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Calculation of diffusion effect for arbitrary pulse sequences

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Abstract

A method is presented for calculating the nuclear spin magnetization created by an arbitrary number of short radio frequency pulses and of piecewise constant gradient applied in a selected direction. The isotropic diffusion, the transverse and longitudinal relaxations as well as the global transport are taken into account. A thorough analysis of the magnetization density evolution results in an algorithm for the analytical calculation of final NMR signal. Computationally, it requires only accumulating numerical coefficients in the found analytical structure. For arbitrary sequences this is done with a computer program. This approach, which can be classified as symbolical computations, results in a high performance and in a practically unlimited accuracy. Results for sample pulse sequences are presented.

1. Introduction

Implementation of any new pulse sequence implies understanding of the way in which the basic MR parameters of a homogeneous sample are represented in the measured signal. While the account for the finite relaxation times is available for all sequences in use, finding the diffusion effect remains a challenging problem. It is only resolved for the gradient echo and spin echo techniques [1,2], for the stimulated echo [3] and for the steady-state precession with pulsed gradients [4–7].

In this paper, the NMR signal is found for a large class of pulse sequences characterized by short radio frequency (RF) pulses and a short gradient rise time. The exact meaning of these limitations and a way to release them are discussed below.

The presented calculation method is based on an analytical solution to the Bloch–Torrey equation for a constant gradient of magnetic field in the absence of RF pulses. A generalization for the switched gradients and an arbitrary number of RF pulses is achieved by convolving such solutions, the operation which is performed by symbolical computations in Fourier space.

The developed technique is applied to two illustrative examples. The first one is a train of pulses with an arbitrary flip angle. The diffusion effect for such a sequence is currently unknown. The other example is a recently developed pulse sequence with smooth transition between pseudo steady states (TRAPS) [8].

2. Method

2.1. Pulse sequences

Consider a pulse sequence shown in Fig. 1. Suppose that the duration of all RF pulses is shorter than any other relevant time such as the diffusion time or the duration of T_2 weighting. In such a case, every RF pulses can be described as an instant spin rotation. A similar assumption for the gradients implies a short gradient rise time. These assumptions are employed throughout this paper and referred to as the instant switching, which can be restriction can be released by representing a long RF pulse with a train of weaker pulses and by a stepwise increasing gradients. An additional limitation on the considered class of sequences is that all gradient pulses are applied in a single selected direction.

To sum up, the considered pulse sequences can be described as a number, N, of events, which are either the RF pulses or the gradient switching (Fig. 1). It is convenient to call all such events the RF pulses assigning a zero flip angle to those which are actually absent.

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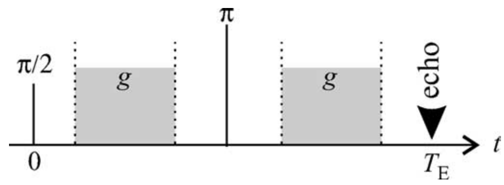

Fig. 1. The Stejskal–Tanner pulse sequence as an example of the assumed sequence description. The applied pulses are shown with the vertical bars. The dashed bars represent the formally added RF pulses with zero flip angle, which serve as separators between the successive time intervals. In each interval the applied gradient is constant, either g or zero.

Keeping this terminology, the pulse sequence is sliced by the instantly acting RF pulses in N successive time intervals. The magnetization evolution in each interval is governed by the diffusion in the constant gradient. An analysis of the arbitrary sequence from this point of view is presented below.

2.2. Basic equations

The observed signal is a sum of all individual spin magnetizations. It is convenient to perform this summation in two steps engaging the notion of spin packets. Consider the sample as consisting of infinitesimally small volume elements, each of them smaller than any relevant length, but still containing a large number of spins. The spin content of each volume element is called the spin packet. The overall sample magnetization in the sample is obtainable by a double summation, first over the spins in each packet and, second, over all packets.

