Journal of Magnetic Resonance 269 (2016) 36–49

Contents lists available at ScienceDirect

Journal of Magnetic Resonance

journal homepage: www.elsevier.com/locate/jmr

Instantaneous signal attenuation method for analysis of PFG fractional diffusions

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ARTICLE INFO

Article history:
Received 16 January 2016
Revised 15 April 2016
Accepted 12 May 2016
Available online 13 May 2016

Keywords:
NMR
MRI
Propagator
Fractional diffusion
PFG

ABSTRACT

An instantaneous signal attenuation (ISA) method for analyzing pulsed field gradient (PFG) fractional diffusion (FD) has been developed, which is modified from the propagator approach developed in 2001 by Lin et al. for analyzing PFG normal diffusion. Both, the current ISA method and the propagator method have the same fundamental basis that the total signal attenuation (SA) is the accumulation of all the ISA, and the ISA is the average SA of the whole diffusion system at each moment. However, the manner of calculating ISA is different. Unlike the use of the instantaneous propagator in the propagator method, the current method directly calculates ISA as $A(K(t'), t' + dt')/A(K(t'), t')$, where $A(K(t'), t' + dt')$ and $A(K(t'), t')$ are the SA. This modification makes the current method applicable to PFG FD as the instantaneous propagator may not be obtainable in FD. The ISA method was applied to study PFG SA including the effect of finite gradient pulse widths (FGPW) for free FD, restricted FD and the FD affected by a non-homogeneous gradient field. The SA expressions were successfully obtained for all three types of free FDs while other current methods still have difficulty in obtaining all of them. The results from this method agree with reported results such as that obtained by the effective phase shift diffusion equation (EPSDE) method. The M-Wright phase distribution approximation was also used to derive an SA expression for time FD as a comparison, which agrees with ISA method. Additionally, the continuous-time random walk (CTRW) simulation was performed to simulate the SA of PFG FD, and the simulation results agree with the analytical results. Particularly, the CTRW simulation results give good support to the analytical results including FGPW effect for free FD and restricted time FD based on a fractional derivative model where there have been no corresponding theoretical reports to date. The theoretical SA expressions including FGPW obtained here such as $E_{\alpha,1}\left[-D_{f_2}\int_0^t K^{\beta}(t')dt'^{\alpha}\right]$ may be applied to analyze PFG FD in polymer or biological systems with improved accuracy where SGP approximation cannot be satisfied. The method can perhaps provide new insight to FD MRI and hence benefit the development of diffusion biomarkers based on fractional derivative.

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1. Introduction

The pulsed field gradient (PFG) diffusion experiment [1–3] has many applications in NMR and MRI. Anomalous dynamical behavior [4] exists in many systems. Unlike the familiar Gaussian characteristics of normal diffusion (ND), the anomalous diffusion often shows non-Gaussian characteristics [5,6]. The non-Gaussian diffusion may be a challenge to be interpreted by the conventional approaches. For example, conventional time-dependent diffusivities may be not sufficient for interpreting the data including large *b*-value in the study of water diffusion in brain tissue by MRI [5,6]. To interpret the anomalous diffusion, the researchers have made many experimental and theoretical efforts such as the propagator representation [7], Gaussian phase distribution (GPD) approximation [8,9], short gradient pulse (SGP) approximation [10], the stretched exponential models [11,12], the walk and spectral dimension parameters method [13], the modified Bloch equations [14–16], the log-normal distribution function [17] and the recently developed effective phase shift diffusion equation (EPSDE) method [18]. These efforts have yielded encouraging results. In the studies of stroke by diffusion MRI, it has been reported that the quantitative parameters related to the degree of diffusion non-Gaussianity are much more sensitive to ischemic changes than the ADC [6]. Nevertheless, the PFG anomalous diffusion is still in the early stages due to the difficulties in the theory and the complexity of the application systems [6]. Therefore, it is still important to develop some theoretical treatments for anomalous diffusion.

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http://dx.doi.org/10.1016/j.jmr.2016.05.011
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Many anomalous diffusion systems have been modeled by the fractional diffusion equations based on fractional derivative or fractal derivative (defined in Appendices B and C) [19–23]. The modified Bloch equations for fractional diffusion based on fractional derivative has been used to obtain the signal attenuation for space-fractional diffusion successfully, which has been applied to study water diffusion in brain tissue by MRI. Based on the fractional derivative, the Mittag–Leffler function attenuation obtained by EPSDE method agrees with molecule diffusing along a curvilinear curve which could exist in the polymer or biological systems [9,18,24]. From the fractional diffusion equation based on a fractional derivative or fractal derivative, the average square displacement of FD does not increase linearly with the diffusion time unlike in ND. FD usually has a non-Gaussian probability distribution function (PDF) such as $t^{-\alpha/\beta}\kappa^{\theta}_{\beta,\alpha}\left(\frac{z}{t^{\alpha/\beta}}\right)$ [19,21], where α is the time derivative order, β is the space derivative order, t is time, z is the position, and the $\kappa^{\theta}_{\beta,\alpha}(x)$ function is defined in Appendix A (when $\alpha = 1$, $\beta = 2$, FD reduces to ND). These non-Gaussian characteristics of FD make it difficult to obtain an analytical SA expression for the PFG FD experiments. First, the effect of finite gradient pulse widths (FGPW) is hard to obtain in some types of FD. The FD may be divided into the following three types: general FD $\{0 < \alpha, \beta \leqslant 2\}$, time FD $\{0 < \alpha \leqslant 2, \beta = 2\}$ and space FD $\{\alpha = 1, 0 < \beta \leqslant 2\}$ [18,19]. Currently, even using the EPSDE and other methods, it is still difficult to obtain analytical SA expressions that include the FGPW effect for the two types of FD—time and general FD—based on the fractional derivative model [18]. For instance, from the fractal derivative model, the EPSDE method gives the complete SA expression $\exp\left[-D_f\int_0^{\tau}K^{\beta}(t)dt^{\alpha}\right]$ for describing free FD, where $K(t)$ is the wavenumber. However, the SA expression including the FGPW effect by the EPSDE method based on the fractional derivative was obtained only in the space FD case [18]. Secondly, there is no analytical SA expression for restricted diffusion including FGPW effects reported in the literature. Thirdly, many different experimental variables may be taken into account, such as that FD may be affected by an inhomogeneous field [25]. It would be helpful to have an intuitive and general method to address these challenges and improve our understanding.

