



About the origins of NMR diffusion-weighting induced by frequency-swept pulses

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ABSTRACT

In the present work, the non-linear phase dispersion induced by slice selective frequency-swept pulses is analyzed, in order to assess NMR signal attenuation due to molecular diffusion during such pulses. In particular, theoretical considerations show that diffusion-weighting can be calculated based on the non-linear phase spatial derivative (i.e. the phase gradient), and that the phase of B_1 field at the instant of the flip does not contribute to phase scrambling and diffusion-weighting, yielding a simple analytical expressions. The theory is validated by confrontation with numerical simulations of the Bloch equations including diffusion, performed for a pair of hyperbolic secant pulses and a pair of CHIRP pulses. The simple though general conceptual framework developed here should be useful for the understanding and the exact calculation of diffusion-weighting in NMR sequences using frequency-swept pulses.

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1. Introduction

Adiabatic pulses provide an efficient way to perform broadband and homogeneous magnetization flip, even in the presence of strong B_1 inhomogeneities [1]. This property has for example been exploited to perform slice or volume selection, such as in the LASER spectroscopy sequence [2], in the Pseudo-LASER spectroscopic imaging sequence [3] or in various imaging sequences [4–7]. Furthermore, trains of adiabatic pulses may be used to generate contrasts based on relaxation in the rotating frame [8,9].

When applied in conjunction with a slice selection gradient, an adiabatic pulse generates a non-linear phase throughout the selected slice along the direction of the gradient. This is due to the frequency-swept nature of adiabatic pulses, where the magnetization is flipped when the frequency of the pulse is equal to the Larmor frequency Ω . This phase can then be refocused by a second, identical pulse [10,11], in order to prevent signal loss due to incoherent averaging throughout the slice. It has been argued that the phase dispersion created by an adiabatic pulse might induce diffusion-weighting. In their pioneer work [12], Sun and Bartha proposed an expression for diffusion-weighting induced by trains of hyperbolic secant pulses, assuming a quadratic phase dispersion (such as induced by a CHIRP pulse [13]).

When “zooming” into the elementary events occurring during frequency-swept pulses, two components can be identified in the

non-linear phase: the phase acquired in the slice selection gradient, depending on the gradient strength and on the instant of the flip t_Ω , and the phase induced by the B_1 field orientation itself, depending on the B_1 phase at the instant of the flip. In the present work, we propose to revisit the origins of the non-linear phase dispersion to assess if both the phase variation of the B_1 field during the sweep and the phase acquired in the slice selection gradient should be explicitly considered when calculating diffusion-weighting. To address these questions, a formalism is proposed that allows general calculation of diffusion-weighting when frequency-swept pulses are used. An analytical expression is then derived for diffusion-weighting induced by a pair of slice selective hyperbolic secant pulses and CHIRP pulses. These expressions are validated by numerical simulation of the Bloch equations including diffusion.

2. Theory

2.1. The phase induced during a frequency-swept pulse

An exact evaluation of the rotation induced by an arbitrary pulse requires composing rotation operators over suitably small time intervals to account for elementary rotations around a step-wise constant effective field, rapidly leading to complex analytical expressions. However, during a frequency-swept pulse, the magnetization can be assumed to be flipped around the B_1 field at the instant t_Ω when the frequency of the pulse is equal to its Larmor frequency Ω [3,6,7,14]. This approximation provides a simple yet accurate description of magnetization's behavior during the pulse,

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which was verified by many numerical simulations and experiments [3,6,7,14]. It allows for example the calculation of the magnetization's phase during the pulse [3,6,7,14]. Let us consider for example a frequency-swept pulse of duration T_p performing slice-selective refocusing. Considering a gradient of magnitude G_{slice} oriented along x , the phase evolution for magnetization with Larmor frequency $\Omega = \gamma G_{\text{slice}} x$ and flipped at t_{Ω} is given by [3,7], Φ_{B_1} being the phase of the \mathbf{B}_1 field (Fig. 1):

$$\begin{aligned} 0 < t < t_{\Omega} : \phi(x, t) &= \gamma G_{\text{slice}} t x \\ t_{\Omega} < t < T_p : \phi(x, t) &= 2\phi_{B_1}(t_{\Omega}) + \gamma G_{\text{slice}}(t - 2t_{\Omega})x \end{aligned} \quad (1)$$

