

A Study of Persistence in Different Non-Equilibrium Systems

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the degree of Doctor of Philosophy



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Certificate of Examination

This is to certify that the dissertation titled '*A Study of Persistence in different Non-Equilibrium systems*' submitted by Mr. Anirban Ghosh (Reg. No. PH14039) for the partial fulfillment of Doctor of Philosophy programme of the Institute, has been examined by the thesis committee duly appointed by the Institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

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Declaration

The work presented in this thesis has been carried out by me under the guidance of Dr. Dipanjan Chakraborty at the Indian Institute of Science Education and Research Mohali. This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bona fide record of original work done by me and all sources listed within have been detailed in the bibliography.

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In my capacity as the supervisor of the candidate's thesis work, I certify that the above statements by the candidate are true to the best of my knowledge.

Dr. Dipanjan Chakraborty

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कर्मण्येवाधिकारस्ते मा फलेषु कदाचन।
मा कर्मफलहेतुर्भूर्मा ते सङ्गोऽस्त्वकर्मणि॥

*karmany-evādhikāras te mā phaleṣhu kadāchana
mā karma-phala-hetur bhūr mā te saṅgo 'stvakarmaṇi*

*You have the right to work only but never to its fruits.
Let not the fruits of action be your motive, nor let your
attachment be to inaction.*

Shree Bhagvat Gita, Chapter 2 Verse 47

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Abstract

Considerable interest has been generated recently in understanding the statistics of first passage events in spatially extended non-equilibrium systems. A persistence probability $P(t)$, is defined as the probability that the position of the step edge at a point along a fluctuating step does not return to its initial value (at time $t = 0$) over time t is found in these studies to decay in time as a power-law, $P(t) \sim t^{-\theta}$, for large t , where θ is the so-called persistence exponent. Similar power-law behavior of the persistence probability has also been found in experiments for other physical processes. The persistence probability has been obtained both analytically and numerically for a large class of stochastic processes, Markovian as well as non-Markovian. For single particle systems such as the Brownian motion, which is also Markovian in nature, the persistence probability is easy to calculate since the stationary correlator of such a process decays exponentially at all times. For many body systems where the field ϕ has a space dependence, the calculation of the zero crossing probability becomes complicated.

In the first part (Chapter 2 and Chapter 3) of the thesis, we investigate the persistence probability $p(t)$ of the position of a Brownian particle with shape asymmetry in two dimensions. We explicitly consider two cases diffusion of a free particle and that of a harmonically trapped particle. The latter is particularly relevant in experiments that use trapping and tracking techniques to measure the displacements. We provide analytical expressions of $p(t)$ for both the scenarios and show that in the absence of shape asymmetry, the results reduce to the case of an isotropic particle. The analytical expressions of $p(t)$ are further validated against a numerical simulation of the underlying overdamped dynamics. We also illustrate that $p(t)$ can be a measure to determine the shape asymmetry of a colloid and the translational and rotational diffusivities can be estimated from the measured persistence probability. The advantage of this method is that it does not require the tracking of the orientation of the particle.

In the second part of the work Chapter 4, we have studied the persistence of the active asymmetric rigid Brownian particle in two dimensions. Nowadays self-propelled systems are an interesting topic of research. Active matter systems are any systems either of biological or artificial origin where the individual components can take up energy from their environment and use it to move automatically. The energy they consume helps them to perform the task of self-movement. These types of systems form patterns and exhibit several interesting properties. We have studied the persistence of such active asymmetric free particle and that in a harmonic trap. We have calculated

the analytical expressions of the persistence and thereafter validated those analytical expressions with numerical simulations.

In the third part of the work Chapter 5, we study the persistence probability $p(t)$ of stochastic models of surface growth that are restricted by finite system size. Surface growth is an important stochastic phenomenon that is found in a large class of physical systems ranging from a few nanometers to a few micrometers. That is why this process is of so much interest to study its persistence for finite-size lattice. We look at two specific models of surface growth - the linear Edwards-Wilkinson(EW) model and the non-linear Kardar-Parisi-Zhang(KPZ) model. In this chapter, we have analytically studied the persistence of the finite-size system.

1

Introduction

A brief introduction of the concept of persistence probability for the stochastic processes has been presented in this chapter. The discussion includes the description of the stochastic process, Fokker-Planck equation, Langevin formalism, and basic concept of the persistence probability. In addition to that, results of persistence probability of a few non-equilibrium systems which were calculated earlier by other researchers, have also been included in this chapter. Basically, this chapter speaks the basics of the whole findings.

A stochastic or random variable is a quantity X , defined by a set of possible values $\{x\}$, and a probability distribution on this set. Let us consider an example of dice; after each throw, the number in the upper face corresponds to variable X , with possible outcomes $x = \{1, 2, 3, 4, 5, 6\}$ and probabilities of each side is $p = \frac{1}{6}$ (for an unbiased dice) for each value of x . The set of possible outcomes (range or set of states) could be discrete, or continuous, finite or infinite. If the range is discrete (as for the case of dice), the probability distribution will be given by a set of non-negative numbers $\{p_n\}$, such that $\sum p_n = 1$.

When the range corresponds to an interval $[a, b]$ over the x -axis, the probability distribution is determined by a non-negative function $P(x)$, with $P(x)dx$ the probability of $X \in [x, x + dx]$, and such that,

$$\int_a^b dx P(x) = 1 \quad (1.1)$$

This function is called probability density, and the possibility that it contains one or more delta-like contributions, should not be discarded. As a matter of fact, a discrete distribution may be written as a continuous one, but only composed of delta contributions.

Every quantity which is dependent on any stochastic variable is also a stochastic variable. In any mathematical object, if we add an auxiliary variable t , and we get $Y = f(x, t)$. t could be the time or some other parameter. Such $Y(t)$ is called a stochastic process. It could be considered as a set of functions or realizations $y(t) = f(x, t)$, each one obtained when we fix X in one of its possible values. Let X be a stochastic variable defined on the range $(-\infty, +\infty)$ and the distribution $P(x)$. The average of the function $f(x)$ over the distribution is,

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} dx f(x) P(x) \quad (1.2)$$

The moment of the variable X can be defined as,

$$\mu_m = \langle X^m \rangle = \int_{-\infty}^{+\infty} dx x^m P(x) \quad (1.3)$$

Let us introduce characteristic function,

$$G(k) = \langle e^{i\mathbf{k}\cdot\mathbf{x}} \rangle = \int_{-\infty}^{+\infty} dx e^{i\mathbf{k}\cdot\mathbf{x}} P(x) \quad (1.4)$$

The moment generating function is,

$$G(k) = \sum \frac{(ik)^m}{m!} \mu_m \quad (1.5)$$

where,

$$\mu_m = (-i)^m \frac{\partial^m}{\partial k^m} G(k=0) \quad (1.6)$$

Another quantity cumulant κ_m is defined as,

$$\ln[G(k)] = \sum \frac{(ik)^m}{m!} \kappa_m = \ln \left[\sum \frac{(ik)^m}{m!} \mu_m \right] \quad (1.7)$$

The first cumulant is the same as the first moment of the stochastic variable $\kappa_1 = \mu_1 = \langle x \rangle$, this is the mean of the variable. The second cumulant is, $\kappa_2 = \mu_2 - \mu_1^2 = \sigma^2$, that is called variance.

We extend all these notions for several variables as well. Considering $X = (x_1, x_2, \dots, x_n)$, with a probability distribution $P(x_1, x_2, \dots, x_n)$, also called joint probability distribution. It gives the probability that the set of variables have their values within $(x_1, x_1 + dx_1)$ and $(x_2, x_2 + dx_2)$ etc. Defining moments of this quantity,

$$\langle X_1^\mu X_2^\nu \dots X_n^\eta \rangle = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} dx_1 dx_2 \dots dx_n x_1^\mu x_2^\nu \dots x_n^\eta P(x_1, x_2, \dots, x_n) \quad (1.8)$$

In terms of moments, the generating function can be expressed as,

$$G(k) = \langle e^{ikx} \rangle = \sum_{\mu} \sum_{\nu} \dots \sum_{\eta} \frac{(ik)^\mu}{\mu!} \frac{(ik)^\nu}{\nu!} \dots \frac{(ik)^\eta}{\eta!} \langle X_1^\mu X_2^\nu \dots X_n^\eta \rangle \quad (1.9)$$

Correspondingly, in terms of generalized cumulants, it is,

$$G(k) = \exp \left\{ \sum_{\mu} \sum_{\nu} \dots \sum_{\eta} \frac{(ik)^\mu}{\mu!} \frac{(ik)^\nu}{\nu!} \dots \frac{(ik)^\eta}{\eta!} \kappa_{\mu} \kappa_{\nu} \dots \kappa_{\eta} \right\} \quad (1.10)$$

1.2 Stochastic Differential Equation

One of the most natural, and most important, stochastic differential equations is given by,

$$\begin{aligned} \dot{X}(t) &= bX(t) + B(X(t))\xi(t) \\ X(0) &= x_0 \end{aligned} \quad (1.11)$$

where B is a function of $X(t)$ ($m \times n$ dimensional matrix) and $\xi = m$ -dimensional "white noise".

Let us make a study Eq.(1.11) in the case for $m = n$, $x_0 = 0$, $b = 0$, and $B \equiv I$. The solution becomes an n -dimensional Brownian motion, denoted by W . Therefore a Brownian motion can be denoted as,

$$\dot{W}(\cdot) = \xi(\cdot)$$

So we can easily assert that "white noise" is the time derivative of Brownian motion.

The general form of Eq.(1.11) becomes,

$$\frac{dX(t)}{dt} = bX(t) + BX(t) \frac{dW(t)}{dt} \quad (1.12)$$

formally multiplying the above equation with 'dt',

$$\begin{aligned} dX(t) &= bX(t)dt + B(X(t))dW(t) \\ X(0) &= x_0 \end{aligned} \quad (1.13)$$

The terms " dX " and " BdW " are called stochastic differentials, and the expression is called as a Stochastic Differential Equation. We can find the solution for all $t > 0$ as,

$$X(t) = x_0 + \int_0^t b(X(s))ds + \int_0^t B(X(s))dW \quad (1.14)$$

Let us assume $n = m = 1$ and $X(t)$ solves the SDE,

$$dX = b(X)dt + dW \quad (1.15)$$

Suppose there is a given smooth function $u = u(x)$. Stochastic differential equation becomes (when $t \geq 0$),

$$Y(t) = u(X(t)) \quad (1.16)$$

Using this Eq.(1.16) in Eq.(1.15), we get

$$dY = u' dX = u' b dt + u' dW \quad (1.17)$$

If we compute dY and keep all terms of order dt or $(dt)^{1/2}$, we get,

$$\begin{aligned} dY &= u' dX + \frac{1}{2} u'' (dX)^2 + \dots \\ &= u' (bdt + u' dW) + \frac{1}{2} u'' (bdt + dW)^2 + \dots \\ &= (u'b + \frac{u''}{2}) dt + u' dW \end{aligned} \quad (1.18)$$

By an analogy, it can be said $(dW)^2 = dt$. So

$$du(X) = (u'b + \frac{u''}{2}) dt + u' dW \quad (1.19)$$

The extra term " $\frac{u''}{2} dt$ " is not present in ordinary calculus. This is called chain rule or Ito's formula.

A stochastic differential equation is an Ordinary Differential equation, which is forced by an irregular stochastic process such as Gaussian noise. It is written as Stochastic differential and is interpreted according to Ito or Stratonovich Stochastic Integrals. Ito description of a stochastic integral is of the form $\int_{t_0}^t f(x(t'), t') dW(t')$ where $f(x(t), t)$ is any arbitrary function and $W(t)$ is a Wiener process, is written as,

$$\int_{t_0}^t f(x(t'), t') dW(t') = \lim_{n \rightarrow \infty} \sum_{i=1}^n f(x(t_{i-1}), t_{i-1}) [W(t_i) - W(t_{i-1})] \quad (1.20)$$

In the Stratonovich approach, the same stochastic integral has the form,

$$\int_{t_0}^t f(x(t'), t') dW(t') = \lim_{n \rightarrow \infty} \sum_{i=1}^n \frac{1}{2} [f(x(t_i), t_i) + f(x(t_{i-1}), t_{i-1})] [W(t_i) - W(t_{i-1})] \quad (1.21)$$

In the Ito Stochastic integral, the function f is evaluated first at the earlier time while in the Stratonovich approach, the function is averaged. The difference between the two approaches changes the form of the stochastic differential equation, the SDE of the form,

$$dx(t) = A(x, t) dt + B(x, t) dW \quad (1.22)$$

Ito description has the form,

$$dx(t) = \left[A(x, t) - \frac{1}{2} B(x, t) \frac{\partial B}{\partial x} \right] dt + B(x, t) dW \quad (1.23)$$

Conversely Stratonovich SDE of the form,

$$dx(t) = A'(x, t) + \frac{1}{2} B'(x, t) dW \quad (1.24)$$

is equivalent to the Ito SDE,

$$dx(t) = \left[A'(x,t) + \frac{1}{2} B'(x,t) \frac{\partial B'}{\partial x} \right] dt + B'(x,t) dW \quad (1.25)$$

In nonequilibrium statistical physics, Langevin SDE may be written as,

$$F(\ddot{\phi}, \dot{\phi}, \phi', \phi'', \phi) = \xi \quad (1.26)$$

1.3 Joint and Conditional Probabilities

We consider the concept $P(A \cap B)$, where $A \cup B$ is non-empty. An event ω that satisfies $\omega \in A$ will only satisfy $\omega \in A \cap B$ if $\omega \in B$ as well. Thus, $P(A \cap B) = P\{(\omega \in A) \text{ and } (\omega \in B)\}$, and $P(A \cap B)$ is called the joint probability, that the event ω is contained in both classes, or, alternatively, that both the events $\omega \in A$ and $\omega \in B$ occur. Joint probabilities occur naturally in two ways,

(a) When the event is specified by a vector e.g., m mice and n tigers. The probability of this event is the joint probability of [m mice (and any number of tigers)] and [n tigers (and any number of mice)]. All vector specifications are implicitly joint probabilities in this sense.

(b) When more than one time is considered; what is the probability that (at time t_1 there are m_1 tigers and n_1 mice) and (at time t_2 there are m_2 tigers and n_2 mice). To consider such a probability, we have effectively created out of the events at time t_1 and events at time t_2 , joint events involving one event at each time. In essence, there is no difference between these two cases except for the fundamental dynamical role of time.

We may specify a condition on the events we are interested in, and consider only these e.g. the probability of 21 deer given that we know there are 100 tigers. We will be interested only in those events contained in the set $B = \{\text{all events where exactly 100 tigers occur}\}$. This means that we define conditional probabilities, which are defined only on the collection of all sets contained in B . We define the conditional probability as,

$$P(A|B) = \frac{P(A \cap B)}{P(B)} \quad (1.27)$$

and this satisfies our intuitive conception that the conditional probability that $\omega \in A$ (given that we know $\omega \in B$), is given by dividing the probability of joint occurrence by

the probability of $\omega \in B$. We can define in both directions i.e. we have,

$$P(A \cap B) = P(A/B)P(B) = P(B/A)P(A) \quad (1.28)$$

There is no particular conceptual difference between say, the probability of {(21 deers) gives (100 tigers)} and the reversed concept. However, when two times are involved, we do see a difference. For example, the probability that a particle is at position x_1 at time t_1 , given that it was at x_2 at the previous time t_2 . The converse sounds strange, i.e the probability that a particle is at position x_1 at time t_1 , given that it will be at position x_2 at a later time t_2 .

Let us have a stochastic process $Y(t)$. We write,

$$P_n(y_1, t_1; y_2, t_2; \dots, y_n, t_n) dy_1 dy_2 \dots dy_n$$

for the probability that $Y(t_1)$ is within the interval $(y_1, y_1 + dy_1)$, $Y(t_2)$ in $(y_2, y_2 + dy_2)$, and so on. These P_n may be defined for $n = 1, 2, \dots$ and only for different times. This hierarchy has the following properties,

(a) $P_n \geq 0$

(b) P_n is invariant under permutations of pair (y_i, t_i) and (y_j, t_j) (c) $\int dy_n P_n = P_{n-1}$ and $\int dy_1 P_1 = 1$

According to the theorem due to Kolmogorov, it is possible to prove that the inverse is also true. Stochastic process are those sets of functions that satisfy the above conditions. An alternative characterization of the stochastic processes through the hierarchy of moments,

$$\mu_n(t_1, t_2, \dots, t_n) = \langle Y(t_1)Y(t_2)\dots Y(t_n) \rangle = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} dy_1 dy_2 \dots dy_n y_1 y_2 \dots y_n P_n(y_1, t_1; y_2, t_2; \dots; y_n, t_n) \quad (1.29)$$

Another very important quantity is the conditional probability density $P_{n/m}$, which corresponds to the probability of having the value y_1 at time t_1 , y_2 at time t_2, \dots, y_n at time t_n , provided that we have $Y(t_{n+1}) = y_{n+1}, Y(t_{n+2}) = y_{n+2}, \dots, Y(t_{n+m}) = y_{n+m}$, it has definition,

$$P_{n/m}(y_1, t_1; \dots; y_n, t_n | y_{n+1}, t_{n+1}; \dots; y_{n+m}, t_{n+m}) = \frac{P_{n+m}(y_1, t_1; \dots; y_n, t_n; y_{n+1}, t_{n+1}; \dots; y_{n+m}, t_{n+m})}{P_m(y_{n+1}, t_{n+1}; \dots; y_{n+m}, t_{n+m})}$$

For a stochastic process $Y(t)$, the conditional probability $P_{1/1}(y_2, t_2 | y_1, t_1)$ is the probability that $Y(t_2)$ has the value of y_2 , provided $Y(t_1)$ has taken the value of y_1 . In terms of this quantity one can express P_2 as,

$$P_2(y_1, t_1; y_2, t_2) = P_1(y_1, t_1) P_{1/1}(y_2, t_2 | y_1, t_1)$$

To construct the higher order P_n , we need transition probabilities $P_{n/m}$ of higher order, e.g. $P_3(y_1, t_1; y_2, t_2; y_3, t_3) = P_2(y_1, t_1; y_2, t_2) P_{1/2}(y_3, t_3 | y_1, t_1; y_2, t_2)$. A stochastic process is called Markov process, if for any set of n successive times $t_1 < t_2 < \dots < t_n$, one has,

$$P_{1/n-1}(y_n, t_n | y_1, t_1; \dots; y_{n-1}, t_{n-1}) = P_{1/1}(y_n, t_n | y_{n-1}, t_{n-1})$$

Physically speaking, the conditional probability distribution of y_n at t_n , given the value y_{n-1} at t_{n-1} is uniquely determined and is not affected by any knowledge of the values earlier times. A Markov process is determined by the two distributions $P_1(y, t)$ and $P_{1/1}(y', t' | y, t)$, from which the entire hierarchy $P_n(y_1, t_1; \dots; y_n, t_n)$ can be constructed. For instance, consider $t_1 < t_2 < t_3$; P_3 can be written as,

$$\begin{aligned} P_3(y_1, t_1; y_2, t_2; y_3, t_3) &= P_2(y_1, t_1; y_2, t_2) P_{1/2}(y_3, t_3 | y_1, t_1; y_2, t_2) \\ &= P_2(y_1, t_1; y_2, t_2) P_{1/1}(y_3, t_3 | y_2, t_2) \\ &= P_1(y_1, t_1) P_{1/1}(y_2, t_2 | y_1, t_1) P_{1/1}(y_3, t_3 | y_2, t_2) \end{aligned} \quad (1.30)$$

The single-time-step memory characterizing a Markov process is equivalent to saying that the future state of the process is only dependent on its present state, and not on the history of how the process reached the present state. It implies at once that all the joint PDF of a Markov process are expressible as products of just two independent PDFs as single-time $P_1(y, t)$ and a two-time conditional PDF $P_{1/1}(y, t | y', t')$ (where $t' < t$) according to,

$$\begin{aligned} P_n(y_n, t_n; y_{n-1}, t_{n-1}; \dots; y_1, t_1) &= P_{1/1}(y_n, t_n | y_{n-1}, t_{n-1}) \times P_{1/1}(y_{n-1}, t_{n-1} | y_{n-2}, t_{n-2}) \times \dots \\ &\quad \times P_{1/1}(y_2, t_2 | y_1, t_1) P_1(y_1, t_1) \end{aligned} \quad (1.31)$$

The Markov process is stationary, then $P_1(y, t) = P(y)$ and $P_{1/1}(y, t | y', t') = P_{1/1}(y, t - t' | y')$ (a function of the difference $(t - t')$).

1.5

Ornstein-Uhlenbeck Process

It is defined in the region $-\infty < y < +\infty$, $-\infty < t < +\infty$ and $(t_2 - t_1) = \tau > 0$ through,

$$P_1(y, t) = [2\pi]^{-1/2} \exp\{-y^2/2\} \quad (1.32)$$

$$P(y_2, t_2 | y_1, t_1) = [2\pi(1 - e^{-2\tau})]^{-1/2} \exp\left\{-\frac{[y_2 - y_1 e^{-\tau}]^2}{2(1 - e^{-2\tau})}\right\}$$

This process defines the velocity of a Brownian particle and is also Gaussian. It is stationary as well, which means

$$P_n(y_1, t_1; \dots; y_n, t_n) = P_n(y_1, t_1 + \tau; \dots; y_n, t_n + \tau) \quad (1.33)$$

According to a theorem defined by Doob, it is the only simultaneously Markovian, Gaussian and stationary process.

The self-correlation function of this process is given by

$$\langle y(t_1)y(t_2) \rangle = \exp\{-|t_2 - t_1|\}$$

Let us put $Y(t) = aL(t)$, $t = b$, and take the limit $b \rightarrow \infty$ and $a \rightarrow \infty$, but in such a way that $2a^2/b \simeq 1$, we find,

$$\langle L(t_1)L(t_2) \rangle = \delta(t_1 - t_2) \quad (1.34)$$

This is called white noise or the Langevin process. Even if $L(t)$ is not a true stochastic process, its integral corresponds to the Wiener process.

1.6

Chapman-Kolmogorov Equation

Let us now derive an important identity that must be obeyed by the transition at any Markov process. On integrating over y_2 , it is obtained ($t_1 < t_2 < t_3$),

$$P_2(y_1, t_1; y_3, t_3) = P_1(y_1, t_1) \int dy_2 P(y_2, t_2 | y_1, t_1) P(y_3, t_3 | y_2, t_2) \quad (1.35)$$

Using Baye's rule,

$$\frac{P_2(y_1, t_1; y_3, t_3)}{P_1(y_1, t_1)} = P(y_3, t_3 | y_1, t_1) = \int dy_2 P(y_3, t_3 | y_2, t_2) P(y_2, t_2 | y_1, t_1) \quad (1.36)$$

This is called the Chapman-Kolmogorov equation. The time ordering is essential; t_2 must lie between t_1 and t_3 for this equation to hold. We can rewrite particular case $P_1(y_2, t_2) = \int dy P_2(y_2, t_2; y_1, t_1)$ of the relation among the distributions of the hierarchy as,

$$P_1(y_2, t_2) = \int dy_1 P(y_2, t_2 | y_1, t_1) P_1(y_1, t_1) \quad (1.37)$$

This is an additional relation involving the two probability distributions characterizing a Markov process.

1.7 Wiener-Levy Process

It can be defined that, in the range $-\infty < y < +\infty$ and $t \geq 0$, through

$$P_1(y, t) = [2\pi t]^{-1/2} \exp\{-y^2/2t\} \quad (1.38)$$

$$P(y_2, t_2 | y_1, t_1) = [2\pi(t_2 - t_1)]^{-1/2} \exp\left\{-\frac{[y_2 - y_1]^2}{2(t_2 - t_1)}\right\}$$

These functions very easily fulfill the Chapman-Kolmogorov equation. We can show the self-correlation function as,

$$\langle y(t_1)y(t_2) \rangle = \min(t_1, t_2) \quad (1.39)$$

This process defines the position of a Brownian particle in one dimension. It is categorized as a Gaussian process indicating that all P_n are Gaussian distributions.

