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A closed form solution of magnetic nanoparticles in rotating drift spectroscopy

T. Kampf[a,b,*] · M. A. Rückert[a] · A. Vilter[a] · V. J. F. Sturm[c] · P. Vogel[a] · V. C. Behr[a]

[a]Department of Experimental Physics 5 (Biophysics), University of Würzburg, 97074, Würzburg, Germany
[b]Department of Diagnostic and Interventional Neuroradiology, University Hospital Würzburg, 97080, Würzburg, Germany
[c]Department of Diagnostic and Interventional Neuroradiology, University Hospital Heidelberg, 69120, Heidelberg, Germany
[*]Corresponding author, email: kampf_t@ukw.de

Abstract

Accurate prediction of experimental results is one of the main goals in scientific research. With higher complexity this relies increasingly on accurate numerical simulations. The inductive detection of magnetic nanoparticles often relies on the nonlinear magnetization response of these particles on externally applied time-varying magnetic fields. However, in some cases a closed analytical solution for special cases can be found and used for calibration as well as testing numerical codes. Furthermore, they allow the systematic study of the system and can be starting points for perturbation theory. In this work an analytical solution for the simplest Rotating Drift Sectroscopy (RDS)-experiment for magnetic nanoparticles in solution with full 3D motion is presented and compared to the known case of 2D-confined rotation of the nanoparticles.

I. Introduction

The detection of magnetic nanoparticles (MNPs) has been in the focus of research in recent years. Their biocompatibility has sparked many applications in life science. Especially Magnetic Particle Imaging (MPI) has gained a lot of interest as it allows the background free detection of the magnetic particle tracers [1]. It has shown its versatility in preclinical research and is now on the brink of clinical application [2-4]. Related to this well-known method is rotational drift spectroscopy (RDS). Contrary to MPI it does not rely on the nonlinear saturation behavior of the magnetic response of MNPs to external time varying magnetic fields. In RDS the MNP follows an external rotating magnetic field. In rotating magnetic fields below a critical field strength, the MNP can't rotate synchronously with the external magnetic field due to viscous friction and an asynchronous rotational drift will occur. This was first investigated in a 2D confined geometry for the particle motion and detected optically [5]. In these optical experiments the frequency of asynchronous nanoparticles rotation proofed as a very sensitive sensor for the effective particle size or the viscous properties of the liquid solvent and was applied to the detection of MNPs binding to bacteria surfaces. Recently the inductive detection of the RDS signal was demonstrated for MNPs suspensions [6,7]. This improvement circumvents the issues of optical particle detection which was limited to single magnetic particles confined to a surface. However, understanding the RDS signal for unrestricted MNPs in liquid suspension requires the full 3D motion of the particles in these conditions. The simplest RDS experiment, a MNP in rotating external field with constant amplitude and rotation frequency has been investigated before [10]. They numerically determined the rotation axes and angle for each time step

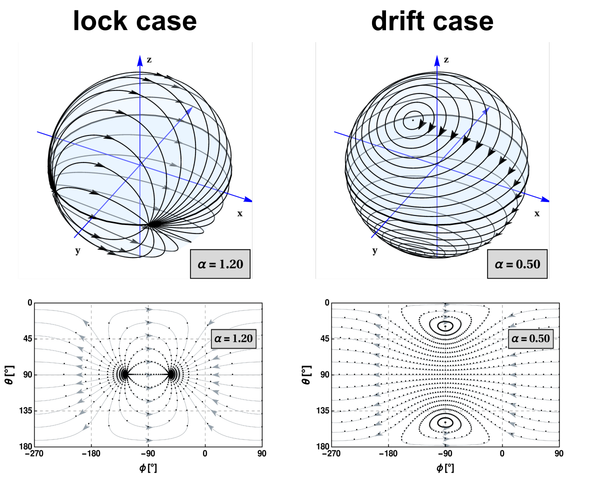

Figure 1: Exemplary trajectories of the MNP magnetization. The upper row shows the 3-D motion in the rotating frame of reference when the magnetic field axis points along the x-direction. In the lower row the same motion is shown in polar and azimuthal angle coordinates. The parameter $\alpha = mB/\xi\omega_0$ with ω_0 as the rotation frequency of the external magnetic field describes the interplay between magnetic and geometric/viscose properties of the particle/liquid.

