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Stochastic Dynamics of Ferroelectric Fluid

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Abstract

Ferroelectric fluid is a colloidal suspension of ferroelectric grains, i.e. electrical counterpart of ferrofluids. In order to discuss the dynamics of ferrolectric particle suspended in homogeneous fluid, continuous time random walk theory has been implemented in this article. We are considering external field is giving delta-kicks to the stochastic particles of the medium. Translation and rotation in time domain has been studied. Dynamic frequency response has also been developed. Fokker-Planck equations of rotation and translation have also been solved numerically, correlation functions calculated and a comparative study between these two theories has also been demonstrated.[1]

Keywords—Ferrofluid, Autocorrelation, Brownian Dynamics, Fokker-Planck, Langevin approach

1 Introduction

A ferroelectric fluid is a colloidal suspension of ferroelectric particles dispersed in a solvent with the help of surfactant. For the stability of such dispersions[1, 2] aggregation must be avoided and the attractive Van-der-Waals forces must be counterbalanced by steric or electrostatic repulsive forces. Each particle of a ferroelectric fluid possesses a permanent electric dipole moment so that the ferroelectric colloids have much in common with dipolar[2, 10, 11] liquids.

In order to discuss our problem relating to the dynamics of a ferroelectric fluid, by comparing ferrofluids (colloidal suspension of ferromagnetic particles) , we at first consider a particle under the influence of collisions or δ kicks from the particles of the medium , due to their Brownian motion. Under this circumstance the particle under consideration can have only two types of motion ; displacement and rotation. Here

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we try to apply the principle of Continuous Time Random Walk (CTRW) to this case in order to treat the problem at hand (i.e. to find the position and final spin/ magnetization of the particle after time t)[1, 2, 3, 4, 5].

Firstly we make some assumptions , we take that each collision changes the position of the particle by an amount either in the positive or the negative x direction(i.e. we consider only the one dimensional displacement of the particle.) . This is similar to the basic CTRW idea to regard the stochastic process as a chain made up of primary events or collisions , in a generalized sense. The process s viewed as an ongoing renewal of a stochastic sequence. The strategy is to break up the time interval (0,t) into sub intervals specified by the points t_1,t_2,t_3,. . .,t_n at which the system is assumed to be subject to certain events or collisions or δ-kicks as in this case. The situation is schematically shown below.

Also we treat the spin independently of the displacement . i.e. we try to go for the decoupled approach[8]. The justification behind this is that the rotational transition of the particle between two spin states has such a fast process that upon comparison with the process of displacement it can be treated as an instantaneous event. In our consideration a spin change operator changes the spin between up (+1) and down(-1) states. Strictly speaking here we have made another assumption. If we consider the particle as an extended rigid body then the rotation should be continuous but in our model we take the particle such that the time it takes to reorient itself from $\theta = 0$ to $\theta = \pi$ or from $\theta = \pi$ to $\theta = 0$ is much much smaller in comparison to he time it remains in one of its equilibrium positions ($\theta = 0$ or $\theta = \pi$) (viz. similar to the superparamagnetic relaxation phenomena[1]). Thus allowing us to treat the process of spin change as an instantaneous jump process and also preparing the way for the application of the Two-level Jump Process (TJP) to our problem at hand both for the spin and the displacement part since we are going for the decoupled approach[12].

2 Theoretical framework

Two collsion operators, denoted by $\hat{\mathbf{D}}(x)$ and $\hat{\mathbf{S}}(\theta)$ are operating on ferroelectric fluid particle causing translation and in rotation respectively. Translation and rotation are delta-kicked process as in CTRW. (i) No collision term: The conditional probability

Figure 1: Schematic diagram of TJP

for this event is $\delta(x_0 - x_1)exp(-\lambda t)$ This comes from the fact that for a poisson process, $exp(-\lambda t)$ measures the probability of no collision in time t.Where λ is the mean pulse rate.So the corresponding operator would be $\mathbf{1}exp(-\lambda t)$.