1.8 The Master equation

The master equation is a differential equation for the transition probability. Chapman Kolmogorov equation for equal time arguments,

$$P(y_3, t_3 | y_1, t) = \int dy_2 P(y_3, t_3 | y_2, t) P(y_2, t | y_1, t) \quad (1.40)$$

where $P(y_2, t | y_1, t) = \delta(y_2 - y_1)$ which is the zeroth-order term in the short-time behavior of $P(y', t' | y, t)$. Short-time transition probability,

$$P(y_2, t + \Delta t | y_1, t) = \delta(y_2 - y_1)[1 - a^{(0)}(y, t)\Delta t] + W_t(y_2 | y_1)\Delta t + \mathcal{O}[(\Delta t)^2] \quad (1.41)$$

where $W_t(y_2 | y_1)$ is interpreted as the transition probability per unit time from y_1 to y_2 at time t . Then, the coefficient $[1 - a^{(0)}(y, t)\Delta t]$ is to be interpreted as the probability that no

transition takes place during Δt . From the normalization of $P(y_2, t_2 | y_1, t_1)$ one has,

$$1 = \int dy_2 P(y_2, t + \Delta t | y_1, t) \simeq 1 - a^{(0)}(y, t) \Delta t + \int dy_2 W_t(y_2 | y_1) \Delta t \quad (1.42)$$

Therefore, to first order in Δt , it is found, $a^{(0)}(y, t) = \int dy_2 W_t(y_2 | y_1)$. Interpretation of $a^{(0)}(y, t) \Delta t$ is the total probability of escape from y_1 is the time interval $(t, t + \Delta t)$, and thus $1 - a^{(0)}(y, t) \Delta t$ is the probability that no transition takes place during this time.

Inserting differential equation for the transition probability from the Chapman-Kolmogorov equation, the above short-time expression for the transition probability into it yields,

$$\begin{aligned} P(y_3, t_2 + \Delta t | y_1, t_1) &= \int dy_2 P(y_3, t_2 + \Delta t | y_2, t_2) P(y_2, t_2 | y_1, t_1) \\ &\simeq [1 - a^{(0)}(y_3, t_2) \Delta t] P(y_3, t_2 | y_1, t_1) + \Delta t \int dy_2 W_{t_2}(y_3 | y_2) P(y_2, t_2 | y_1, t_1) \end{aligned} \quad (1.43)$$

Replacing the value of $a^{(0)}(y_3, t_2)$ we get,

$$\frac{1}{\Delta t} [P(y_3, t_2 + \Delta t | y_1, t_1) - P(y_3, t_2 | y_1, t_1)] \simeq \int dy_2 [W_{t_2}(y_3 | y_2) P(y_2, t_2 | y_1, t_1) - W_{t_2}(y_2 | y_3) P(y_3, t_2 | y_1, t_1)] \quad (1.44)$$

If $\Delta t \rightarrow 0$ and changing notations $((y_1, t_1 \rightarrow y_0, t_0), (y_2, t_2 \rightarrow y', t), y_3 \rightarrow y)$, the master equation,

$$\frac{\partial}{\partial t} P(y, t | y_0, t_0) = \int dy' [W_t(y | y') P(y', t | y_0, t_0) - W_t(y' | y) P(y, t | y_0, t_0)] \quad (1.45)$$

It is an integro-differential equation. The master equation is a differential form of the Chapman-Kolmogorov equation. Therefore, it is an expression of the transition probability $P(y, t | y_0, t_0)$ but not for $P_1(y, t)$. An equation for $P_1(y, t)$ can be obtained by using the concept of extraction of a sub-ensemble. Suppose $Y(t)$ is a stationary Markov process characterized by $P_1(Y)$ and $P(y, t | y_0, t_0)$. Let us define a non-stationary Markov process $Y^*(t)$ for $t \geq t_0$ by setting,

$$\begin{aligned} P_1^*(y, t_1) &= P(y_1, t_1 | y_0, t_0) \\ P^*(y_2, t_2 | y_1, t_1) &= P(y_2, t_2 | y_1, t_1) \end{aligned} \quad (1.46)$$

This is a sub-ensemble of $Y(t)$ characterized by taking the sharp value y_0 at t_0 , since $P_1^*(y_1, t_0) = \delta(y_1 - y_0)$. More generally, we may extract a sub-ensemble in which at a given time t_0 the values of $Y^*(t_0)$ are distributed according to a given probability distri-

bution $p(y_0)$.

$$P_1^*(y_1, t_1) = \int dy_0 P(y_1, t_1 | y_0, t_0) p(y_0) \quad (1.47)$$

Physically, the extraction of a sub-ensemble means that one 'prepares' the system in a certain non-equilibrium state at t_0 . The above $P_1^*(y_1, t_1)$ obey the same differential equation naming Master equation.

$$\frac{\partial P(y, t)}{\partial t} = \int dy' [W(y|y')P(y', t) - W(y'|y)P(y, t)] \quad (1.48)$$

If the range of Y is a discrete set of states labeled with n the equation reduces to,

$$\frac{dP_n(t)}{dt} = \sum_{n'} [W_{nn'} P_{n'}(t) - W_{n'n} P_n(t)] \quad (1.49)$$

The master equation is a balanced (gain-loss) equation for the problem of each state. The first term represents gain due to transitions from other states n' to n , and the second term is the loss due to transitions into other configurations. The master equation can be extended to the case of a multi-component Markov process $Y_i(t)$, $i = 1, 2, \dots, N$ on noting that the Chapman-Kolmogorov equation is valid as it stands by merely replacing y by $\mathbf{y} = (y_1, \dots, y_N)$. Then we get the multivariate counterpart of the master equation,

$$\frac{\partial P(\mathbf{y}, t)}{\partial t} = \int d\mathbf{y}' [W(\mathbf{y}|\mathbf{y}')P(\mathbf{y}', t) - W(\mathbf{y}'|\mathbf{y})P(\mathbf{y}, t)] \quad (1.50)$$

1.9 Kramers-Moyal expansion and Fokker Planck equation

Let us first express the transition probability W as a function of the size r of the jump from one configuration y' to another one y , and of the starting point y' ,

$$W(y|y') = W(y'; r), \quad r = y - y'$$

The Master equation becomes,

$$\frac{\partial P(y, t)}{\partial t} = \int dr W(y - r; r) P(y - r, t) - P(y, t) \int dr W(y; -r) \quad (1.51)$$

Where the sign change is associated with the change of variables $y' \rightarrow r = y - y'$, is absorbed in the boundaries, by considering a symmetrical integration interval extending from $-\infty$ to $+\infty$,

$$\int_{-\infty}^{+\infty} dy' f(y') = - \int_{y+\infty}^{y-\infty} dr f(y - r) = - \int_{+\infty}^{-\infty} dr f(y - r) = \int_{-\infty}^{+\infty} dr f(y - r)$$

Moreover, since finite integration limits would incorporate an additional dependence on y , we shall restrict our attention to problems to which the boundary is irrelevant. Let us now assume that the changes on y occur via small jumps, i.e. that $W(y'; r)$ is a sharply peaked function of r but varies slowly enough with y' . Another assumption is that $P(y, t)$ itself also varies slowly with y . It is then possible to deal with the shift from y to $y - r$ in the first integral in the equation using the Taylor's expansion,

$$\begin{aligned} \frac{\partial P(y, t)}{\partial t} &= \int dr W(y; r) P(y, t) + \sum_{m=1}^{\infty} \frac{(-1)^m}{m!} \int dr r^m \frac{\partial^m}{\partial y^m} [W(y; r) P(y, t)] - P(y, t) \int dr W(y; -r) \\ &= \sum_{m=1}^{\infty} \frac{(-1)^m}{m!} \frac{\partial^m}{\partial y^m} \left\{ \left[\int dr r^m W(y; r) \right] P(y, t) \right\} \end{aligned} \quad (1.52)$$

Where we have used the first and third terms on the right-hand side of the first equation cancel each other. Finally introducing jump moments,

$$a^{(m)}(y, t) = \int dr r^m W(y; r)$$

One gets Kramers-Moyal expansion of the master equation,

$$\frac{\partial P(y, t)}{\partial t} = \sum_{m=1}^{\infty} \frac{(-1)^m}{m!} \frac{\partial^m}{\partial y^m} [a^{(m)}(y, t) P(y, t)] \quad (1.53)$$

If the situation is $m > 2$, $a^{(m)}(y, t)$ is identically zero or terms are negligible. In this case,

$$\frac{\partial P(y, t)}{\partial t} = -\frac{\partial}{\partial y} [a^{(1)}(y, t) P(y, t)] + \frac{1}{2} \frac{\partial^2}{\partial y^2} [a^{(2)}(y, t) P(y, t)] \quad (1.54)$$

This is widely known as the Fokker-Planck equation. The first term is drift or transport term and the second term is diffusion term, while $a^{(1)}(y, t)$ and $a^{(2)}(y, t)$ are drift and diffusion coefficients.

1.10 SDE and Fokker-Planck equations

Let us establish the mathematical relationship between the Stochastic differential equation of the Langevin type, and Fokker-Planck equations. The general form of SDE is,

$$\dot{x}(t) = \frac{d}{dt} x(t) = f[x(t), t] + g[x(t)] \xi(t) \quad (1.55)$$

Here $\xi(t)$ is white noise with conditions $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = D\delta(t-t')$, taking $D = 1$, relation becomes $\langle \xi(t)\xi(t') \rangle = \delta(t-t')$. The assumption is that the process is Gaussian. Let us integrate Eq.(1.55) over a short time interval δt ,

$$x(t + \delta t) - x(t) = f[x(t), t]\delta t + g[x(t), t]\xi(t)\delta t \quad (1.56)$$

As $x(t)$ is a Markov process, we can determine its probability distribution $P_1(x, t)$ as well as conditional probability distribution $P(x, t|x', t')$ for $t > t'$. Let us define a conditional average corresponding to the average of a function of the stochastic variable x , given that x has the value y at $t' < t$;

$$\langle F[x(t)]|x(t') = y \rangle = \langle \langle F[x(t)] \rangle \rangle = \int dx' F(x') P(x', t|y, t') \quad (1.57)$$

Due to the property $P(x, t|x', t) = \delta(x - x')$, we have

$$\langle F(x(t))|x(t) = y \rangle = \int dx' F(x') P(x', t|y, t) = \int dx' F(x') \delta(x - x') \quad (1.58)$$

We will use this definition to find the first few conditional moments of $x(t)$,

$$\begin{aligned} \langle \langle F[x(t)] \rangle \rangle &= \langle x(t + \delta t)|x(t) = x \rangle = \int dx' F(x') \delta(x - x') P(x', t + \delta t|x, t) \\ &= \langle \langle f[x(t), t]\delta t \rangle \rangle + \langle \langle g[x(t), t]\xi(t)\delta t \rangle \rangle \end{aligned} \quad (1.59)$$

It is clear that the first term on the r.h.s.

$$\langle \langle f[x(t), t]\delta t \rangle \rangle = f[x(t), t]\delta t \quad (1.60)$$

and the second term is,

$$\langle \langle g[x(t), t]\xi(t)\delta t \rangle \rangle = g[x(t), t]\langle \langle \xi(t) \rangle \rangle \delta t \quad (1.61)$$

Based on Langevin's argument, $\langle x\xi \rangle = 0$, which gives

$$\langle \langle \Delta x(t) \rangle \rangle = \int dx' (x - x') P(x', t + \delta t|x, t) = f[x(t), t]\delta t \quad (1.62)$$

For the second moment,

$$\begin{aligned}
\langle\langle \Delta x(t)^2 \rangle\rangle &= \int dx' (x-x')^2 P(x', t + \delta t | x, t) \\
&= \langle\langle [f[x(t), t] \delta t + g[x(t), t] \xi(t) \delta t]^2 \rangle\rangle \\
&= \langle\langle [f[x(t), t] \delta t]^2 \rangle\rangle + \langle\langle 2f[x(t), t]g[x(t), t] \xi(t) \delta t^2 \rangle\rangle \\
&\quad + \langle\langle [g[x(t), t] \xi(t) \delta t]^2 \rangle\rangle \\
&= [f[x(t), t] \delta t]^2 + 2f[x(t), t]g[x(t), t] \langle\langle \xi(t) \rangle\rangle \delta t^2 \\
&\quad + g[x(t), t]^2 \langle\langle [\xi(t) \delta t]^2 \rangle\rangle
\end{aligned} \tag{1.63}$$

Using the properties of the Wiener process,

$$\xi(t) \delta t = \int_t^{t+\delta t} dt' \xi(t') = \Delta W(t)$$

Where $W(t)$ is the Wiener process, and $\langle\langle [\xi(t) \delta t]^2 \rangle\rangle \simeq \langle\langle \Delta W(t)^2 \rangle\rangle = \Delta t$, renders

$$\langle\langle \Delta x(t)^2 \rangle\rangle = \int dx' (x-x')^2 P(x', t + \delta t | x, t) = g[x(t), t]^2 \delta t + \mathcal{O}(\delta t^2) \tag{1.64}$$

We can show that in general,

$$\langle\langle \Delta x(t)^v \rangle\rangle \simeq \mathcal{O}(\delta t^v), v \geq 2$$

Let us make consideration of an arbitrary function $R(x)$, and evaluate its conditional average. Using the Chapman-Kolmogorov equation,

$$\begin{aligned}
\int dx R(x) P(x, t + \delta t | y, s) &= \int dx R(x) \int dz P(x, t + \delta t | z, t) P(z, t | y, s) \\
&= \int dz P(z, t | y, s) \int dx R(x) P(x, t + \delta t | z, t)
\end{aligned} \tag{1.65}$$

Expanding $R(x)$ in Taylor series around z , as for $\delta t \simeq 0$ we find that, $P(x, t + \delta t | z, t) \simeq \delta(x-z)$, and only a neighborhood of z will be relevant,

$$\begin{aligned}
\int dx R(x) P(x, t + \delta t | y, s) &= \int dz P(z, t | y, s) \\
&\quad \int dx \left[R(z) + (x-z)R'(z) + \frac{1}{2}R''(z)(x-z)^2 + \dots \right] P(x, t + \delta t | z, t)
\end{aligned} \tag{1.66}$$

Putting the normalization condition for $P(z, t | y, s)$, we get

$$\begin{aligned}
&= \int dz P(z, t | y, s) R(z) + \int dz R'(z) P(z, t | y, s) \int dx (x-z) \\
&\quad + \int dz \frac{1}{2} R''(z) P(z, t | y, s) \int dx (x-z)^2 P(x, t + \delta t | z, t) + \dots
\end{aligned} \tag{1.67}$$

integrating by parts and using Eqs. (1.62), (1.64) we get,

$$\int dx R(x) P(x, t + \delta t | y, s) = \int R(x) + \left[P(x, t | y, s) - \frac{\partial}{\partial x} [f(x, t) P(x, t | y, s)] \right] \delta t + \frac{1}{2} \frac{\partial^2}{\partial x^2} [g(x, t)^2 P(x, t | y, s)] \delta t + \mathcal{O}(\delta t^2) \quad (1.68)$$

Arranging terms and taking the limit $\delta t \rightarrow 0$, gives

$$\begin{aligned} 0 &= \int dx R(x) \left[\frac{\partial}{\partial t} P(x, t | y, s) - \left(-\frac{\partial}{\partial x} [f(x, t) P(x, t | y, s)] + \frac{1}{2} \frac{\partial^2}{\partial x^2} [g(x, t)^2 P(x, t | y, s)] \right) \right] \\ \frac{\partial}{\partial t} P(x, t | y, s) &= -\frac{\partial}{\partial x} [f(x, t) P(x, t | y, s)] + \frac{1}{2} \frac{\partial^2}{\partial x^2} [g(x, t)^2 P(x, t | y, s)] \end{aligned} \quad (1.69)$$

This is the desired Fokker-Planck equation for the transition probability $P(x, t | y, s)$ associated with the stochastic process driven by the SDE Eq. (1.55).

1.11 Brownian Motion

In this section, we will take a break from our mathematical treatments of the stochastic processes and look back at their origins. In fact, the whole content of this thesis can be regarded as the continuation of the analysis of the Brownian motion conceptualized by Einstein, Smoluchowski, and Langevin. Let us see the historical background of the Brownian motion.

In 1827, the botanist Robert Brown observed in his microscope the small pollen grains suspended in water, perform an irregular, jittery motion. He could not explain the origins of the motion. The explanation came later, in 1905, with the theoretical treatments by Einstein and Smoluchowski. Einstein derives the mathematics behind Brownian motion which was able to define many concepts introduced earlier.

The motion observed occurs due to very frequent collisions between the molecules of the suspension and the pollen grain. An accurate description of these collisions is not possible that's why we are more interested in treating them statistically. Let us see it in one-dimensional setup. Let us consider the density of the particles per unit volume is $n(x, t)$. In a small interval dt , each particle will experience a shift Δ due to the collision effect. The probability $p(\Delta)$ of a certain shift shall be independent for every particle, independent from its past, and symmetric in nature, $p(-\Delta) = p(\Delta)$, it will have a sharp

peak around $\Delta = 0$. So, the density for the time $t + dt$ is,

$$n(x, t + dt) = \int d\Delta n(x - \Delta, t) p(\Delta) \quad (1.70)$$

This formulation is similar to the Chapman-Kolmogorov equation (1.37), which is derived assuming that collisions have no memory.

Now, we expand the LHS of Eq. (1.70) for small dt

$$n(x, t + dt) = n(x, t) + dt \frac{\partial n}{\partial t} \quad (1.71)$$

This is an important step in deriving the master equation. Let us assume a sharp peak in $p(\Delta)$, Einstein calculated his version of the Kramers-Moyal expansion:

$$n(x - \Delta, t) = n(x, t) - \Delta \frac{\partial n}{\partial x} + \frac{\Delta^2}{2} \frac{\partial^2 n}{\partial x^2} - \dots \quad (1.72)$$

Using the results of Eq. (1.72) in Eq. (1.70) and using the symmetry and the normalization of $p(\Delta)$, Einstein gets the diffusion equation, which is Fokker-Planck equation:

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} \quad (1.73)$$

So, the diffusion coefficient from Fick's law of diffusion

$$D = \frac{1}{dt} \int d\Delta \frac{\Delta^2}{2} p(\Delta) \quad (1.74)$$

Einstein describes a random walk of the pollen grain with infinitely small steps and shows how this is related to diffusion. The biggest contribution of Einstein and Smoluchowski is finding the relation of the diffusion coefficient D with the temperature T and the coefficient of Stokes's friction γ and the solution for a spherical particle is:

$$D = \frac{k_B T}{\gamma} \quad (1.75)$$

where k_B is Boltzmann's constant.

1.12 Langevin Formalism

Let us discuss Langevin formalism in brief for Non-equilibrium statistical mechanics. The well-defined non equilibrium system is the theory of Brownian motion. The basic

equation of Langevin equation consists of two parts, frictional part which is a systematic force and random forces, which is fluctuating force. Both the friction and random forces generated from the interaction of the Brownian particles with their environment. The equation of motion for Brownian motion is thus given by,

$$m \frac{d}{dt} \mathbf{v}(\mathbf{t}) = -\xi \mathbf{v}(\mathbf{t}) + \delta \mathbf{F}(\mathbf{t}) \quad (1.76)$$

It can be written as,

$$m\dot{v} = -\xi v(t) + \eta(t) \quad (1.77)$$

between impacts in any two distinct time intervals. As the frictional force depends merely on the velocity of the particle and not on its earlier values, we are describing a Markovian process. The random force behaves as,

$$\langle \delta \mathbf{F}(\mathbf{t}) \rangle = 0 \quad (1.78)$$

and also,

$$\langle \delta F^i(t) \delta F^j(t') \rangle = 2B \delta_{ij} \delta(t - t') \quad (1.79)$$

Where B is the measure of the strength of the fluctuating force. Eq. (1.78) tells us that the average of the random force is measured as zero and from Eq. (1.79) we conclude that there is no correlation between impacts in any two distinct time intervals. As the frictional force depends merely on the velocity of the particle and not on its earlier values, we are describing a Markovian process. The velocity of the particle decays to zero in the absence of random force, but here it doesn't happen. At thermal equilibrium, $\langle v^2 \rangle_{eq} = kT/m$. The Langevin equation which is a linear, first order, inhomogeneous differential equation in nature can be solved as,

$$v(t) = e^{-\xi t/m} v(0) + \int_0^t dt' e^{-\xi(t-t')/m} \delta F(t')/m \quad (1.80)$$

The first term states the exponential decay of the initial velocity and the second term gives the extra velocity produced because of the random noise force. Let us calculate mean squared velocity. We get from Eq. (1.80) the value of $\langle v^2(t) \rangle$ as,

$$\langle v^2(t) \rangle = e^{-2\xi t/m} v^2(0) + \frac{B}{\xi m} (1 - e^{-2\xi t/m}) \quad (1.81)$$

In the long time limit, exponential terms drop out, and the quantity tends to the value $B/\xi m$. But in the long time limit mean squared velocity must approach its equilibrium

value kT/m , consequently, we find $B = \xi kT$. This is known as Fluctuation-dissipation theorem. It is a relation between the strength B of the random force or fluctuating force with the magnitude of friction force ξ . It expresses the balance between friction, which drives any system to a completely "dead state", and the noise which keeps the system "alive".

Let us rewrite the Langevin equation of Eq.(1.76)

$$\frac{d}{dt}\dot{x} = -\xi\dot{x} + \eta(t) \quad (1.82)$$

We will evaluate the r.m.s. displacement. Multiply Eq. (1.82) by x , we get,

$$x\frac{d}{dt}\dot{x} = \frac{d}{dt}(x\dot{x}) - \dot{x}^2 = -\xi x\dot{x} + x\eta(t) \quad (1.83)$$

Langevin's original argument was to assume that $\eta(t)$ and $x(t)$ were uncorrelated,

$$\langle x(t)\eta(t) \rangle = 0 \quad (1.84)$$

Now we take the average of Eq. (1.83)

$$\left\langle \frac{d}{dt}(x\dot{x}) \right\rangle = \frac{d}{dt}\langle x\dot{x} \rangle = \frac{kT}{m} - \xi \langle x\dot{x} \rangle \quad (1.85)$$

We get,

$$\langle x(t)\dot{x}(t) \rangle = Ce^{-\xi t} + \frac{kT}{\xi m} \quad (1.86)$$

If x measures the displacement from the origin (where we consider all the Brownian particles at $t = 0$), we find the condition $0 = C + \frac{kT}{\xi m}$, that gives

$$\langle x(t)\dot{x}(t) \rangle = \frac{d}{dt}\langle x^2 \rangle = \frac{kT}{\xi m}(1 - e^{-\xi t}) \quad (1.87)$$

Integrating again, we find,

$$\langle x^2(t) \rangle = \frac{2kT}{\xi m} \left[t - \frac{1}{\xi}(1 - e^{-\xi t}) \right] \quad (1.88)$$

Now, let us consider two limiting cases,

(a) Initial transient regime: $t \ll \frac{1}{\xi}$, where we can expand $e^{-\xi t} \simeq 1 - \xi t + \frac{1}{2}(\xi t)^2 - \dots$,

and we get

$$\langle x^2(t) \rangle \simeq \frac{kT}{m} t^2 \quad (1.89)$$

that is the inertial motion of the particle during the initial transient(when thermal velocity $\bar{v} = \sqrt{\frac{kT}{m}}$)

(b) Asymptotic regime: $t \gg \frac{1}{\xi}$, where we can approximate $e^{-\xi t} \simeq 0$, and then

$$\langle x^2(t) \rangle \simeq \frac{2kT}{m} t \quad (1.90)$$

this is the characteristic of a diffusive motion.