The first RF pulse, which is applied at time $t = 0$, initiates the evolution of nuclear magnetization. The spin carrying molecules freely diffuse in the applied gradient. Each spin is affiliated with its original spin packet regardless its actual Brownian trajectory for $t > 0$. Let $\Psi(\mathbf{r}, \mathbf{r}_0, t)$ be the magnetization density produced to a time moment t at a point $\mathbf{r}$ by a spin packet originated at a point $\mathbf{r}_0$. Initially $\Psi(\mathbf{r}, \mathbf{r}_0, 0) = \delta(\mathbf{r} - \mathbf{r}_0)$. This implies that the equilibrium magnetization density is set to unity, which is the assumed normalization. In terms of $\Psi(\mathbf{r}, \mathbf{r}_0, 0)$, the total NMR signal, $S(t)$, takes the following form:

$$S(t) = \int \mathrm{d}\mathbf{r}_0 \, \mathrm{d}\mathbf{r} \, \Psi(\mathbf{r}, \mathbf{r}_0, t). \tag{1}$$

Here $\int \mathrm{d}\mathbf{r} \Psi(\mathbf{r}, \mathbf{r}_0, t) \equiv m(\mathbf{r}_0, t)$ is the total spin packet magnetization, while $\int \mathrm{d}\mathbf{r}_0$ accounts for all spin packets. In the homogeneous medium all spin packets are equivalent up to the phase factor, $\mathrm{e}^{\mathbf{ikr}_0}$, with $\mathbf{k}$ defined by the applied gradient. Thus $S(t)$ is equal to the Fourier transform of the sample shape with a weight given by $m(0, t)$. This signal is zero for infinitely large homogeneous sample considered here unless the spin echo is formed. In such a case, the spin packet magnetization, $m(\mathbf{r}_0, t)$, has an $\mathbf{r}_0$-independent component. The total signal, which is then proportional to the sample volume, can be represented by the magnetization $m(0, t)$ of a single spin packet positioned at the origin $\mathbf{r}_0 = 0$. The aim of the following analysis is to find this quantity for the considered pulse sequence.

The spin magnetization evolves according to the Bloch–Torrey equation [9] during each interpulse interval. Being a three-dimensional vector, the spin packet magnetization depends on variables $\mathbf{r}$ and t, and on $\mathbf{r}_0$ as a parameter. The appropriate form of Bloch–Torrey equation reads

$$\frac{\partial \psi}{\partial t} = D\nabla^2 \psi + \mathbf{igrI}_z \psi - \frac{1}{T_2} \mathbf{I}_z^2 \psi - \frac{1}{T_1} \left(\mathbf{1} - \mathbf{I}_z^2\right) \psi \tag{2}$$

for the low-frequency magnetization. Here ψ is the difference between the current and the equilibrium magnetization densities. Its exact meaning as well as that of other quantities is as follows.

The first term on the right-hand side of Eq. (2) describes the conventional isotropic diffusion of magnetization with a constant D. Laplacian operator ∇^2 acts on the variable $\mathbf{r}$.

The next term describes the spin precession caused by the applied gradient. The vector $\mathbf{g}$ is the gradient of the Larmore frequency (which is the gradient of the magnetic field measured, e.g., in mT/m multiplied with the gyromagnetic ratio, γ). The combination $\mathbf{gr}$ is a scalar product of the two vectors. The 3×3 matrix $\mathbf{I}_z$ generates the variation of magnetization vectors by the infinitesimal rotations around the z-axis, which is selected in the direction of the main field. The vector ψ rotated by a small angle ϵ is equal to $(\mathbf{1} + \mathrm{i}\epsilon\mathbf{I}_z)\psi$ plus the higher order terms in ϵ. Here $\mathbf{1}$ is the 3×3 unity matrix. The explicit form of $\mathbf{I}_z$ and one of its useful properties read

$$\mathbf{I}_z = \begin{pmatrix} 0 & \mathrm{i} & 0 \\ -\mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{I}_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{3}$$