$$P = \delta(x_0 - x_1)\delta(\theta_0 - \theta_1)exp(-\lambda t) \quad (1)$$

(ii) Single collision term: Here the probability is that a collision occurs at time t_1 in the interval $(t_1, t_1 + dt_1)$ which is multiplied by the probability that no further collision occurs between t_1 and t

$$P = \int_0^t exp[-\lambda(t - t_1)]\lambda dt_1(x, \theta|\hat{\mathbf{J}}|x_0, \theta_0)exp(-\lambda t_1) \tag{2}$$

where $\hat{\mathbf{J}} = \hat{\mathbf{D}}\hat{\mathbf{S}}$ which gives

$$\begin{aligned} P &= \int_0^t exp[-\lambda(t - t_1)]\lambda dt_1(x, \theta|\hat{\mathbf{D}}\hat{\mathbf{S}}|x_0, \theta_0) \\ &\quad \times exp(-\lambda t_1) \end{aligned} \tag{3}$$

(iii)Two collision term: The conditional probability for this event is

$$\begin{aligned} P &= \sum_{x_1} \int_0^t dt_2 \int_0^{t_2} dt_1 exp[-\lambda(t - t_2)]\lambda(x, \theta|(\hat{\mathbf{D}}\hat{\mathbf{S}})|x_1, \theta_1) \\ &\quad \times exp[-\lambda(t_2 - t_1)\lambda(x_1, \theta_1|(\hat{\mathbf{D}}\hat{\mathbf{S}})|x_0, \theta_0) \end{aligned} \tag{4}$$

(iv)n- colliion term: We can see now that the conditional probability for n-collisional events is

$$\begin{aligned} P &= \sum_{x_1,\theta_1 x_2,\theta_2,x_3,\theta_3,\ldots,x_{n-1},\theta_{n-1}} \int_0^t dt_n \int_0^{t_n} dt_{n-1}\ldots \\ &\quad \times \int_0^{t_2} dt_1 exp[-\lambda(t - t_n)]\lambda \\ &\quad \times (x, \theta|(\hat{\mathbf{D}}\hat{\mathbf{S}})|x_{n-1}, \theta_{n-1}) \end{aligned} \tag{5}$$

So the collision probability operator has the form

$$\hat{\mathbf{P}}(\mathbf{t}) = \sum_{n=0}^{\infty} f_n(t)(\hat{\mathbf{D}}\hat{\mathbf{S}})^n \tag{6}$$

2.1 APPLICATION OF TJP FOR DISPLACEMENT

The simplest Stationary Markov Process is the TJP.Here the stochastic variable x is a stepwise constant process which jumps between two discrete values $x_0$and $-x_0$ with equal probability (ref fig.)

It can be shown that the collision matrix $\hat{\mathbf{J}}$ for such a TJP is given by $\hat{\mathbf{J}} = \hat{\mathbf{D}}\hat{\mathbf{S}}$ where

$$\hat{\mathbf{S}} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \tag{7}$$

also

$$\hat{\mathbf{D}} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \tag{8}$$

$\hat{\mathbf{J}}$ here is an idempotent matrix (this property helps us to construct the conditional probability matrix) $\mathbf{P}(\hat{\mathbf{t}})$.

$$\hat{\mathbf{P}}(\mathbf{t}) = exp[\lambda(\hat{\mathbf{J}} - \mathbf{1})t] \tag{9}$$

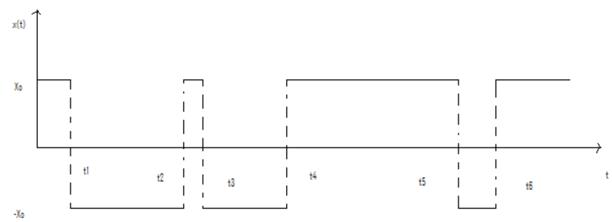

Figure 2: Schematic diagram of TJP

Hence using a direct power series expansion and the property that $\hat{\mathbf{J}}$ is an idempotent matrix we obtain

$$\begin{aligned} \hat{\mathbf{P}}(\mathbf{t}) &= exp(-\lambda t)[\mathbf{1} - \hat{\mathbf{J}} + \sum_{k=0}^{\infty}((\lambda t)^k/k!)\hat{\mathbf{J}}] \\ &= exp(-\lambda t)[\mathbf{1} - \hat{\mathbf{J}} + \hat{\mathbf{J}}exp(\lambda t)] \end{aligned} \tag{10}$$

Which gives with some simple algebra

$$\hat{\mathbf{P}}(\mathbf{t}) = \begin{pmatrix} 1 & 1 - exp(-\lambda t) \\ 1 - exp(-\lambda t) & 1 \end{pmatrix} \tag{11}$$

We work in a 2 dim vector space spanned by the orthonormal set $|n)$ with the matrix representation