Another way to define Brownian motion is to consider the probability distribution of finding the system within a given velocity range $(v, v + dv)$, taking velocity v_0 at the initial time t_0

$$Pdv = P(v, t | v_0, t_0) dv \quad (1.91)$$

We know that

$$\lim_{\delta t \rightarrow 0} P(v, t + \delta t | v', t) = \delta(v - v') \quad (1.92)$$

The normalized PDF corresponding to the OU distribution is,

$$p(v, t | v_0) = \left[\frac{m}{2\pi kT(1 - e^{-2\gamma t})} \right]^{1/2} \exp\left[\frac{-m(v - v_0 e^{-\gamma t})^2}{2kT(1 - e^{-2\gamma t})} \right] \quad (1.93)$$

In the limit of very large value of time, we get,

$$\lim_{\delta t \rightarrow \infty} P(v, t + \delta t | v', t) = \left(\frac{m}{2\pi kT} \right)^{1/2} e^{-\frac{mv^2}{2kT}} \quad (1.94)$$

In the Kramers-Moyal expansion of the master equation, when the moments of order greater than two are zero, we get a Fokker-Planck equation. In this case, the master equation indicates the gain and loss contributions within the interval $(v, v + dv)$. According to the average values found for $\langle v \rangle$ and $\langle v^2 \rangle$, we get

$$\frac{\partial}{\partial t} P(v, t | v_0, t_0) = -\frac{\partial}{\partial v} \xi v P(v, t | v_0, t_0) + \frac{D}{2} \frac{\partial^2}{\partial v^2} P(v, t | v_0, t_0) \quad (1.95)$$

We may impose a condition on $\eta(t)$, which is a Gaussian process. It means that all

the odd moments are zero and even moments can be written in terms of the second moment,

$$\begin{aligned}\langle \eta(t_1)\eta(t_2)\eta(t_3)\eta(t_4) \rangle &= \langle \eta(t_1)\eta(t_2) \rangle \langle \eta(t_3)\eta(t_4) \rangle + \langle \eta(t_1)\eta(t_3) \rangle \langle \eta(t_2)\eta(t_4) \rangle + \dots \\ &= D^2 \{ \delta(t_1 - t_2)\delta(t_3 - t_4) + \dots \}\end{aligned}\quad (1.96)$$

1.13 Fokker Planck Equation

Let us consider a stochastic differential equation,

$$dx(t) = A(x,t)dt + B(x,t)dW \quad (1.97)$$

The differential of a function $f(x(t))$ according to the Ito representation is written as

$$\begin{aligned}df(x(t)) &= f(x(t)) + dx(t) - f(x) \\ &= f'(x(t))dx(t) + \frac{1}{2}f''(x(t))dx(t)^2 \\ &= f'(x(t))[A(x,t)dt + B(x,t)dW] + \frac{1}{2}f''(x(t))B^2(x,t)dW^2\end{aligned}\quad (1.98)$$

Using $dW^2 = dt$, we get

$$df(x(t)) = A(x,t)f'(x(t))dt + \frac{1}{2}f''(x(t))B^2(x,t)dt + B(x,t)f'(x(t))dW \quad (1.99)$$

Let us divide Eq. (1.99) by dt and take the noise average,

$$\frac{\langle df(x(t)) \rangle}{dt} = \left\langle \frac{df(x(t))}{dt} \right\rangle = \langle A(x,t)f' + \frac{1}{2}f''B^2(x,t) \rangle \quad (1.100)$$

If $P(x,t|x_0,t_0)$ is the conditional probability for the process $x(t)$ then the left-hand side of Eq. (1.100) is written as

$$\left\langle \frac{df}{dt} \right\rangle = \int dx f(x(t)) \frac{\partial P}{\partial x} \quad (1.101)$$

Right-hand side may be written as,

$$\langle A(x,t)f' + \frac{1}{2}f''B^2(x,t) \rangle = \int dx [A(x,t)f' + \frac{1}{2}f''B^2(x,t)]P(x,t|x_0,t_0) \quad (1.102)$$

Now we can integrate by parts and neglect the surface terms

$$\int dx f(x(t)) \frac{\partial x}{\partial t} = \int dx \left[-\frac{\partial A(x,t)P}{\partial x} + \frac{1}{2} \frac{\partial^2 B^2(x,t)P}{\partial x^2} \right] f(x(t)) \quad (1.103)$$

As $f(x(t))$ is arbitrary, the above equation for conditional probability becomes

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x} \left(A(x,t)P \right) + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left(B^2(x,t)P \right) \quad (1.104)$$

Eq. (1.104) is known as the Fokker-Planck equation for the conditional probability. The first term is the drift term and the second term is the diffusion term.

1.14 Different Problems of Persistence

The persistence of a continuous stochastic process has recently generated much interest in a wide variety of non-equilibrium systems including various models of phase ordering kinetics, fluctuating interfaces, diffusion, and reaction-diffusion process. The persistence probability $p(t)$ of a stochastic variable is the probability that the variable has not changed sign up to time t . That means, the survival-persistence probability is that a stochastic process $X(t)$ does not cross zero up to time t is a quantity of long-standing interest in probability theory which has many practical applications. The derivative of the persistence probability $F(t) = -dp(t)/dt$ is the first-passage probability¹. Physically the persistence property has been investigated both theoretically²⁻¹⁰ and experimentally¹⁰⁻¹⁶ in spatially extended systems that are out of equilibrium. Let us define the precise concept of persistence probability. Let us take a non-equilibrium field fluctuating in space and time $\phi(x,t)$. It may be simply a diffusing field starting from a random initial configuration or the height of a fluctuating interface. Persistence of such fluctuating field can simply be defined as, the probability at a fixed point in space, the quantity $\text{sgn}[\phi(x,t) - \langle \phi(x,t) \rangle]$ does not change up to time t . In a wide class of non-equilibrium systems this probability decays algebraically with an exponent θ ¹⁷. This exponent has been studied in systems like a free random walk in homogeneous and disordered media¹⁸, diffusion in two dimensions¹⁹, fluctuating interface⁵, KPZ interface²⁰, critical dynamics²¹, surface growth^{7,20}, diffusive processes with random initial conditions²², advected diffusive processes²³, and finance^{24,25}.

The persistence probability of spatially extended systems decays as a power law $p(t) \sim t^{-\theta}$, when θ is a non-trivial exponent. This algebraic decay of $p(t)$ is applicable for a wide class of non-equilibrium systems. The calculation of the exponent θ for

a general stochastic process is extremely difficult, and the exact form of $p(t)$ exists in very few cases. In the Brownian systems, $X(t)$ is Gaussian as well as Markovian, and the non-stationary process can be mapped into a stationary Ornstein-Uhlenbeck process $\bar{X}(T)$ through suitable transformation $X \rightarrow \bar{X}$ and $t \rightarrow T$ with the consequence that the correlator $C(t) \equiv \langle \bar{X}(T)\bar{X}(0) \rangle$ decays exponentially at all times. Slepian theory says that if the stationary correlator $C(t)$ of a Gaussian stochastic process decays purely exponentially at all times, the persistence probability of $X(t)$ is proportional to $C(T)$ at late times and $p(t)$ can then be constructed back by the inverse of the time transformation $t \rightarrow T$. In the case when the correlation function $C(T)$ of a Gaussian stochastic process does not decay exponentially at all times, the exponent θ can be extracted using the independent interval approximation provided the density of zero crossing remains finite.

The route to calculating the persistence probability is through the non stationary two-time correlation function. The Lamperti transformation converts the non stationary correlator to a stationary process. For a Gaussian Markovian stochastic process, the persistence probability can be directly calculated using Slepian theorem²⁶. In contrast, when the process is non-Markovian, $p(t)$ is evaluated either using the Independent Interval Approximation (IIA) when the density of zero crossings stays finite or using a perturbative expansion. It should be emphasized that IIA or the perturbative expansion works only for Gaussian stochastic processes.

1.14.1 Some Known Results

Let us consider $X(T)$ a Gaussian Stationary process (GSP), where correlation can be written as $f(\tau) = \langle X(T)X(T + \tau) \rangle$ and we denote $P(T, f(\tau))$ as the persistence probability in the time variable T . The scaling form

$$P(T, \lambda f(\tau)) = P(T, f(\tau)) \quad (1.105)$$

$$P(T, f(\lambda \tau)) = P(\lambda T, f(\tau)) \quad (1.106)$$

The first scaling law implies that we may normalize the correlation function such that $f(0) = 1$. The second scaling law denotes a normalization of the time scale. By the way, this is not possible for all classes of correlation functions. So, we consider processes for which $[f(\tau) - 1]$, for small τ behaves as $|\tau|^\alpha$, when α positive. Under such circumstances the covariance $f(\tau)$ is said to be class- α if τ approaches 0,

$$f(\tau) = 1 - \frac{|\tau|^\alpha}{\Gamma(\alpha + 1)} \quad (1.107)$$

and $f(\tau)$ is strictly monotone in the neighborhood of the origin. The gamma function in the denominator comes due to the normalization of the time scale and $0 \leq \alpha \leq 2$. We have

$$(1) \quad f(\tau) = e^{-|\tau|} \quad \text{for } 0 \leq \tau \leq \infty$$

$$P(T, f(\tau)) = \frac{2}{\pi} \text{Sin}^{-1}[f(\tau)] \quad (1.108)$$

$$(2) \quad f(\tau) = 1 - \beta^2 \sin^2(\tau/2\beta) \quad \text{for } 0 \leq \tau \leq \infty \quad \text{and } 0 \leq \beta \leq 1$$

$$P(T, f(\tau)) = \frac{1}{2} - \frac{T}{4\pi} - \frac{1}{2\pi} \text{sin}^{-1}[\beta \text{sin}(\frac{T}{2\beta})] \quad \text{for } 0 \leq \frac{T}{\beta} \leq 2\pi \quad (1.109)$$

$$= \frac{1}{2}(1 - \beta) \quad \text{for } 2\pi \leq T < \infty$$

$$(3) \quad f(\tau) = 1 - |\tau| \quad \text{for } |\tau| \leq 1$$

$$= 0 \quad |\tau| \geq 1 \quad (1.110)$$

$$P(T, f(\tau)) = \frac{1}{4} + \frac{1}{2\pi} [\text{sin}^{-1}(1 - T) - \sqrt{T(2 - T)}]$$

Further, if two different processes which are characterized by the correlation function $f(\tau)$ and $g(\tau)$, then Slepian's inequality says that if

$$f(\tau) \leq g(\tau) \quad \text{for } 0 \leq \tau \leq T \quad (1.111)$$

then

$$P(T, f(\tau)) \leq P(T, g(\tau)) \quad (1.112)$$

The stationary correlator decays exponentially at all times for a Markovian process and by using Eq. (1.108) we can show that persistence probability also decays exponentially. For the non-Markovian process, correlation does not decay exponentially at all the time.

1.14.2 Random Walk Model

The simplest non-equilibrium system is Random Brownian Walker Model²⁷. Let us consider $\phi(t)$, which represents the position of a 1-D Brownian walker at time t . The position evolves as

$$\frac{d\phi}{dt} = \eta(t) \quad (1.113)$$

Where $\eta(t)$ is a value of white noise with zero mean and δ -correlation $\langle \phi(t)\phi(t') \rangle = \delta(t-t')$. The persistence $P_0(t)$ is simply the probability that $\phi(t)$ does not change sign up to time t . We find from Eq. (1.113)

$$\langle \phi(t_1)\phi(t_2) \rangle = 2Dt_2 \quad t_2 < t_1 \quad (1.114)$$

ϕ is a Gaussian non-stationary process. Normalizing this process

$$X(t) = \frac{\phi(t)}{\sqrt{\langle \phi^2(t) \rangle}} \quad (1.115)$$

Taking time transformation we get

$$T = \ln t \quad (1.116)$$

and non-stationary correlator becomes

$$\langle X(T_1)X(T_2) \rangle = e^{-\frac{1}{2}(T_1-T_2)} \quad (1.117)$$

As the stationary correlator decays exponentially for all times, by Eq. (1.108) the persistence probability in time variable T decays as $P(T) \sim e^{-T/2}$. Now we transform back to the real-time, the persistence probability decays as

$$p(t) \sim t^{-1/2} \quad (1.118)$$

So, persistence exponent $\theta = 1/2$ for the Random walk model.

1.14.3 Random acceleration Model

The equation of motion for a randomly accelerated particle is

$$\frac{d^2\phi}{dt^2} = \eta(t) \quad (1.119)$$

Where η is white Gaussian noise. The solution for $\phi(t)$ is

$$\phi(t) = \int_0^t dt' \delta(t-t') \eta(t') \quad (1.120)$$

Using the same transformation in Eq. (1.115) and Eq. (1.116) the stationary correlator makes the form

$$f(\tau) = \langle X(T)X(T+\tau) \rangle = \frac{3}{2}e^{-\frac{1}{2}\tau} - \frac{1}{2}e^{-\frac{3}{2}\tau} \quad (1.121)$$

It is of class-2. The exact result has been found by Sinai and Burkhardt is $\theta = 1/4$ ²⁷.

1.14.4 Brownian Particle in a shear flow

We consider the motion of a Brownian particle, with a unit mass, in an unbounded solvent moving in two-dimensional planar geometry. We consider a stationary distribution of velocity,

$$\mathbf{u} = (0, ax) \quad (1.122)$$

The force on the Brownian particle from the imposed flow is given by, $\mathbf{F} = -\zeta(\mathbf{v} - \mathbf{u})$, where \mathbf{v} is the instantaneous velocity of the particle and ζ is Stoke's friction on the colloid. The Langevin equation for the position of a colloid $\mathbf{r} \equiv (x, y)$ in the overdamped limit takes the form,

$$\begin{aligned} \frac{dx}{dt} &= \eta_x(t) \\ \frac{dy}{dt} &= ax + \eta_y(t) \end{aligned} \quad (1.123)$$

When $\eta \equiv (\eta_x, \eta_y)$ these are Gaussian White noise and the correlations are,

$$\begin{aligned} \langle \eta \rangle &= 0 \\ \langle \eta(t) \otimes \eta(t') \rangle &= 2D\mathbf{I}\delta(t-t') \end{aligned} \quad (1.124)$$

Where \mathbf{I} is the identity matrix and \otimes is the outer product of a vector quantity. $D = k_B T / \zeta$ diffusion constant, which is the strength of the noise. Two time correlation functions,

$$\langle x(t_1)x(t_2) \rangle = 2Dt_2 \quad (1.125)$$

and

$$\langle y(t_1)y(t_2) \rangle = 2Dt_2 + a^2D \left(t_1 t_2^2 - \frac{t_2^3}{3} \right) \quad (1.126)$$

Cross-correlation functions are,

$$\langle x(t_1)y(t_2) \rangle = Dat_2^2 \quad (1.127)$$

$$\langle y(t_1)x(t_2) \rangle = 2Da \left(t_1 t_2 - \frac{t_2^2}{2} \right) \quad (1.128)$$

When $t_1 = t_2 = t$ we get motion along x -direction purely diffusive, while Mean square displacement along y -direction is,

$$\langle y^2(t) \rangle = 2Dt + \frac{2}{3}a^2Dt^3 \quad (1.129)$$

for short time, $t \ll a^{-1}$ motion along y -direction becomes purely diffusive. For $t \gg a^{-1}$ Means Square Displacement scales t^3 , similar to a randomly accelerated particle. Cross-correlation becomes,

$$\langle x(t)y(t) \rangle = Dat^2 \quad (1.130)$$

Now the persistence probability has been calculated from the correlation function. The fundamental idea is to map non-stationary process $y(t)$ to a stationary O-U process \bar{Y} . Stationary correlator $C(t)$ for \bar{Y} decays exponentially for all times and the persistence probability can be shown to decay as $P(T) \sim \frac{2}{\pi} \sin^{-1}[C(T)]$. Transformation, $\bar{Y} = y(t)/\sqrt{\langle y^2(t) \rangle}$, which yields,

$$\langle \bar{Y}(t_1)\bar{Y}(t_2) \rangle = \frac{\langle y(t_1)y(t_2) \rangle}{\sqrt{\langle y^2(t_1) \rangle \langle y^2(t_2) \rangle}} = \frac{2Dt_2 + a^2D \left(t_1 t_2^2 - \frac{t_2^3}{3} \right)}{\sqrt{\left(2Dt_1 + \frac{2}{3}a^2Dt_1^3 \right) \left(2Dt_2 + \frac{2}{3}a^2Dt_2^3 \right)}} \quad (1.131)$$

for $t \ll a^{-1}$, the motion of the particle is purely diffusive and neglects the $\mathcal{O}(t^3)$ terms,

$$\langle \bar{Y}(t_1)\bar{Y}(t_2) \rangle = \sqrt{\frac{t_2}{t_1}} \quad (1.132)$$

for $t \gg a^{-1}$, we get

$$\langle \bar{Y}(t_1)\bar{Y}(t_2) \rangle = \frac{3}{2} \left(\frac{t_2}{t_1} \right)^{1/2} - \frac{1}{2} \left(\frac{t_2}{t_1} \right)^{3/2} \quad (1.133)$$

Using the time transformation $e^T = t$, Eq. (1.132) and Eq. (1.133) become

$$\begin{aligned} C(T) &= e^{-T/2} \quad \text{for } t \ll a^{-1} \\ &= \frac{3}{2}e^{-T/2} - \frac{1}{2}e^{-3T/2} \quad \text{for } t \gg a^{-1} \end{aligned} \quad (1.134)$$

As the stationary correlator for $t < a^{-1}$ decays exponentially, the persistence probability in the transformed variable T is $P(T) \sim e^{-T/2}$ and in real-time $p(t) \sim t^{-1/2}$. In the

asymptotic regime, the correlation function corresponds to that of a randomly accelerated particle when the persistence probability is known from the works of Sinai and Burkhardt, decays as $p(t) \sim t^{-1/4}$ ^{16,28}.

1.14.5 Harmonically confined Brownian Particle in shear flow

Like the last system, we have applied a harmonic potential $U(r) = \frac{1}{2}kr^2$. The harmonic confinement naturally takes place in the experiments of optical tweezers. The stationary velocity profile equation is found by using the Langevin equation as

$$\frac{dx}{dt} = -kx + \eta_x(t) \quad (1.135)$$

$$\frac{dy}{dt} = -ky + \eta_y(t) + ax \quad (1.136)$$

The time evolution of the x, y coordinates is given by,

$$\begin{aligned} x(t) &= \int_0^t dt' e^{-k(t-t')} \eta_x(t') \\ y(t) &= \int_0^t dt' e^{-k(t-t')} [x(t') + \eta_y(t')] \end{aligned} \quad (1.137)$$

Correlation functions are,

$$\langle x(t_1)x(t_2) \rangle = \frac{D}{k} [e^{-k(t_1-t_2)} - e^{-k(t_1+t_2)}] \quad (1.138)$$

and

$$\begin{aligned} \langle y(t_1)y(t_2) \rangle &= \frac{a^2 D}{2k^3} \left[(e^{-k(t_1-t_2)} - e^{-k(t_1+t_2)}) - k((t_1+t_2)e^{-k(t_1+t_2)} - (t_1-t_2)e^{-k(t_1-t_2)}) \right. \\ &\quad \left. - 2k^2 t_1 t_2 e^{-k(t_1+t_2)} \right] + \frac{D}{k} [e^{-k(t_1-t_2)} - e^{-k(t_1+t_2)}] \end{aligned} \quad (1.139)$$

The mean-square displacement for $y(t)$ becomes,

$$\langle y^2(t) \rangle = \frac{a^2 D}{2k^3} [(1 - e^{-2kt}) + 2kte^{-2kt} - 2k^2 t^2 e^{-2kt}] + \frac{D}{k} [1 - e^{-2kt}] \quad (1.140)$$

If we make Taylor's series expansion of Eq. (1.139) for $t < k^{-1}$, shows that the dynamics at short time scales as $2Dt + (2/3)a^2Dt^3$, and in the asymptotic regime, mean-square displacement saturates to a value $D/k + a^2D/k^3$. In the asymptotic regime, a suitable time transformation is not found to convert the process $y(t)$ to a Gaussian stationary

process. Persistence can only be found in the time domain which is smaller than k^{-1} . In this domain, persistence probability decays initially as $t^{-1/2}$, followed by a decay of $t^{-1/4}$ ²⁸.

1.14.6 Persistence exponents for fluctuating interfaces

In this paper⁵ the first passage properties of the fluctuating interfaces have been studied. The large-scale behavior model of interest is described here by the linear Langevin equation,

$$\frac{\partial h}{\partial t} = -(-\nabla^2)^{z/2}h + \eta \quad (1.141)$$

for the height field $h(x, t)$. Here the dynamic exponent z (usually $z = 2$ or 4) characterizes the relaxation mechanism, while $\eta(x, t)$ is a Gaussian noise term, possibly with spatial correlations. It is assumed that the system starts from a flat interface i.e. $h(x, 0) = 0$. As Eq.(1.141) is linear and $h(x, t)$ is Gaussian and its temporal statistics at an arbitrary fixed point in space is fully specified by the auto-correlation function computed from Eq.(1.141)

$$A(t, t') = \langle h(x, t)h(x, t') \rangle = K \left[(t' + t)^{2\beta} - |t' - t|^{2\beta} \right] \quad (1.142)$$

where K is some positive constant, and β denotes the dynamic roughness exponent, which depends on z and the type of noise considered.

A normalized random variable $X = h/\sqrt{\langle h^2 \rangle}$ is introduced and a time transformation $T = \ln t$ is taken. Now this Gaussian process is stationary by construction i.e $f_0(T - T') = \langle X(T)X(T') \rangle$, the correlation function f_0 can be obtained from Eq(1.142) as,

$$f_0(T) = \cosh(T/2)^{2\beta} - |\sinh(T/2)|^{2\beta} \quad (1.143)$$

Similarly, a normalized stationary process has been associated with the steady-state problem. The height difference variable is defined as,

$$H(x, t; t_0) = h(x, t + t_0) - h(x, t_0) \quad (1.144)$$

the autocorrelation function has been computed in the limit $t_0 \rightarrow \infty$

$$\begin{aligned} A_s(t, t') &= \lim_{t \rightarrow \infty} \langle H(x, t; t_0)H(x, t'; t_0) \rangle \\ &= K \left[t^{2\beta} + t'^{2\beta} - |t' - t|^{2\beta} \right] \end{aligned} \quad (1.145)$$

this is precisely the correlator of fractional Brownian motion with Hurst exponent β ²⁹.

Next $A_s(t, t')$ is normalized $\sqrt{A_s(t, t)A_s(t', t')}$ and rewritten in terms of $T = \ln t$, this gives,

$$f_s(T) = \cosh(\beta T) - \frac{1}{2}|2 \sinh(T/2)|^{2\beta} \quad (1.146)$$

So the short time singularity

$$f_{0,s}(T) = 1 - \mathcal{O}(|T|^{2\beta}) \quad (1.147)$$

this is applicable for $T \rightarrow 0$, which places them in the class $\alpha = 2\beta$. For large T , they decay with different rates, $f_{0,s}(T) \sim \exp(-\lambda_{0,s}T)$ for $T \rightarrow \infty$, where $\lambda_0 = 1 - \beta$ and $\lambda_s = \min[\beta, 1 - \beta]$, can be interpreted, in analogy with phase ordering kinetics, as the autocorrelation exponents of the two processes.

For a stationary Gaussian process with a general autocorrelator $f(T)$, the calculation of the decay exponent θ of the persistence probability is very hard. Approximate results can be derived for certain classes of autocorrelators $f(T)$. In such cases the density of zero crossings is finite and an independent interval approximation (IIA) gives a very good estimate of θ ^{30,31}.

