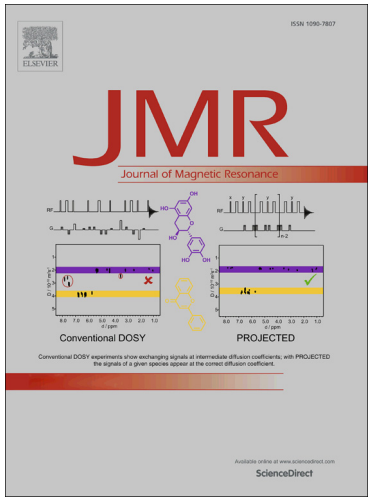

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PII: S1090-7807(17)30025-3
DOI: http://dx.doi.org/10.1016/j.jmr.2017.01.018
Reference: YJMRE 6032

To appear in: *Journal of Magnetic Resonance*

Received Date: 5 October 2016
Revised Date: 24 January 2017
Accepted Date: 25 January 2017

Please cite this article as: I. Seroussi, D.S. Grebenkov, O. Pasternak, N. Sochen, Microscopic Interpretation and Generalization of the Bloch-Torrey Equation for Diffusion Magnetic Resonance, *Journal of Magnetic Resonance* (2017), doi: http://dx.doi.org/10.1016/j.jmr.2017.01.018

Microscopic Interpretation and Generalization of the Bloch-Torrey Equation for Diffusion Magnetic Resonance

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Abstract

In order to bridge microscopic molecular motion with macroscopic diffusion MR signal in complex structures, we propose a general stochastic model for molecular motion in a magnetic field. The Fokker-Planck equation of this model governs the probability density function describing the diffusion-magnetization propagator. From the propagator we derive a generalized version of the Bloch-Torrey equation and the relation to the random phase approach. This derivation does not require assumptions such as a spatially constant diffusion coefficient, or ad-hoc selection of a propagator. In particular, the boundary conditions that implicitly incorporate the microstructure into the diffusion MR signal can now be included explicitly through a spatially varying diffusion coefficient. While our generalization is reduced to the conventional Bloch-Torrey equation for piecewise constant diffusion coefficients, it also predicts scenarios in which an additional term to the equation is required to fully describe the MR signal.

1. *Introduction*

Measuring molecular self-diffusion in magnetic resonance (MR) experiments is an important tool for understanding the geometrical structure of materials ranging from porous media to brain tissue. Translational diffusion within an inhomogeneous magnetic field causes dephasing in a spin-echo experiment [1]. The macroscopic MR signal decay is related to the average overall molecular spin phases [2]. The molecular displacement depends on random thermal forces (Brownian motion), however it is also affected by the boundaries dictated by the geometric structure of the specimen, such as cellular membranes or the edges of pores, which modulate the motion of molecules. The goal of diffusion MR is ultimately to recover information about geometrical structure from the macroscopic, voxel scale, MR signal [3]. This structure can be encoded through effective diffusion coefficients, or Probability Density Functions (PDF), which are defined over a large population of molecules.

The leading approach to relate the microstructure to the macroscopic MR signal is the Bloch–Torrey (BT) equation [4], in which the phenomenological Bloch equation [5] is expanded by accounting for the behavior of a population of spins, explicitly modeled by the diffusion coefficient, D, yielding

$$\frac{\partial}{\partial t}\langle \mathbf{m} \rangle = \gamma(\langle \mathbf{m} \rangle \times \mathbf{H}) - \nabla\left(\mathbf{v}\langle \mathbf{m} \rangle\right) + \nabla\left(D\nabla\langle \mathbf{m} \rangle\right), \quad (1)$$

where $\langle \mathbf{m} \rangle$ is the average magnetization (throughout the paper, boldface describes three-dimensional vectors), $\mathbf{H}$ is the applied magnetic field[2], γ is the gyromagnetic ratio, and $\mathbf{v}$ is the velocity of the spins due to the flow of the medium within which the spins are embedded [6]. The complete equation also includes T_1 and T_2 weighted terms: $-\frac{\langle m_x \rangle \hat{\mathbf{x}} + \langle m_y \rangle \hat{\mathbf{y}}}{T_2} - \frac{\langle m_z \rangle - \langle m_0 \rangle}{T_1}\hat{\mathbf{z}}$, where T_1 is the longitudinal (spin–lattice) relaxation time, T_2 is the transverse (spin–spin) relaxation time [5], and $\langle m_0 \rangle$ is the thermal equilibrium magnetization of the sample in the presence of a magnetic field. In our analysis we assume that T_1 and T_2 are spatially invariant, in which case these relaxation mechanisms affect all the nuclei in the same way and their contribution can be factored out by comparing the diffusion-weighted signal to a reference signal (e.g., without a diffusion gradient). In what follows, we will omit these relaxation terms, concentrating on the diffusion related terms.

The macroscopic MR signal is obtained by integrating the solution of the BT equation over the whole sample or over a given voxel. The BT equation provides an explicit description of the combined effects of diffusion, flow and spin dephasing, whereas the microstructure is incorporated *implicitly* through boundary conditions imposed on interfaces between various tissue components or solid-fluid phases in porous media. This makes analytical and even numerical solutions of the BT equation challenging [7–9]. In particular, analytical approaches that solve the

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[2] As in the Bloch equation, Eq. (1) refers to the case of a large static field H_z in the $\hat{z}$ direction, plus possible small components which may be variable in the transverse plane.