term of $(\omega_1^{\max}/A)^2$, we have $a \rightarrow i\frac{R\pi}{2\beta}$ and $b \rightarrow 0$. Under this condition, the solution for an initial magnetization in the z direction can be reduced to (for details see Appendix I in Supporting Information)

$$\begin{aligned} \lim_{\sqrt{\frac{R\pi}{\beta}} \frac{\omega_1^{\max}}{A} \ll 1} \frac{M_{xy}}{M_0} &= \lim_{\substack{a \rightarrow i\frac{R\pi}{2\beta} \\ b \rightarrow 0}} \frac{2f}{1+|f|^2} \approx 2f \\ &= \sqrt{\frac{R\pi}{\beta}} \frac{\omega_1^{\max}}{A} \lim_{b \rightarrow 0} \frac{iS(t)F\left(i\frac{R\pi}{2\beta} + 1, 1, c+1; p\right)}{4\sqrt{\frac{R\pi}{\beta}} c} \\ &\simeq O\left(\sqrt{\frac{R\pi}{\beta}} \frac{\omega_1^{\max}}{A}\right) \simeq O(\theta) \end{aligned} \quad [30]$$

where $\omega_1(t) = \omega_1^{\max} S(t)$ was used. Notice that the last step is directly related to the result of

Eq. [26]. Equation [30] shows that if $\sqrt{\frac{R\pi}{\beta}} \frac{\omega_1^{\max}}{A} \ll 1$, the leading term of the analytical

solution is in the first order of θ , as expected from the fact that $\frac{M_{xy}}{M_0} = \sin\theta$. It can also be proved that Eq. [30] is the solution of Eq. [28] (see Appendix II appearing in Supporting Information), implying that the solution derived from the small-tip approximation (Eq. [29]) becomes equivalent to the complete analytical solution under the condition that

$\sqrt{\frac{R\pi}{\beta}} \frac{\omega_1^{\max}}{A} \ll 1$, as long as all the higher-order terms are neglected. For a self-consistency

check, it is worthwhile to note that, with the same approximation, i.e., by keeping only the leading-order term, the Bloch-Riccati equation (Eq. [7]) is also reduced to

$$\frac{df}{dt} + i\Omega f - \frac{i}{2}\omega_1(t) = 0, \quad [31]$$

which is identical to Eq. [28].

Simulation

The analytical solution presented here describes spin excitation for an arbitrary initial state of the magnetization when using one HS pulse or any combination of HS pulses in a sequence. Various simulations were performed for demonstration of various conditions, including different frequency offsets, different initial magnetization states, and different flip angles. To validate the derived analytical solution, a numerical simulation of the Bloch equation was also performed using the Runge-Kutta method and compared with the analytical solution. In addition, an example of combined HS pulses, e.g., a $\pi/2$ pulse successively followed by a π pulse, was investigated for different pulse cutoff (β) values, whose effect on spin evolution has not been investigated before. Lastly, comparisons between the derived analytical solution and the solution from the small-tip approximation were made to ascertain the limitation of the small-tip approximation by varying the flip angle.

RESULTS

Examples of the temporal evolution of M_{xy} are shown in Fig. 2 for two different initial states ($M_{xy0} = 0, M_{z0} = 1; M_{xy0} = 1, M_{z0} = 0$) at two different frequencies ($\Omega/2\pi = 0$ and 6 kHz) during execution of a single HS pulse with $R = 32$ and 16 kHz-bandwidth. One initial state ($M_{xy0} = 0, M_{z0} = 1$) was intended for $\pi/2$ excitation and the other one ($M_{xy0} = 1, M_{z0} = 0$) for π refocusing. Since the pulse bandwidth is wide enough to cover the 6-kHz frequency offset, as well as the on-resonance frequency, the $\pi/2$ excitation and π refocusing cause the magnitude of M_{xy} go to 1 from 0 and 1, respectively, at the end of the pulse duration. By comparing the plots for $\Omega/2\pi = 0$ and 6 kHz, it is apparent that the evolution patterns of M_{xy} differ substantially and the frequency offset causes the largest temporal variations in $\text{Re}(M_{xy})$ and $\text{Im}(M_{xy})$.

In Fig. 3, the difference between the analytical solution and the numerical solution obtained using the Runge-Kutta method is plotted for the same simulation setups as in Fig. 2. The overall difference between the analytical and numerical solutions is marginal; the difference was less than 1% for the $\pi/2$ HS pulse and less than ~2% for the π HS pulse, supporting the validity of the analytical solution derived here.

Figure 4 presents an example of applying the $\pi/2$ HS pulse successively followed by the π HS pulse (6), for two different β values which satisfy $\text{sech}(\beta_1) = 0.01$ and $\text{sech}(\beta_2) = 0.0001$, respectively. The initial magnetization was assumed to be along the z axis. HS pulses of $R = 128$ and 64 were used for $\pi/2$ excitation and π refocusing, respectively, having the same

bandwidth of 31.25 kHz. While the use of a different β has only a limited influence on the time evolution of M_{xy} during the first $\pi/2$ HS pulse, the choice of β value has considerable affect during the following π HS pulse. This is a consequence of the phase of M_{xy} (including the initial phase) having dependence on β (Eq. [20]), and when the initial magnetization is not along the z axis as is the case before the application of the π HS pulse in this simulation, the time evolution of M_{xy} is fairly sensitive to the choice of β .