For perturbation theory near $\beta = 1/2$, when persistence probability of a process whose correlation function differs perturbatively from the Markov process, i.e. whose autocorrelation function is

$$f(T) = \exp(-\lambda|T|) + \varepsilon\phi(T) \quad (1.148)$$

maybe then calculated from an understanding of the eigenstates of the quantum harmonic oscillator. In such processes, the exponents are found as⁵,

$$\begin{aligned} \theta_0 &= \frac{1}{2} - \varepsilon(2\sqrt{2} - 1) + \mathcal{O}(\varepsilon^2) \\ \theta_s &= \frac{1}{2} - \varepsilon + \mathcal{O}(\varepsilon^2) \end{aligned} \quad (1.149)$$

1.14.7 Persistence Probabilities of German DAX and Shanghai Index

Here, a detailed analysis of the persistence probability distributions in financial dynamics has been studied. Compared with the auto-correlation function, the persistence probability distributions describe dynamic correlations non-local in time. Universal and non-universal behaviors of the German DAX and Shanghai Index are analyzed here, and numerical simulations of some microscopic models are also done. At the fixed

point, $z_0 = 0$; the interacting herding model produces the scaling behavior of the real markets²⁵.

Nowadays physicists are paying much interest in the dynamics of financial markets. In many body systems, interactions among agents and producers may generate long range temporal correlations in financial dynamics, and thus results in the dynamic scaling behavior.

In this work, the value of and index(DAX or Shanghai) has been taken as $y(t')$ at the time t' , and the magnitude of the logarithm price change in a fixed time interval Δt as $Z(t', \Delta t) \equiv |\ln y(t' + \Delta t) - \ln y(t')|$. The persistence probability $P_+(t)(P_-(t))$ has been defined persistence probability as the probability that $Z(t' + \tilde{t}, \Delta t)$ has always been above(below) $Z(t', \Delta t)$ in time t , i.e. $Z(t' + \tilde{t}, \Delta t) > Z(t', \Delta t)(Z(t' + \tilde{t}, \Delta t) < Z(t', \Delta t))$ for all $\tilde{t} < t'$. Here $Z(t', \Delta t)$ is defined as the magnitude of the variation of $\ln y(t')$.

The persistence probabilities describe the temporal correlation of $Z(t', \Delta t)$ non-local in time, while the auto-correlation function describes the temporal correlation local in time. Since $Z(t', \Delta t)$ in financial dynamics is long-range correlated in time, one expects a non-trivial dynamic behavior. In this work, they first perform the measurements using the minute-to-minute data of the German Dax from December 1993 to July 1997. The total number of the records during this period of time is about 350 000. In the measurements, $\Delta t = 1 \text{ min}$ has been taken. Plot of the persistence probabilities have been done on a log-log scale. It is obvious that $P_-(t)$ obeys a power law up to four orders of magnitude, while $P_+(t)$ decays to zero rather fast. Compared with the auto-correlation function calculated with the same data, $P_+(t)$ and $P_+(t)$ are much less fluctuating. Different behaviors of $P_+(t)$ and $P_+(t)$ indicate the high-low asymmetry in the time series of $y(t')$. For $P_-(t)$, it is assumed as power law, $P_-(t) \sim t^{-\theta_p}$, θ_p is the so-called persistence exponent. Carefully looking at the curve of $P_-(t)$ of the German DAX, they observe a quasi-periodic dropping in the first 2000 minutes. When one measures the slope in a time interval [500, 20000], the persistence exponent of $P_-(t)$ is $\theta_p = 0.88(2)$, clearly different from a random walk. This indicates that $Z(t', \Delta t)$ is indeed long-range correlated in time.

They have also performed the measurements with the data of the Shanghai Index from January 1998 to July 2003. The time interval between successive records is 5 minute. Similar to the case of the German DAX, $P_-(t)$ obeys a power law and $P_+(t)$ decays faster. A quasi-periodic dropping of $P_-(t)$ in early times is also observed, but the period now is less than 300 minutes, because the working day in China is about or less than five hours in those years. If one measures the slope of the curve in the time interval [500, 20000] the persistence exponent $\theta_p = 0.97(2)$ is obtained.

For further understanding the dynamic behavior of financial markets, they introduce more general persistence probability distributions. Assuming that z_0 is a real positive number, they define the generalized persistence probability $P_+(t, z_0)$ ($P_-(t, z_0)$) as the probability that $Z(t' + \tilde{t}, \Delta t)$ has never been down(up) to $Z(t', \Delta t) - z_0$ ($Z(t', \Delta t) + z_0$) in time t , for all $\tilde{t} < t$. At $z_0 = 0$, $P_+(t, z_0)$ and $P_-(t, z_0)$ coincide with the persistence probabilities found in observational studies. For $P_-(t, z_0)$, a generalized dynamics scaling form can be written as, $P_-(t, z_0) = t^{-\theta_p} F_-(t^{\alpha-} z_0)$, $\alpha-$ is an exponent describing the scaling behavior of z_0 .

In conclusions, they have investigated the persistence probabilities $P_{\pm}(t, z_0)$ defined with the magnitude of the logarithm price change of the financial index, using the data of the German DAX and Shanghai Index. A power-law behavior is observed for $P_-(t, z_0 = 0)$ up to some months for both indices. The minute-to-minute data and daily data of the German DAX consistently yield a same persistence exponent while the minutely data and daily data of the Shanghai Index do not give a same persistence exponent. These results indicate that both the German DAX and Shanghai Index are indeed long-range correlated in time, but they very probably belong to different universality classes.

Appendices

A.1 Slepian's theory

Let $X(t)$ be a real continuous parameter Gaussian process, stationary and continuous in the mean. It is assumed through out that $\langle X(t) \rangle = 0$ and $r(\tau) = \langle X(t)X(t + \tau) \rangle$. Assume that it is being dealt with a separable measurable version of the process. The main concern is the probability $P[T, r(\tau)]$ that $X(t)$ be non-negative for $0 \leq t \leq T$. This quantity is of interest as a means of describing the duration of the excursions taken by the process from its mean. From $P[T, r(\tau)]$ the distribution function $F[\lambda, r(\tau)]$ of the interval between successive zeros of the process can be determined by differentiation.

From its definition, it is clear that $P[T, r(\tau)]$ is a non increasing function of T . It assumes the value $\frac{1}{2}$ for $T = 0$. It obeys the scaling laws,

$$\begin{aligned} P[T, \lambda r(\tau)] &= P[T, r(\tau)] \\ P[T, r(\lambda \tau)] &= P[\lambda T, r(\tau)] \\ \lambda &> 0 \end{aligned} \tag{A.1}$$

It is to be noted, however, that $P[T, r(\tau)]$ for $0 \leq T \leq T_0$ depends only on the "piece" of the covariance function $r(\tau)$, $0 \leq \tau \leq T_0$.

The first scaling law of Eq.(A.1) suggests normalizing the covariances to be considered so that $r(0) = 1$. The second scaling law of Eq.(A.1) suggests that a normalization of the time scale is in order.

According to Slepian, when the scaling laws of Eq.(A.1) are taken into account, there are 'only three distinct covariances for which $P[T, r(\tau)]$ is known explicitly. These are,

(1)

$$\begin{aligned} r_1(\tau) &= e^{-|\tau|}, 0 \leq \tau \leq \infty, \\ P[T, r_1(\tau)] &= \frac{2}{\pi} \sin^{-1} e^{-T}, 0 \leq T < \infty \end{aligned}$$

(2)

$$\begin{aligned} r_2(\beta, \tau) &= 1 - \beta^2 + \beta^2 \cos \tau/\beta, \quad 0 \leq \tau \leq \infty, \quad 0 \leq \beta \leq 1 \\ P[T, r_2(\beta, \tau)] &= \frac{1}{2} - \frac{T}{4\pi} - \frac{1}{2\pi} \sin^{-1} \left[\beta \sin \left(\frac{T}{2\beta} \right) \right], \quad 0 \leq \frac{T}{\beta} \leq 2\pi \\ &= \frac{1}{2} [1 - \beta], \quad 2\pi \leq \frac{T}{\beta} < \infty \end{aligned}$$

(3)

$$\begin{aligned} r_3(\tau) &= 1 - |\tau|, & |\tau| \leq 1 \\ &= 0, & |\tau| \geq 1 \end{aligned}$$

$$P[T, r_3(\tau)] = \frac{1}{4} + \frac{1}{2\pi} \left[\sin^{-1}(1 - T) - \sqrt{T(2 - T)} \right], \quad 0 \leq T \leq 1$$

The process with covariance $r_1(\tau)$ is Markovian, and it is this special property that permits determination of $P[T, r_1(\tau)]$.

Case(2) corresponds to the stochastic process

$$X(t) = A + B \cos \left[\frac{t}{\beta} + \phi \right]$$

with A , B and ϕ independent random variables, the two former being normal with mean zero and variances $1 - \beta^2$ and β^2 respectively, and the latter being distributed uniformly in $(0, 2\pi)$. The determination of P in this case is an exercise in integration and elementary probability theory that will be omitted here. For the obvious generalization of this case, namely,

$$X(t) = A + \sum_1^N B_i \cos \left[\frac{t}{\beta_i} + \phi_i \right]$$

$P[T, r(\tau)]$, can be expressed in principle as a $(2N + 1)$ -fold integral. Except in the case $N = 1$ presented, the integrals appear untractable.

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2

Persistence in Brownian motion of a Free ellipsoidal particle in two dimension

We will investigate the persistence probability $p(t)$ of the position of a Brownian particle with shape asymmetry in two dimensions. The persistence probability is defined as the probability that a stochastic variable has not changed its sign in the given time interval. We explicitly consider two cases- diffusion of a free particle and that of a harmonically trapped particle. The latter is particularly relevant in experiments that use trapping and tracking techniques to measure the displacements. We provide analytical expressions of $p(t)$ that are further validated against numerical simulation and the underlying overdamped dynamics. We also illustrate that $p(t)$ can be a measure to determine the shape asymmetry of a colloid and the translational and rotational diffusivities can be estimated from the measured persistence probability. The advantage of this method is that it does not require the tracking of the orientations of the particle.

Particles that exhibit a shape asymmetry are abundant in nature with sizes ranging from few nanometers to few micrometers. Over the last decade, accelerated by the advancement in particle chemistry, a plethora of such particles with enhanced transport properties have been developed in an attempt to mimic nature. These synthetically engineered colloids with multi-functional properties often find wide ranging applications in photonics, nano and biotechnology, drug delivery and other bio-medical uses. Unlike an isotropic particle, the shape asymmetry leads to different transport properties along the symmetry axes of the particle and any real-life application would require the knowledge of these transport properties. Perhaps, the most crucial of these transport properties are the translational and rotational diffusivities that characterize their stochastic dynamics. For example, the diffusive dynamics of such particles are completely characterized by the mobility matrix.

In this chapter, we determine the persistence probability¹⁻³⁴ of such an extended object. We choose the simplest asymmetric particle – an ellipsoid and look at its two dimensional Brownian motion. The quasi-two-dimensional confinement is assumed to be strong, so that the equations of motion in two-dimensions can be applied. Since the dynamics of the translational and the orientational degrees of freedom are stochastic due to the thermal fluctuations from the bath, the position and the orientation are both random variables in time. We use the stochastic nature of the position to calculate the persistence probability $p(t)$ of the particle. The method has the potential application of extracting the diffusion coefficients along the two symmetry axes of the particle as well the rotational diffusion constant. The method, however, is restrictive due to the non-gaussian nature of the position in the lab frame and is applicable for asymmetric particles with weak anisotropy.

The theory of Brownian motion of a free spherical particle is well studied, but here the study of ellipsoidal particle has been conducted. For ellipsoidal or cylindrical particles, a first-order approximation to a wide variety of asymmetrical molecules, has also been studied. The analysis of Brownian motion of asymmetrical particles is more complicated as compared to that of a spherical particle, as the coupling of rotational and translational motion takes place in this case. In precise, the dependence of the instantaneous translational diffusion coefficient on the current orientation of the particle leads to anisotropic motion for the short time. This will produce substantial changes and complications in solving the Langevin and the Fokker-Planck descriptions of the problem.

These complications are usually overcome by assuming that anisotropic diffusion lasts only for very short times and the isotropic diffusion is recovered for all reasonable times, where we can use simply the mathematical formalism valid for a spherical Brownian particle. The transition in dynamical behavior with time is because of the fact that rotational diffusion ultimately washes out the initial anisotropic translational motion of the particle. The translational diffusion coefficient in long-time equals the average of the translational diffusion coefficients along the two semi-axes of the ellipsoidal or cylindrical particle.

All the results here are mentioned for free asymmetrical particles. In this chapter, we seek to understand how the intrinsic asymmetry of molecules or aggregates affects the persistence probability of a Brownian particle. This study gives us an yet another alternative to determine the diffusion coefficients of such extended object.

This chapter is organized as follows. In Section 2.2 we have presented the Langevin model of the system with detailed Equations in both the body frame and lab frame. The detailed calculation of diffusion coefficients in various situations has been calculated and shown in Section 2.3. The important property persistence has been calculated for the free particle and the simulation results with plots have been placed in the Section 2.4. Finally, a brief conclusion is presented in Section 2.5.

2.2 The Langevin Equations For an Ellipsoidal Particle

We consider an ellipsoidal particle in two dimension with mobilities Γ_{\parallel} and Γ_{\perp} along the x and y direction respectively and a single rotational mobility Γ_{θ} . The particle is immersed in a bath at a temperature T , so that the translational diffusion coefficients along the two directions are given by $D_x = k_B T \Gamma_{\parallel}$, $D_y = k_B T \Gamma_{\perp}$ and the rotational diffusion constant $D_{\theta} = k_B T \Gamma_{\theta}$. In a frame fixed to the particle, the translational and rotational motion of the particle is completely decoupled. However, in the lab-frame, the shape asymmetry of the particle leads to a coupling between the translational and rotational motions of the particle. In the body frame the equations of motion of the particle take the form

$$\begin{aligned}\Gamma_x^{-1} \frac{\partial \tilde{x}}{\partial t} &= F_x \cos \theta(t) + F_y \sin \theta(t) + \tilde{\eta}_x(t) \\ \Gamma_y^{-1} \frac{\partial \tilde{y}}{\partial t} &= F_y \cos \theta(t) + F_x \sin \theta(t) + \tilde{\eta}_y(t) \\ \Gamma_{\theta}^{-1} \frac{\partial \theta}{\partial t} &= \tau + \tilde{\eta}_{\theta}\end{aligned}\tag{2.1}$$

where F_x and F_y are the forces acting on the particle along the x and y directions and τ is the torque acting on the particle. The correlations of the thermal fluctuations in the body frame are given by,

$$\begin{aligned}\langle \tilde{\eta}_i \rangle &= 0 \\ \langle \tilde{\eta}_i(t) \tilde{\eta}_j(t') \rangle &= 2D_i \delta_{ij} \delta(t - t')\end{aligned}\quad (2.2)$$

where $i, j = x, y, \theta$. In the lab frame, the displacements are related to the body frame as,

$$\begin{aligned}\delta x &= \cos \theta \delta \tilde{x} - \sin \theta \delta \tilde{y} \\ \delta y &= \cos \theta \delta \tilde{y} + \sin \theta \delta \tilde{x}\end{aligned}\quad (2.3)$$

Using the transformation relation of Eq. 2.3 we can convert equations of motion in Eq.

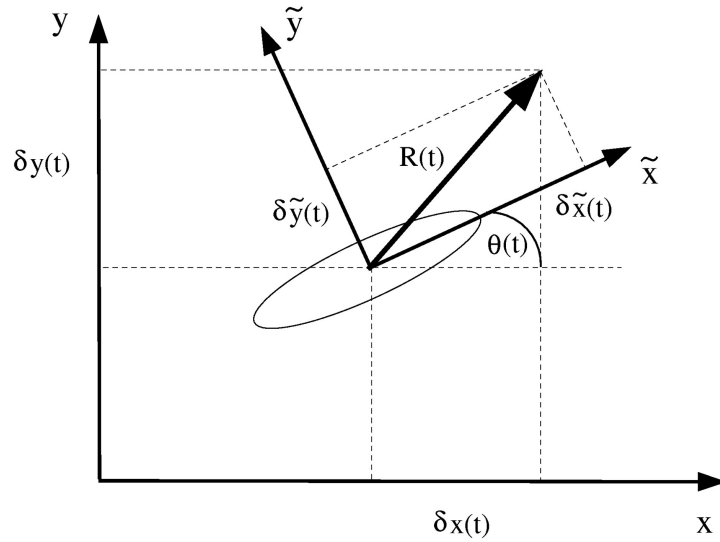


Figure 2.1 Representation of an ellipsoid in the $x - y$ lab frame and the $\tilde{x} - \tilde{y}$ body frame. The angle between two frames is θ . The displacement \mathbf{R} can be decomposed as $(\delta \tilde{x}, \delta \tilde{y})$ or $(\delta x, \delta y)$.

2.1 as

$$\begin{aligned}\frac{\partial x(t)}{\partial t} &= F_x \left[\bar{\Gamma} + \frac{\Delta \Gamma}{2} \cos 2\theta \right] + F_y \frac{\Delta \Gamma}{2} \sin 2\theta + \eta_x(t) \\ \frac{\partial y(t)}{\partial t} &= F_x \frac{\Delta \Gamma}{2} \sin 2\theta + F_y \left[\bar{\Gamma} - \frac{1}{2} \Delta \Gamma \cos 2\theta(t) \right] + \eta_y(t) \\ \frac{\partial \theta(t)}{\partial t} &= \Gamma_\theta \tau + \eta_\theta(t)\end{aligned}\quad (2.4)$$

with the quantities $\bar{\Gamma} = (\Gamma_{\parallel} + \Gamma_{\perp})/2$ and $\Delta \Gamma = \Gamma_{\parallel} - \Gamma_{\perp}$, are the average and difference mobilities of the body, respectively.

Using Eq. (2.1), the corresponding Langevin equation in the lab frame is given by,

$$\frac{\partial x_i}{\partial t} = -\Gamma_{ij} \frac{\partial U}{\partial x_j} + \eta_i \quad (2.5)$$

where $U(\mathbf{r})$ is the external potential and $\mathbf{\Gamma}$ is the mobility tensor given by,

$$\overline{\overline{\mathbf{\Gamma}}} = \begin{bmatrix} \overline{\Gamma} + \frac{\Delta\Gamma}{2} \cos 2\theta & \frac{\Delta\Gamma}{2} \sin 2\theta \\ \frac{\Delta\Gamma}{2} \sin 2\theta & \overline{\Gamma} - \frac{\Delta\Gamma}{2} \cos 2\theta \end{bmatrix} \quad (2.6)$$

In the component form, the mobility tensor is given by $\Gamma_{ij} = \overline{\Gamma} \delta_{ij} + \frac{\Delta\Gamma}{2} \Delta\mathcal{R}_{ij}[\theta(t)]$, where the form of $\Delta\mathcal{R}$ is given by

$$\Delta\overline{\overline{\mathcal{R}}} = \begin{bmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{bmatrix} \quad (2.7)$$

Using the correlation of the thermal fluctuations from Eq. (2.2), the moments of the stochastic forces are given by,

$$\langle \eta_i \rangle = 0 \quad (2.8)$$

$$\langle \eta_i(t) \eta_j(t') \rangle_{\theta(t)}^{\eta_x, \eta_y} = 2k_B T \Gamma_{ij}[\theta(t)] \delta(t - t') \quad (2.9)$$

$$\langle \eta_\theta(t) \eta_\theta(t') \rangle^{\eta_\theta} = 2D_\theta \delta(t - t') \quad (2.10)$$

The statistical averages have superscripts to indicate over which noise is the average taken and subscripts denote that quantities which are kept fixed. It is to be noted that the movement in the x and y directions are not independent of each other but they are coupled through the angular position of the particle. Thus particle's translational diffusion couples to its rotational diffusion and the strength of this coupling behaviour increases proportionally with particle shape asymmetry, but this is zero for spherical particle. Inspection of Eq. (2.4) reveals that this phenomenon cannot affect the long-time average velocity of the particle but could affect the long-time mean square displacements.

2.3 Diffusion Coefficients of Ellipsoidal Particle in a Constant Field Force

In this section, we are aiming to calculate the temporal variation of the diffusion coefficients of an ellipsoidal particle under constant force field which is constrained to move in a plane. We shall calculate the three translational diffusion coefficients, namely, the one along x direction (D_{11}), the one in the y direction (D_{22}), and the cross-diffusion co-

efficient ($D_{12} = D_{21}$). The general formula for diffusion coefficient is,

$$D_{ij}(t) = \frac{\langle \Delta x_i(t) \Delta x_j(t) \rangle_{\theta_0}^{\eta_x, \eta_y, \eta_\theta} - \langle \Delta x_i(t) \rangle_{\theta_0}^{\eta_x, \eta_y, \eta_\theta} \langle \Delta x_j(t) \rangle_{\theta_0}^{\eta_x, \eta_y, \eta_\theta}}{2t} \quad (2.11)$$

Here $(x_1, x_2) = (x, y)$.

Let us now calculate D_{11} in details. Let us integrate Eq. (2.4) with respect to time, we get

$$\Delta x_1(t) = F_x \bar{\Gamma} t + \frac{\Delta \Gamma}{2} F_x \int_0^t \cos 2\theta(t') dt' + \frac{\Delta \Gamma}{2} F_y \int_0^t \sin 2\theta(t') dt' + \int_0^t \eta_x(t') dt' \quad (2.12)$$

Now we will calculate the average displacement in the x direction. The ensemble average of the sinusoidal functions can be calculated by considering the angular displacement $\Delta\theta(t) = \theta(t) - \theta_0$ is a Gaussian random variable, in which case the listed identity is valid:

$$\langle e^{i[m\Delta\theta(t') \pm n\Delta\theta(t'')] } \rangle_{\theta_0}^{\eta_\theta} = e^{-D_\theta [m^2 t' + n^2 t'' \pm 2mn \min(t', t'')]} \quad (2.13)$$

This implies $\langle \cos n\theta(t) \rangle_{\theta_0}^{\eta_\theta} = \cos n\theta_0 e^{-n^2 D_\theta t}$ and $\langle \sin n\theta(t) \rangle_{\theta_0}^{\eta_\theta} = \sin n\theta_0 e^{-n^2 D_\theta t}$. And the average of the translational noise η_x is zero. Now we can find average displacement along x direction from Eq. (2.12), which is

$$\begin{aligned} \langle \Delta x_1(t) \rangle &= F_x \bar{\Gamma} t + \frac{\Delta \Gamma}{2} F_x \int_0^t \langle \cos 2\theta(t') \rangle dt' + \frac{1}{2} \Delta \Gamma F_y \int_0^t \langle \sin 2\theta(t') \rangle dt' \\ &= F_x \bar{\Gamma} t + \frac{\Delta \Gamma}{2} F_x \int_0^t \cos 2\theta_0 e^{-4D_\theta t'} dt' + \frac{1}{2} \Delta \Gamma F_y \int_0^t \sin 2\theta_0 e^{-4D_\theta t'} dt' \\ &= F_x \bar{\Gamma} t + \frac{\Delta \Gamma}{2} F_x \cos 2\theta_0 \frac{1}{4D_\theta} (1 - e^{-4D_\theta t}) + \frac{1}{2} \Delta \Gamma F_y \sin 2\theta_0 \frac{1}{4D_\theta} (1 - e^{-4D_\theta t}) \\ &= F_x \bar{\Gamma} t + \frac{\Delta \Gamma}{2} F_x \cos 2\theta_0 \tau_4(t) + \frac{1}{2} \Delta \Gamma F_y \sin 2\theta_0 \tau_4(t) \end{aligned} \quad (2.14)$$

Where we have considered $\tau_n = \frac{1}{nD_\theta} (1 - e^{-4D_\theta t})$

To compute mean-squared displacement we take square of Eq. (2.12) and average it, thus we get

$$\begin{aligned} \langle \Delta x_1^2(t) \rangle &= F_x^2 \bar{\Gamma}^2 t^2 + \frac{1}{4} \Delta \Gamma^2 F_x^2 \int_0^t \int_0^t \langle \cos 2\theta(t') \cos 2\theta(t'') \rangle dt' dt'' \\ &\quad + \frac{1}{4} \Delta \Gamma^2 F_y^2 \int_0^t \int_0^t \langle \sin 2\theta(t') \sin 2\theta(t'') \rangle dt' dt'' + \int_0^t \int_0^t \langle \eta_x(t') \eta_x(t'') \rangle dt' dt'' \\ &\quad + \frac{1}{2} F_x^2 \bar{\Gamma} \Delta \Gamma t \int_0^t \langle \cos 2\theta(t') \rangle dt' + \frac{1}{2} F_x F_y \Delta \Gamma \bar{\Gamma} t \int_0^t \langle \sin 2\theta(t') \rangle dt' \\ &\quad + \frac{1}{4} \Delta \Gamma^2 F_x F_y \int_0^t \int_0^t \langle \cos 2\theta(t') \sin 2\theta(t'') \rangle dt' dt'' \end{aligned} \quad (2.15)$$

We have removed two integrals comprising products of sinusoidal functions of the particle's angle $\theta(t)$ and of translational noise η_x , as these two terms are zero. Now, we will calculate the integrals separately. Let us first calculate the second integral.

