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# Brownian Rotational Motion of Ferromagnetic Nanoparticle in Liquid

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Langevin and Fokker Planck equations are considered for stochastic spherical motion of the ferromagnetic fine particle with frozen magnetic moment in a viscous carrier. Special attention devotes to the correspondence between dissipative and diffusive terms of these equations. For the case when the particle moment of inertia is negligible small, the effective system of Langevin equation for spherical coordinates is obtained. This system contains two equations with additive noises and can be readily treated numerically. We confirm our analytical finding by numerical simulation.

**Keywords:** Ferrofluid, Spherical motion, Brownian motion, Langevin equation, Fokker-Planck equation.

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## 1. INTRODUCTION

The problem of the dynamics of ferromagnetic nanoparticles, dispersed in viscous carried, is important for both theoretical and applied reasons. From one hand, the ensemble of such particles is a remarkable example of a complex system, where a lot of dynamical and stochastic effects can take a place. From another hand, these ensembles are nothing other than ferrofluids [1]. Therefore, dynamic of particles determines response of ferrofluid on an external action, and, hence, ferrofluid properties.

The motions of a nanoparticle can be represented as superposition of two types of motion: 1) displacement of a particle center of mass, 2) rotation of a particle about fixed center of mass, or spherical motion. Since the average size of nanoparticles in real ferrofluid usually is ~10 nm [2], the spherical motion is stochastic at room temperature and, also called Brownian rotation.

Two approaches to description of stochastic dynamics exist: Langevin equation (LE) and Fokker-Plank equation (FPE) [3]. The first one is the base of numerical analysis, while second is used for analytical evaluation of statistical properties. Despite the difference in methodology, the correspondence between LE and FPE is present. There are a lot of investigations where LE was examined for the problem of stochastic rotation of fine particles in fluid [4-7]. However, FPE was written only in the case of validity of Boltzmann distribution [4]. The last is not applicable when the time-dependent external field is applied to the ferrofluid.

The correct FPE let to verify the results of numerical simulation, based on LE, and gives the possibility to obtain some statistical characteristics in simplest cases. But also, using FP one can develop new simulation techniques, which more powerful and suitable for description the collective effects in a large nanoparticle ensembles [8]. That is why in our analysis we devote a special attention to the full accordance with LE and FPE without any additional suppositions.

## 2. MODEL AND MAIN EQUATIONS

### 2.1 System of equations with inertia term

We study rotational motion of spherical ferromagnetic nanoparticle of radius $R$, whose magnetic moment $\boldsymbol{\mu}$ is locked to the crystal axis, or, so-called particle with frozen magnetic moment. The corresponding system of LEs is represented by the angular momentum equation and on the equations of spherical motion [9, 7]

$$\begin{cases} \dfrac{d}{dt}\boldsymbol{\omega} = \dfrac{1}{\tau_0^2}\mathbf{m}\times\mathbf{h} - \dfrac{1}{\tau_r}\boldsymbol{\omega} + \dfrac{1}{I}\boldsymbol{\xi}(t), \\ \dfrac{d}{dt}\mathbf{m} = \boldsymbol{\omega}\times\mathbf{m}, \end{cases} \tag{2.1}$$

where $\boldsymbol{\omega}$ is the angular velocity, $\mathbf{m} = \boldsymbol{\mu}/M$ is the reduced magnetic moment, $M$ is the particle material magnetization, $h = \mathbf{H}(t)/M$ is the reduced external field ($\mathbf{H}(t)$ is the external field), $\tau_0 = (I/\mu_0 M^2 V)^{1/2}$, $\tau_r = I/6\eta V$ are the characteristic time, $I = {}^2/_5 DVR^2$ is the particle moment of inertia, $D$ is the particle density, $V = {}^3/_4\pi R^3$ is the particle volume, $\eta$ is the liquid viscosity, $\mu_0 = 4\pi 10^{-7}$ H·m is the magnetic constant, $\boldsymbol{\xi}(t)$ is the random torque, which represent the interaction with a heat bath. We assume that random torque $\boldsymbol{\xi}(t)$ is approximated by a Gaussian white noise of zero mean and delta correlation.

