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Attenuation of the NMR signal in a field gradient due to stochastic dynamics with memory

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Abstract

The attenuation function $S(t)$ for an ensemble of spins in a magnetic-field gradient is calculated by accumulation of the phase shifts in the rotating frame resulting from the displacements of spin-bearing particles. The found $S(t)$, expressed through the particle mean square displacement, is applicable for any kind of stationary stochastic motion of spins, including their non-markovian dynamics with memory. The known expressions valid for normal and anomalous diffusion are obtained as special cases in the long time approximation. The method is also applicable to the NMR pulse sequences based on the refocusing principle. This is demonstrated by describing the Hahn spin echo experiment. The attenuation of the NMR signal is also evaluated providing that the random motion of particle is modeled by the generalized Langevin equation with the memory kernel exponentially decaying in time.

Keywords: NMR; Diffusion; Brownian motion; Generalized Langevin equation; Induction signal; Spin echo

1. Introduction

Nuclear magnetic resonance (NMR) has proven to be an effective method of studying molecular self-diffusion and diffusion in various materials and has a wide range of applications ranging from characterization of solutions to inferring microstructural features in biological tissues [1–13]. The effect of diffusion on the NMR signal was incorporated by Torrey into the Bloch equations for the spin magnetization of an excited sample placed in a magnetic field [14]. By solving these equations the NMR signal is obtained as a product of the time evolution of the magnetization without the influence of diffusion and the diffusion suppression function $S(t)$. The function $S(t)$ can also be evaluated through the time-dependent resonance frequency offset in the frame rotating with the resonance frequency [1–4, 10, 15–23]. Evidently, the results based on the first approach do not go beyond the Einstein–Fick theory of diffusion. The second approach needs more attention. Most calculations of $S(t)$ within this approach are valid within the long-time approximation. This means that only experiments on spin-bearing particles undergoing diffusion in liquids or gases, when their mean square displacement (MSD) is recorded at times t much larger than the characteristic frictional time of the particles [24], can be interpreted within the current

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