Let us use $\Delta\theta(t) = \theta(t) - \theta_0$ in the second integral, which becomes

$$\begin{aligned}
& \int_0^t \int_0^t \langle \cos 2\theta(t') \cos 2\theta(t'') \rangle dt' dt'' \\
&= \frac{1}{2} \int_0^t \int_0^t \left[\langle \cos(4\theta_0 + 2\Delta\theta(t') + 2\Delta\theta(t'')) \rangle + \langle \cos(2\Delta\theta(t') - 2\Delta\theta(t'')) \rangle \right] dt' dt'' \\
&= \frac{1}{2} \int_0^t \int_0^t \left[\cos 4\theta_0 e^{-4D_\theta[t'+t''+2\min(t',t'')]} + e^{-4D_\theta[t'+t''-2\min(t',t'')]} \right] dt' dt'' \\
&= \cos 4\theta_0 I_a + I_b
\end{aligned} \tag{2.16}$$

We have calculated integrals I_a and I_b of Eq. (2.16) separately.

$$\begin{aligned}
I_a &= \frac{1}{2} \int_0^t dt' \int_0^{t'} dt'' e^{-4D_\theta[3t''+t']} + \frac{1}{2} \int_0^t dt'' \int_0^{t''} dt' e^{-4D_\theta[3t'+t'']} \\
&= \frac{3 + e^{-16D_\theta t} - 4e^{-4D_\theta t}}{192D_\theta^2}
\end{aligned} \tag{2.17}$$

$$\begin{aligned}
I_b &= \frac{1}{2} \int_0^t dt' \int_0^{t'} dt'' e^{-4D_\theta(t'-t'')} + \frac{1}{2} \int_0^t dt'' \int_0^{t''} dt' e^{-4D_\theta(t''-t')} \\
&= \frac{4D_\theta t + e^{-4D_\theta t} - 1}{16D_\theta^2}
\end{aligned} \tag{2.18}$$

Similarly we have calculated

$$\int_0^t \int_0^t \langle \sin 2\theta(t') \sin 2\theta(t'') \rangle dt' dt'' = I_b - \cos 4\theta_0 I_a \tag{2.19}$$

$$\int_0^t \int_0^t \langle \sin 2\theta(t') \cos 2\theta(t'') \rangle dt' dt'' = \sin 4\theta_0 I_a \tag{2.20}$$

The integral $\int_0^t dt' \int_0^t dt'' \langle \eta_x(t') \eta_x(t'') \rangle$ can be calculated as

$$\begin{aligned}
\int_0^t dt' \int_0^t dt'' \langle \eta_x(t') \eta_x(t'') \rangle &= 2k_B T \int_0^t dt' \int_0^t dt'' \langle \Gamma_{ii}[\theta(t')] \rangle_{\eta_\theta} \delta(t' - t'') \\
&= 2k_B T \int_0^t dt' \left[\bar{\Gamma} + \frac{\Delta\Gamma}{2} \langle \cos 2\theta(t') \rangle_{\eta_\theta} \right] \\
&= 2k_B T \bar{\Gamma} t + k_B T \Delta\Gamma \cos 2\theta_0 \frac{1 - e^{-4D_\theta t}}{4D_\theta} \\
&= 2\bar{D}t + \Delta D \cos 2\theta_0 \frac{1 - e^{-4D_\theta t}}{4D_\theta}
\end{aligned} \tag{2.21}$$

We have considered diffusion coefficients of the particle in directions parallel and per-

pendicular to its longest axis are $D_{\parallel} = k_B T \Gamma_{\parallel}$ and $D_{\perp} = k_B T \Gamma_{\perp}$, respectively. Here, $\bar{D} = k_B T \bar{\Gamma}$ and $\Delta D = k_B T \Delta \Gamma$.

Using all values of Eqs. (2.16) (2.17), (2.18), (2.19), (2.20), (2.21) we can calculate the value of mean-square displacement along x direction of Eq. (2.15).

$$\begin{aligned}
\langle \Delta x_1^2(t) \rangle &= 2\bar{D}t + \frac{\Delta D}{4D_{\theta}} \cos 2\theta_0 (1 - e^{-4D_{\theta}t}) + F_x^2 \bar{\Gamma}^2 t^2 + \frac{1}{4} \Delta \Gamma^2 F_x^2 \left(\cos 4\theta_0 \frac{3 + e^{-16D_{\theta}t} - 4e^{-4D_{\theta}t}}{192D_{\theta}^2} + \right. \\
&\quad \left. \frac{4D_{\theta}t + e^{-4D_{\theta}t} - 1}{16D_{\theta}^2} \right) + \frac{1}{4} \Delta \Gamma^2 F_y^2 \left(\frac{4D_{\theta}t + e^{-4D_{\theta}t} - 1}{16D_{\theta}^2} - \cos 4\theta_0 \frac{3 + e^{-16D_{\theta}t} - 4e^{-4D_{\theta}t}}{192D_{\theta}^2} \right) \\
&\quad + \frac{1}{2} F_x^2 \bar{\Gamma} \Delta \Gamma t \cos 2\theta_0 \frac{1}{4D_{\theta}} (1 - e^{-4D_{\theta}t}) + \frac{1}{2} F_x F_y \Delta \Gamma \bar{\Gamma} t \sin 2\theta_0 \frac{1}{4D_{\theta}} (1 - e^{-4D_{\theta}t}) \\
&\quad + \frac{1}{4} \Delta \Gamma^2 F_x F_y \sin 4\theta_0 \frac{3 + e^{-16D_{\theta}t} - 4e^{-4D_{\theta}t}}{192D_{\theta}^2}
\end{aligned} \tag{2.22}$$

Now to calculate D_{11} we have calculated the value of $\langle \Delta x_1(t) \rangle \langle \Delta x_1(t) \rangle$, we use Eq. (2.14) and it becomes

$$\begin{aligned}
\langle \Delta x_1(t) \rangle \langle \Delta x_1(t) \rangle &= F_x^2 \bar{\Gamma}^2 t^2 + \frac{1}{4} \Delta \Gamma^2 F_x^2 \cos^2 2\theta_0 \frac{1}{16D_{\theta}^2} (1 - e^{-4D_{\theta}t})^2 \\
&\quad + \frac{1}{4} \Delta \Gamma^2 F_y^2 \sin^2 2\theta_0 \frac{1}{16D_{\theta}^2} (1 - e^{-4D_{\theta}t})^2 + \frac{1}{4D_{\theta}} F_x^2 \Delta \Gamma t \bar{\Gamma} \cos 2\theta_0 (1 - e^{-4D_{\theta}t}) \\
&\quad + \frac{1}{4D_{\theta}} F_x F_y \Delta \Gamma \bar{\Gamma} t \sin 2\theta_0 (1 - e^{-4D_{\theta}t}) + \frac{1}{4} \Delta \Gamma^2 F_x F_y \cos 2\theta_0 \sin 2\theta_0 \frac{1}{16D_{\theta}^2} (1 - e^{-4D_{\theta}t})^2
\end{aligned} \tag{2.23}$$

from these two Eq. (2.22) and Eq. (2.23) we find D_{11} from Eq. (2.11)

$$\begin{aligned}
D_{11} &= \bar{D} + \frac{\Delta \Gamma^2}{32D_{\theta}} (F_x^2 + F_y^2) + \frac{1}{2t} \left[\frac{\Delta \Gamma^2 \cos 4\theta_0}{768D_{\theta}^2} (F_x^2 - F_y^2 + 2F_x F_y \tan 4\theta_0) \right. \\
&\quad \times (3 + e^{-16D_{\theta}t} - 4e^{-4D_{\theta}t}) + \frac{\Delta \Gamma^2 (F_x^2 + F_y^2)}{64D_{\theta}^2} (e^{-4D_{\theta}t} - 1) + \frac{\Delta D \cos 2\theta_0}{4D_{\theta}} (1 - e^{-4D_{\theta}t}) \\
&\quad \left. - \frac{\Delta \Gamma^2}{64D_{\theta}^2} (1 - e^{-4D_{\theta}t})^2 (F_x \cos 2\theta_0 + F_y \sin 2\theta_0)^2 \right]
\end{aligned} \tag{2.24}$$

Similarly we can calculate the average displacement along y direction from Eq. (2.4)

$$\Delta y_1(t) = F_y \bar{\Gamma} t - \frac{1}{2} F_y \Delta \Gamma \int_0^t \cos 2\theta(t') dt' + \frac{\Delta \Gamma}{2} F_x \int_0^t \sin 2\theta(t') + \int_0^t \eta_y(t') dt'$$

By a similar calculation, one obtains the translational diffusion coefficient in the y -direction (D_{22}) and the cross-diffusion coefficient (D_{12}). The expression for D_{22} can be

obtained from that for D_{11} by interchanging F_x and F_y , and replacing $\cos 2\theta_0$ by $-\cos 2\theta_0$.

The cross-diffusion term is given by³⁵,

$$D_{12} = \frac{\Delta D \sin 2\theta_0}{8D_{\theta}t} + \frac{1}{2t} \left[\frac{F_x F_y \Delta \Gamma^2 \cos 4\theta_0}{D_{\theta}^2} \left(\frac{1}{128} - \frac{1}{48} e^{-4D_{\theta}t} + \frac{1}{64} e^{-8D_{\theta}t} - \frac{1}{384} e^{-16D_{\theta}t} \right) \right. \\ \left. + \frac{(F_x^2 - F_y^2) \Delta \Gamma^2 \sin 4\theta_0}{D_{\theta}^2} \left(\frac{1}{256} - \frac{1}{96} e^{-4D_{\theta}t} + \frac{1}{128} e^{-8D_{\theta}t} - \frac{1}{768} e^{-16D_{\theta}t} \right) \right]$$

For the case of zero forces the above expression reduces to the simple forms,

$$\begin{aligned} D_{11}(t) &= \bar{D} + \frac{\Delta D}{8D_{\theta}t} \cos 2\theta_0 (1 - e^{-4D_{\theta}t}) \\ D_{22}(t) &= \bar{D} - \frac{\Delta D}{8D_{\theta}t} \cos 2\theta_0 (1 - e^{-4D_{\theta}t}) \\ D_{12}(t) &= \frac{\Delta D}{8D_{\theta}t} \sin 2\theta_0 (1 - e^{-4D_{\theta}t}) \end{aligned} \quad (2.25)$$

2.4 Calculation of Persistence of a free ellipsoidal Particle

We first look at the case of a free ellipsoidal particle. Setting the external potential to zero, the formal solution to the equation of motion takes the form

$$x_i(t) = \int_0^t \eta_i(t') + x_i(0) \quad (2.26)$$

The mean-square displacement of the particle, averaged over the orientational noise can be explicitly calculated from the above equation as,

$$\begin{aligned} \langle \Delta x_i^2 \rangle_{\eta_{\theta}} &= \int_0^t dt' \int_0^t dt'' \langle \eta_i(t') \eta_i(t'') \rangle \\ &= 2k_B T \int_0^t dt' \int_0^t dt'' \langle \Gamma_{ii}[\theta(t')] \rangle_{\eta_{\theta}} \delta(t' - t'') \\ &= 2k_B T \int_0^t dt' \langle \Gamma_{ii}[\theta(t')] \rangle_{\eta_{\theta}} \end{aligned} \quad (2.27)$$

Using the explicit form of Γ_{xx} the mean-square displacement along the x -direction reads

$$\langle \Delta x_1^2 \rangle_{\eta_{\theta}} = 2k_B T \int_0^t dt' \left[\bar{\Gamma} + \frac{\Delta \Gamma}{2} \langle \cos 2\theta(t') \rangle_{\eta_{\theta}} \right] \quad (2.28)$$

The ensemble average of $\cos \theta(t)$ over the thermal fluctuations in the orientational degrees of freedom can be done explicitly by noting the fact that $\Delta \theta = \theta(t) - \theta_0$ is a

Gaussian random variable and consequently the following identity holds:

$$\langle e^{\pm \beta m \Delta \theta(t')} \rangle = e^{-m^2 D_\theta t'} \quad (2.29)$$

Using Eq.(2.29) in Eq. (2.28), we finally arrive at

$$\langle \Delta x^2 \rangle_{\eta_\theta} = 2k_B T \left[\bar{\Gamma} t + \frac{\Delta \Gamma}{2} \cos 2\theta_0 \left(\frac{1 - e^{4D_\theta t}}{4D_\theta} \right) \right] \quad (2.30)$$

and

$$\langle \Delta y^2 \rangle_{\eta_\theta} = 2k_B T \left[\bar{\Gamma} t - \frac{\Delta \Gamma}{2} \sin 2\theta_0 \left(\frac{1 - e^{4D_\theta t}}{4D_\theta} \right) \right] \quad (2.31)$$

The above results are well known^{35,36} and have also been experimentally verified³⁶. However, our interest lies in the persistence probability of this system. The route to determine the persistence probability using the results of Slepian is applicable for a Gaussian stochastic process³⁷. In contrast, the body-frame coordinates are non-Gaussian in nature. The non-Gaussian parameter is defined as

$$\phi(t, \theta_0) = \frac{\langle \Delta x(t)^4 \rangle}{3 \langle \Delta x(t)^2 \rangle^2} - 1 \quad (2.32)$$

$$\begin{aligned} \langle \Delta x_i(t) \Delta x_j(t) \rangle_{\theta_0} &= 2\bar{D}t + \Delta D M_{ij}(\theta_0) \int_0^t dt' e^{-4D_\theta t'} \\ &= 2\bar{D}t + \Delta D M_{ij}(\theta_0) \tau_4(t) \end{aligned} \quad (2.33)$$

and

$$\begin{aligned} \langle \Delta x(t)^4 \rangle &= \int_0^t dt_1 \dots dt_4 \langle \eta_x(t_1) \eta_x(t_2) \eta_x(t_3) \eta_x(t_4) \rangle \\ &= 12(k_B T)^2 \int_0^t dt_1 \int_0^t dt_2 \langle \Gamma_{xx}(\theta(t_1)) \Gamma_{xx}(\theta(t_2)) \rangle_{\eta_\theta} \\ &= 12(k_B T)^2 \int_0^t dt_1 \int_0^t dt_2 \left(\bar{\Gamma}^2 + \frac{1}{2} \Delta \Gamma \bar{\Gamma} \langle \cos 2\theta(t_1) + \cos 2\theta(t_2) \rangle + \frac{1}{4} (\Delta \Gamma)^2 \langle \cos 2\theta(t_1) \cos 2\theta(t_2) \rangle \right) \\ &= 12 \left[\bar{D}^2 t^2 + \Delta D \bar{D} t \cos 2\theta_0 \tau_4(t) + \frac{(\Delta D)^2}{8} \left(\tau_\theta(t - \tau_4(t)) + \cos 4\theta_0 \frac{\tau_\theta(\tau_4(t) - \tau_{16}(t))}{3} \right) \right] \end{aligned} \quad (2.34)$$

We have used,

$$\langle \cos 2\theta_1 \cos 2\theta_2 \rangle = \frac{1}{2} [\langle \cos 2(\theta_1 - \theta_2) \rangle + \langle \cos 2(\theta_1 + \theta_2) \rangle] \quad (2.35)$$

and

$$\begin{aligned}\langle \cos 2[\theta(t_1) - \theta(t_2)] \rangle &= e^{-4D_\theta |t_1 - t_2|} \\ \langle \cos 2[\theta(t_1) + \theta(t_2)] \rangle &= \cos 4\theta_0 e^{-4D_\theta [t_1 + t_2 + 2\min(t_1, t_2)]}\end{aligned}\quad (2.36)$$

Using Eq.(2.33) and Eq.(2.34) non-Gaussian parameter takes the form,

$$\phi(t, \theta_0) = \frac{1}{24} \left(\frac{\Delta D}{D} \right)^2 \frac{[3(\tau_\theta t - \tau_\theta \tau_4(t) - \tau_4(t)^2) + (\tau_\theta \tau_4(t) - \tau_\theta \tau_1 6(t) - 3\tau_4(t)^2) \cos 4\theta_0]}{\left[t + \left(\frac{\Delta D}{D} \right) \tau_4(t) \cos 2\theta_0 \right]^2} \quad (2.37)$$

where $\tau_\theta = 1/2D_\theta$ and $\tau_n(t) = \int_0^t dt' e^{-4D_\theta t'} = (1 - e^{-nD_\theta t})/nD_\theta$. An average over the initial orientation leads to the result,

$$\bar{\phi}(t) = \frac{1}{8} \left(\frac{\Delta D}{\bar{D}} \right)^2 \frac{\tau_\theta (t - \tau_4(t))}{t^2} \quad (2.38)$$

Clearly, for a weak asymmetry, the non-Gaussian parameter is vanishingly small. $\phi(t, \theta_0)$ exhibits a maximum at $t = \tau_\theta$ and vanishes for $t \ll \tau_\theta$ as well as $t \gg \tau_\theta$. Hence, for large and small times, the body-frame coordinates remain a Gaussian stochastic process.

To calculate the persistence of a free ellipsoidal Brownian particle, we start with Eq.(2.26) and choose $x_i(0) = 0$. The calculation of the two time correlation function

$$\langle x(t_1)x(t_2) \rangle_{\eta_\theta} = \int_0^{t_1} dt' \int_0^{t_2} dt'' \langle \eta_x(t') \eta_x(t'') \rangle_{\eta_\theta} \quad (2.39)$$

Taking $t_1 > t_2$, the integral evaluates to the following expression for the two time correlation,

$$\langle x(t_1)x(t_2) \rangle_{\eta_\theta} = 2k_B T \bar{\Gamma} t_2 \left[1 + \frac{\Delta \Gamma}{2\bar{\Gamma}} \cos \theta_0 \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta t_2} \right) \right] \quad (2.40)$$

In order to transform the non-stationary correlation into a stationary correlation we first make the transformation $\bar{X}(t) = x(t)/\sqrt{\langle x^2(t) \rangle_{\eta_\theta}}$, and the correlation $\langle \bar{X}(t_1)\bar{X}(t_2) \rangle_{\eta_\theta}$ reads as

$$\langle \bar{X}(t_1)\bar{X}(t_2) \rangle_{\eta_\theta} = \sqrt{\frac{2\bar{D}t_2}{2\bar{D}t_1}} \sqrt{\frac{\left[1 + \frac{\Delta \Gamma}{2\bar{\Gamma}} \cos \theta_0 \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta t_2} \right) \right]}{\left[1 + \frac{\Delta \Gamma}{2\bar{\Gamma}} \cos \theta_0 \left(\frac{1 - e^{-4D_\theta t_1}}{4D_\theta t_1} \right) \right]}} \quad (2.41)$$

We now define the transformation in time as

$$e^T = 2\bar{D}t \left[1 + \frac{\Delta D}{2\bar{D}} \cos \theta_0 \left(\frac{1 - e^{-4D_\theta t}}{4D_\theta t} \right) \right] \quad (2.42)$$

and Eq. (2.41) takes the simple form of

$$\langle \bar{X}(T_1) \bar{X}_2(T_2) \rangle_{\eta_\theta} = e^{-(T_1 - T_2)/2} \quad (2.43)$$

Following Slepian³⁷, if the correlation function of a stochastic variable $X(T)$ decays exponentially for all times $C_{XX}(T) = e^{-\lambda T}$, then the persistence probability is given by

$$P(T) \sim \sin^{-1} e^{-\lambda T} \quad (2.44)$$

Asymptotically, $P(T)$ takes the form $P(T) \sim e^{-\lambda T}$. Consequently, looking at Eq. (2.38) and transforming back in real time t , the persistence probability reads as

$$p(t) \sim \frac{1}{\sqrt{2Dt}} \frac{1}{\sqrt{1 + \frac{\Delta D}{2D} \cos \theta_0 \left(\frac{1 - e^{-4D\theta t}}{4D\theta t} \right)}} \quad (2.45)$$

In the absence of any asymmetry, the expression for $p(t)$ correctly reproduces the persistence probability of that of a random walker³⁸. Rearranging Eq. (2.45), the quantity $t^{1/2}p(t)$ can be recast as

$$t^{1/2}p(t) \sim \frac{1}{\sqrt{2D}} \left[1 + \frac{\Delta D}{2D} \cos \theta_0 \left(\frac{1 - e^{-4\tau}}{8\tau} \right) \right]^{-1/2} \quad (2.46)$$

In the limit of $\Delta D \rightarrow 0$, the persistence probability reduces to that of a random walker $p(t) \sim t^{-1/2}$.

To test Eq.(2.45), we performed numerical integration of the equations of the equations of motion using an Euler scheme for discretization. The initial condition was chosen from a Gaussian distribution with a very small width, so that the sign of $\mathbf{r}(0)$ is clearly defined. The trajectories was evolved in time with an integration time-step of $\delta t = 0.001$. At every instant the survival of the particle was checked by looking at the sign of $\mathbf{r}(t)$. Fraction of trajectories for which the position did not change its sign up to time t gave the survival probability $p(t)$. A total of 10^9 trajectories were used in estimating the survival probability. A comparison of the measured $p(t)$ with that of the predictions of Eq.(2.45) is shown Fig.(2.2) and Fig.(4.3). The comparison in Fig.(2.2) clearly shows that the survival probability can pick up the asymmetry in particle shape even when the difference in the diffusivities is as small as 5%.

The process to extract the diffusion coefficients is as follows:

The first step would be to determine the overall constant is given by $\mathcal{A} = (2/\pi)\sqrt{2\bar{\Gamma}\delta t}$.