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{12}$$

$$|2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{13}$$

The fluctuating variable x may then be regarded as an operator $\hat{\mathbf{X}}$whose matrix is diagonal in the above representation

$$\hat{\mathbf{X}} = \begin{pmatrix} x_0 & 0 \\ 0 & -x_0 \end{pmatrix} \tag{14}$$

average value of x in the stationary state is

$$< x(0)x(t) >= \sum_{n,m=1}^{2} p_n(n|\hat{\mathbf{X}}|n) = 0 \tag{15}$$

where $p_n = 1/2$
and the autocorrelation of x is given by

$$< x(0)x(t) >= \sum_{n,m=1}^{2} p_n(n|\hat{\mathbf{X}}|n)(m|\mathbf{P}\hat{(\mathbf{t})}|n)(m|\hat{\mathbf{X}}|m) \tag{16}$$

which is calculated to be

$$< x(0)x(t) >= {x_0}^2 exp(-\lambda t) \tag{17}$$

also

$$< x^2 >= \sum_{n=1}^{2} p_n(n|\hat{\mathbf{X}}^2|n) = x_0^2 \tag{18}$$

So eqn(17) can be recast into the form

$$< x(0)x(t) >=< x^2 > exp(-\lambda t) \tag{19}$$

Now the correlation time τ_c of this stochastic process is given by

$$\tau_c = (1/ < x^2 >) \int_0^\infty dt < x(0)x(t) >= 1/\lambda \tag{20}$$

2.2 APPLICATION OF TJP FOR ROTATION

As seen in the magnetization of a superparamagnetic material the magnetic enregy of the particle has its origin in the anisotropy energy of the particles. We can assume that our case of ferrofluid particle is also quite similar to that model.So the application of the two level jump process (TJP) in this case will be analogous to that applied for a superparamagnetic relaxation phenomena.
Here the stochastic variable at hand is the angle of rotationθ.Which has the matrix representation of the operator as $\hat{\theta}$

$$\hat{\theta} = \begin{pmatrix} \theta_0 & 0 \\ 0 & -\theta_0 \end{pmatrix} \tag{21}$$

applying a similar treatment as we did in the case of displacement we have the following results

$$\begin{aligned} < \theta > &= 0 & (22)\\ < \theta^2 > &= {\theta_0}^2 & (23)\\ < \theta(0)\theta(t) > &= {\theta_0}^2 exp(-\lambda t) & (24) \end{aligned}$$

Since

$$\mu = V M_0 cos\theta \tag{25}$$

thus we have

$$\begin{aligned} < \mu > &= 0 & (26)\\ < \mu^2 > &= {\theta_0}^2 V^2 M_0^2 & (27)\\ < \mu(0)\mu(t) > &= {\theta_0}^2 V^2 M_0^2 exp(-\lambda t) & (28) \end{aligned}$$

We know the linear response to a constant magnetic field along Z is given by the response function

$$\begin{aligned} \psi(t) &= \beta(< \mu^2 > - < \mu(0)\mu(t) >) \\ &= \beta {\theta_0}^2 V^2 M_0^2 [1 - exp(-\lambda t)] \end{aligned} \tag{29}$$

On the other hand, the relaxation function is obtained from the response correlation function for generalized susceptibility

$$\psi_{AB}(t) = \phi_{AB}(t=0) - \phi_{AB}(t) \tag{30}$$

to be

$$\begin{aligned} \phi(t) &= \psi(t=\infty) - \psi(t) \\ &= \beta{\theta_0}^2 V^2 M_0^2 exp(-\lambda t) \end{aligned} \tag{31}$$

Finally the frequency-dependent response is derived by substituting equation (29) into equation (30)[1] :

$$\chi(\omega) = \beta{\theta_0}^2 V^2 M_0^2 \lambda(\lambda - i\omega)^{-1} \tag{32}$$

which can be written in the alternative form

$$\chi(\omega) = \beta{\theta_0}^2 V^2 M_0^2 \lambda(1 - i\omega\tau)^{-1} \tag{33}$$

