Journal of Magnetic Resonance 308 (2019) 106555

Contents lists available at ScienceDirect

Journal of Magnetic Resonance

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

Comments on "Larmor frequency in heterogeneous media"

A recent theoretical paper by Kiselev [1] sheds some new lights on the Larmor frequency shift calculations from magnetized inclusions with a constant susceptibility tensor in a porous media and in the pure diffusion regime. The paper is interesting and it is also heavily mathematical oriented. Following the derivations in [1], it appears that Eq. (10) can be re-derived more rigorously, with a re-defined correlation function in Eq. (11) and its Fourier transform in Eq. (13). This short communication is meant to show these different and subtle derivations.

Starting with Eq. (7) in [1], which is repeated here, the local Larmor frequency offset within the mesoscopic sphere is given by the longitudinal projection of the susceptibility-induced magnetic field, $\mathbf{B}^{macro}(\mathbf{r})$,

$$\Omega(\mathbf{r}) = \gamma n_a B_a^{macro}(\mathbf{r}) \tag{1}$$

where $\gamma = 2\pi \cdot 42.58$ MHz/T and $\mathbf{n} = \mathbf{B}_0/B_0$ is the unit vector in the direction of the main magnetic field B_0.

The measured Larmor frequency, $\overline{\Omega}$, is obtained from averaging the complex signals within a spherical volume V over the space occupied by water and magnetic inclusions,

$$\begin{aligned}
\overline{\Omega} &= \arg\left(\frac{1}{\mathrm{V}}\int d^3\mathbf{r} M(\mathbf{r})\exp\{i\Omega(\mathbf{r})t\}\right)/t \\
&\approx \arg\left(\frac{1}{\mathrm{V}}\int d^3\mathbf{r} M(\mathbf{r})(1+i\Omega(\mathbf{r})t)\right)/t \\
&= \begin{cases} \dfrac{1}{\mathrm{V}}\displaystyle\int d^3\mathbf{r}\,\Omega(\mathbf{r}) & \text{if } M(\mathbf{r}) \text{ is a constant} \\ \dfrac{1}{\mathrm{V}(1-\zeta)}\displaystyle\int d^3\mathbf{r}\,\Omega(\mathbf{r})[1-v(\mathbf{r})] & \text{if } M(\mathbf{r}) = 0 \text{ inside inclusions but a constant outside} \end{cases}
\end{aligned} \tag{2}$$

where $M(\mathbf{r})$ represents the magnitude signal from spins at each spatial point, ζ is the volume fraction of inclusions inside the volume V, and $v(\mathbf{r})$ is an indicator function, which is unity inside any magnetic inclusion and zero otherwise. The integrals are performed over volume V, which can be considered as the size of a voxel for the purpose of measurements, and the induced local phase needs to be small enough for a valid expansion. The magnitude signals inside inclusions have been assumed to be zero in [1] in order to be consistent with Eq. (8) of [1]. If magnitude signals inside and outside inclusions are the same, but the induced magnetic fields inside inclusions are zero, both formulas derived in the above Eq. (2) will have $1 - v(\mathbf{r})$ in the integrands but the normalized volume in the denominator becomes V without the $1-\zeta$ factor. An application of this situation will be briefly discussed at the end of this comment.

In addition, under the diffusion narrowing regime, if its time scale is much shorter than the sampling time during MRI data acquisition, it may be more appropriate to estimate $\overline{\Omega}$ directly from the induced local Larmor frequency $\Omega(\mathbf{r})$. This is because when a subject is placed inside an MRI machine, even without turning on any sequence, magnetic field $\mathbf{B}^{macro}(\mathbf{r})$ will already be induced inside the subject. Again, if the induced magnetic fields inside inclusions are zero, which is true for spherical inclusions regardless of their magnitude signals, $\overline{\Omega}$ will be $\int d^3\mathbf{r}\,\Omega(\mathbf{r})/\mathrm{V} = \int d^3\mathbf{r}\,\Omega(\mathbf{r})[1-v(\mathbf{r})]/\mathrm{V}$.

