A mixed basis perturbation method for fast calculations of obstructed diffusion

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ABSTRACT: By the use of numerical methods it is possible to express the solution to the diffusion equation, in not only the trivial cases, but also for complex obstructing geometries, in terms of eigenfunction expansions. Using this approach, relations such as time-dependent diffusion coefficients, effective diffusion constants and relaxation rates can be directly related to geometrical properties [1]. The calculation of the eigenfunctions can however be a tedious work and require either heavy computational work or complex implementations. We have recently developed a new perturbation method [2,3] for calculating approximations to the eigenfunctions of the diffusion operator in general obstructing geometries. By the form of the method, we call it a *mixed basis* method and it is relatively easy to implement. The resulting approximations to the eigenfunctions are given as linear combinations of Fourier modes (free diffusion) and special functions describing the influence of the boundaries – surface modes. As the weight of the Fourier component for each eigenfunction is calculated, the method is well suited in applications involving a Fourier transform of the eigenfunctions such as in diffusion NMR. In this talk we will introduce you to this method, show how it can be used to calculate various diffusion properties in materials and show an application of the method in diffusion NMR.

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[2] Nordin, M., Nydén, M., & Nilsson Jacobi, M. A mixed basis perturbation approach to approximate the spectrum of Laplace operator. Proceedings of ITP-09 2009 Interdisciplinary Transport Phenomena VI, Volterra, Italy, October 4-9, (2009). [arXiv:0909.0935v1]

[3] Nordin, M., Nydén, M., & Nilsson Jacobi, M. A mixed basis approach in the SGP-limit. JMR. 212 (2) (2011) 274-279