In the case $|\mathbf{m}| = \text{const}$ and using spherical coordinates system, equations (2.1) can be rewritten as

$$\begin{cases} \dfrac{d\theta}{dt} = \omega_y\cos\varphi - \omega_x\sin\varphi, \\ \dfrac{d\varphi}{dt} = \omega_z - \left(\omega_x\cos\varphi + \omega_y\sin\varphi\right)\cot\theta, \\ \dfrac{d\omega_x}{dt} = \dfrac{1}{\tau_0^2}\left(h_z\sin\theta\sin\varphi - h_y\cos\theta\right) - \dfrac{1}{\tau_r}\omega_x + \dfrac{1}{I}\xi_x, \\ \dfrac{d\omega_y}{dt} = \dfrac{1}{\tau_0^2}\left(h_x\cos\varphi - h_z\sin\theta\cos\varphi\right) - \dfrac{1}{\tau_r}\omega_y + \dfrac{1}{I}\xi_y, \\ \dfrac{d\omega_z}{dt} = \dfrac{1}{\tau_0^2}\left(h_y\sin\theta\cos\varphi - h_x\sin\theta\sin\varphi\right) - \dfrac{1}{\tau_r}\omega_z + \dfrac{1}{I}\xi_z, \end{cases} \tag{2.2}$$

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where $\theta$ and $\varphi$ is the angular coordinates of the nanoparticle; $\omega_x$, $\omega_y$, $\omega_z$ are the angular velocity projection on laboratory *xyz* coordinate system axis; $h_x$, $h_y$, $h_z$ are the external field projections on laboratory coordinate system axis; $\xi_x$, $\xi_y$, $\xi_z$ are same projection of the random torque.

The corresponding to (2.1) FPE [3] one can be written as

$$\frac{\partial}{\partial t}P+(\boldsymbol{\omega}\times\mathbf{m})\frac{\partial}{\partial\mathbf{m}}P+\frac{\partial}{\partial\boldsymbol{\omega}}\left(\frac{1}{\tau_0^2}\mathbf{m}\times\mathbf{h}-\frac{1}{\tau_r}\boldsymbol{\omega}\right)P-$$
$$-\frac{\Delta}{I^2}\sum_i\frac{\partial^2}{\partial\omega_i^2}P=0, \qquad (2.3)$$

where $P=P(t,\ \boldsymbol{\omega},\ \mathbf{m})$ is the time-dependent probability density of $\mathbf{m}$ states, and $\Delta$ is the noise intensity. Expression (2.3) can be presented in the scalar form

$$\frac{\partial P}{\partial t}+\frac{\partial}{\partial\theta}\left(\omega_y\cos\varphi-\omega_x\sin\varphi\right)P+$$
$$+\frac{\partial}{\partial\varphi}\left[\omega_z-\left(\omega_x\cos\varphi+\omega_y\sin\varphi\right)\cot\theta\right]P$$
$$+\frac{\partial}{\partial\omega_x}\left[\frac{1}{\tau_0^2}\left(h_z\sin\theta\sin\varphi-h_y\cos\theta\right)-\frac{1}{\tau_r}\omega_x\right]P+$$
$$+\frac{\partial}{\partial\omega_y}\left[\frac{1}{\tau_0^2}\left(h_x\cos\varphi-h_z\sin\theta\cos\varphi\right)-\frac{1}{\tau_r}\omega_y\right]P+ \qquad (2.4)$$
$$+\frac{\partial}{\partial\omega_z}\left[\frac{1}{\tau_0^2}\left(h_y\sin\theta\cos\varphi-h_x\sin\theta\sin\varphi\right)-\frac{1}{\tau_r}\omega_z\right]P-$$
$$-\frac{\Delta}{I^2}\sum_i\frac{\partial^2}{\partial\omega_i^2}P=0,$$

which will be corresponding in statistical sense to the equation (2.3). When external field is constant, the stationary probability density $P_{st}$ should be defined by Boltzmann distribution. This fact let us to obtain the explicit forms of $P_{st}$ and $\Delta$