The way this formalism works is made clear by selection only the precession term on the right-hand side of Eq. (2):

$$\frac{\partial \psi}{\partial t} = \mathbf{igrI}_z \psi. \tag{4}$$

This equation has a simple solution

$$\psi(t) = \mathrm{e}^{\mathbf{igr}t\mathbf{I}_z} \psi(0). \tag{5}$$

Here the exponential function of matrix arises as a multiple product of $\mathbf{1} + \mathbf{igrI}_z \, \mathrm{d}t$. This function can be calculated as the Taylor expansion with an account for the second property stated in Eq. (3):

$$\begin{aligned} \mathrm{e}^{\mathrm{i}\alpha\mathbf{I}_z} &= \mathbf{1} - \mathbf{I}_z^2 + \mathbf{I}_z^2 \cos\alpha + \mathrm{i}\mathbf{I}_z \sin\alpha \\ &= \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{6}$$

This is the conventional rotation matrix. $\mathbf{I}_z$ is proportional to its derivative with respect to α. This property explains the mathematical name of $\mathbf{I}_z$ which is the generator of rotations around the z-axis.

The third and the fourth terms on the right-hand side of Eq. (2) describe the transverse and the longitudinal relaxations, respectively. They result in a factor in ψ in the form

$$\begin{pmatrix} e^{-t/T_2} & 0 & 0 \\ 0 & e^{-t/T_2} & 0 \\ 0 & 0 & e^{-t/T_1} \end{pmatrix}. \tag{7}$$

This multiplier is for simplicity omitted in the following intermediate expressions.

Eq. (2) can now be solved for any initial condition. To this end it is convenient to use a regular way consisting in finding the unique fundamental solution of Eq. (2) and convolving it with the given initial condition. Since both the latter and the resulted magnetization are three-dimensional vectors, the fundamental solution should be a 3×3 matrix. This solution, which is called the Green function or the propagator, is selected by the initial condition

$$\psi(\mathbf{r}, \mathbf{r}_0, 0) = \mathbf{1} \cdot \delta(\mathbf{r} - \mathbf{r}_0). \tag{8}$$

The solution of Eq. (2) for a magnetization density $\eta(\mathbf{r}, t)$ takes the following form for the given initial condition $\eta(\mathbf{r}, 0)$

$$\eta(\mathbf{r}, t) = \int d\mathbf{r}_0 \psi(\mathbf{r}, \mathbf{r}_0, t)\eta(\mathbf{r}_0, 0). \tag{9}$$

Here the convolution is performed for both the continuous coordinate $\mathbf{r}_0$ (the integration) and the discrete vector index of η (by the action of matrix ψ).

The explicit form of $\psi(\mathbf{r}, \mathbf{r}_0, t)$ is known for each interpulse interval, that is for the constant gradient without any RF pulses. A straightforward substitution in Eq. (2) proves that

$$\begin{aligned} \psi(\mathbf{r}, \mathbf{r}_0, t) &= \frac{1}{(4\pi D t)^{3/2}} \\ &\exp\left(-\frac{(\mathbf{r}-\mathbf{r}_0)^2}{4Dt} + \mathrm{i}\mathbf{g}t\frac{\mathbf{r}-\mathbf{r}_0}{2}\mathbf{I}_z - \frac{D\mathbf{g}^2t^3}{12}\mathbf{I}_z^2 \right) e^{\mathrm{i}\mathbf{g}\mathbf{r}_0 t\mathbf{I}_z} \\ &\equiv \phi(\mathbf{r}-\mathbf{r}_0, t)e^{\mathrm{i}\mathbf{g}\mathbf{r}_0 t\mathbf{I}_z}. \end{aligned} \tag{10}$$

The latter form is introduced to display the structure of ψ consisting of ϕ, which is a function of displacement $\mathbf{r} - \mathbf{r}_0$, and of the $\mathbf{r}_0$-dependent phase factor. This factor is a matrix which can be calculated using Eq. (6). The meaning of the three columns of $\psi(\mathbf{r}, \mathbf{r}_0, t)$ is the magnetization density of the initially δ-functional spin packets magnetized in the directions of x, y, and z, respectively.

