A matrix formalism: an efficient numerical tool for diffusion NMR

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A matrix formalism was originally developed for computation of the pulsed-gradient spin-echo signal attenuated due to restricted diffusion of nuclei in simple isolated domain such as a slab, a cylinder and a sphere[1-4]. More recently, this approach was also applied to equilateral triangles[5,6] and multilayered structures[7] (e.g., multiple slabs, cylindrical or spherical shells), in which individual layers are characterized by (different) diffusion coefficients and relaxation times, while boundaries between adjacent layers are characterized by (different) permeabilities. The explicit form of Laplacian eigenfunctions in these domains allows one to incorporate the effects of restricted diffusion and of gradient encoding through two matrices. The signal is then represented in a compact matrix form and the explicit analytical formulas for the elements of the underlying matrices are derived. Arbitrary temporal profile of the applied magnetic field gradient can be incorporated. The implemented algorithm is faster and much more accurate than classical techniques such as Monte Carlo simulations or finite-element or finite-difference numerical resolutions of the Bloch-Torrey equation. The algorithm can be applied for studying restricted diffusion in biological systems which exhibit a multilayered structure such as composite tissues, axons and living cells. The relative roles of inter-layer diffusive exchange, surface relaxivity, and strong gradients can be investigated in depth with unprecedented accuracy. In particular, this method was used to analyze the non-Gaussian stretched-exponential behavior of the signal at high gradients in the so-called localization regime[8].

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