3 Rotation translation coupling and Fokker Planck approach

Rotation and translational dynamics of ferrofluid can also be portrayed by means of Fokker Planck Equation. Two state Brownian motion will be enough to discuss a simplistic model with such external delta kicks as described earlier. The initial coupled distribution (rotation as well as translation) will be $\delta(x_0 - x_1)\delta(\theta_0 - \theta_1)$ (as no collision term at t=0 in previous section). When distribution spreads in absence of any potential, that will follow

$$\begin{aligned} P(x,\theta,t) &= P_{rot}(\theta,t)P_{trans}(x,t) \\ &= \frac{1}{2\pi\sqrt{D_x D_\theta}} exp\left(-\frac{(x_0 - x)^2}{2D_x}\right) \\ &\quad \times exp\left(-\frac{(\theta_0 - \theta)^2}{2D_\theta}\right) exp(-\lambda t) \end{aligned} \tag{34}$$

The corresponding Fokker-Planck equation is given by

$$\frac{\partial P_\theta}{\partial t} = -\frac{\partial}{\partial \theta}[F_0 f(\theta)\delta_T(t)P_\theta] + D_0\frac{\partial^2 P}{\partial \theta^2} \tag{35}$$

$$\frac{\partial P_x}{\partial t} = -\frac{\partial}{\partial x}[F_0 \phi(x)\delta_T(t)P_x] + D_0\frac{\partial^2 P}{\partial x^2} \tag{36}$$

Now $V_1\phi(\theta)$ is rotational potential
and $V_2\phi(x)$ is the translational potential
also

$$f(\theta) = \frac{\partial V_1}{\partial \theta} \tag{37}$$

$$f(\theta) = \frac{\partial V_2}{\partial x} \tag{38}$$

Suppose rotational potential is harmonic potential

$$f(\theta) = -\frac{\partial V(\theta)}{\partial \theta} = k\theta \tag{39}$$

We consider the rotational potential to be ratchet potential.

$$\phi(x) = cos(kx) \tag{40}$$

so the Fokker-Planck equation (FPE) for rotational motion is

$$\frac{\partial P_\theta}{\partial t} = -\frac{\partial}{\partial \theta}[kF_0\theta\delta_T(t)P_\theta] + D_0\frac{\partial^2 P}{\partial \theta^2} \tag{41}$$

Now as we are considering external force is giving aperiodic delta kicks to the ferrofluid particle [5, 6]

$$\begin{aligned} \delta_T(t) &= \sum_{n=-\infty}^{\infty}\delta(t-\eta T) \\ &= \frac{1}{T} + \frac{2}{T}\sum_{m=1}^{\infty}cos(\frac{2\pi mt}{T}) \end{aligned} \tag{42}$$

where T is the period of the external force. Therefore the equations are

$$\frac{\partial P_\theta}{\partial t} = -\frac{\partial}{\partial \theta}[kF_0\theta\delta_T(t)P_\theta] + D_{0\theta}\frac{\partial^2 P}{\partial \theta^2} \tag{43}$$

$$\frac{\partial P_x}{\partial t} = -\frac{\partial}{\partial x}[F_0cos(kx)\delta_T(t)P_x] + D_{0x}\frac{\partial^2 P}{\partial x^2} \tag{44}$$