The subtraction and the addition of the equilibrium magnetization is done with the relation

$$\Psi(\mathbf{r}, \mathbf{r}_0, t) = \mathbf{M}_0 + \psi(\mathbf{r}, \mathbf{r}_0, t), \tag{11}$$

where $\Psi(\mathbf{r}, \mathbf{r}_0, t)$ is the total magnetization matrix, and

$$\mathbf{M}_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix}. \tag{12}$$

The goal of this paper can now be formulated as to find the function $\Psi(\mathbf{r}, \mathbf{r}_0, t)$ in the presence of RF pulses. The solution is simple in principle. The magnetization created right after an RF pulse should be considered as the initial condition for the evolution during the following interpulse interval according to Eqs. (11), (9), and (10). This procedure repeats itself after the next RF pulse. Starting with the initial equilibrium magnetization, it is possible to find $\Psi(\mathbf{r}, \mathbf{r}_0, t)$ for the arbitrary combination of RF and gradient pulses provided the assumption of the instant switching is met. This program is fulfilled in the next section.

2.3. Evolution of magnetization in Fourier space

It is convenient to perform all calculations in Fourier space in which the convolution Eq. (9) turns in a product. Consider an interpulse interval assigning $t = 0$ to its beginning. Let now $\eta(\mathbf{r}_0, 0)$ in Eq. (9) be the previously developed Green function of the Bloch–Torrey equation (which is now the 3×3 matrix). Performing the convolution in Eq. (9) for the function defined in Eq. (10) results in the following relation for the Fourier transforms:

$$\tilde{\psi}(\mathbf{k}, t) = \int d\mathbf{p}\tilde{\phi}(k, t)\delta(\mathbf{k} - \mathbf{p} - \mathbf{g}t\mathbf{I}_z)\tilde{\eta}(\mathbf{p}, 0). \tag{13}$$

Here the tilde marks the Fourier transform of the corresponding quantities. The δ-function arises due to the phase factor in Eq. (10). It should be understood as the matrix Eq. (6) integrated with the additional phase factors. It reads explicitly

$$\begin{aligned} &\delta(\Delta k - \mathbf{g}t\mathbf{I}_z) \\ &= \frac{1}{2}\begin{pmatrix} \delta_- + \delta_+ & \mathrm{i}\delta_- - \mathrm{i}\delta_+ & 0 \\ -\mathrm{i}\delta_- + \mathrm{i}\delta_+ & \delta_- + \delta_+ & 0 \\ 0 & 0 & 2\delta(\Delta k) \end{pmatrix} \equiv \Delta, \end{aligned} \tag{14}$$

where $\delta_\pm = \delta(\Delta k \pm \mathbf{g}t)$. The presence of the δ-functions in Eq. (13) removes the integration over $\mathbf{p}$ thus reducing the convolution to a product. It is convenient to postpone this step keeping Eq. (13) for the following analysis.

The evolution of magnetization density $\tilde{\Psi}(\mathbf{k}, t)$, which is the Fourier transform of $\Psi(\mathbf{r}, 0, t)$, can be summarized as a sequence of elementary operations on $\tilde{\Psi}(\mathbf{k}, t)$. Consider a building block of the pulse sequence, that is an RF pulse with the following interpulse interval. In each such block $\tilde{\Psi}(\mathbf{k}, t)$ can be calculated through the following steps:

$$\begin{aligned}
&\tilde{\Psi} := O_\varphi(\alpha)\cdot\tilde{\Psi} \quad \text{rotation by the RF pulse,}\\
&\tilde{\Psi} := \tilde{\Psi} - \tilde{M}_0 \quad \text{subtraction of equilibrium magnetization,}\\
&\tilde{\Psi} := \Delta\cdot\tilde{\Psi} \quad \text{action of matrix consisting of } \delta\text{-functions,}\\
&\tilde{\Psi} := \tilde{\phi}\cdot\tilde{\Psi} \quad \text{evolution between the pulses,}\\
&\tilde{\Psi} := \tilde{\Psi} + \tilde{M}_0 \quad \text{addition of equilibrium magnetization.}
\end{aligned} \tag{15}$$

Here the symbol $:=$ denotes the assignment from the right to the left-hand side. Matrix $O_\varphi(\alpha)$ performs the global spin rotation by the angle α around the axis with the phase φ in the xy plane. It can be calculated as follows:

$$O_\varphi(\alpha) = \mathrm{e}^{-\mathrm{i}\varphi\mathbf{I}_z}\,\mathrm{e}^{\mathrm{i}\alpha\mathbf{I}_x}\,\mathrm{e}^{\mathrm{i}\varphi\mathbf{I}_z}, \tag{16}$$

where $\mathbf{I}_x$ is the matrix similar to Eq. (6), but generating rotations around the x-axis

$$\mathrm{e}^{\mathrm{i}\alpha\mathbf{I}_x} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix}. \tag{17}$$

The equilibrium magnetization $\tilde{M}_0$ takes the form

$$\tilde{M}_0 = M_0\delta(k). \tag{18}$$

The meaning of the product in Eq. (15) depends on the context. It is the regular matrix product in the first and the fourth lines. In the third line, it implies the convolution as defined in Eq. (13).

The steps listed in Eq. (15) should be repeated for all interpulse intervals. The initial value of $\tilde{\Psi}$ before the very first RF pulse defines the identity matrix

$$\tilde{\Psi} = \mathbf{1}\cdot\delta(\mathbf{k}), \tag{19}$$

which corresponds to the homogeneous magnetization. The final $\tilde{\Psi}$ should be taken at $k = 0$ according to Eq. (1) (this is the condition of echo formation).

It is the key issue of the present method that the evolution matrix $\tilde{\Psi}$ keeps its following form on each step of procedure described in Eq. (15). $\tilde{\Psi}$ is a 3×3 matrix consisting of elements $\tilde{\Psi}_{ij}$, $i, j = 1, 2, 3$, which are linear combinations of δ-functions:

$$\tilde{\Psi}_{ij}(k,t) = \sum_a C^a_{ij}\delta(k - \kappa^a_{ij}), \tag{20}$$

where κ^a_{ij} are some real numbers and the running index a counts all terms with different κ^a_{ij}. This statement can be proved by the mathematical induction as follows. First note that the initial condition Eq. (19) falls in the form Eq. (20). The same is valid for $\tilde{M}_0$. Thus the operations in the first, the second, and the last lines of Eq. (15) preserve this form. The multiplication with Δ is performed according to Eq. (13), which turns into the following rule:

$$\int \mathrm{d}p\,\delta(k - p - \kappa_1)\delta(p - \kappa_0) = \delta(k - \kappa_1 - \kappa_0). \tag{21}$$

Here the first δ-function comes from Δ, while the second is a term of $\tilde{\Psi}$. This operation is equivalent to incrementing the previously accumulated κ_0 by the new contribution κ_1. The coefficients in front of the δ-functions should be obviously multiplied. The form Eq. (20) is also preserved by the multiplication with a function $\tilde{\phi}(k)$ in the fourth line of Eq. (15). It modifies solely the coefficients C^a_{ij} in Eq. (20), since the function argument can be replaced with the value defined by the δ-function. This completes the proof.

