

Accurate RTOP Estimation from PFG-NMR Signal

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The return to the origin probability (RTOP) for diffusing molecules is a valuable indicator of porous media microstructure [1-2]. For example, in isolated pores with non-relaxing walls, the pore volume is related to the RTOP at long diffusion times. Similarly, in disordered media, the temporal scaling of the RTOP is necessary in the estimation of the fractal dimension of the medium [3]. However, the RTOP is related to the pulsed field gradient (PFG) NMR signal via an integration over the entire q -space. The unavailability of data at large wavevectors is a serious problem particularly in restricted domains where the NMR signal does not attenuate significantly even at relatively large wavenumbers.

In principle, the extrapolation of the signal values can be performed by model fitting to data. However, very different signal profiles are possible depending on the particular specimen under examination whose structure is not known *a priori*. Another alternative is the cumulant expansion, which may fail to converge to the true signal attenuation. Fig. 1a shows the failure of both the cumulant expansion and sometimes used biexponential fitting in describing the theoretical signal attenuation from rectangular pores at long diffusion times.

In this work, we propose to represent the PFG-NMR signal in terms of a complete set of Hermite functions. The basis possesses many interesting properties relevant to q -space NMR, such as the ability to represent both the signal and its Fourier transform. Unlike the previously employed methods, this approach is linear and capable of reproducing complicated signal profiles, e.g., those exhibiting diffraction peaks. The estimation of the coefficients is fast and accurate while the representation lends itself to a direct reconstruction of ensemble average propagators as well as calculation of useful descriptors of it, such as the RTOP and its moments.

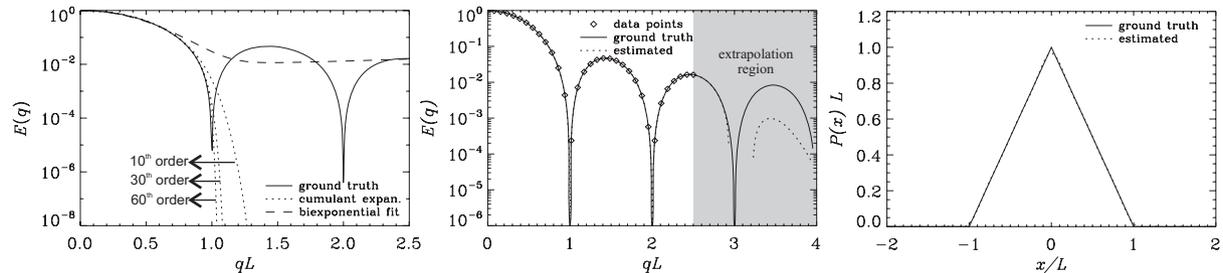


Fig. 2: PFG-NMR signal attenuation curves from rectangular pores at long diffusion times. (a) Cumulant expansion of and biexponential fit to simulated data. (b) The performance of the proposed approach with the same data. (c) Propagator reconstructed from the basis functions whose value at $x=0$ is the RTOP.

We performed simulations to assess the performance of the RTOP estimations for one-, two- and three-dimensional, isotropic, restricted media as well as mono- and bi-exponential decays and even the presence of flow was considered. RTOP values in 1-, 2- and 3- dimensions all yielded very accurate results (<6% error in restricted geometries, <1% in others). The proposed approach is expected to improve the accuracy of RTOP estimates and parameters deduced from it.

References:

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