An efficient eigenfunction approach to calculate spin-echo signals in heterogeneous porous media

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In the late 90ies, Caprihan et al. [1], Callaghan [2] and Barzykin [3] (among others) developed a framework for treating finite gradient pulses using eigenfunction expansions (see [4] for a review). But still, fifteen years later, few use this approach in practice. The main reason is that calculating the eigenfunctions is itself a difficult numerical problem, in particular when the problem size and complexity grows. Nevertheless, several groups in applied mathematics [5] strive for standardizing the code and procedure for efficient eigenfunction solvers and this leads us to the question, *how can the NMR-community benefit from this*?

We have developed a novel approach for calculating the eigenfunctions in confined geometries [6] relying on one of the fastest methods known to solve electrostatic problems – the fast multipole method. In our mixed basis method, the eigenfunctions are approximated as linear combinations of Fourier modes (describing the bulk diffusion) and surface modes (describing the influence of the boundaries). Previous work has shown how the mixed basis method can be used in NMR calculations when the spatial labeling of the spins is instant - the so called short gradient limit [7]. In this work, we extend this method to cover time-dependent gradient forms. We will focus on heterogeneous porous media and show how the spin-echo decay can be efficiently calculated using the mixed basis method (see figure 1 below for a two-dimensional example). The talk will be accompanied with illustrative examples (e.g. different gradient forms and pulse sequences) and the benefits and drawbacks of the approach will be discussed. In many NMR experiments in heterogeneous media the origin of the experimental signal and its relation to the geometrical structure of the medium are still poorly understood, and therefore the ability of modeling such experiments is important.

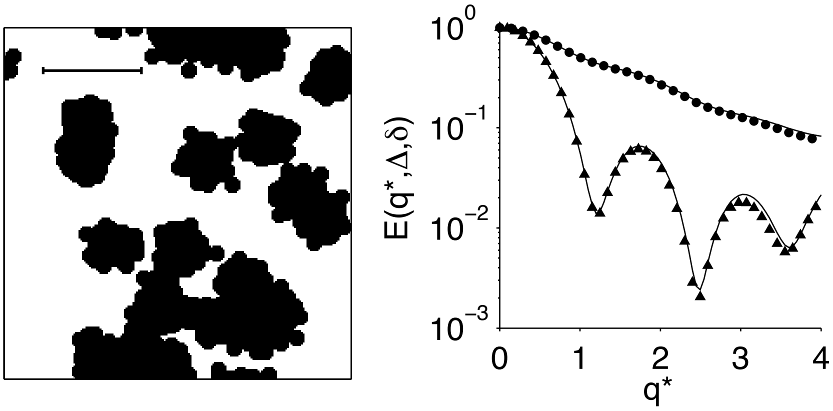

Fig. 1: The image to the left shows a two-dimensional test structure (200^2 grid points) (from [7]) where spins diffuse in the white regions and bounce off the perimeter between white and black (Neumann conditions). The graph to the right shows spin echo signals for a Stejskal-Tanner sequence with a square gradient form (with area δg) for $\Delta=\delta$ (circles) and $\Delta\rightarrow\infty$ (triangles). The diffusion length during the gradient $l=2(D\delta)^{1/2}$ has been marked as a line in the image to the left and $q^*=\gamma g\delta a^3/(D2\pi)$, where a is the box side length. The reference signals (shown by symbols) have been calculated using Barzykin's approach with the first 200 eigenfunctions (obtained by a standard eigensolver in MATLAB). The signals calculated using the mixed basis method are shown as solid lines for the two times respective, and where calculated using the first 50 approximate eigenfunctions. The efficiency is striking, given the fact that the approximate eigenfunctions were retrieved using calculations on the perimeter only (the curves between black and white).

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