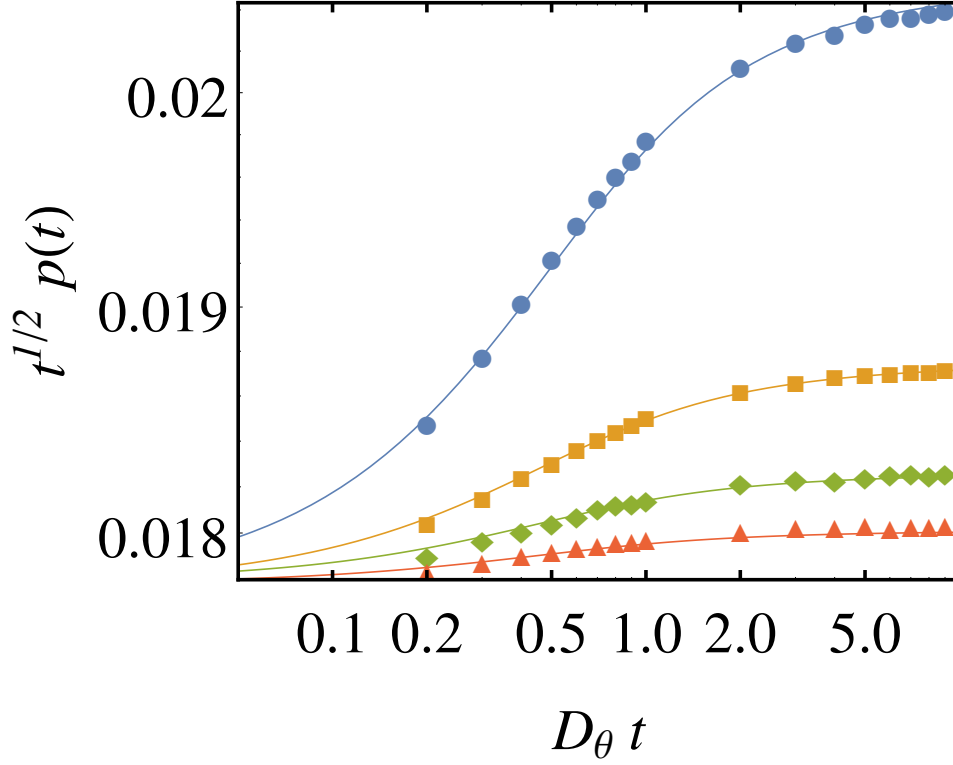


Figure 2.2 Plot of $t^{1/2}p(t)$ for different choices of translational diffusivities of the anisotropic particle: $D_{\parallel} = 1, D_{\perp} = 0.5$ (blue circles); $D_{\parallel} = 1, D_{\perp} = 0.8$ (orange squares); $D_{\parallel} = 1, D_{\perp} = 0.9$ (green diamonds); and $D_{\parallel} = 1, D_{\perp} = 0.95$ (red triangles). The rotational diffusion constant and the initial angle θ_0 , respectively. The solid lines are fit to the data using Eq.(2.46). The fit yields the overall constant \mathcal{A} . The estimated values of \mathcal{A} from the fit are 0.025132 ± 0.000014 for $D_{\parallel} = 1, D_{\perp} = 0.5$, 0.025144 ± 0.000011 for $D_{\parallel} = 1, D_{\perp} = 0.8$, 0.025166 ± 0.000012 for $D_{\parallel} = 1, D_{\perp} = 0.9$ and 0.025148 ± 0.000019 for $D_{\parallel} = 1, D_{\perp} = 0.95$

In Fig.5, we show a plot of \mathcal{A} as a function of the scaled variable $\sqrt{\frac{8\bar{\Gamma}\delta t}{\pi^2}}$. Since the value of $\bar{\Gamma}$ is a priori not known. \mathcal{A} can be fixed by fitting the data with the form of $p(t)$ given in the Eq.(2.45). This fit yields the value of \mathcal{A} . In Fig.(2.2), we have shown this fitting for different choices of diffusivities with \mathcal{A} as the fit parameter. The value of \mathcal{A} is solely determined by the integration time step used to estimate $p(t)$, and the estimated values from the fit are given in the caption of Fig.(2.2). An alternative way to determine \mathcal{A} is to measure the persistence probability of an isotropic particle in which case $p(t) \sim \mathcal{A}/\sqrt{2Dt}$. Once this number is known, we look at the quantity $t^{1/2}p(t)/\mathcal{A}$. In the limit of $t \rightarrow 0$, $t^{1/2}p(t)/\mathcal{A} \rightarrow (2\bar{D} + \Delta D)^{-1/2}$, and in the limit of $t \rightarrow \infty$, $t^{1/2}p(t)/\mathcal{A} \rightarrow (2\bar{D})^{-1/2}$.

Once we know the two diffusivities and therefore \bar{D} , the rotational diffusion constant

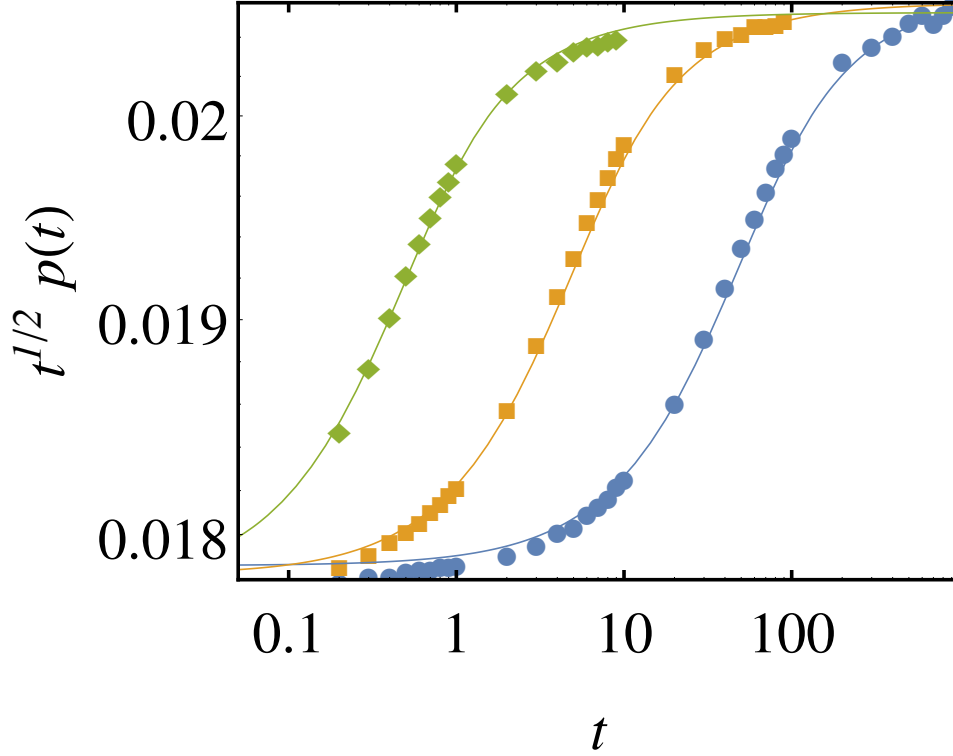


Figure 2.3 Plot of $t^{1/2}p(t)$ for different choices of the rotational diffusion constant of the anisotropic particle: $D_\theta = 0.01$ (blue circles), $D_\theta = 0.1$ (orange squares), and $D_\theta = 1$ (green diamonds). The translational diffusion constants in all three cases were $D_{\parallel} = 1$ and $D_{\perp} = 0.5$, and the initial orientation was fixed at $\theta_0 = 0$

can be determined from the quantity $\left(\mathcal{A}/\sqrt{2\bar{D}t}p(t)\right)^2$, which goes as

$$\tilde{p}(t) \equiv \left(\frac{\mathcal{A}}{\sqrt{2\bar{D}t}p(t)}\right)^2 = 1 + \left(\frac{\Delta D}{\bar{D}}\right) \left(\frac{1 - e^{-4D_\theta t}}{8D_\theta t}\right) \quad (2.47)$$

A fit to $\tilde{p}(t)$ with D_θ as a fit parameter would yield the value of the rotational diffusion coefficient. This is illustrated in the Fig.(2.5). In fact, fitting the data for \tilde{p} with $\Delta D/\bar{D}$ and D_θ as fit parameters yields very good estimates for $\Delta D/\bar{D}$ and D_θ . A comparison of these values obtained from the fit with the actual values is shown on the Table 2.1

It should be pointed out that the values of $\Delta D/\bar{D}$ and D_θ obtained from the fit are sensitive to the value \mathcal{A} , and a careful estimation of \mathcal{A} is of paramount importance.

Before we conclude, we would like to remark on the expression for the persistence

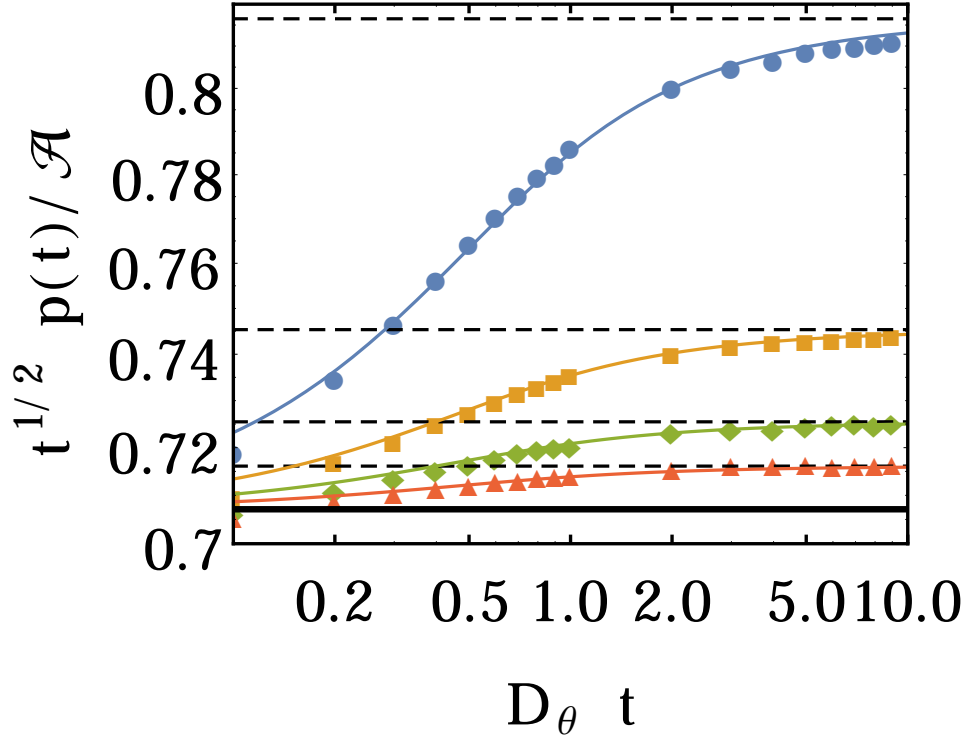


Figure 2.4 Plot of $t^{1/2} p(t) / \mathcal{A}$ for different choices of translational diffusivities of the anisotropic particle: $D_{\parallel} = 1, D_{\perp} = 0.5$ (blue circles); $D_{\parallel}, D_{\perp} = 0.9$ (green diamonds); $D_{\parallel} = 1, D_{\perp} = 0.95$ (red triangles). The rotational diffusion constant and the initial orientation were fixed at $D_{\theta} = 1$ and $\theta_0 = 0$, respectively. The black solid line indicates the value of $1/\sqrt{2\bar{D} + \Delta\bar{D}} = 1/\sqrt{D_{\parallel}} = 1/\sqrt{2}$, whereas the dashed lines indicates the values of $1/\sqrt{2\bar{D}}$. For the choice translational diffusivities, the indicated values from top are $1/\sqrt{2\bar{D}} \approx 0.8165, 0.7454, 0.7255$, and 0.7161 .

$\Delta D/\bar{D}$	D_{θ}	Estimated $\Delta D/\bar{D}$	Estimated D_{θ}
	0.01	0.6698 ± 0.0018	0.0117 ± 0.0002
2/3	0.10	0.6799 ± 0.002	0.1146 ± 0.0009
	1.00	0.681 ± 0.0295	1.076 ± 0.06

Table 2.1 A comparison of the actual values of $\Delta D/\bar{D}$ and D_{θ} used in the simulations to those obtained from the fit of the data for $\mathcal{A}/2\bar{D}t p^2(t)$

probability when the rotational motion is decoupled from the translational motion of the colloid. The trivial scenario when this happens is when the particle is isotropic and the difference in mobilities vanish. Consequently, $p(t) \sim t^{-1/2}$ and $\tilde{p}(t) \rightarrow 1$. The other scenario when this happens is when the rotational diffusion coefficient is large and the particle rotates very fast. As a result, the term $e^{-4D_{\theta}t}$ decays faster and $\tilde{p}(t) \sim t^{-1}$ asymptotically.

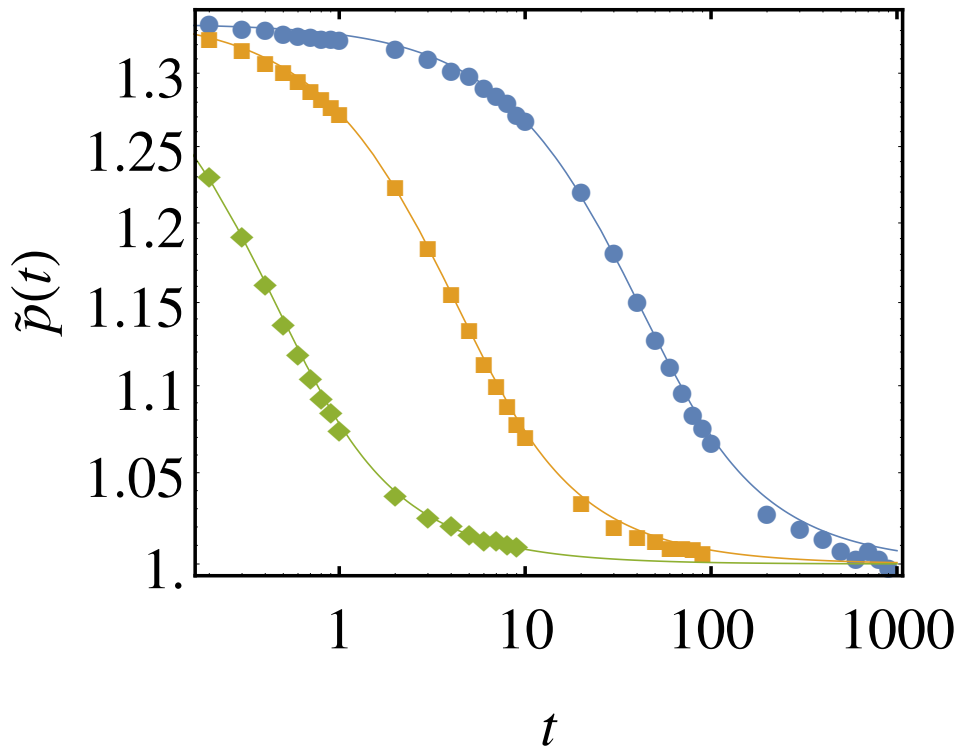


Figure 2.5 Plot of the dimensionless quantity $\tilde{p}(t)$ [see Eq. (2.47)] as a function of time for different choices of the rotational diffusion constant of the anisotropic particle: $D_\theta = 0.01$ (blue circles), $D_\theta = 0.1$ (orange squares), and $D_\theta = 1$ (green diamonds). The translation diffusion constants in all cases were $D_{\parallel} = 1$ and $D_{\perp} = 0.5$. The initial orientation in all the cases were fixed at $\theta_0 = 0$. The solid lines are fit to the data using (Eq. (2.47)) using $\Delta D/\bar{D}$ and D_θ as fit parameters. The estimated values of these parameters from the fit are compared with the actual values used in the simulation in Table

2.5 Conclusion

In this chapter, we have explored the effects of shape asymmetry on the dynamics of particle movement. In particular, we have studied the diffusion coefficient and persistence of a free ellipsoidal particle. It is well known that for short times the behavior is anisotropic but becomes isotropic for a longer time. It is usually assumed that for practical purposes the short-time behavior can be neglected. The movement of an asymmetric particle can be described by the Langevin Equations for a point particle with an isotropic translational diffusion coefficient given by the average of the diffusion coefficients along the major axis of the ellipsoidal particle. The two main results studied here are,

- The translational diffusion coefficients of an asymmetrical free particle. The determination of the rotational and the translational diffusion coefficients has been

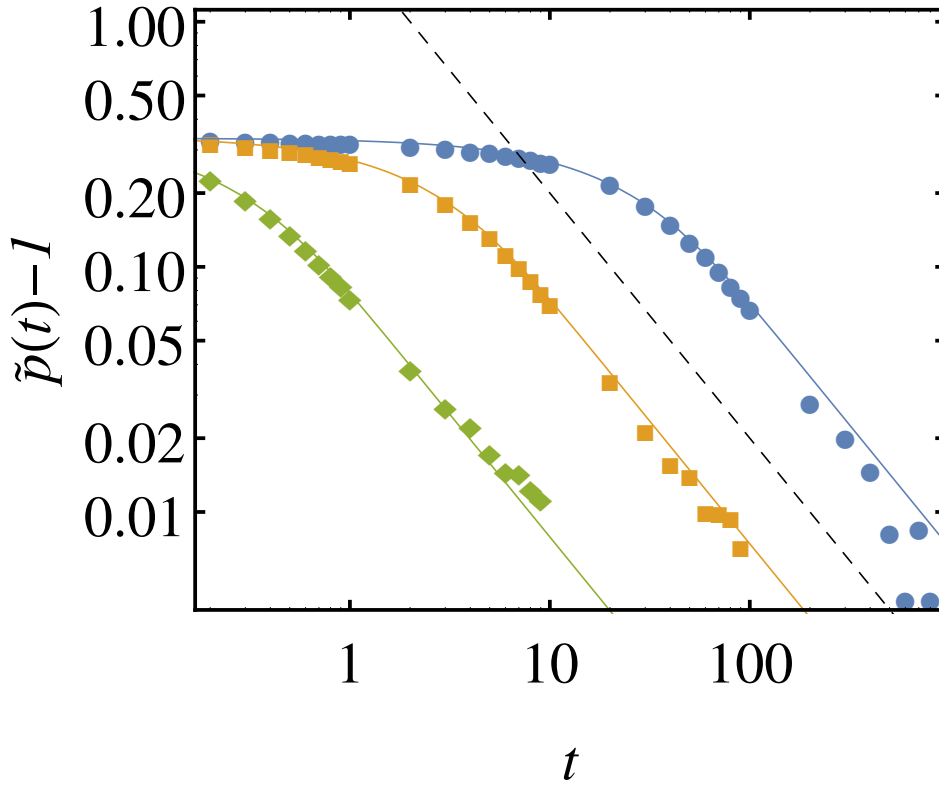


Figure 2.6 Plot of the dimensionless quantity $\tilde{p}(t) - 1$ [see Eq. (2.47)] as a function of time for different choices of the rotational diffusion constant of the anisotropic particle: $D_\theta = 0.01$ (blue circles), $D_\theta = 0.1$ (orange squares), and $D_\theta = 1$ (green diamonds). The translation diffusion constants in all cases were $D_\parallel = 1$ and $D_\perp = 0.5$. The initial orientation in all the cases were fixed at $\theta_0 = 0$. The solid lines are fit to the data using (Eq. (2.47)) using $\Delta D/\bar{D}$ and D_θ as fit parameters. The dashed line is a plot of t^{-1} indicating the asymptotic decay given in Eq. (2.47)

explicitly carried out for an anisotropic particle that undergoes free Brownian motion.

- Persistence probability of the free ellipsoidal particle. The persistence probability is computed from the two-time correlation function using a suitable transformation in space and time. Additionally, the analytical expression for $p(t)$ has been confirmed by the numerical simulation of the underlying stochastic dynamics.

The phenomena studied here, suggest that there exists a strong relationship between molecular asymmetry and the kinetics of diffusion-limited reactions on the surfaces, membranes or in crowded environments which are found inside cells.

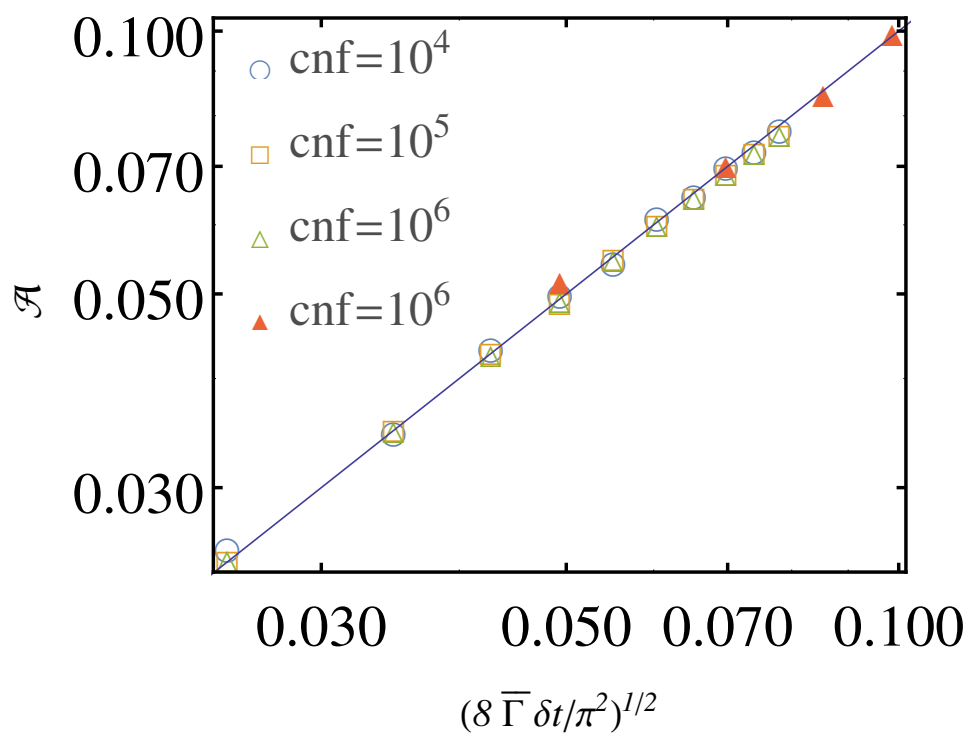


Figure 2.7 Scaled plot of the overall constant \mathcal{A} for different independent configurations, as indicated in the legend for diffusivities $D_{\parallel} = 1.0$, $D_{\perp} = 0.5$ and $D_{\parallel} = 4$, $D_{\perp} = 2$. In both cases, the rotational diffusivity was fixed at $D_{\theta} = 1$. The solid line is a plot of $y = x$.

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3

Persistence in Brownian motion of a Harmonically Trapped Ellipsoidal Particle

In this chapter, we are going to study the persistence of the ellipsoidal Brownian particle in a harmonic potential. This chapter tells the theory used for experimental purposes that use trapping and tracking techniques to measure the displacements. In experiments, the tracking of colloidal particles is usually done with laser traps and consequently, it is pertinent to discuss the scenario where an ellipsoidal particle is trapped in a harmonic trap is isotropic and there is no preferential direction of alignment. Further, if we suppose strong confinement, then at late times the deviations from the mean position of the particle are practically zero. Accordingly, the particle rotates freely so that the angular displacements obey Gaussian statistics. We have provided the analytical expression of $p(t)$ for the ellipsoidal particle in a harmonic potential and study the shape asymmetry and later on, we show that in the absence of shape asymmetry, the result reduces to the case of an isotropic particle. The analytical expression of $p(t)$ is validated with the numerical simulation.

3.1 Introduction

We now present the results of a study of a Brownian particle in a harmonic potential. This model is used to define a Brownian particle in the equilibrium position of a potential and a small displacement is considered to be harmonic. The particles we are using are of the dimension of a few micrometers and they are in a thermal bath.

In the experiments, the tracking of colloidal particles is usually conducted with the help of laser trapping, therefore it is a very much useful physical phenomenon to discuss the scenario where an ellipsoidal particle is trapped in a harmonic trap. In this chapter, we assume that the harmonic trap is isotropic in nature which means that there will be no preferential direction of alignment. We also are assuming that the rotational dynamics is decoupled from the translational degrees of freedom. This is most certainly true for a weak confinement of the particle or a small asymmetry. If the confinement is taken very strong, then at later times, the orientational degrees of freedom undergo a rotational Brownian motion with a renormalized diffusion coefficient¹. We confirmed these from a separate molecular dynamic simulation of anisotropic bodies that preserve the hydrodynamics in the fluid.

The main aim of this chapter is to study the persistence²⁻³⁵ of an ellipsoidal Brownian particle in a harmonic trap. The effect of the harmonic confinement has been studied using the perturbative expansion method and we have studied the effect of the shape asymmetry as well. We have studied the effect of the large rotational diffusion constant of the asymmetric particle on the mean-squared displacement.