This phase dispersion can then be refocused by a second, identical slice selective pulse. Looking at Eq. (1), two components can be identified in the non-linear phase: the phase acquired in the slice selection gradient, depending on the gradient strength and on the instant of the flip t_{Ω} , and the phase induced by the \mathbf{B}_1 field orientation itself, depending on the \mathbf{B}_1 phase at the instant of the flip. Since diffusion-weighting is based on phase scrambling, both components may *a priori* contribute to signal attenuation. Without further analysis, the effect of the \mathbf{B}_1 phase cannot be taken into account. We will now try to clarify how this \mathbf{B}_1 phase contributes to diffusion-weighting induced by frequency-swept pulses.

2.2. Diffusion in an arbitrary phase gradient

The usual definition of $\mathbf{k}(t)$ as the moment of a \mathbf{B}_0 gradient \mathbf{G} will be used:

$$\mathbf{k}(t) = \gamma \int_0^t \mathbf{G}(t') dt' \quad (2)$$

Using this notation, the signal attenuation due to diffusion during duration t in \mathbf{B}_0 gradients is (\mathbf{D} being the diffusion tensor):

$$A(t) = \exp\left(-\int_0^t \mathbf{k}^T(u) \times \mathbf{D} \times \mathbf{k}(u) du\right) \quad (3)$$

It is important to note that the phase induced by a gradient along x is $\phi(x, t) = k_x(t)x$, $k_x(t)$ being therefore the phase gradient $\partial\phi/\partial x$ (independent of x). Starting from here, let us consider now a more general case, where the phase $\phi(x, t)$ is not solely induced by \mathbf{B}_0 gradients, but by any other phenomenon, such as frequency-swept pulses. $\phi(x, t)$ is now an arbitrary function of x and t , with $\partial\phi/\partial x$ *a priori* depending on x and t . However, there is still a strong physical analogy between this arbitrary phase gradient $\partial\phi/\partial x$ and a \mathbf{B}_0 gradient moment k_x along x . Indeed, the effect of diffusion will be to scramble phase and induce signal loss, as induced by a \mathbf{B}_0 gradient. Using the gradient operator $\vec{\nabla}$, the phase gradient is given by:

$$\vec{\nabla}\phi(\mathbf{r}, t) = \left(\frac{\partial\phi}{\partial x}(\mathbf{r}, t), \frac{\partial\phi}{\partial y}(\mathbf{r}, t), \frac{\partial\phi}{\partial z}(\mathbf{r}, t)\right)^T \quad (4)$$

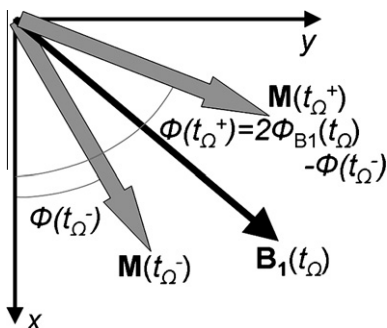


Fig. 1. Evolution of the transverse magnetization \mathbf{M} at the instant of the flip t_{Ω} during a 180° frequency-swept pulse. \mathbf{M} is considered to be instantaneously flipped by 180° around \mathbf{B}_1 .

