Journal of Magnetic Resonance 308 (2019) 106556

Contents lists available at ScienceDirect

Journal of Magnetic Resonance

journal homepage: www.elsevier.com/locate/jmr

Response to Comment on "Larmor Frequency in Heterogeneous Media"

In his comment [1] Dr. Cheng discusses the derivation of Eq. (9) in my article [2] and suggests a correction to the main result arising from a modified definition of the medium correlation function. While a brief response is given in the following two paragraphs, more comments are made in the rest of this note intended for a curious reader.

In brief, after a discussion of media with NMR-reporting inclusions, Dr. Cheng derives his Eq. (4) that coincides with Eq. (9) in my original article. While misconceptions in his derivation are commented upon below, this agreement suggests stopping the discussion of this issue and turn to the second one.

The second point of Dr. Cheng's comment concerns the definition of the correlation function of microbeads,

$$\Gamma(\mathbf{r}) = \int \frac{\mathrm{d}^3\mathbf{r}_0}{V}\, v(\mathbf{r}_0+\mathbf{r})\, v(\mathbf{r}_0) - \zeta^2, \tag{1}$$

where V is the volume of the mesoscopic sphere, v the indicator function of inclusions and ζ their volume fraction. An alternative definition used by Dr. Cheng does not include the subtraction of ζ^2. While definitions may be a subject of convention, the present one is operational in Dr. Cheng's calculations removing the factor $1-\zeta$ in the final result. To give a brief response, the constant $-\zeta^2$ affects only the Fourier component with $\mathbf{k}=0$. Note that $\Gamma(\mathbf{k})$ enters the final result in the product with the dipole field, $\mathcal{Y}_{ab}(\mathbf{k})$. The latter is explicitly set to zero at the point $\mathbf{k}=0$ by the reason given below with more details in a recent review [3]. Therefore, the value of the correlation function at this point is irrelevant.

To give more details to the first issue, the starting point of Dr. Cheng's derivation, Eq. (2) of his comment, is the averaging of the phase factor, $\exp\{i\Omega(\mathbf{r})t\}$, over the medium. This is misleading, since we consider the diffusion narrowing regime in which each spin samples a large portion of the medium, therefore not having a constant value of $\Omega(\mathbf{r})$. It is the essence of the diffusion narrowing that the time-averaged field experiences by spins equals the space averaging of $\Omega(\mathbf{r})$.

In the same vein, the introduction of the "magnitude signal at each spatial point" contradicts the essence of the diffusion narrowing. If we wish to consider NMR-visible inclusion, it is the local density of NMR-visible spins that can be used, say ρ_0 and ρ_1 inside and outside the inclusions, respectively. In the absence of exchange between these compartments and to the first order in $\Omega(\mathbf{r})$, the overall frequency shift is the weighted mean over the compartments,

$$\overline{\Omega} = \frac{\zeta\rho_0}{\zeta\rho_0+(1-\zeta)\rho_1}\Omega_0 + \frac{(1-\zeta)\rho_1}{\zeta\rho_0+(1-\zeta)\rho_1}\Omega_1, \tag{2}$$

where Ω_0 and Ω_1 are the compartment-averaged Larmor frequency offsets for the volume inside and outside the inclusions, respectively:

$$\Omega_0 = \int \frac{\mathrm{d}^3\mathbf{r}}{\zeta V}\, v(\mathbf{r})\Omega(\mathbf{r}),\ \Omega_1 = \int \frac{\mathrm{d}^3\mathbf{r}}{(1-\zeta)V}[1-v(\mathbf{r})]\Omega(\mathbf{r}). \tag{3}$$

The general formula, Eq. (2), coincides with Eq. (9) in my publication derived for the originally considered case of $\rho_0=0$ and with the last but one expression in Eq. (2) in Dr. Cheng's comment in the case $\rho_0=\rho_1$. The same equality justifies his inline expression for the case of zero frequency shift inside the inclusions. This case is however unrealistic for dense media in which each inclusion is exposed to the field induced by all other ones.

Turning to the second issue raised by Dr. Cheng, consider the above definition of $\Gamma(\mathbf{r})$, which was used in [2]. For very large separation, $\mathbf{r}$, the local forms of the indicator function $v(\mathbf{r}_0+\mathbf{r})$ and $v(\mathbf{r}_0)$ become statistically independent and can be replaced by their mean, ζ, which makes the integral equal ζ^2. Since this cancels against the second term in Eq. (1), the correlation function tends to zero for large separations. Provided this occurs faster than $1/r^3$, such a function has a non-singular Fourier transform, $\Gamma(\mathbf{k})$. Discarding the constant term in Eq. (1) results in the addition of the delta-function, $(2\pi)^3\zeta^2\delta(\mathbf{k})$ to the so far non-singular $\Gamma(\mathbf{k})$. The same is clear from the relation in the Fourier space, Eq. (13) in [2] if the comment about the $\mathbf{k}=0$ component is ignored,

$$\Gamma(\mathbf{k}) = \frac{v(\mathbf{k})\, v(-\mathbf{k})}{V}. \tag{4}$$

Indeed, when calculating the components with $\mathbf{k}=0$, $v(\mathbf{r})$ can be replaced with its mean value, ζ, which gives ζV for $v(\mathbf{k}=0)$. The resulted contribution in $\Gamma(\mathbf{k})$ is $\zeta^2 V$, which is precisely the magnitude of the above delta-function for $k=0$. As supplemental material to this response, a Matlab script is provided to illustrate the properties of correlation function, both $\Gamma(\mathbf{r})$ and $\Gamma(\mathbf{k})$ in one spatial dimension.

The $\mathbf{k}=0$ component of the elementary dipole field, $\mathcal{Y}_{ab}(\mathbf{k})$, is proportional to the spatially constant component of the field. Solving the magnetostatic equations for any given source distribution within the mesoscopic sphere leaves this component arbitrary, which is normally fixed by the boundary conditions on the sphere surface. Since the field from the sources outside the mesoscopic sphere is taken into account separately (Fig. 1 in [2]), this field should not be double counted, which is equivalent to considering the mesoscopic sphere with no outside sources (Fig. 1 in [2]). In principle, the sources inside the sphere could induces a constant field component thus contributing to $\mathcal{Y}_{ab}(\mathbf{k})$ for $\mathbf{k}=0$. However, this component must be zero to obey the well-know fact that

DOI of original article: https://doi.org/10.1016/j.jmr.2019.07.042

https://doi.org/10.1016/j.jmr.2019.07.043

the field offset within a sphere is zero with account for the field of the classical Lorentz sphere on the molecular scale. More detailed discussion can be found in [3].

Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.jmr.2019.07.042.

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Available online 18 July 2019

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