In Fig. 5, magnitude and phase comparisons between the analytical solution of the Bloch equation and the solution from the small-tip approximation are shown with respect to flip angle for HS excitation with initial state $M_{xy0} = 0$ and $M_{z0} = 1$. The simulations of Figs. 5a and 5b were performed by varying the R value of the HS pulse from $R = 10$ to 128 by an increment of 10. Figure 5a is a 3D plot of the simulation results and some examples of three different R values (10, 20, and 128) are representatively shown in Fig. 5b. While the magnitude of M_{xy} predicted by the small-tip approximation shows a deviation from the exact solution less than 5% for flip angles less than $\sim 30^\circ$, the deviation is more than 10% when the flip angle is larger than $\sim 40^\circ$ and keeps increasing as the flip angle increases regardless of the R value. Besides the difference in the M_{xy} amplitude, difference in phase is also shown through the difference in the real part of M_{xy} ($\text{Re}(M_{xy})$) between the small-tip approximation and the exact analytical solution (Fig. 5c – 5h). Three different flip angles (8° , 40° , 80°) were tested for simulation. While Figs. 5c, 5d, and 5e present the time evolution of $\text{Re}(M_{xy})$ for a frequency offset of 31.25 kHz, Figs. 5f, 5g, and 5h show the signals (the sum of $M_{xy}(t)$ over all isochromats during excitation) acquired from a 1D square object simulating the SWIFT sequence (8). For comparison purposes, the M_{xy} amplitude for the small-tip approximation case was rescaled to that of the analytical solution. Differences were not apparent between the two solutions during the spin pre-releasing period ($t < 0.8$ ms) for the three flip angles. A difference begins to be noticeable at 40° and becomes more apparent at the higher flip angle of 80° . In practice, such error in the small-tip approximation may be problematic for SWIFT reconstruction (8). Specifically, in image reconstruction of SWIFT data, a correlation procedure is needed to effectively remove the non-linear phase contamination caused by the frequency modulation of the HS pulse. Since the validity of such correlation procedure relies on the assumption of the linear response of a spin system, the solution from the small-tip approximation has been used in SWIFT image reconstruction. However, for high flip angles (e.g. higher than 40° in settings as in Fig. 5d), the linear approximation no more holds, and thus, the complete analytical solution should be used in the algebraic reconstruction of SWIFT data (25).

DISCUSSIONS

In this paper, a full theoretical solution (M_{xy} and M_z) of the Bloch equation using the HS pulse for spin resonance was derived for an arbitrary initial magnetization state. The derived solution can be used with any combination of HS pulses including a single HS pulse for spin excitation, refocusing, and inversion. This analytic solution has utility for explicitly revealing and thereby understanding the dependence of spin dynamics on pulse parameters when using the HS pulse.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Fig. 1.

(a–d) Representative plots of the HS pulse with $R = 32$ and $T_p = 2.048$ ms: (a) Trajectory of the $B_1(t)$ field in a reference frame rotating at a constant carrier frequency (also known as the phase-modulated frame); (b) The plots of the $B_1(t)$ components, $B_{1x}(t)$ and $B_{1y}(t)$, in x and y directions, respectively; (c) & (d) are the amplitude- and frequency-modulated functions of the HS pulse as in the format of Eq. [2]; The pulse power spectral density (PSD) of HS pulses with different R and β values showing different sharpness of the transition region: (e) $R = 32$; (f) $\text{sech}(\beta) = 0.01$.

Fig. 2.

Transverse time evolutions of a spin isochromat for two different initial states at two different frequency offsets ($\Omega/2\pi = 0$ and 6 kHz), respectively, during the HS pulse duration. The HS pulse of $R = 128$ and $\text{sech}(\beta) = 0.01$ was used, with $BW = 62.5$ kHz and $T_p = 2.048$ ms. For the left two columns, flip angle was $\pi/2$ and the initial magnetization was in the z axis ($M_{xy0} = 0$, $M_{z0} = 1$). For the right two columns, flip angle was π and the initial magnetization was in the xy plane ($M_{xy0} = 1$, $M_{z0} = 0$).

Fig. 3.

The difference between the derived analytical solution and the numerical solution obtained using the Runge-Kutta method for the same simulation setups as in Fig. 2. The overall difference was marginal, that is, less than 1% for $\pi/2$ HS pulse and less than $\sim 2\%$ for π HS pulse, supporting the validity of the analytical solution derived here.

Fig. 4.

The real, imaginary and magnitude of $M_{xy}(t)$ on resonance (a, b & c) or at 6 kHz frequency offset (d, e & f) during two successive pulses for two different β values satisfying $\text{sech}(\beta_1)=0.01$ and $\text{sech}(\beta_2)=0.0001$. The two HS pulses have the same bandwidth: $\pi/2$ pulse, $R = 128$, $T_p = 4.096$ ms; π pulse, $R = 64$, $T_p = 2.048$ ms. The phase shift due to different β values is apparent, especially during the π pulse.

Fig. 5.

3D (a) and 2D (b) plots of the percentage difference of $\text{abs}(M_{xy})$ between the small-tip approximation and the derived analytical solution with respect to flip angle and R value of the HS pulse. The difference is less than 5% only for flip angles lower than 30° , whereas it becomes more than 10% when the flip angle is larger than 40° . (c)–(h) Comparison between the derived analytic solution (marked in red) and the solution from the small-tip approximation (marked in blue). The M_{xy} amplitude for the small-tip approximation case was rescaled to that of the analytical solution. While (c), (d) and (e) show the time evolution of the real part of M_{xy} for a spin offset with $\Omega = 31.25$ kHz, (f), (g) and (h) are the sum of the signals acquired from a 1D square object with spins at $\Omega \in [-31.25, 31.25]$ kHz simulating the SWIFT sequence. The HS pulse was used for spin excitation having $R = 128$ and $T_p = 2.048$ ms.