The algorithm formulated in Eq. (15) with the form for the elements of Ψ as defined in Eq. (20) provide a regular analytical way to compute the signal for any pulse sequence of the considered class. In praxis, the calculations quickly become cumbersome as the number of pulses increases thus hindering the pure analytical calculus. To overcome this trouble, the routine computations can be delegated to a computer. This implies keeping the analytical structure of all involved quantities with only the coefficients C^a_{ij} and κ^a_{ij} in Eq. (20) computed numerically. These values are subjected to addition and multiplication only. Consequently, there is no inherent method error. The accuracy is limited by the rounding error, which is typically of the order of 10^{-16} for the double precision numbers. In practical computations the required accuracy should be reduced by several orders of magnitude in order to reliably collect similar terms. This method yields the magnetization matrix $\tilde{\Psi}(k,t)$ to the time moment of signal acquisition. Only the terms which are proportional to $\delta(k)$ contribute to the signal according to the condition of echo formation. Finally the third column of $\tilde{\Psi}$ is selected, that yields the magnetization of spins, which have been initially polarized along the z-direction. The above method has been implemented as a C++ program in which the objects entering Eq. (15) are described by means of C++ classes.

2.4. Account for global transport

The above approach can be extended to account for uniform motion of all spins with a velocity $\mathbf{v}$. Consider the transport part of Eq. (2). It follows from the equation for the magnetization balance supplemented with a formula for the magnetization flux density $\mathbf{j}$:

$$\frac{\partial\psi}{\partial t} = -D\nabla\mathbf{j}, \tag{22}$$

$$\mathbf{j} = -D\nabla\psi + \mathbf{v}\psi. \tag{23}$$

Substitution of Eq. (23) in Eq. (22) results in

$$\frac{\partial\psi}{\partial t} = D\nabla^2\psi - \mathbf{v}\nabla\psi + \mathbf{igrI}_z\psi + \cdots, \tag{24}$$

where dots stand for the relaxation terms in Eq. (2). The solution to this equation takes the form of Eq. (10) with the function ϕ replaced with

$$\phi_v(\mathbf{r}-\mathbf{r}_0, t) = \phi(\mathbf{r}-\mathbf{r}_0-\mathbf{v}t, t)\mathrm{e}^{-\mathrm{i}\mathbf{g}\mathbf{v}t^2\mathbf{I}_z/2}. \tag{25}$$

Here the modified argument of ϕ takes into account the transport and the exponential factor describes the phase acquired by spins moving in the constant gradient. The Fourier transform of $\phi(\mathbf{r}-\mathbf{r}_0-\mathbf{v}t)$ is $\tilde{\phi}(\mathbf{k}, t)\mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{v}t}$. Since any change in $\mathbf{k}$ is proportional to $\mathbf{g}$ (according to Eq. (14)), the result actually depend on the component $\mathbf{v}$ in the direction of $\mathbf{g}$. Other velocity components do not cause any encoding. Thus the problem is reduced to considering the motion in the direction of applied gradient. To sum up, the uniform transport does not change the calculation scheme Eq. (15) resulting only in the above modification of $\tilde{\phi}$.

3. Sample results

Application of the developed method to the Stejskal–Tanner, stimulated echo and CPMG pulse sequences has shown a perfect agreement with the analytically known results. The computational performance depends on whether the phases acquired in the applied gradients are commensurate. In the extreme case of all commensurate phases, that is for the CPMG pulse sequences, the computation time scales proportionally to the number of applied RF pulses. On a 2 GHz Pentium PC running under Linux, it takes about 3 s for 4096 RF pulses with 275 KB memory allocated.

