The drum is visible in nuclear magnetic resonance diffusion experiments

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Introduction

In 1966, Kac asked the famous question: "Can you hear the shape of a drum?" [1], or more tangibly, can the shape of the boundary for an arbitrary closed domain be computed if the spectrum of the Laplace operator is known? He conjectured that it was not possible and was proven right in 1992, when Gordon et al. presented differently shaped domains with the same spectrum of the Laplace operator [2]. In this work, we tackle the unresolved questions, whether the mathematically closely related NMR diffusion experiments can reveal the shape of the pore space function and whether the diffusion weighted signal can bear a phase.

Theory

For that, we use temporally asymmetric diffusion weighting gradient profiles $\mathrm{G(t) = G}$ for $0 < \mathrm{t} < \delta_1 \cdot \mathrm{T}$ and $\mathrm{G(t)} = -\mathrm{G}\delta_1/\delta_2$ for $(1-\delta_2) \cdot \mathrm{T} < t < T$ (see Fig. 2). Here, T is the complete duration of the temporal gradient profile; δ_1 and δ_2 are dimensionless. Following Mitra et al. [3], the signal can be interpreted as $\mathrm{S(q)} = \langle \exp[\mathrm{iq}(\mathrm{x_{cm,1}} - \mathrm{x_{cm,2}})] \rangle$, where $\mathrm{q} = \gamma \mathrm{GT}\delta_1$. $\mathrm{x}_{cm,1} = \frac{1}{\mathrm{T}\delta_1}\int_0^{\mathrm{T}\cdot\delta_1} \mathrm{x(t)dt}$ and $\mathrm{x_{cm,2}} = \frac{1}{\mathrm{T}\delta_2}\int_{\mathrm{T}\cdot(1-\delta_2)}^{\mathrm{T}} \mathrm{x(t)dt}$ are the centers of mass of the particle random walk during the first and second gradient, respectively. For closed domains and long gradient durations, the particle was at every position within the boundary with an equal probability. Thus, the expectation values are $\langle \mathrm{x_{cm,1}} \rangle = \langle \mathrm{x_{cm,2}} \rangle = \mathrm{x_{cm}}$, where $\mathrm{x_{cm}}$ is the center of mass of the pore space function $\chi(\mathrm{x})$, which is 1 inside and 0 outside the domain. If the second gradient is narrow, it follows that $\mathrm{S(q)} = \langle \exp[\mathrm{iq}(\mathrm{x_{cm}} - \mathrm{x(T)})] \rangle = \exp[\mathrm{iqx_{cm}}] \int_\Omega \mathrm{dx} \exp(-\mathrm{iqx})\, \mathrm{P(x)}$. Here, $\mathrm{P(x)dx}$ is the probability that the particle is located in the volume element dx at time T, and the integration is performed over the domain Ω. Since it is assumed that the diffusion process is in the long time limit, the particle is at any position with equal probability, independently of the starting position. Hence, $\mathrm{P(x)} = \chi(\mathrm{x})/|\Omega|$, where $|\Omega|$ denotes the volume of the domain. Thus, the pore space function can be determined exactly by inverse Fourier transformation.

Methods

We validated these theoretical results using the matrix approach described in [4,5], which very efficiently calculates the effect of arbitrary temporal diffusion gradients on the diffusion-weighted signal. Spatially linear gradients were considered for the equilateral triangle [6] (Fig. 1). **L** is the length of the edges.

Results

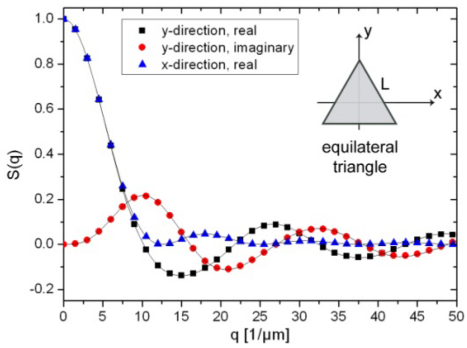

Fig. 1. Diffusion-weighted normalized signal (dots) for very asymmetric temporal gradient profile (δ_2=1-δ_1=1E-6) in the long time limit (L=1 µm, D=1 µm²/ms, T=100 ms, DT/L²=100) and the Fourier transform of the pore space function (line) are in perfect agreement. Thus, the pore space function can be obtained by measuring the diffusion-weighted signal.

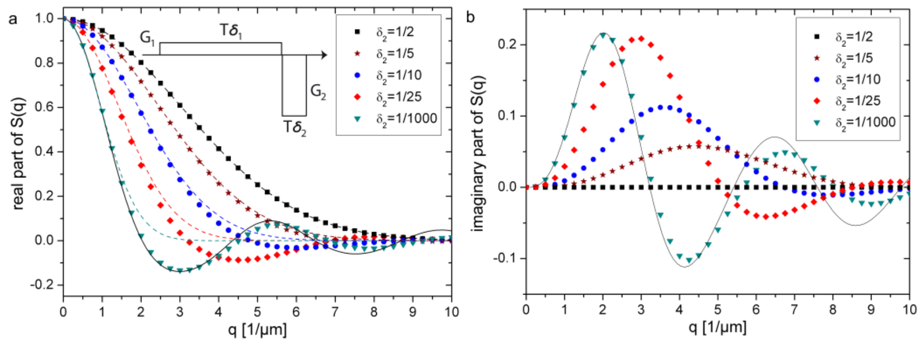

Fig. 2. Real and imaginary parts of the diffusion weighted normalized signal (dots) for a diffusion gradient along the y-direction (L=5 µm, D=1 µm²/ms, T=100 ms, DT/L²=4). The solid line is the Fourier transform of $\chi(\mathrm{x})$; the dotted line is the signal calculated in the Gaussian phase approximation (GPA). A slow transition from diffusion (GPA) to imaging type behavior (solid line) can be observed. Unlike in Fig. 1, the signal for short δ_2=1-δ_1 does not overlap exactly with the Fourier transform of $\chi(\mathrm{x})$ since DT/L² is smaller.

Discussion

If the first gradient is applied over a sufficient long time, the random walker acquires a phase identical to that of a particle located at the center of mass. On the other hand, the rephasing gradient is too short for diffusion dynamics to be of any importance. It merely produces a linear phase dispersion, as does an ordinary imaging gradient. Therefore, the experiment presents itself as a diffusion experiment, but the dynamics are completely lost. It is actually an imaging experiment in disguise! Hence, it follows naturally that the diffusion-weighted signal may bear a phase, just as the signal does in k-space imaging. And thus, most excitingly, the drum is visible in NMR diffusion experiments.

References

[1] Kac. Am. Math. Monthly 73, 1 (1966) [2] Gordon et al. Bull. Am. Math. Soc. 27, 134 (1992) [3] Mitra et al. J. Magn. Res. A 113, 94 (1995) [4] Barzykin. J. Magn. Reson. 139, 342 (1999) [5] Grebenkov. Rev. Mod. Phy. 79, 1077 (2007) [6] Laun et al. ISMRM 2010, p.1581