The displacement correlation tensor from double wave vector diffusion experiments encodes information about pore microstructure and ensemble properties

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Introduction: Pulsed field gradient diffusion sequences with multiple diffusion encoding blocks have recently gained renewed interest in the magnetic resonance community**.** Some of the properties that appear promising in terms of applications are the ability to measure pore sizes, detect anisotropic pores in macroscopically isotropic media, and the enhancement of diffraction peaks [1-3]. Here we consider the cumulant expansion of the double wave vector diffusion signal, and introduce the displacement correlation tensor [4]. This formalism leads to a number of new theoretical insights, for example enabling the detection of fiber curvature [4], or allowing a precise and compact description of the interplay between compartmental anisotropy and ensemble anisotropy. We demonstrate this latter property by comparing to simulations of diffusion in distributions of ellipsoidal pores.

Theory: Under the narrow pulse approximation, Eq. (1) expresses the normalized signal from the double wave vector diffusion sequence (Fig. 1) with diffusion wave vectors $\mathbf{q}_1$ and $\mathbf{q}_2$, where $\mathbf{R}_1 = \mathbf{r}(\Delta) - \mathbf{r}(0)$ and $\mathbf{R}_2 = \mathbf{r}(2\Delta+\tau) - \mathbf{r}(\Delta+\tau)$ are the spin displacements during the two diffusion epochs, and Greek subscripts label Cartesian components with sum over repeated indices implied. The tensor $\mathrm{Q}_{\alpha\beta}(\Delta,\tau) = \langle R_{1\alpha} R_{2\beta} \rangle$ is an explicit measure of correlation between spin displacements in the two periods – the displacement correlation tensor. It can be extracted conveniently using pairs of double diffusion wave vector experiments by fitting to Eq. (2). In the short diffusion time regime, Q is sensitive to the pore space surface to volume ratio *S/V*, as shown by Eq. (3) for $\tau = 0$. In the large diffusion time regime on the other hand, -Q approaches the radius of gyration tensor, $-\mathrm{Q} \approx \langle r_\alpha r_\beta \rangle - D_{\alpha\beta}(\tau)\tau$. Here we consider Q in an ensemble of identical pores of prolate ellipsoidal shapes, where Q is given by Eq. (4) in which I is the identity matrix,T is the scatter matrix of the orientation distribution, and *A* and *B* are eigenvalues of the single pore displacement correlation tensor. Thus, Q encodes information about orientation distribution properties (e.g. ensemble anisotropy) via T, and pore shape (e.g. microscopic anisotropy) via *A* and *B*.

$$S(\mathbf{q}_1,\mathbf{q}_2) = \exp\left(-1/2\left(q_{1\alpha}q_{1\beta} + q_{2\alpha}q_{2\beta}\right)\langle R_{1\alpha}R_{1\beta}\rangle + q_{1\alpha}q_{2\beta}\langle R_{1\alpha}R_{2\beta}\rangle\right) \quad (1)$$

$$\log S(\mathbf{q},\mathbf{q}) - \log S(\mathbf{q},-\mathbf{q}) = 2\mathbf{q}^T \mathrm{Q}\mathbf{q} \quad (2)$$

$$\mathrm{Tr}(\mathrm{Q}) = -(S/V)8\left(\sqrt{2}-1\right)/(3\sqrt{\pi})(D\Delta)^{3/2} + O\left((D\Delta)^2\right) \quad (3)$$

$$\mathrm{Q}(\Delta,\tau) = A(\Delta,\tau)\mathrm{I} + \mathrm{T}\left(A(\Delta,\tau) - B(\Delta,\tau)\right) \quad (4)$$

Methods: Simulations for diffusion in ellipsoids were implemented in Matlab using Monte Carlo methods with 500,000 particles, a diffusion constant of 2 µm²/ms, and time step 0.001 ms. The ellipsoids were cylindrically symmetric with a long axis of 10 µm and short axis 5 µm. 500 unit vectors were generated from a Watson distribution with concentration parameters between 0 and 33, and were used as the directions of the long axes of 500 ellipsoids. The parallel and anti-parallel double wave vector diffusion experiment with $\tau = 0$ was simulated for a wave vector magnitude of 0.1 μm^{-1} and diffusion times 2 and 10 ms. Half the hemisphere of the "24 point spherical 7-design" (set of 24 directions [5]) was used as the basis for selecting the directions of **q**, and a nonlinear least squares Levenberg-Marquardt fitting procedures supplied by Matlab was used on Eq. 2 to estimate Q. The scatter matrix T was estimated empirically by averaging the outer product over the 500 unit vectors. Eigenvalues of Q and T were matched by matching the eigenvectors, and values for *A(Δ)* and *B(Δ)* were obtained numerically by diagonalizing Q obtained from a single ellipsoid.

Fig. 1

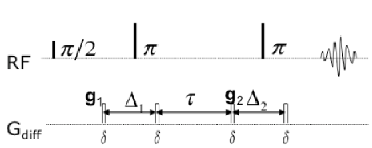


Fig. 2

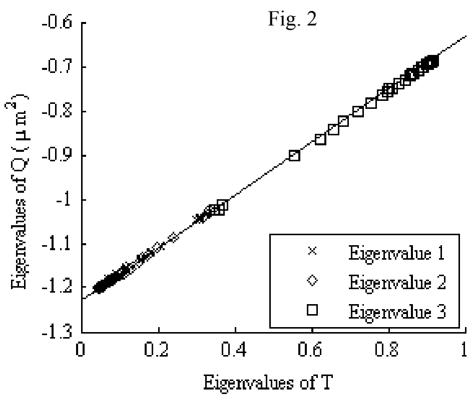
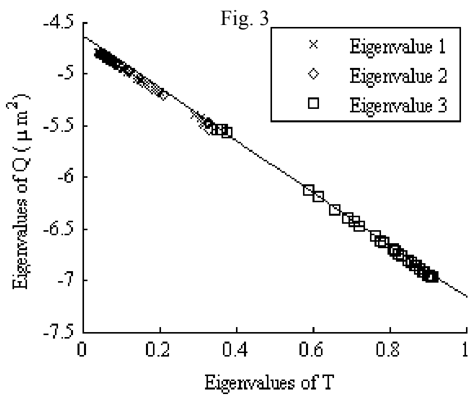


Fig. 3



Results: In Figs. 2 (Δ=2ms) and 3 (Δ=10ms), we demonstrate the linear relationship between the eigenvalues of Q and T expected from Eq. 4 (solid line). The simulations are in excellent agreement with the theory. Note that the slope of the line depends on the diffusion time, and can be either negative or positive. One consequence of this is that for a certain diffusion time, the signal will not depend on the scatter matrix, and the signal will thus appear as if arising from spherical pores.

Conclusions: We introduced the displacement correlation tensor on the basis of the Gaussian approximation to the double wave vector diffusion signal. A number of interesting properties were noted. In particular an exact formula revealing the dependence of the signal on compartmental and ensemble characteristics was presented. This result was corroborated by numerical simulations of diffusion in ellipsoids. The results contribute to the understanding of the properties of the double wave vector diffusion experiment, and can be potentially used to characterize pore shape and dimensions, and to separately characterize compartmental anisotropy and ensemble anisotropy.

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