It is demonstrated in Appendix A that, since ϕ can generally be considered locally linear (i.e. the phase gradient $\partial\phi/\partial x$ is constant) over the distance experienced by diffusing spins during the sequence (see Appendix B for the validity of this assumption), the attenuation due to diffusion is given by:

$$A(\mathbf{r}, t) = \exp\left(-\int_0^t \vec{\nabla}\phi^T(\mathbf{r}, u) \times \mathbf{D} \times \vec{\nabla}\phi(\mathbf{r}, u) du\right) \quad (5)$$

Therefore, there is a formal analogy between \mathbf{k} and $\vec{\nabla}\phi$ regarding diffusion-weighting. However, due to its more general form compared to Eq. (3), Eq. (5) can now be used to rigorously evaluate the effect of the phase induced by a frequency-swept pulse on diffusion-weighting.

2.3. Phase gradient induced during a frequency-swept pulse

The phase gradient evolution during the pulse is given by differentiating Eq. (1):

$$\begin{aligned} 0 < t < t_{\Omega} : \frac{\partial\phi}{\partial x} &= \gamma G_{\text{slice}} t = k_{\text{slice}}(t) \\ t_{\Omega} < t < T_p : \frac{\partial\phi}{\partial x} &= \underbrace{2 \frac{\partial\phi_{B_1}}{\partial t}(t_{\Omega}) \frac{\partial t_{\Omega}}{\partial x}}_{k_{B_1}} - 2\gamma G_{\text{slice}} x \frac{\partial t_{\Omega}}{\partial x} + \underbrace{\gamma G_{\text{slice}}(t - 2t_{\Omega})}_{k_{\text{slice}}(t)} \end{aligned} \quad (6)$$

In Eq. (6) two components can be identified: the usual slice gradient moment k_{slice} (whose sign is changed at t_{Ω} by the 180° rotation), and a “radiofrequency” term k_{B_1} including \mathbf{B}_1 contribution. However, during frequency-swept pulses, the magnetization is flipped when the pulse frequency is equal to Ω , which can be written as $\partial\phi_{B_1}/\partial t(t_{\Omega}) = \gamma G_{\text{slice}} x$. Inserting in Eq. (6) yields the following simplification:

$$\begin{aligned} 0 < t < t_{\Omega} : \frac{\partial\phi}{\partial x} &= \gamma G_{\text{slice}} t = k_{\text{slice}}(t) \\ t_{\Omega} < t < T_p : \frac{\partial\phi}{\partial x} &= \gamma G_{\text{slice}}(t - 2t_{\Omega}) = k_{\text{slice}}(t) \end{aligned} \quad (7)$$

In the end, the contribution of the \mathbf{B}_1 field orientation is cancelled out when calculating the spatial derivative of the non-linear phase, so that only the phase induced by the gradient needs to be considered for diffusion-weighting. In short, when considering diffusion-weighting, the effect of a 180° frequency-swept pulse is simply to change the sign of gradient moment \mathbf{k} at the instant t_{Ω} .

Note that a similar conclusion is reached if the pulse induces a 90° excitation rather than a 180° refocusing. Indeed, the phase is simply zero before the excitation ($0 < t < t_{\Omega}$), then the magnetization is instantaneously flipped around \mathbf{B}_1 and starts precessing for $t > t_{\Omega}$ [6]:

$$\begin{aligned} 0 < t < t_{\Omega} : \phi(x, t) &= 0 \\ t_{\Omega} < t < T_p : \phi(x, t) &= \phi_{B_1}(t_{\Omega}) + \frac{\pi}{2} + \gamma G_{\text{slice}}(t - t_{\Omega})x \end{aligned} \quad (8)$$

In that case the phase gradient simplifies as well to:

$$\begin{aligned} 0 < t < t_{\Omega} : \frac{\partial\phi}{\partial x} &= 0 \\ t_{\Omega} < t < T_p : \frac{\partial\phi}{\partial x} &= \gamma G_{\text{slice}}(t - t_{\Omega}) = k_{\text{slice}}(t) \end{aligned} \quad (9)$$

3. Methods

3.1. Analytical calculation of diffusion-weighting during a pair of slice-selective frequency-swept pulses

Following the analysis detailed in the Theory section, diffusion-weighting induced during a pair of slice selective frequency-swept

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