This chapter is organized as follows, the first section 3.2 tells about the basic mathematical model of the particle using the Langevin dynamic equation, in the second section 3.2.1, we have studied the perturbation effect in the general solution, and using that perturbative expansion we have calculated the correlation of different variables of different orders. In the third section 3.3, we have studied the Mean-squared displacement for large rotational diffusion constant. In the fourth section 3.4, we have studied the persistence of the ellipsoidal particle in a harmonic trap and at last, we concluded with section 3.5

3.2 Harmonically Trapped Ellipsoidal Particle

We consider an ellipsoidal particle in two-dimensions having mobilities Γ_{\parallel} and Γ_{\perp} along the longer and the shorter axes of the particle. We denoted the body frame x and y direc-

tions as the longer and the shorter axes respectively. The particle has a single rotation mobility Γ_θ . The particle is immersed in a heat bath of a temperature T . So the translational diffusion coefficients are given by $D_{\parallel} = k_B T \Gamma_{\parallel}$, $D_{\perp} = k_B T \Gamma_{\perp}$ and $D_\theta = k_B T \Gamma_\theta$. The potential confinement has the form $U(x, y) = \kappa(x^2 + y^2)/2$ and the corresponding Langevin equation from Eq.(2.4) takes the form,

$$\begin{aligned}\frac{\partial x}{\partial t} &= -\kappa x \left(\bar{\Gamma} + \frac{1}{2} \Delta\Gamma \cos \theta(t) \right) - \frac{1}{2} \kappa y \Delta\Gamma \sin \theta(t) + \eta_x(t) \\ \frac{\partial y}{\partial t} &= -\kappa x \Delta\Gamma \sin \theta(t) - \kappa y \left(\bar{\Gamma} - \frac{1}{2} \Delta\Gamma \cos \theta(t) \right) + \eta_y(t) \\ \frac{\partial \theta}{\partial t} &= \eta_\theta\end{aligned}\tag{3.1}$$

Here $\bar{\Gamma} = (\Gamma_{\parallel} + \Gamma_{\perp})/2$ and $\Delta\Gamma = \Gamma_{\parallel} - \Gamma_{\perp}$ and the correlation of the thermal noise follows Eq.(2.2) and Eq.(2.9). In the lab frame, the displacements are related to the body frame as Eq.(2.3).

3.2.1 Perturbative Expansion

Defining the vector $\mathbf{R} \equiv (x, y)^T$, the equation takes the simple form

$$\dot{\mathbf{R}} = \kappa \left[\bar{\Gamma} \mathbf{1} + \frac{\Delta\Gamma}{2} \overline{\overline{\mathcal{R}}}(t) \right] \mathbf{R}(t) + \boldsymbol{\eta}(t)\tag{3.2}$$

Where

$$\overline{\overline{\mathcal{R}}} = \begin{bmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{bmatrix}\tag{3.3}$$

Eq.(3.1) reduces to that of isotropic particle in absence of any asymmetry and the correction term due to asymmetry comes from the combination of $\kappa\Delta\Gamma/2$. Eq.(3.1) is basically non-Markovian in nature. Since our interest is to calculate persistence, the non-Markovian nature of the process plays a significant role in determining $p(t)$. We used here weak confinement, which gives κ values small.

To solve the above equation, we use the perturbative expansion

$$\mathbf{R}(t) = \mathbf{R}_0(t) - \left(\frac{\kappa\Delta\Gamma}{2} \right) \mathbf{R}_1(t) + \left(\frac{\kappa\Delta\Gamma}{2} \right)^2 \mathbf{R}_2(t) + \mathcal{O} \left(\frac{\kappa\Delta\Gamma}{2} \right)^3\tag{3.4}$$

Substituting Eq.(3.4) in Eq.(3.2) and keeping up to the linear order in $\kappa\Delta\Gamma/2$ we obtain

the equations for $\mathbf{R}(t)$ and $\mathbf{R}_1(t)$ as

$$\begin{aligned}\dot{\mathbf{R}}_0 &= -\kappa\bar{\Gamma}\mathbf{R}_0(t) + \eta(t) \\ \dot{\mathbf{R}}_1 &= -\kappa\bar{\Gamma}\mathbf{R}_1(t) + \overline{\overline{\mathcal{R}}}(t)\mathbf{R}_0(t) \\ \dot{\mathbf{R}}_2 &= -\kappa\bar{\Gamma}\mathbf{R}_2(t) + \overline{\overline{\mathcal{R}}}(t)\mathbf{R}_1(t)\end{aligned}\tag{3.5}$$

The solutions for the Eq.(3.5) together with the initial condition $\mathbf{R}(0) = 0$ take the form

$$\begin{aligned}\mathbf{R}_0(t) &= \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \eta(t') \\ \mathbf{R}_1(t) &= \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \overline{\overline{\mathcal{R}}}(t') \mathbf{R}_0(t') \\ \mathbf{R}_2(t) &= \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \overline{\overline{\mathcal{R}}}(t') \mathbf{R}_1(t')\end{aligned}\tag{3.6}$$

In explicit form, the equal time correlation matrix $R_i(t)R_j(t)$ is then given by

$$\begin{aligned}\langle R_i(t)R_j(t) \rangle_{\eta,\theta} &= \langle R_{0,i}(t)R_{0,j}(t) \rangle_{\eta,\theta} - \left(\frac{\kappa\Delta\Gamma}{2} \right) \langle R_{0,i}(t)R_{1,j}(t) \rangle_{\eta,\theta} \\ &+ \left(\frac{\kappa\Delta\Gamma}{2} \right)^2 \left[\langle R_{1,i}(t)R_{1,j}(t) \rangle_{\eta,\theta} + 2\langle R_{0,i}(t)R_{2,j}(t) \rangle_{\eta,\theta} \right] \\ &+ \mathcal{O}\left(\frac{\kappa\Delta\Gamma}{2} \right)^3\end{aligned}\tag{3.7}$$

where we have used the fact that $\langle R_{0,i}R_{1,j} \rangle = \langle R_{0,j}R_{1,i} \rangle$. Further, note that the thermal noise correlation given in Eq.(2.8) and Eq.(2.9) gives an additional factor of $\kappa\Delta\Gamma/2$ in the correlation terms $\langle R_{\alpha,i}(t)R_{\beta,j}(t) \rangle$, where α, β denotes the order of the perturbation series.

We next proceed to calculate this equal time correlation matrix using the solutions in Eq.(3.6). The correlation matrix of $\mathbf{R}_0(t)$ averaged over the translational and the rotational noise is then given by,

$$\langle \mathbf{R}_0(t)\mathbf{R}_0(t) \rangle_{\eta,\theta} = \int_0^t dt' \int_0^t dt'' e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t-t'')} \langle \eta(t')\eta(t'') \rangle_{\eta,\theta}\tag{3.8}$$

where in correlation of the thermal noise is understood as an outer product of the

variable η_x and η_y . Using Eq.(2.8) and Eq.(2.9), the calculation is straight forward.

$$\begin{aligned}
\langle \mathbf{R}_0(t)\mathbf{R}_0(t) \rangle_{\eta,\theta} &= \int_0^t dt' \int_0^{t'} dt'' e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t-t'')} \left[\bar{\Gamma}\mathbf{1} + \frac{\Delta\Gamma}{2} \overline{\overline{\mathcal{R}}}(t') \right] \delta(t-t') \\
&= 2k_B T e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' e^{2\kappa\bar{\Gamma}t'} \left[\bar{\Gamma}\mathbf{1} + \frac{\Delta\Gamma}{2} \langle \overline{\overline{\mathcal{R}}}(t') \rangle_{\eta,\theta} \right] \\
&= \frac{k_B T}{\kappa} \mathbf{1} \left(1 - e^{-2\kappa\bar{\Gamma}t} \right) + 2k_B T e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' e^{2\kappa\bar{\Gamma}t'} \frac{\Delta\Gamma}{2} \overline{\overline{\mathcal{R}}}(\theta_0) e^{-4D_\theta t'} \\
&= \frac{k_B T}{\kappa} \mathbf{1} \left(1 - e^{-2\kappa\bar{\Gamma}t} \right) + \Delta D \overline{\overline{\mathcal{R}}}(\theta_0) e^{-2\kappa\bar{\Gamma}t} \left(\frac{e^{(2\kappa\bar{\Gamma}-4D_\theta)t} - 1}{2\kappa\bar{\Gamma} - 4D_\theta} \right) \\
&= \frac{k_B T}{\kappa} \mathbf{1} \left(1 - e^{-2\kappa\bar{\Gamma}t} \right) + \Delta D \overline{\overline{\mathcal{R}}}(\theta_0) \left(\frac{e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma} - 4D_\theta} \right)
\end{aligned} \tag{3.9}$$

More explicitly, the mean-square displacement along the x and y direction are given by

$$\langle x_0^2(t) \rangle_{\eta,\theta} = \frac{k_B T}{\kappa} (1 - e^{-2\kappa\bar{\Gamma}t}) + \Delta D \cos 2\theta_0 \left(\frac{e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma} - 4D_\theta} \right) \tag{3.10}$$

and

$$\langle y_0^2(t) \rangle_{\eta,\theta} = \frac{k_B T}{\kappa} (1 - e^{-2\kappa\bar{\Gamma}t}) - \Delta D \cos 2\theta_0 \left(\frac{e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma} - 4D_\theta} \right) \tag{3.11}$$

The cross-correlation function $x_0(t)y_0(t)$ reads

$$\langle x_0(t)y_0(t) \rangle_{\eta,\theta} = \Delta D \sin 2\theta_0 \left(\frac{e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma} - 4D_\theta} \right) \tag{3.12}$$

In the limit of $\kappa \rightarrow 0$, Eqs.(3.10),(3.11) and (3.12) reproduce the correct result of a free diffusion of an anisotropic particle given in Eqs.(2.30) and (2.31). On the other hand, for $\Delta\Gamma \rightarrow 0$ Eqs.(3.10), (3.11) and (3.12) yields the correlation matrix for an isotropic Brownian particle in a harmonic trap.

Our next attempt is to look into the correction to the above expression that comes from $\mathbf{R}_1(t)$ and $\mathbf{R}_2(t)$. For this, we rewrite the solutions for $\mathbf{R}_1(t)$ and $\mathbf{R}_2(t)$ in explicit form as

$$\begin{aligned}
R_{1,i}(t) &= \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \sum_j \mathcal{R}_{ij}(t') R_{0,j}(t') \\
R_{2,i}(t) &= \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \sum_j \mathcal{R}_{ij}(t') R_{1,j}(t')
\end{aligned} \tag{3.13}$$

where the subscripts are for the two spatial dimensions and can take the values 1 and 2. Using Eq.(3.7), we proceed to calculate the terms $\langle R_{0,i}(t)R_{0,j}(t) \rangle_{\eta,\theta}$, $\langle R_{1,i}(t)R_{1,j}(t) \rangle_{\eta,\theta}$ and $\langle R_{2,i}(t)R_{2,j}(t) \rangle_{\eta,\theta}$. The detailed calculation of the three terms are calculated here.

3.2.1.1 Calculation of $\langle R_{0,i}(t)R_{1,j}(t) \rangle$

$$\begin{aligned}
\langle R_{0,i}(t_1)R_{0,j}(t_2) \rangle_\eta &= \int_0^{t_1} dt'_2 \int_0^{t_2} dt'_1 e^{-\kappa\bar{\Gamma}(t_1-t'_1)} e^{-\kappa\bar{\Gamma}(t_2-t'_2)} \langle \eta_i(t'_1)\eta_j(t'_2) \rangle_\eta \\
&= 2k_B T e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_1} dt'_2 \int_0^{t_2} dt'_1 e^{-\kappa\bar{\Gamma}(t'_1+t'_2)} \left[\bar{\Gamma}\delta_{ij} + \frac{\Delta\Gamma}{2} \mathcal{R}_{ij}(t'_1) \right] \delta(t'_1 - t'_2) \\
&= 2k_B T \bar{\Gamma} \delta_{ij} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_1} dt'_2 \int_0^{t_2} dt'_1 e^{-\kappa\bar{\Gamma}(t'_1+t'_2)} \delta(t'_1 - t'_2) \\
&\quad + 2k_B T \frac{\Delta\Gamma}{2} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_1} dt'_2 \int_0^{t_2} dt'_1 e^{-\kappa\bar{\Gamma}(t'_1+t'_2)} \mathcal{R}_{ij}(t'_1) \delta(t'_1 - t'_2) \\
&= 2k_B T \bar{\Gamma} \delta_{ij} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{\min(t_1,t_2)} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} \\
&\quad + 2k_B T \frac{\Delta\Gamma}{2} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{\min(t_1,t_2)} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} \mathcal{R}_{ij}(t'_1) \\
&= \frac{k_B T}{\kappa} \delta_{ij} [e^{-\kappa\bar{\Gamma}|t_1-t_2|} - e^{-\kappa\bar{\Gamma}(t_1+t_2)}] + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{\min(t_1,t_2)} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} \mathcal{R}_{ij}(t'_1)
\end{aligned} \tag{3.14}$$

$$\begin{aligned}
\langle R_{0,i}(t)R_{1,j}(t) \rangle_{\eta,\theta} &= \left\langle R_{0,i}(t) \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \sum_k \mathcal{R}_{jk}(t') R_{0,k}(t') \right\rangle_{\eta,\theta} \\
&= \left\langle \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \sum_k \mathcal{R}_{jk}(t') \langle R_{0,i}(t)R_{0,k}(t') \rangle_\eta \right\rangle_\theta
\end{aligned} \tag{3.15}$$

Using the final form of $\langle R_{0,i}(t_1)R_{0,j}(t_2) \rangle$ from Eq.(3.14) and identifying $t_1 \equiv t$, $t_2 \equiv t'$ with $t' < t$ we get

$$\langle R_{0,i}(t)R_{0,k}(t') \rangle = \frac{k_B T}{\kappa} \delta_{ik} [e^{-\kappa\bar{\Gamma}(t-t')} - e^{-\kappa\bar{\Gamma}(t+t')}] + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t+t')} \int_0^{t'} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} \mathcal{R}_{ik}(t'_1) \tag{3.16}$$

Substituting Eq.(3.16) in Eq.(3.15) we get

$$\begin{aligned}
\langle R_{0,i}(t)R_{1,j}(t) \rangle_{\eta,\theta} &= \left\langle \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \sum_k \mathcal{R}_{jk}(t') \left[\frac{k_B T}{\kappa} \delta_{ik} (e^{-\kappa\bar{\Gamma}(t-t')} \right. \right. \\
&\quad \left. \left. - e^{-\kappa\bar{\Gamma}(t+t')}) + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t+t')} \int_0^{t'} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} \mathcal{R}_{ik}(t'_1) \right] \right\rangle_\theta \\
&= \left(\frac{k_B T}{\kappa} \right) \mathcal{R}_{ji}(\theta_0) e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' e^{-4D\theta t'} (e^{2\kappa\bar{\Gamma}t'} - 1) + k_B T \Delta\Gamma e^{-2\kappa\bar{\Gamma}t} \\
&\quad \int_0^t dt' \int_0^{t'} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} \left\langle \sum_k \mathcal{R}_{jk}(t') \mathcal{R}_{ik}(t'_1) \right\rangle_\theta \\
&= \left(\frac{k_B T}{\kappa} \right) \mathcal{R}_{ji}(\theta_0) e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' (e^{(2\kappa\bar{\Gamma}-4D\theta)t'} - e^{-4D\theta t'}) \\
&\quad + k_B T \Delta\Gamma e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^{t'} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} \left\langle \sum_k \mathcal{R}_{jk}(t') \mathcal{R}_{ik}(t'_1) \right\rangle_\theta
\end{aligned} \tag{3.17}$$

For the mean-square displacement along the x and the y direction, the second term in the last line of Eq.(3.17) yeilds

$$\begin{aligned} \left\langle \sum_k \mathcal{R}_{ik}(t') \mathcal{R}_{ik}(t'_1) \right\rangle_{\theta} &= \langle \cos 2\theta(t') \cos 2\theta(t'_1) + \sin 2\theta(t') \sin 2\theta(t'_1) \rangle_{\theta} = \langle \cos 2(\theta(t') - \theta(t'_1)) \rangle_{\theta} \\ \left\langle \sum_k \mathcal{R}_{ik}(t') \mathcal{R}_{ik}(t'_1) \right\rangle_{\theta} &= e^{-4D_{\theta}(t'-t'_1)} \end{aligned} \quad (3.18)$$

On the other hand for $i \neq j$, the term $\langle \sum_k \mathcal{R}_{jk}(t') \mathcal{R}_{ik}(t'_1) \rangle_{\theta} = 0$. Using Eq.(3.18) the contribution to the mean-square displacement along the x -direction becomes

$$\begin{aligned} \langle x_0(t)x_1(t) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa} \right) \cos 2\theta_0 e^{-2\kappa\bar{\Gamma}t} \left(\frac{e^{(2\kappa\bar{\Gamma}-4D_{\theta})t} - 1}{(2\kappa\bar{\Gamma} - 4D_{\theta})} - \frac{1 - e^{-4D_{\theta}t}}{4D_{\theta}} \right) \\ &\quad + k_B T \Delta \Gamma e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^{t'} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} e^{-4D_{\theta}(t-t'_1)} \\ &= \left(\frac{k_B T}{\kappa} \right) \cos 2\theta_0 \left(\frac{e^{-4D_{\theta}t} - e^{-2\kappa\bar{\Gamma}t}}{(2\kappa\bar{\Gamma} - 4D_{\theta})} - \frac{e^{-2\kappa\bar{\Gamma}t} - e^{(2\kappa\bar{\Gamma}+4D_{\theta})t}}{4D_{\theta}} \right) \\ &\quad + k_B T \Delta \Gamma e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' e^{-4D_{\theta}t'} \frac{e^{(2\kappa\bar{\Gamma}+4D_{\theta})t'} - 1}{2\kappa\bar{\Gamma} + 4D_{\theta}} \\ &= \left(\frac{k_B T}{\kappa} \right) \cos 2\theta_0 \left(\frac{e^{-4D_{\theta}t} - e^{-2\kappa\bar{\Gamma}t}}{(2\kappa\bar{\Gamma} - 4D_{\theta})} - \frac{e^{-2\kappa\bar{\Gamma}t} - e^{(2\kappa\bar{\Gamma}+4D_{\theta})t}}{4D_{\theta}} \right) \\ &\quad + k_B T \Delta \Gamma e^{-2\kappa\bar{\Gamma}t} \left(\frac{e^{2\kappa\bar{\Gamma}t} - 1}{2\kappa\bar{\Gamma}(2\kappa\bar{\Gamma} + 4D_{\theta})} - \frac{1 - e^{-4D_{\theta}t}}{4D_{\theta}(2\kappa\bar{\Gamma} + 4D_{\theta})} \right) \\ &= \left(\frac{k_B T}{\kappa} \right) \cos 2\theta_0 \left(\frac{e^{-4D_{\theta}t} - e^{-2\kappa\bar{\Gamma}t}}{(2\kappa\bar{\Gamma} - 4D_{\theta})} - \frac{e^{-2\kappa\bar{\Gamma}t} - e^{(2\kappa\bar{\Gamma}+4D_{\theta})t}}{4D_{\theta}} \right) \\ &\quad + k_B T \Delta \Gamma \left(\frac{1 - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma}(2\kappa\bar{\Gamma} + 4D_{\theta})} - \frac{e^{-2\kappa\bar{\Gamma}t} - e^{-(2\kappa\bar{\Gamma}+4D_{\theta})t}}{4D_{\theta}(2\kappa\bar{\Gamma} + 4D_{\theta})} \right) \end{aligned} \quad (3.19)$$

and that along the y -direction takes the form

$$\begin{aligned} \langle y_0(t)y_1(t) \rangle_{\eta,\theta} &= - \left(\frac{k_B T}{\kappa} \right) \cos 2\theta_0 \left(\frac{e^{-4D_{\theta}t} - e^{-2\kappa\bar{\Gamma}t}}{(2\kappa\bar{\Gamma} - 4D_{\theta})} - \frac{e^{-2\kappa\bar{\Gamma}t} - e^{(2\kappa\bar{\Gamma}+4D_{\theta})t}}{4D_{\theta}} \right) \\ &\quad + k_B T \Delta \Gamma \left(\frac{1 - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma}(2\kappa\bar{\Gamma} + 4D_{\theta})} - \frac{e^{-2\kappa\bar{\Gamma}t} - e^{-(2\kappa\bar{\Gamma}+4D_{\theta})t}}{4D_{\theta}(2\kappa\bar{\Gamma} + 4D_{\theta})} \right) \end{aligned} \quad (3.20)$$

3.2.1.2 Calculation of $\langle R_{1,i}(t)R_{1,j}(t) \rangle$

The correlation matrix now takes the form

$$\langle R_{1,i}(t)R_{1,j}(t) \rangle_{\eta,\theta} = \int_0^t dt' \int_0^t dt'' e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t-t'')} \left\langle \sum_k \mathcal{R}_{ik}(t') R_{0,k}(t') \sum_l \mathcal{R}_{jl}(t'') R_{0,l}(t'') \right\rangle_{\eta,\theta} \quad (3.21)$$

Rearranging and averaging first over the translational noise we get,

$$\langle R_{1,i}(t)R_{1,j}(t) \rangle_{\eta,\theta} = \int_0^t dt' \int_0^t dt'' e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t-t'')} \left\langle \sum_{k,l} \mathcal{R}_{ik}(t') \mathcal{R}_{jl}(t'') \langle R_{0,k}(t') R_{0,l}(t'') \rangle_{\eta} \right\rangle_{\theta} \quad (3.22)$$

$$\begin{aligned} \langle R_{1,i}(t)R_{1,j}(t) \rangle_{\eta,\theta} &= 2k_B T \int_0^t dt' \int_0^t dt'' e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t-t'')} \\ &\left\langle \sum_{k,l} \mathcal{R}_{ik}(t') \mathcal{R}_{jl}(t'') \int_0^{t'} dt'_1 \int_0^{t''} dt'_2 e^{-\kappa\bar{\Gamma}(t'-t'_1)} e^{-\kappa\bar{\Gamma}(t''-t'_2)} \left[\bar{\Gamma} \delta_{kl} + \frac{\Delta\Gamma}{2} \mathcal{R}_{kl}(t'_1) \right] \delta(t'_1 - t'_2) \right\rangle \end{aligned} \quad (3.23)$$

Integrating over delta function and ignoring the term proportional to $\Delta\Gamma$ we get

$$\begin{aligned} \langle R_{1,i}(t)R_{1,j}(t) \rangle_{\eta,\theta} &= 2k_B T \bar{\Gamma} e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^t dt'' \int_0^{\min(t',t'')} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} \left\langle \sum_{k,l} \mathcal{R}_{ik}(t') \mathcal{R}_{jl}(t'') \delta_{kl} \right\rangle_{\theta} \\ \langle R_{1,i}(t)R_{1,j}(t) \rangle_{\eta,\theta} &= 2k_B T \bar{\Gamma} e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^t dt'' \int_0^{\min(t',t'')} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} \left\langle \sum_{k,l} \mathcal{R}_{ik}(t') \mathcal{R}_{jk}(t'') \right\rangle_{\theta} \end{aligned} \quad (3.24)$$

In order to proceed further, we look at $\langle x_1^2(t) \rangle_{\eta,\theta}$ and $\langle y_1^2(t) \rangle_{\eta,\theta}$ by setting $i = j$ and subsequently using Eq.(3.24)

$$\langle x_1^2(t) \rangle_{\eta,\theta} = 2k_B T \bar{\Gamma} e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^t dt'' \int_0^{\min(t',t'')} dt'_1 e^{2\kappa\bar{\Gamma}t'_1} \langle \cos 2[\theta(t') - \theta(t'')] \rangle_{\theta} \quad (3.25)$$

General form of the identity used as

$$\langle e^{im\Delta\theta(t') - in\Delta\theta(t'')} \rangle_{\theta} = e^{-D_{\theta}(m^2 t' + n^2 t'' - 2mn \min(t', t''))} \quad (3.26)$$