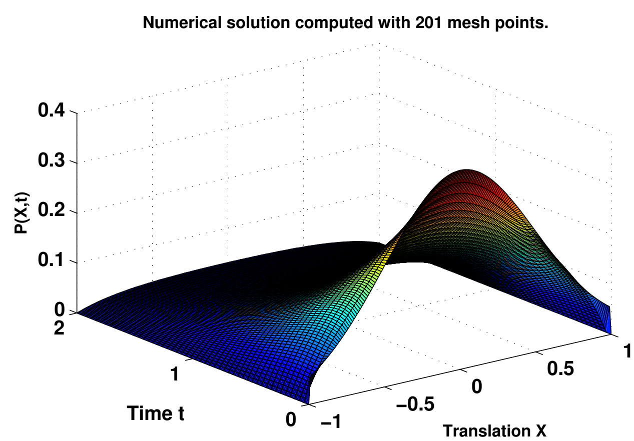

Figure 3: Numerical simulation of the probability with 201 mesh points

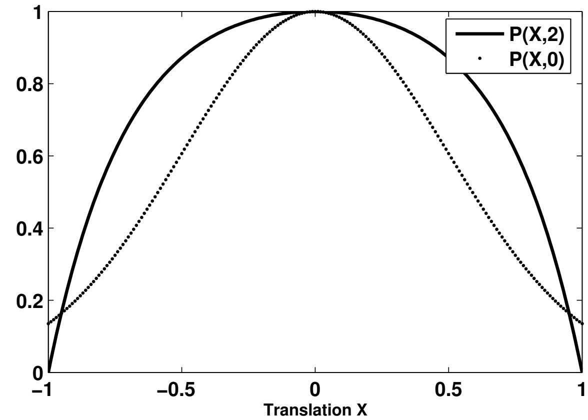

Figure 4: Translational probability at t=2 and t=0

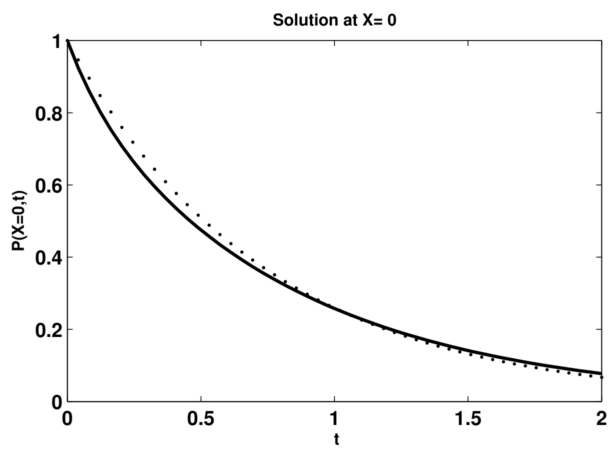

Figure 5: Solid line indicates Translational Probability at x=0 and dotted line is according to CTRW

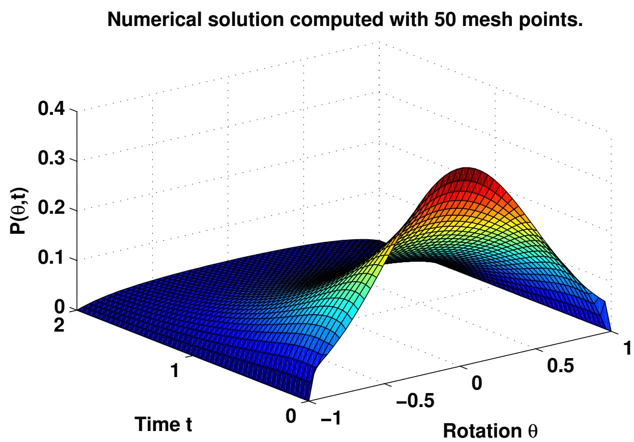

Figure 6: Numerical simulation of the probability with 50 mesh points

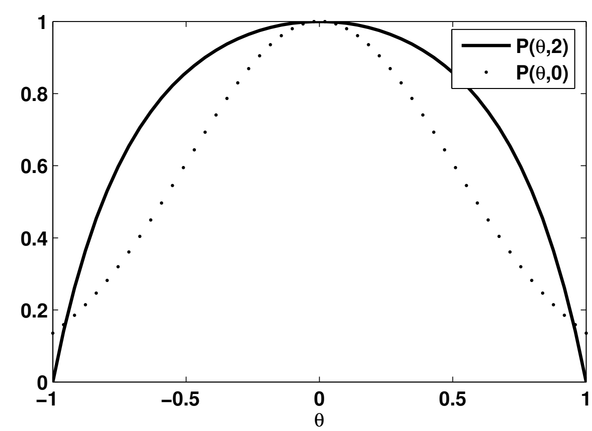

Figure 7: Rotational probability at t=2 and t=0

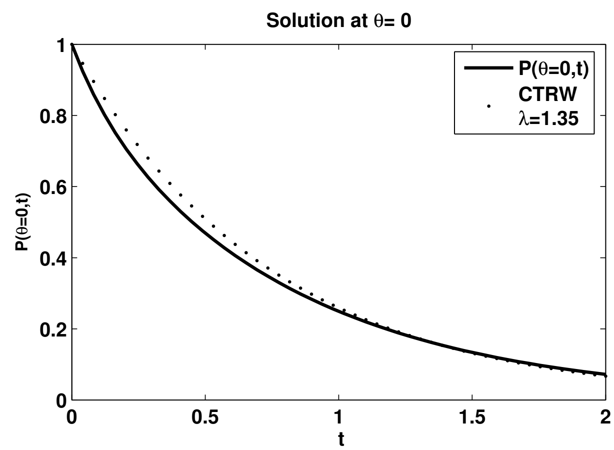

Figure 8: Solid line indicates Rotational Probability at x=0 and dotted line is according to CTRW

where $D_{0\theta}$ and D_{0x} are the rotational[3, 7] and the translational diffussion coefficient respectively.By solving the above stochastic differential equations with initial condition we can get the probabilities $P(\theta, t)$,$P(x, t)$ and study their variation with time and with θ and x respectively.These results have been graphically depicted in Figs. 3,4,5,6 and 7.