3.1. Train of RF pulses with arbitrary flip angle

Sample calculations were applied to trains of N α-pulses with a $\pi/2$ phase difference between the first and all other pulses and a constantly applied gradient g (the cursive letters denote the magnitudes of corresponding vectors). The T_1 and T_2 relaxations were neglected. The transverse magnetization in units of equilibrium magnetization, which is called hereafter the signal, S, is shown in Fig. 2 as a function of N and α. The signal for $N = 1$ (Fig. 2, left) vanishes since no echo is formed. For large N the magnetization reaches the steady state. No signal is present for $\alpha = 0$ and $\alpha = \pi$ (Fig. 2, right), as such pulses create no transverse magnetization. For all other flip angles, the signal dependence on the applied gradient is singular at $g = 0$, the feature which is well known for the stimulated echo. In the absence of any gradient ($g = 0$ in the figure) all spin are flipped coherently. The final magnetization is just $s = (1 - (\cos\alpha\cos(N-1)\alpha)^2)^{1/2}$. In the infinite sample, any finite gradient eliminates the signal from the magnetization components which do not form the echo to the moment of acquisition. In praxis, the gradient takes effect when gt is larger than the inverse sample or voxel size. As it is seen in Fig. 2 right, the signal never exceeds 0.5, the value reached for the stimulated echo.

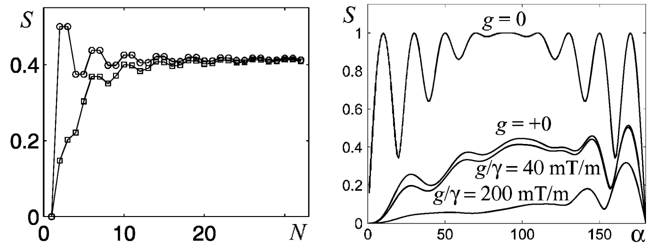

Fig. 2. The signal, S, for the α-pulse train described in Section 3.1. Left: The signal 40 ms after the first pulse as a function of N for $\alpha = \pi/2$, $D = 0$ (top line) and $D = 2\,\mu\mathrm{m}^2/\mathrm{ms}$ (bottom line). Right: The signal as a function of α for $N = 10$, $D = 2\,\mu\mathrm{m}^2/\mathrm{ms}$ and gradient indicated in the figure. The label $g = 0$ implies the absence of any gradient. The line labeled with $g = +0$ shows the limit for small, but finite g.

For given N and α the signal depends on a dimensionless parameter $Dg^2\Delta t^3$, where Δt is the interpulse interval. This gives reason for the notion of the b-factor. Its effective value, which is defined as $-(\ln S)/D$, is shown in Fig. 3 as a function of α. It reaches the maximum near $\alpha = 30$ grad, with the maximal value about fivefold smaller than that of the spin echo sequence.

The effect of global transport is illustrated in Fig. 4. Note the signal increase for some values of α. This can be understood as a constructive interference between the transport-related dephasing and the multiple spin flipping in the applied gradient. For a given velocity, increasing the gradient results in complex oscillations of the signal magnitude (Fig. 5). The characteristic period can be assessed by treating the signal as a function of dimensionless parameter gvt^2.

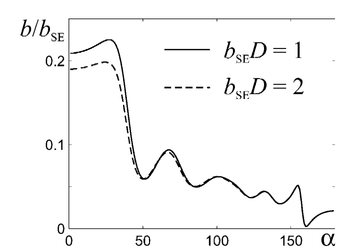

Fig. 3. Ratio of effective b-factor to the b-factor of the spin echo sequence, b_{SE}, with similar T_{E} and g as a function of α for $N = 10$.

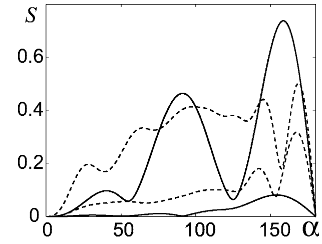

Fig. 4. Effect of global transport for the same sequence as in Fig. 2 right. The curves for $g = 40\,\mathrm{mT/m}$ and $g/\gamma = 200\,\mathrm{mT/m}$ for $v = 0$ are reproduced with the dashed lines. The solid lines show the corresponding dependencies for $v = 5\,\mathrm{mm/s}$.

