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Diffusion-mediated dephasing in the dipole field around a single spherical magnetic object

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In this work, the time evolution of the free induction decay caused by the local dipole field of a spherical magnetic perturber is analyzed. The complicated treatment of the diffusion process is replaced by the strong-collision-approximation that allows a determination of the free induction decay in dependence of the underlying microscopic tissue parameters such as diffusion coefficient, sphere radius and susceptibility difference. The interplay between susceptibility- and diffusion-mediated effects yields several dephasing regimes of which, so far, only the classical regimes of motional narrowing and static dephasing for dominant and negligible diffusion, respectively, were extensively examined. Due to the asymmetric form of the dipole field for spherical objects, the free induction decay exhibits a complex component in contradiction to the cylindrical case, where the symmetric local dipole field only causes a purely real induction decay. Knowledge of the shape of the corresponding frequency distribution is necessary for the evaluation of more sophisticated pulse sequences and a detailed understanding of the off-resonance distribution allows improved quantification of transverse relaxation.

1. Introduction

Generally, in magnetic resonance imaging, transverse relaxation is highly sensitive to microscopic properties of the underlying tissue. Representative imaging modalities that are based on these effects are BOLD imaging [1], signal alterations in neurodegenerative disease [2] or the development of iron-oxide contrast agents [3]. The main physical principle of these applications is the susceptibility difference between microscopic magnetic perturbers and the surrounding tissue that contains the spin-bearing particles. Especially in the case of small magnetic objects, the contribution of diffusion of the respective spins on signal formation is not negligible. However, susceptibility and diffusion have opposing effects on signal formation: while static line broadening in NMR is based on susceptibility effects, the influence of diffusion leads to a motional narrowing of the line shape [4]. Therefore, a concise knowledge of the interplay between susceptibility- and diffusion-related effects is important for quantifying accumulations of microscopic magnetic tissue inhomogeneities. The susceptibility-induced local magnetic field inhomogeneities can be described by a multipole expansion whereby the dominating contribution stems from the dipole field. The case of negligible diffusion, also known as static dephasing regime, has first been analyzed by Brown [5] for three-dimensional dipole fields and also later in the seminal work of Yablonskiy and Haacke [6] where the free induction decay and corresponding relaxation times are analyzed for cylindrical and spherical perturbers. By adapting the density-of-states concept known from statistical physics it is possible to study the frequency distribution of the local Larmor frequency around the magnetic objects. The first steps of analyzing such frequency distributions arose in the field of lung imaging, where the frequency density of states was calculated in terms of the histogram method by subdividing the dephasing volume in smaller subvoxels [7]. A detailed study of the dipole field signal formation of spherical magnetic pertubers was provided by Cheng et al. [8] who derived an analytical expression for the frequency distribution. Further experimental evidence for the frequency distribution in the static dephasing regime can be found in Ref. [9]. Objects with a more

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complex shape were considered in Ref. [10]; further findings were reviewed in detail in Ref. [11]. So far, theoretical results could be confirmed experimentally in various ways, especially for lung tissue where three-dimensional dipole fields are the underlying geometrical structures that are generated by air-filled alveoli [12,13]. Recently, the investigation of cylindrical objects and their influence on signal formation became a focus of interest for cardiac magnetic resonance imaging since myocardial architecture mainly consists of capillaries that generate two-dimensional dipole fields due to paramagnetic properties of deoxygenized hemoglobin [14]. By adapting the well-known methods for the case of spherical objects, it was possible to analogously analyze the frequency distribution around cylindrical objects theoretically [15] and experimentally [16].

However, the influence of diffusion on the line-shape of the frequency distribution is essential to understand diffusion-mediated signal decay and the respective relaxation process. With increasing diffusion, the line-shape narrows (also known as diffusion-narrowing) and the frequency distribution can be approximated by a Lorentzian line shape and the free induction decay by a mono-exponential decay. The influence of diffusion and susceptibility on relaxation times has been analyzed in Refs. [17–19]. In general, the combination of susceptibility effects and diffusion effects on transverse magnetization can be described by the Bloch–Torrey equation [20]. A step towards analytical quantification of the free-induction decay has been carried out by Bauer et al. [14,21] who established the strong-collision-approximation in replacing the diffusion operator in the Bloch–Torrey-equation by a simpler stochastic process operator. Incorporating the strong-collision-approximation into the frequency density-of-states concept allows examining diffusion effects on the line shape and free-induction decay. For cylindrical magnetic objects, the frequency distribution exhibits a typical pattern with two symmetric peaks in the static dephasing regime while narrowing to a Lorentzian shaped peak occurs with increasing diffusion [16]. These symmetric peaks reveal analogies to beat frequency phenomena as known from the harmonic oscillator [22]. They allow the classification of diffusion regimes through the presence of an oscillating or decaying time evolution of the free induction decay, corresponding to the existence of one or two peaks in the frequency distribution, respectively. Beside the strong-collision-approximation several other approximation were applied to the Bloch–Torrey-equation. The Gaussian approximation [23] is valid for weak magnetic inhomogeneities as well as the weak field approximation of Jensen and Chandra [24]. For dominating susceptibility effects the slow diffusion approximation of Kiselev and Posse [25,26] and the strong field approximation allow predictions of the free induction decay.