4 Rotation and translation: Langevin aproach

Rotation and translational dynamics of ferro-fluid can be portrayed by means of Langevin Equation as well.We persist our discussion with the two state Brownian motion which would be a simplistic model with such external delta kicks as described earlier.

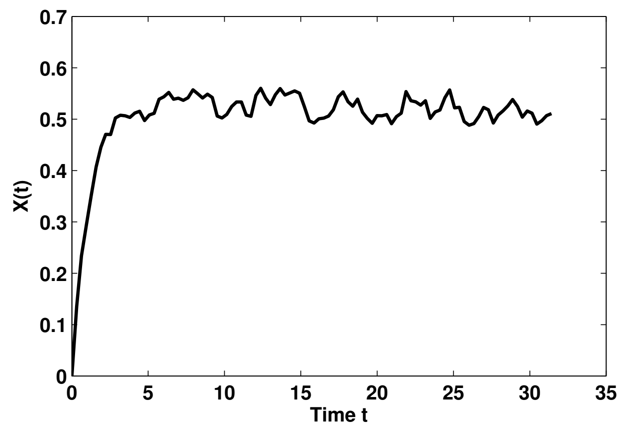

Figure 9: Translation in time

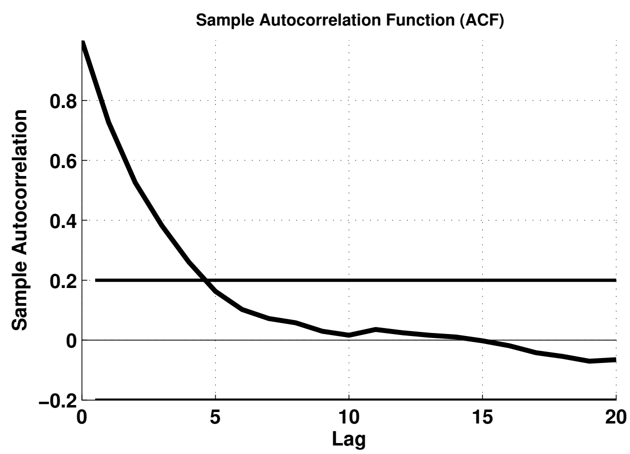

Figure 10: Sample temporal autocorrelation of translation

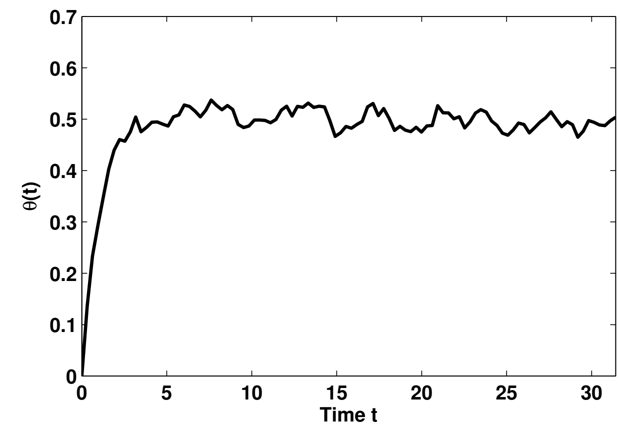

Figure 11: Rotation in time

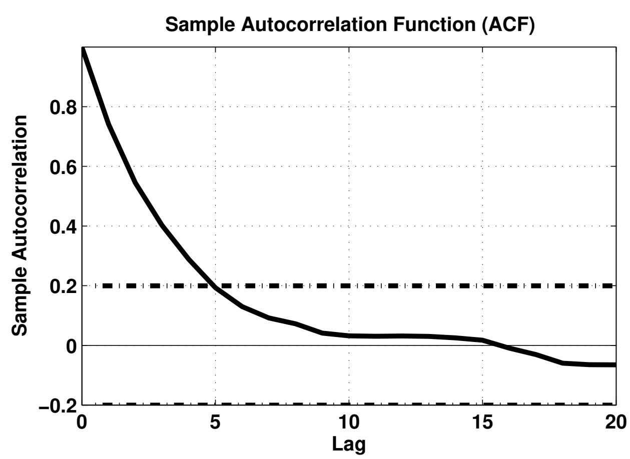

Figure 12: Sample temporal auto-correlation of rotation

The initial coupled distribution (rotation as well as translation) will be $\delta(x_0 - x_1)\delta(\theta_0 - \theta_1)$ (as no collision term at t=0 in previous section). When distribution spreads in absence of any potential, that will follow