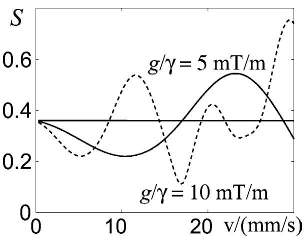

Fig. 5. Effect of diffusion weighting gradient on the signal as a function of the transport velocity for $\alpha = 75$ grad. The horizontal line corresponds to the vanishing gradient, in which case the signal does not depend on velocity. Increasing the gradient results in oscillations illustrated for $g/\gamma = 5\,\mathrm{mT/m}$ (solid line) and $g/\gamma = 10\,\mathrm{mT/m}$ (dashed line).

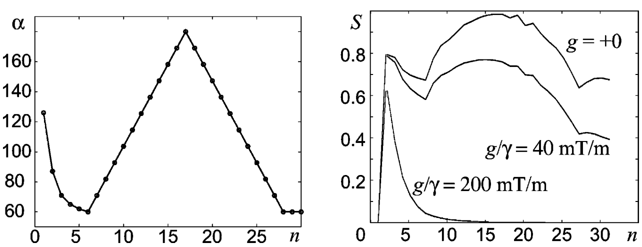

Fig. 6. An illustrative application of developed method to a TRAPS sequence. The sequence consists of a $\pi/2$-pulse (not shown) followed by a train of RF pulses with the phase $\pi/2$ relative to the first one. Their flip angles are shown in the left figure. The first interpulse interval is $\Delta t/2$, all other are equal to Δt. The right figure presents the result for low, but nonzero gradient ($g = +0$), for $g/\gamma = 40\,\mathrm{mT/m}$ and for $g/\gamma = 200\,\mathrm{mT/m}$. Other parameters are $\Delta t = 8\,\mathrm{ms}$ and $D = 2\,\mu\mathrm{m}^2/\mathrm{ms}$.

3.2. *TRAPS sequence*

The sequences employing the smooth transition between pseudo steady states (TRAPS) [8] consist of a preparation period, during which the nuclear magnetization reaches a pseudo steady state, followed by a train of pulses with gradually changing flip angle (Fig. 6, left). When interlaced with readout gradients, this allows for imaging with a good contrast to noise ratio and a significantly reduced specific absorption rate. In the present example the gradient is constant simulating either an applied or a susceptibility induced gradient.

The calculation result is presented in Fig. 6 in which the echo magnitude is shown as a function of interpulse interval number. The relatively small diffusion effect can be explained as a consequence of the large flip angles involved that have a noticeble refocusing effect.

4. Discussion

The present method is useful for calculating the spin magnetization in homogeneous media created by complex sequences of RF and gradient pulses. It combines the advantages of numerical calculations with the analytical accuracy. The instant switching of the both kind of pulses is assumed. This restriction can be released by replacing the RF pulses with trains of low-flip-angle pulses and by the stepwise gradient variation. This would require additional computation resources and a proper simulation of realistic pulses. The method can be extended to account for the gradients and transport in arbitrary directions and for the off-resonance precession. This should not result in any significant reduction in the performance or accuracy. Application to complex practically used sequences such as hyperecho [10] will be discussed elsewhere.

The analytical part of the developed method complements the phase path technique [11] which is invaluable for theoretical analysis, but results in increasingly cumbersome calculations for complicated pulse sequences. The presented method does not explicitly count the phase paths. Instead, it employs the Green function, the quantity that gives rise to them. The correspondence between the two methods is transparent in view of Eq. (20). The values κ_{ij}^a define the modes of magnetization in k-space which are present to the given time moment. The coefficients C_{ij}^a define their weights. Plotting κ_{ij}^a as functions of time would reproduce the conventional phase graph up to the obvious linear transformation which is conventionally applied in the phase graph technique in order to diagonalize the rotation matrix defined in Eq. (6).

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