By plugging Eq. (1) into Eq. (2) and with

$$B_a^{macro}(\mathbf{r}) = \int d^3\mathbf{r_0}\, \mathscr{Y}_{ab}(\mathbf{r}-\mathbf{r_0})\chi_{bc} v(\mathbf{r_0}) n_c B_0 \tag{3}$$

described in [1], where $\mathscr{Y}_{ab}$ is the Green's function or the dipole fields provided by [1] (although a factor of $1/(4\pi)$ should be multiplied if SI system is used) and χ_{bc} is the susceptibility tensor of inclusions, Eq. (9) in [1] is derived:

$$\frac{\overline{\Omega}}{\Omega_0} = \int \frac{d^3\mathbf{r_1}}{\mathrm{V}(1-\zeta)} d^3\mathbf{r_0}[1-v(\mathbf{r_1})]n_a\mathscr{Y}_{ab}(\mathbf{r_1}-\mathbf{r_0})\chi_{bc}n_c v(\mathbf{r_0}) \tag{4}$$

where $\Omega_0 = \gamma B_0$ is the nominal Larmor frequency. The limits of the two integrals over $\mathbf{r_0}$ and $\mathbf{r_1}$ are within the same spherical volume V.

As the author of [1] has stated, the integral result of the first term is zero. After that, this outcome allows the limits of the two integrals to be extended to infinity, because the function v only

DOI of original article: https://doi.org/10.1016/j.jmr.2018.12.008

https://doi.org/10.1016/j.jmr.2019.07.042

defines inclusions inside the volume V and υ is zero outside V. Thus, we now change the variable in Eq. (4) and rewrite Eq. (10) to be

$$\begin{aligned}\frac{\overline{\Omega}}{\Omega_0} &= -\int \frac{d^3\mathbf{r}d^3\mathbf{r_0}}{\mathrm{V}(1-\zeta)}\upsilon(\mathbf{r_0}+\mathbf{r})\upsilon(\mathbf{r_0})n_a\mathscr{Y}_{ab}(\mathbf{r})\chi_{bc}n_c \\ &= -\frac{1}{1-\zeta}\int d^3\mathbf{r}\, n_a\mathscr{Y}_{ab}(\mathbf{r})\chi_{bc}n_c\Gamma(\mathbf{r})\end{aligned} \quad (5)$$

where

$$\Gamma(\mathbf{r}) \equiv \int \frac{d^3\mathbf{r_0}}{\mathrm{V}}\upsilon(\mathbf{r_0}+\mathbf{r})\upsilon(\mathbf{r_0}) \quad (6)$$

and the limits of all integrals are from minus infinity to plus infinity, rather than within finite mesoscopic volumes. This will enable the proper Fourier transform of $\Gamma(\mathbf{r})$ and a recalculation of $\Gamma(\mathbf{k})$ at $\mathbf{k}=0$. If the limits of integrals in the original Eq. (10) are finite, it is unclear whether the original Eq. (10) can be rewritten to Eq. (14) still with definitions given by Eq. (11) and Eq. (13) in [1]. In addition, physics requires $\Gamma(\mathbf{r})$ to vanish when $|\mathbf{r}|$ is longer than the diameter of the spherical volume V (i.e., outside V). The above Eq. (6) satisfies this physics requirement, but the original Eq. (11) does not.

Finally, the Fourier transform of Eq. (6) is still Eq. (13) in [1], but with $\Gamma(\mathbf{k}=0)=\zeta^2\mathrm{V}$. This now makes $\Gamma(\mathbf{k})$ a continuous function over the $\mathbf{k}=0$ point. In addition, based on Eq. (6), the result of Eq. (C.2), $\Gamma^{(2d)}(\mathbf{r}=0)$, will become ζ instead of $\zeta(1-\zeta)$. This elimination of the factor $1-\zeta$ unfortunately will lead to the same factor offset in relevant results shown in Sections 3.2 and 3.3 of [1]. However, that should not be seen as a critical drawback of the work presented in [1]. The combination of all these subtle revisions above leads to a more general derivation of the original equations without using any statistical arguments. On the other hand, if inclusions have zero frequencies under aforementioned certain scenarios, the above Eq. (2) will also drop the factor $1-\zeta$ in the denominator. In the scenario that inclusions have magnitude signals but zero frequencies, which may be closer to the presence of magnitude signals in white matter microstructures [2] and optic nerves [3], results shown in Sections 3.2 and 3.3 of [1] and its conclusion actually remain the same.

Acknowledgements

This work was supported in part by the Department of Radiology at Wayne State University and grant support from NIH/NIA R56 AG060822-01A1. The content is solely the responsibility of the author and does not necessarily represent the official views of the National Institutes of Health.

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Available online 18 July 2019