$$\begin{cases}P_{st}=C\sin\theta\exp\left(-\dfrac{I}{2k_\mathrm{B}T}\boldsymbol{\omega}^2+\dfrac{\mu_0VM^2}{k_\mathrm{B}T}\mathbf{m}\cdot\mathbf{h}\right),\\ C=\left(\dfrac{I}{2\pi k_\mathrm{B}T}\right)^{\frac{3}{2}}\cdot\dfrac{\mu_0VM^2h}{4\pi k_\mathrm{B}T}\cdot\dfrac{1}{\sinh\left(\mu_0VM^2h/k_\mathrm{B}T\right)},\end{cases} \qquad (2.5)$$

$$\Delta=6\eta Vk_\mathrm{B}T\ , \qquad (2.6)$$

Where $k_\mathrm{B}$ is the Boltzmann constant, T is the thermodynamic temperature. The validity of (2.5) was approved by numerical simulation using the direct solution of system (2.2), where the noise intensity was defined by relationship (2.6).

## 2.2 Reduced system of equations

The direct numerical solution of system (2.2) is consumes considerable computing resources, because of presence of five equations, including stochastic ones. It is a main restriction for using (2.2) for simulation ensembles with large number of nanoparticles.

The typical average size of fine particle in a ferrofluid is ~ 10 nm [10]. That is why the particle moment of inertia $I$ is too small, and one can neglect the inertia terms in (2.1) and (2.2). Therefore, we can rewrite equation (2.1) in the following form:

$$\frac{d}{dt}\mathbf{m}=-\frac{\tau_r}{\tau_0^2}\mathbf{m}\times\left(\mathbf{m}\times\mathbf{h}\right)-\frac{\tau_r}{I}\mathbf{m}\times\xi(t)\ . \qquad (2.7)$$

In turn, vector equation (2.7), when the magnetic moment is constant by magnitude, is reduced to the system of two equations for spherical angles

$$\begin{cases}\dfrac{d\theta}{dt}=\dfrac{\tau_r}{\tau_0^2}\left(h_x\sin\theta\cos\varphi+h_y\sin\theta\sin\varphi+h_z\cos\theta\right)\cot\theta-\\ \quad-\dfrac{\tau_r}{\tau_0^2}h_z\dfrac{1}{\sin\theta}+\dfrac{\tau_r}{I}\left(\xi_y\cos\varphi-\xi_x\sin\varphi\right),\\ \dfrac{d\varphi}{dt}=\dfrac{\tau_r}{\tau_0^2}\left(h_y\cos\varphi-h_x\sin\varphi\right)\dfrac{1}{\sin\theta}-\\ \quad-\dfrac{\tau_r}{I}\left(\xi_x\cos\varphi+\xi_y\sin\varphi\right)\cot\theta+\dfrac{\tau_r}{I}\xi_z.\end{cases} \qquad (2.8)$$

The corresponding to LE (2.8) FPE [3] have the form

$$\frac{\partial}{\partial t}P+\frac{\tau_r}{\tau_0^2}\frac{\partial}{\partial\theta}\left[\left(h_x\cos\varphi-h_y\sin\varphi\right)\cos\theta-\right.$$
$$\left.-h_z\sin\theta+\frac{\tau_0^2}{\tau_r}\frac{1}{\tau}\cot\theta\right]P+$$
$$+\frac{\tau_r}{\tau_0^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}\left(h_y\cos\varphi-h_x\sin\varphi\right)P- \qquad (2.9)$$
$$-\frac{1}{\tau}\frac{\partial^2P}{\partial\theta^2}-\frac{1}{\tau}\frac{1}{\sin^2\theta}\frac{\partial^2P}{\partial\varphi^2}=0,$$

where $P=P(t,\ \theta,\ \varphi)$ is the time-dependent probability density of the magnetic moment states, parameter $\tau$ is defined by noise intensity. In the way, described below and using the Boltzmann distribution, we derived it as

$$\tau=6\eta V/k_\mathrm{B}T\ . \qquad (2.10)$$

The expression (2.8) contais only two equatios instead of five in (2.3). However, the integration of (2.8) is obstructed. By physical reasons, we need to use here the white noise in Stratonovich interpretation. At the same time, the widely used numerical methods [11] are developed for LE with noises in Ito interpretation. This problem is not actual, when noises are additive, and one can used all these method regardless of the interpretation of the noise. But, in our case, expressions in (2.8) contain multiplicative noises.