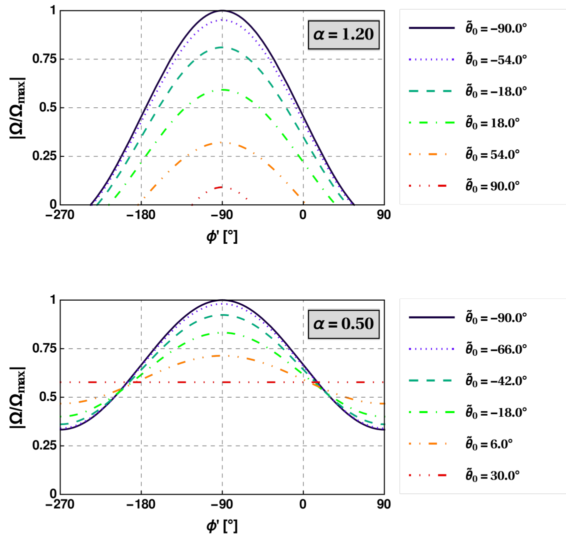

Figure 2: Angular velocity Ω of MNPs for different starting angles in the respective local frame of reference. Upper row exemplary for a lock case and lower row exemplary for a drift case value of α. Please note that in the local frame of reference for the lock case the phase angle depends on the chosen trajectory represented by $\tilde{\theta}_0$.

and simulated the motion by applying the corresponding rotation matrix for each discrete time step. In this work the closed form solution of this experiment is presented.

II. Material and methods

Here, the motion of MNPs in an external magnetic field with constant amplitude and frequency performing a uniaxial rotation is considered. For simplicity a spherical particle with magnetization locked to its lattice is assumed. The particle can move freely around all three axes as in liquid suspension, however, stochastic effects like random collisions leading to random torques and thus thermal noise and rotational diffusion are neglected. Thus, neglecting inertial terms, the particles motion is governed by [11]

$$\frac{d\mathbf{n}}{dt} = \frac{m}{\xi}(\mathbf{n}\times\mathbf{B})\times\mathbf{n},$$

with fixed amplitude m and direction $\mathbf{n}$ of the MNP's magnetic moment, the rotating external magnetic field with constant amplitude $\mathbf{B}$, and the constant ξ, which depends on the particle size and shape as well as the dynamic viscosity of the surrounding liquid.

This equation describes a rotation of the magnetization around a current time and magnetization dependent angular frequency $m(\mathbf{n}\times\mathbf{B})/\xi$. However, transformation into the rotating frame of the external magnetic field reveals that the corresponding axis of rotation becomes stationary in this frame.

III. Results and discussion

The mathematical analysis shows that one can choose a local frame of reference with z-axis parallel to the rotation axis, where the magnetization performs a 2D uniaxial rotation with its phase following in local coordinates:

$$\frac{d\phi'}{d\tau'} = -(\alpha'\sin(\phi')+1) \Rightarrow \tau' - \tau'_0 = -\int_{\phi'_0}^{\phi'} \frac{d\Phi}{\alpha'\sin(\Phi)+1}.$$

The solution is straight forward but requires a case by case analysis which is lengthy, but can be looked up in integration tables, e.g. [12]. Thus, the full 3D solution also displays the two general types of motion (see Fig. 1). When the magnetic interaction dominates, the MNP follows the rotating external magnetic field with a locked phase after an initial transient (*lock case*: $\alpha > 1$). If the magnetic interaction is too weak, the MNP rotates asynchronously with the external magnetic field (*drift case*: $\alpha < 1$). In the rotating frame of reference this asynchronous rotation becomes a rotation on fixed orbits around the corresponding stable axis. For two starting points of the magnetic moment the net torque on the magnetization in the rotating frame of reference becomes zero and the orbits degenerate to fixed points. Hence, contrary to the 2D case in 3D even in the drift case a rotation locked to the external magnetic field is possible.

For particles with the same value of ξ the mean frequency of this rotation is independent of the starting position. However, for each orbit the temporal variation

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of the angular velocity is different in the corresponding local frame of reference (see Fig. 2).

The result was compared to numerical results presented earlier demonstrating a good agreement of both results.

IV. Conclusions

In this work a closed form solution for the simplest RDS experiment considering the full 3D motion of a MNP particle in viscose liquid is described. It can be used to test and calibrate numerical code in this special case, which then can be used to investigate more sophisticated experiments that cannot be described in closed form. Currently only single particles without the influence of stochastic collisions with the liquid background are considered. However, the described closed form solution is a necessary precursor to investigate the magnetization of MNP ensembles and the corresponding collective effects. Furthermore, it can be used as starting for perturbation calculations to include additional effects like offset fields or rotational diffusion.

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Author's statement

Conflict of interest: Authors state no conflict of interest.

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