In this paper, an instantaneous signal attenuation method is proposed, which is both a general and intuitive method, that can be applied to analyze PFG free or restricted FD including the FGPW effect. The method is based on the propagator approach developed in 2001 from Ref. [26], which will be referred to as the "original propagator method". However, the original propagator method needs an instantaneous propagator to calculate the ISA expression, which makes it hard to apply to PFG FD, as the instantaneous propagator may be hard to obtain. To overcome this difficulty, the ISA method described here obtains the ISA by comparing two consecutive SAs at t' and $t' + dt'$ without the need for the instantaneous propagator. This method was used to obtain the theoretical SA expressions for free FD, restricted FD and FD with nonlinear field case. The motive to study free and restricted FDs is because, in polymer or biological systems, the investigated short time FD may be approximated as free FD, while the long time FD may be treated as restricted diffusion when the domain size or boundary effect become observable. While the nonlinear field investigated for ND by researchers may have some potential applications for FD too. Additionally, to verify these theoretical SA expressions, continuous-time random walk (CTRW) simulation [27] was performed to simulate the PFG SA for FD. Moreover, the M-Wright phase distribution approximation (see Appendix D) was also used to derive a general SA expression $E_{\alpha,1}\left[-\frac{\Gamma(\alpha+1)\langle\varphi^2\rangle}{2}\right]$ for time FD that agrees with ISA method, the results obtained from the ISA method agree with the simulation results as well as other methods, particularly the EPSDE method. The ISA method introduced provides a simple and accurate way to analyze PFG SA.

2. Theory

2.1. From the propagator approach to the ISA method

2.1.1. The original propagator approach for ND

The principal idea of the original propagator approach in Ref. [26] can be described as follows: because the number of spins in a macroscopic sample can be viewed as infinitely large, the phase difference of the spins diffusing to the same location will be averaged out and cannot be distinguished after mixing for every moment during diffusion. Spatial averaging of the phase shift results in SA. For free diffusion of the spin system at time t' there will be an equal number of spins diffusing to location z from both directions $z + \Delta z$ and $z - \Delta z$. The average phase shift of these mixing spins is the same as that of the spins remaining at location z and can be written as

$$\varphi(z,t') = \int_0^{t'} \gamma g(t'')z dt'' = zK(t'), \tag{1}$$

where

$$K(t') = \int_0^{t'} \gamma g(t'')dt'', \tag{2}$$

where γ is the gyromagnetic ratio, $g(t'')$ is the gradient strength at time t'', and $K(t')$ is a wavenumber that summarizes the gradient effect from the beginning of the first gradient pulse to time t' within the gradient pulse sequence, and its units are rad/m. The ISA $a(z, t', dt')$ (called ISA factor) at z will be [26]

$$a(z,t',dt') = \int_{-\infty}^{+\infty} \sigma(z',t')P(z,dt'|z')\cos[\varphi(z',t') - \varphi(z,t')]dz' \Bigg/ \int_{-\infty}^{+\infty} \sigma(z',t')P(z,dt'|z')dz', \tag{3}$$

where $\sigma(z', t')$ is the spin particle density, and $P(z, dt'|z')$ is the PDF during interval dt' moving from z' to z. As $\sigma(z', t')$ can be assumed homogeneous in the sample for free diffusion, the ISA will then be [26]

$$a(K(t'),t',dt') = \exp(-K^2(t')Ddt'), \tag{4}$$

where z drops out as the ISA is equal everywhere for free diffusion, and we have used $a(K(t'), t', dt')$ rather than $a(z, t', dt')$ for the ISA. The total diffusion SA will be the cumulative multiplicative ISA, which can be expressed as

$$A(t) = \prod_{dt'} a(K(t'),t',dt') = \exp\left[-D\int_0^t K^2(t')dt'\right]. \tag{5}$$

where $A(t)$ is the SA (or so-called attenuation factor) that is defined as $A(t) = S(t)/S(0)$ (S is the signal intensity). The same expression as Eq. (5) was derived already by the Torrey modified Bloch equations and other methods in the literature [18,28,29], and is a convenient method for calculating the SA produced by a PFG pulse sequence [30]. For the pulsed gradient spin echo (PGSE) and the pulsed gradient stimulated-echo (PGSTE) experiments as shown in Fig. 1, from Eq. (5), the SA is $\exp\left[-D\gamma^2 g^2\delta^2\left(\Delta - \frac{1}{3}\delta\right)\right]$, which agrees with established results [31]. When the diffusion coefficient is time-dependent, the SA for free ND can be similarly obtained by the above process,

$$A(t) = \exp\left[-\int_0^t D(t)K^2(t')dt'\right]. \tag{6}$$

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