To overcome this problem, the following effective LE

$$\begin{cases}\dfrac{d\theta}{dt}=\dfrac{\tau_r}{\tau_0^2}\left(h_x\cos\varphi+h_y\sin\varphi\right)\cos\theta-\dfrac{\tau_r}{\tau_0^2}h_z\sin\theta+\\ \quad+\dfrac{1}{\tau}\cot\theta+\sqrt{\dfrac{2}{\tau}}\xi_1\\ \dfrac{d\varphi}{dt}=\dfrac{\tau_r}{\tau_0^2}\left(h_y\cos\varphi-h_x\sin\varphi\right)\dfrac{1}{\sin\theta}+\sqrt{\dfrac{2}{\tau}}\dfrac{1}{\sin\theta}\xi_2\end{cases} \qquad (2.11)$$

was introduced. Here $\xi_{1,2}$ are the gaussian white noise with unit intensity. The last system contains additive noises and corresponding in statistical sense to the FPE in the form (2.9). It let to use the system (2.11) instead of (2.8) in numerical simulation.

To examine the developed approach we considered joined action of the circularly polarized and the static fields

$$\vec{h} = \vec{e}_x h \cos \Omega t + \vec{e}_y h \sin \Omega t + \vec{e}_z h_z \,, \qquad (2.12)$$

where $h$ and $\Omega$ are the rotating field amplitude and frequency respectively, $h_z$ is the static field value. We calculated the average projection of the nanoparticles magnetization the on $z$ axis (see Fig. 1). The results obtained in the case $h_z = 0$ fit to the well-known Langevin function: $\langle m_z \rangle = \coth\alpha - 1/\alpha$, $\alpha = \mu_0 M^2 V h_z / k_B T$.

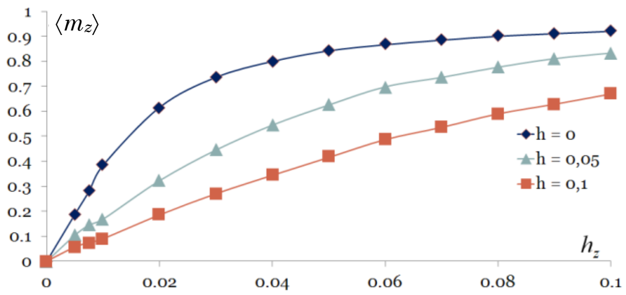


**Fig. 1** – The magnetization curves for the field (2.12) obtained numerically. $M = 3{,}1 \cdot 10^5$ A/m, $R = 10$ nm ,$T = 298$ K

## 3. CONCLUSIONS

The consistent approach for description of Brownian rotational motion of the ferromagnetic fine particle in a viscous liquid was proposed. This approach based on the strong correspondence between dissipative and diffusive terms in Langevin and Fokker Planck equations. Two cases were considered 1) equations of motions contain the inertia terms, 2) the inertia terms were neglected because of the nanoparticle small size.

Using the system of equations of motion without inertia terms let to achieve of significant saving of the computing power during simulation of the large ferrofluid volumes. But such system, written in the spherical coordinates contained the multiplicative noises that complicate the numerical solution. Thereby, the effective system of Langevin equations was obtained. Such system correspond to the same Fokker-Planck equation, that the original system of motion. At the same time, effective system contain only additive noises and suitable enough for conventional numerical techniques.

Using the derived Langevin equations, the numerical simulation was performed. The results obtained were in a good agreement with analytical predictions, which were performed using Fokker-Planck equation in the case of absence of time-dependent external fields.

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