Due to the complex nature of three-dimensional dipole fields, the frequency distribution for spherical objects is not easily obtained. However, similar effects of line narrowing through increased diffusion effects have been observed (see Fig. 7 in Ref. [16]), corresponding to a transition from the asymmetric shape of the static dephasing regime to a symmetric shape in the motional narrowing limit. Likewise, experiments of Mulkern et al. [27] found asymmetric line-shapes for lung tissue. Therefore, the question arises if similar analogies to the harmonic oscillator can be found for the diffusion process in a three-dimensional dipole field. Moreover, the oscillating or monotonically decaying behavior of the free induction decay will be of interest for the quantitative analysis and combination of susceptibility and diffusion weighted imaging.

In the present work we study the effects of diffusion on the dephasing process of a dipole field around a spherical magnetic object. These investigations enable a clear differentiation of diffusion regimes. In addition, the characteristic form of the frequency distribution and the free induction decay allow quantifying microscopic distributions that consist of spherically shaped magnetic components. Furthermore, the calculated free induction decay is compared with other model approximations and experimental measurements of human lung tissue to support the theoretical predictions.

2. Methods

2.1. Diffusion and dephasing in a dipole field

We consider a tissue with embedded spherical magnetic perturbers, such as alveoli in lung tissue. It is then convenient to adapt the well-known Krogh capillary model to the three-dimensional case to allow for an adequate approximative description of the complex geometrical arrangement of such perturbers. In this approximation, the spherical magnetic perturber is treated as a single sphere with radius R that is surrounded by a spherical dephasing volume with radius R_D (see Fig. 1).

Naturally, the superposition of all magnetic field inhomogeneities has to be considered to describe the susceptibility effects of the tissue. Therefore, it is advantageous to use a multipole expansion and keep only the leading term of the dipole moment. This can be included into the model by assuming a homogeneously magnetized inner sphere. Thus, the magnetic dipole field is given by

$$\omega(\mathbf{r}) = \delta\omega R^3 \frac{3cos^2(\theta) - 1}{r^3}, \tag{1}$$

where the characteristic equatorial frequency shift $\delta\omega = |\omega(r = R, \theta = \pi/2)| = \gamma B_{eq}$ and angle θ represent the angle between external magnetic field B_0 and position vector $\mathbf{r} = (r,\theta,\varphi)$ (in spherical coordinates) as sketched in Fig. 1. The equatorial magnetic field B_{eq} can be determined as $B_{eq} = \mu_0 \Delta M/3$ with vacuum permeability μ_0 and the difference in magnetization ΔM between homogeneously magnetized inner sphere and surrounding tissue. The considered spherical magnetic object is assumed to not contain any water molecules that contribute to the signal formation. Spin-bearing particles diffuse in the spherical shell $R \le r \le R_D$ around the local field homogeneity and such a diffusion process is characterized by the diffusion coefficient D. The volume fraction of the magnetic content is defined as

$$\eta = \frac{R^3}{R_D^3}. \tag{2}$$

The assumption of reflecting boundary conditions on the surface of both concentric spheres can be used to account for the complex arrangement of the spherical magnetic perturbers (see Fig. 1 in Ref. [28] and Fig. 1 in Ref. [29]). This single spherical shell model is an established approximation of the tissue (see, e.g., Ref. [30]) and can be used for the description of lung tissue [11]. The model allows calculating analytical expressions of the free induction decay and the frequency distribution.

Generally, the complex-valued local magnetization $m(\mathbf{r},t) = m_x(\mathbf{r},t) - \mathrm{i}m_y(\mathbf{r},t)$ obeys the Bloch–Torrey equation [20].

$$\frac{\partial}{\partial t} m(\mathbf{r}, t) = [D\Delta + \mathrm{i}\omega(\mathbf{r})] m(\mathbf{r}, t) \tag{3}$$

with Laplace operator Δ. The measured signal $M(t)$ consists of the superposition of signals at all points within the dephasing volume and, thus, reads

$$M(t) = \frac{1}{V} \int_V \mathrm{d}^3\mathbf{r}\, m(\mathbf{r}, t). \tag{4}$$