$$\begin{aligned} P(x,\theta,t) &= P_{rot}(\theta,t)P_{trans}(x,t) \\ &= \frac{1}{2\pi\sqrt{D_x D_\theta}} exp\left(-\frac{(x_0 - x)^2}{2D_x}\right) \\ &\quad \times exp\left(-\frac{(\theta_0 - \theta)^2}{2D_\theta}\right) exp(-\lambda t) \end{aligned} \tag{45}$$

The corresponding Langevin equation for a thermal bath at temperature T is given by

$$\frac{\partial x}{\partial t} = -\frac{\partial V(x,\theta)}{\partial x} + \lambda_1 \xi_x(t) + F_x(t) \tag{46}$$

$$\frac{\partial \theta}{\partial t} = -\frac{\partial V(x,\theta)}{\partial \theta} + \lambda_2 \xi_\theta(t) + F_\theta(t) \tag{47}$$

Where ξ_x and ξ_θ are Gaussian white noise for translation and rotation respectively and $F_x(t)$ and $F_\theta(t)$ are the external force (delta kick) for translation and rotation respectively. Now $V_1\phi(\theta)$ is rotational potential
and $V_2\phi(x)$ is the translational potential
also

$$f(\theta) = \frac{\partial V_1}{\partial \theta} \tag{48}$$

$$f(\theta) = \frac{\partial V_2}{\partial x} \tag{49}$$

Suppose rotational potential is harmonic potential

$$f(\theta) = -\frac{\partial V(\theta)}{\partial \theta} = k_2\theta \tag{50}$$

Now the potential $V(x,\theta)$ is of the form
$V(x,\theta)$ =Ratchet Potential for translation + harmonic potential for rotation

$$V(x) = \cos(k_1 x) \tag{51}$$

$$V(\theta) = \frac{1}{2}k_2\theta^2 \tag{52}$$

Now as we are considering external force is giving aperiodic delta kicks to the ferrofluid particle

$$\begin{aligned} \delta_T(t) &= \sum_{n=-\infty}^{\infty} \delta(t-\eta T) \\ &= \frac{1}{T} + \frac{2}{T}\sum_{m=1}^{\infty}\cos(\frac{2\pi m t}{T}) \end{aligned} \tag{53}$$

where T is the period of the external force.By solving the above stochastic differential equations with initial condition we can get $<\theta(0)\theta(t)>$, $<x(0)x(t)>$, and frequency response and susceptibility can be found [9].

5 Result and discussion

In this paper we have started with CTRW method to discuss rotational and translational motion of a analytically discuss the rotational and the translational motion of a ferrofluid particle analytically. Later on we have used the FPE and the Langevin Equation in order to analyze the dynamics using numerical methods to solve these equations. By solving Langevin's stochastic differential equation for both rotation and translation, we have computed the autocorrelation functions and relaxation time.

Resemblance has been found in both approach. CTRW was assumed as Poisson distribution in time, and Langevin equation has also show the same distribution with $\lambda =$. The whole study is quite satisfactory towards understanding the stochastic behavior of ferrofluid particles under delta kicks. In the end we have made a comparitive study between the analytical and the numerical approaches to solve the problem at hand. From figs 3 (and 6) we can understand both the variation of the translational (and rotational) probability with x (and θ)and also the evolution of the distribution with time.The fig 4 (and 7) show the Evolution of the Translational (and rotational) probability with time , here the initial poisson distribution(at t=0) is seen to be spreading out as time evolves.The fig 5 (and 8) give us the solutions at x=0 (and $\theta = 0$)as found out numerically from the FPE , the dotted lines represent our analytical results for $\lambda = 1.35$ the close matching of the two is worth noticing.Finally figures 9 and 11 represent the solutions for x (and θ) obtained numerically from the Langevin approach. We can see the initial transient growth followed by saturation which is of course accompanied by some thermal noise due to fluctuations in the thermal bath.In fig. 10 and 12 the autocorrelation function obtained from the Langevin approach has been depicted.

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