Using the above relation, the averages of the trigonometric functions over the rotational noise take the form

$$\begin{aligned} \langle \cos 2[\theta(t') - \theta(t'')] \rangle_{\theta} &= e^{-4D_{\theta}(t'+t''-2\min(t',t''))} \\ \langle \cos 2[\theta(t') + \theta(t'')] \rangle_{\theta} &= \cos 4\theta_0 e^{-4D_{\theta}(t'+t''+2\min(t',t''))} \\ \langle \sin 2[\theta(t') + \theta(t'')] \rangle_{\theta} &= \sin 4\theta_0 e^{-4D_{\theta}(t'+t''+2\min(t',t''))} \\ \langle \sin 2[\theta(t') - \theta(t'')] \rangle_{\theta} &= 0 \end{aligned} \quad (3.27)$$

Substituting for $\langle \cos 2[\theta(t') - \theta(t'')] \rangle_\theta$ from Eq.(3.27) we get

$$\langle x_1^2(t) \rangle_{\eta, \theta} = 2k_B T \bar{\Gamma} e^{-2\kappa \bar{\Gamma} t} \int_0^t dt' \int_0^t dt'' \int_0^{\min(t', t'')} dt'_1 e^{2\kappa \bar{\Gamma} t'_1} e^{-4D_\theta(t'+t''-2\min(t', t''))} \quad (3.28)$$

$$\langle x_1^2(t) \rangle_{\eta, \theta} = 2k_B T \bar{\Gamma} e^{-2\kappa \bar{\Gamma} t} \int_0^t dt' \int_0^t dt'' \frac{e^{2\kappa \bar{\Gamma} \min(t', t'')} - 1}{2\kappa \bar{\Gamma}} e^{-4D_\theta(t'+t''-2\min(t', t''))} \quad (3.29)$$

$$\begin{aligned} \langle x_1^2(t) \rangle_{\eta, \theta} = & \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa \bar{\Gamma} t} \left[\int_0^t dt' \int_0^{t'} dt'' \left(e^{2\kappa \bar{\Gamma} t''} - 1 \right) e^{-4D_\theta(t'-t'')} \right. \\ & \left. + \int_0^t dt' \int_{t'}^t dt'' \left(e^{2\kappa \bar{\Gamma} t'} - 1 \right) e^{-4D_\theta(t''-t')} \right] \end{aligned} \quad (3.30)$$

$$\begin{aligned} \langle x_1^2(t) \rangle_{\eta, \theta} = & \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa \bar{\Gamma} t} \left[\int_0^t dt' e^{-4D_\theta t'} \int_0^{t'} dt'' \left(e^{(2\kappa \bar{\Gamma} + 4D_\theta)t''} - e^{4D_\theta t''} \right) \right. \\ & \left. + \int_0^t dt' \left(e^{2\kappa \bar{\Gamma} t'} - 1 \right) e^{4D_\theta t'} \int_{t'}^t dt'' e^{-4D_\theta t''} \right] \end{aligned} \quad (3.31)$$

$$\begin{aligned} \langle x_1^2(t) \rangle_{\eta, \theta} = & \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa \bar{\Gamma} t} \left[\int_0^t dt' e^{-4D_\theta t'} \left[\frac{e^{(2\kappa \bar{\Gamma} + 4D_\theta)t'} - 1}{2\kappa \bar{\Gamma} + 4D_\theta} - \frac{e^{4D_\theta t'} - 1}{4D_\theta} \right] \right. \\ & \left. + \int_0^t dt' \left(e^{2\kappa \bar{\Gamma} t'} - 1 \right) e^{4D_\theta t'} \left[\frac{e^{-4D_\theta t'} - e^{-4D_\theta t}}{4D_\theta} \right] \right] \end{aligned} \quad (3.32)$$

$$\begin{aligned} \langle x_1^2(t) \rangle_{\eta, \theta} = & \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa \bar{\Gamma} t} \left[\int_0^t dt' \left(\frac{e^{2\kappa \bar{\Gamma} t'}}{2\kappa \bar{\Gamma} + 4D_\theta} - \frac{e^{-4D_\theta t'}}{2\kappa \bar{\Gamma} + 4D_\theta} - \frac{1 - e^{-4D_\theta t'}}{4D_\theta} \right) \right. \\ & \left. + \int_0^t dt' \left(\frac{e^{2\kappa \bar{\Gamma} t'} - 1}{4D_\theta} \right) - e^{-4D_\theta t} \int_0^t dt' \left(\frac{e^{(2\kappa \bar{\Gamma} + 4D_\theta)t'} - e^{4D_\theta t'}}{4D_\theta} \right) \right] \end{aligned} \quad (3.33)$$

$$\begin{aligned} \langle x_1^2(t) \rangle_{\eta, \theta} = & \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa \bar{\Gamma} t} \left[\left(\frac{e^{2\kappa \bar{\Gamma} t} - 1}{2\kappa \bar{\Gamma} (2\kappa \bar{\Gamma} + 4D_\theta)} - \frac{1 - e^{-4D_\theta t}}{4D_\theta (2\kappa \bar{\Gamma} + 4D_\theta)} - \frac{t}{4D_\theta} + \frac{1 - e^{-4D_\theta t}}{16D_\theta^2} \right) \right. \\ & \left. + \left(\frac{e^{2\kappa \bar{\Gamma} t} - 1}{4D_\theta 2\kappa \bar{\Gamma}} \right) - \frac{t}{4D_\theta} - e^{-4D_\theta t} \left(\frac{e^{(2\kappa \bar{\Gamma} + 4D_\theta)t} - 1}{4D_\theta (2\kappa \bar{\Gamma} + 4D_\theta)} - \frac{e^{4D_\theta t} - 1}{16D_\theta^2} \right) \right] \end{aligned} \quad (3.34)$$

$$\begin{aligned} \langle x_1^2(t) \rangle_{\eta, \theta} = & \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa \bar{\Gamma} t} \left[\left(\frac{e^{2\kappa \bar{\Gamma} t} - 1}{2\kappa \bar{\Gamma} (2\kappa \bar{\Gamma} + 4D_\theta)} - \frac{1 - e^{-4D_\theta t}}{4D_\theta (2\kappa \bar{\Gamma} + 4D_\theta)} - \frac{t}{4D_\theta} + \frac{1 - e^{-4D_\theta t}}{16D_\theta^2} \right) \right. \\ & \left. + \left(\frac{e^{2\kappa \bar{\Gamma} t} - 1}{4D_\theta 2\kappa \bar{\Gamma}} - \frac{t}{4D_\theta} - \frac{e^{2\kappa \bar{\Gamma} t} - 1}{4D_\theta (2\kappa \bar{\Gamma} + 4D_\theta)} - \frac{1 - e^{-4D_\theta t}}{4D_\theta (2\kappa \bar{\Gamma} + 4D_\theta)} - \frac{1 - e^{-4D_\theta t}}{16D_\theta^2} \right) \right] \end{aligned} \quad (3.35)$$

$$\langle x_1^2(t) \rangle_{\eta, \theta} = \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa \bar{\Gamma} t} \left[\frac{e^{2\kappa \bar{\Gamma} t} - 1}{\kappa \bar{\Gamma} (2\kappa \bar{\Gamma} + 4D_\theta)} - \frac{t}{4D_\theta} + \kappa \bar{\Gamma} \frac{1 - e^{-4D_\theta t}}{4D_\theta^2 (2\kappa \bar{\Gamma} + 4D_\theta)} \right] \quad (3.36)$$

$$\langle x_1^2(t) \rangle_{\eta, \theta} = \left(\frac{k_B T}{\kappa} \right) \left[\frac{1 - e^{-2\kappa\bar{\Gamma}t}}{\kappa\bar{\Gamma}(2\kappa\bar{\Gamma} + 4D_\theta)} - \frac{te^{-2\kappa\bar{\Gamma}t}}{4D_\theta} + \kappa\bar{\Gamma} \frac{e^{-2\kappa\bar{\Gamma}t} - e^{-(2\kappa\bar{\Gamma} + 4D_\theta)t}}{4D_\theta^2(2\kappa\bar{\Gamma} + 4D_\theta)} \right] \quad (3.37)$$

3.2.1.3 Calculation Of $\langle R_{0,i}(t)R_{2,j}(t) \rangle$

$$\begin{aligned} \langle R_{0,i}(t_1)R_{1,j}(t_2) \rangle_\eta &= \left\langle R_{0,i}(t_1) \int_0^{t_2} dt'_2 e^{-\kappa\bar{\Gamma}(t_2-t'_2)} \sum_k \mathcal{R}_{jk}(t'_2) R_{0,k}(t'_2) \right\rangle_\eta \\ \langle R_{0,i}(t_1)R_{1,j}(t_2) \rangle_\eta &= \int_0^{t_2} dt'_2 e^{-\kappa\bar{\Gamma}(t_2-t'_2)} \sum_k \mathcal{R}_{jk}(t'_2) \langle R_{0,i}(t_1)R_{0,k}(t'_2) \rangle_\eta \\ \langle R_{0,i}(t_1)R_{1,j}(t_2) \rangle_\eta &= \int_0^{t_2} dt'_2 e^{-\kappa\bar{\Gamma}(t_2-t'_2)} \sum_k \mathcal{R}_{jk}(t'_2) \left[\frac{k_B T}{\kappa} \delta_{ik} \left[e^{-\kappa\bar{\Gamma}(t_1-t'_2)} - e^{-\kappa\bar{\Gamma}(t_1+t'_2)} \right] \right. \\ &\quad \left. + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t'_2)} \int_0^{\min(t_1, t'_2)} dt'' e^{2\kappa\bar{\Gamma}t''} \mathcal{R}_{ik}(t'') \right] \\ \langle R_{0,i}(t_1)R_{1,j}(t_2) \rangle_\eta &= \left(\frac{k_B T}{\kappa} \right) e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 e^{\kappa\bar{\Gamma}t'_2} \mathcal{R}_{ji}(t'_2) \left(e^{\kappa\bar{\Gamma}t'_2} - e^{-\kappa\bar{\Gamma}t'_2} \right) \\ &\quad + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{\min(t_1, t'_2)} dt'' e^{2\kappa\bar{\Gamma}t''} \sum_k \mathcal{R}_{jk}(t'_2) \mathcal{R}_{ik}(t'') \end{aligned} \quad (3.38)$$

$$\begin{aligned} \langle R_{0,i}(t_1)R_{1,j}(t_2) \rangle_{\eta, \theta} &= \left(\frac{k_B T}{\kappa} \right) e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 e^{\kappa\bar{\Gamma}t'_2} \langle \mathcal{R}_{ji}(t'_2) \rangle_\theta \left(e^{\kappa\bar{\Gamma}t'_2} - e^{-\kappa\bar{\Gamma}t'_2} \right) \\ &\quad + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{\min(t_1, t'_2)} dt'' e^{2\kappa\bar{\Gamma}t''} \sum_k \langle \mathcal{R}_{jk}(t'_2) \mathcal{R}_{ik}(t'') \rangle_\theta \\ \langle R_{0,i}(t_1)R_{1,j}(t_2) \rangle_{\eta, \theta} &= \left(\frac{k_B T}{\kappa} \right) \mathcal{R}_{ji}(\theta_0) e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 e^{-4D_\theta t'_2} \left(e^{2\kappa\bar{\Gamma}t'_2} - 1 \right) \\ &\quad + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 \int_0^{\min(t_1, t'_2)} dt'' e^{2\kappa\bar{\Gamma}t''} \sum_k \langle \mathcal{R}_{jk}(t'_2) \mathcal{R}_{ik}(t'') \rangle_\theta \end{aligned} \quad (3.39)$$

$$\begin{aligned}
\langle x_0(t_1)x_1(t_2) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa}\right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 \left(e^{(2\kappa\bar{\Gamma}-4D_\theta)t'_2} - e^{-4D_\theta t'_2} \right) \\
&\quad + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 \int_0^{t'_2} dt'' e^{2\kappa\bar{\Gamma}t''} \sum_k \langle \mathcal{R}_{ik}(t'_2) \mathcal{R}_{ik}(t'') \rangle_\theta \\
\langle x_0(t_1)x_1(t_2) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa}\right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 \left(e^{(2\kappa\bar{\Gamma}-4D_\theta)t'_2} - e^{-4D_\theta t'_2} \right) \\
&\quad + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 \int_0^{t'_2} dt'' e^{2\kappa\bar{\Gamma}t''} \sum_k \langle \cos 2(\theta(t'_2) - \theta(t'')) \rangle_\theta \\
\langle x_0(t_1)x_1(t_2) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa}\right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 \left(e^{(2\kappa\bar{\Gamma}-4D_\theta)t'_2} - e^{-4D_\theta t'_2} \right) \\
&\quad + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 \int_0^{t'_2} dt'' e^{2\kappa\bar{\Gamma}t''} e^{-4D_\theta(t'_2+t''-2\min(t'_2,t''))} \\
\langle x_0(t_1)x_1(t_2) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa}\right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}(t_1+t_2)} \left(\frac{e^{(2\kappa\bar{\Gamma}-4D_\theta)t_2} - 1}{2\kappa\bar{\Gamma} - 4D_\theta} - \frac{1 - e^{-4D_\theta t_2}}{4D_\theta} \right) \\
&\quad + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 \int_0^{t'_2} dt'' e^{2\kappa\bar{\Gamma}t''} e^{-4D_\theta(t'_2-t'')} \\
\langle x_0(t_1)x_1(t_2) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa}\right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_1} \left(\frac{e^{-4D_\theta t_2} - e^{-\kappa\bar{\Gamma}t_2}}{2\kappa\bar{\Gamma} - 4D_\theta} - \frac{e^{-\kappa\bar{\Gamma}t_2} - e^{-(4D_\theta+\kappa\bar{\Gamma})t_2}}{4D_\theta} \right) \\
&\quad + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 \frac{e^{2\kappa\bar{\Gamma}t'_2} - e^{-4D_\theta t'_2}}{2\kappa\bar{\Gamma} + 4D_\theta} \\
\langle x_0(t_1)x_1(t_2) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa}\right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_1} \left(\frac{e^{-4D_\theta t_2} - e^{-\kappa\bar{\Gamma}t_2}}{2\kappa\bar{\Gamma} - 4D_\theta} - \frac{e^{-\kappa\bar{\Gamma}t_2} - e^{-(4D_\theta+\kappa\bar{\Gamma})t_2}}{4D_\theta} \right) \\
&\quad + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \left[\frac{e^{2\kappa\bar{\Gamma}t_2} - 1}{2\kappa\bar{\Gamma}(2\kappa\bar{\Gamma} + 4D_\theta)} - \frac{1 - e^{-4D_\theta t_2}}{4D_\theta(2\kappa\bar{\Gamma} + 4D_\theta)} \right]
\end{aligned} \tag{3.40}$$

$$\begin{aligned}
\langle x_0(t_1)x_1(t_2) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa}\right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_1} \left(\frac{e^{(\kappa\bar{\Gamma}-4D_\theta)t_2} - e^{-\kappa\bar{\Gamma}t_2}}{2\kappa\bar{\Gamma} - 4D_\theta} - \frac{e^{-\kappa\bar{\Gamma}t_2} - e^{(4D_\theta+\kappa\bar{\Gamma})t_2}}{4D_\theta} \right) \\
&\quad + \left(\frac{k_B T}{\kappa}\right) \left(\frac{\Delta\Gamma}{2\bar{\Gamma}}\right) e^{-\kappa\bar{\Gamma}t_1} \left[\frac{e^{\kappa\bar{\Gamma}t_2} - e^{-\kappa\bar{\Gamma}t_2}}{2\kappa\bar{\Gamma} + 4D_\theta} - \frac{2\kappa\bar{\Gamma} e^{-\kappa\bar{\Gamma}t_2} - e^{-(2\kappa\bar{\Gamma}+4D_\theta)t_2}}{\kappa\bar{\Gamma} + 4D_\theta} \right]
\end{aligned} \tag{3.41}$$

$$\begin{aligned}
\langle R_{0,i}(t)R_{2,j}(t) \rangle_{\eta,\theta} &= \left\langle R_{0,i}(t) \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \sum_k \mathcal{R}_{jk}(t') R_{1,k}(t') \right\rangle_{\eta,\theta} \\
&= \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \left\langle \sum_k \mathcal{R}_{jk}(t') \langle R_{0,i}(t) R_{1,k}(t') \rangle_\eta \right\rangle_\theta
\end{aligned} \tag{3.42}$$

$$\begin{aligned}
\langle R_{0,i}(t)R_{1,k}(t') \rangle_\eta &= \left(\frac{k_B T}{\kappa}\right) e^{-\kappa\bar{\Gamma}(t+t')} \int_0^{t'} dt'' e^{\kappa\bar{\Gamma}t''} \mathcal{R}_{ki}(t'_2) \left(e^{\kappa\bar{\Gamma}t'_2} - e^{-\kappa\bar{\Gamma}t'_2} \right) \\
&\quad + k_B T \Delta\Gamma e^{-\kappa\bar{\Gamma}(t+t')} \int_0^{t'} dt'' e^{2\kappa\bar{\Gamma}t''} \sum_l \mathcal{R}_{kl}(t'_2) \mathcal{R}_{il}(t'')
\end{aligned} \tag{3.43}$$

Neglecting the second term in Eq.(3.43), we have

$$\begin{aligned}
\langle R_{0,i}(t)R_{2,j}(t) \rangle_{\eta,\theta} &= \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \left\langle \sum_k \mathcal{R}_{jk}(t') \left(\frac{k_B T}{\kappa} \right) e^{-\kappa\bar{\Gamma}(t+t')} \int_0^{t'} dt'_2 e^{\kappa\bar{\Gamma}t'_2} \mathcal{R}_{ki}(t'_2) \left(e^{\kappa\bar{\Gamma}t'_2} - e^{-\kappa\bar{\Gamma}t'_2} \right) \right\rangle_{\theta} \\
\langle R_{0,i}(t)R_{2,j}(t) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa} \right) \int_0^t dt' \int_0^{t'} dt'_2 e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t+t')} e^{\kappa\bar{\Gamma}t'_2} \left(e^{\kappa\bar{\Gamma}t'_2} - e^{-\kappa\bar{\Gamma}t'_2} \right) \left\langle \sum_k \mathcal{R}_{jk}(t') \mathcal{R}_{ki}(t'_2) \right\rangle_{\theta} \\
\langle R_{0,i}(t)R_{2,j}(t) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^{t'} dt'_2 \left(e^{2\kappa\bar{\Gamma}t'_2} - 1 \right) \left\langle \sum_k \mathcal{R}_{jk}(t') \mathcal{R}_{ki}(t'_2) \right\rangle_{\theta}
\end{aligned} \tag{3.44}$$

For the mean-square displacement along x and y direction, setting $j = i$ and using Eq.(3.18) we get

$$\begin{aligned}
\langle x_0(t)x_2(t) \rangle_{\eta,\theta} &= \langle y_0(t)y_2(t) \rangle_{\eta,\theta} = \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^{t'} dt'_2 \left(e^{2\kappa\bar{\Gamma}t'_2} - 1 \right) \langle \cos 2(\theta(t') - \theta(t'_2)) \rangle_{\theta} \\
&= \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^{t'} dt'_2 \left(e^{2\kappa\bar{\Gamma}t'_2} - 1 \right) e^{-4D_{\theta}(t'-t'_2)} \\
&= \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' e^{-4D_{\theta}t'} \int_0^{t'} dt'_2 \left(e^{(2\kappa\bar{\Gamma}+4D_{\theta})t'_2} - e^{4D_{\theta}t'_2} \right) \\
&= \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' e^{-4D_{\theta}t'} \left(\frac{e^{(2\kappa\bar{\Gamma}+4D_{\theta})t'} - 1}{2\kappa\bar{\Gamma} + 4D_{\theta}} - \frac{e^{-4D_{\theta}t'} - 1}{4D_{\theta}} \right) \\
&= \left(\frac{k_B T}{\kappa} \right) e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \left(\frac{e^{2\kappa\bar{\Gamma}t'} - e^{-4D_{\theta}t'}}{2\kappa\bar{\Gamma} + 4D_{\theta}} - \frac{1 - e^{-4D_{\theta}t'}}{4D_{\theta}} \right) \\
&= \left(\frac{k_B T}{\kappa} \right) \left(\frac{e^{2\kappa\bar{\Gamma}t} - 1}{2\kappa\bar{\Gamma}(2\kappa\bar{\Gamma} + 4D_{\theta})} - \frac{1 - e^{-4D_{\theta}t}}{4D_{\theta}(2\kappa\bar{\Gamma} + 4D_{\theta})} - \frac{t}{4D_{\theta}} - \frac{1 - e^{-4D_{\theta}t}}{16D_{\theta}^2} \right) \\
&= \left(\frac{k_B T}{\kappa} \right) \left[\frac{1 - e^{2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma}(2\kappa\bar{\Gamma} + 4D_{\theta})} - \frac{te^{-2\kappa\bar{\Gamma}t}}{4D_{\theta}} + \frac{2\kappa\bar{\Gamma}}{4D_{\theta}} \left(1 - e^{-4D_{\theta}t} \right) \right]
\end{aligned} \tag{3.45}$$

The final form of the terms $\langle R_{0,i}(t)R_{0,j} \rangle_{\eta,\theta}$, $\langle R_{1,i}(t)R_{1,j}(t) \rangle_{\eta,\theta}$ and $\langle R_{2,i}(t)R_{2,j}(t) \rangle_{\eta,\theta}$ have been calculated here. Detailed steps of the calculation are written above. The final form

$$\begin{aligned}
\langle x_0(t)x_1(t) \rangle_{\eta,\theta} &= \langle y_0(t)y_1(t) \rangle_{\eta,\theta} \\
&= \left(\frac{k_B T}{\kappa} \right) \cos 2\theta_0 \left(\frac{e^{-4D_{\theta}t} - e^{-2\kappa\bar{\Gamma}t}}{(2\kappa\bar{\Gamma} - 4D_{\theta})} - \frac{e^{-2\kappa\bar{\Gamma}t} - e^{-(2\kappa\bar{\Gamma}+4D_{\theta})t}}{4D_{\theta}} \right) \\
&\quad + 2 \left(\frac{k_B T}{\kappa} \right) \left(\frac{\kappa\Delta\Gamma}{2} \right) \left(\frac{1 - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma}(2\kappa\bar{\Gamma} + 4D_{\theta})} - \frac{e^{-2\kappa\bar{\Gamma}t} - e^{-(2\kappa\bar{\Gamma}+4D_{\theta})t}}{4D_{\theta}(2\kappa\bar{\Gamma} + 4D_{\theta})} \right)
\end{aligned} \tag{3.46}$$

$$\begin{aligned}
\langle x_1^2(t) \rangle_{\eta,\theta} &= \langle y_1^2(t) \rangle_{\eta,\theta} \\
&= \left(\frac{k_B T}{\kappa} \right) \left[\frac{1 - e^{-2\kappa\bar{\Gamma}t}}{\kappa\bar{\Gamma}(2\kappa\bar{\Gamma} + 4D_{\theta})} - \frac{te^{-2\kappa\bar{\Gamma}t}}{4D_{\theta}} + \kappa\bar{\Gamma} \frac{e^{-2\kappa\bar{\Gamma}t} - e^{-(2\kappa\bar{\Gamma}+4D_{\theta})t}}{4D_{\theta}^2(2\kappa\bar{\Gamma} + 4D_{\theta})} \right]
\end{aligned} \tag{3.47}$$

$$\begin{aligned}
\langle x_0(t)x_2(t) \rangle_{\eta,\theta} &= \langle y_0(t)y_2(t) \rangle_{\eta,\theta} \\
&= \left(\frac{k_B T}{\kappa} \right) \left[\frac{1 - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma}(2\kappa\bar{\Gamma} + 4D_\theta)} - \frac{te^{-2\kappa\bar{\Gamma}t}}{4D_\theta} + \frac{2\kappa\bar{\Gamma}}{4D_\theta} \left(1 - e^{-4D_\theta t} \right) \right]
\end{aligned} \tag{3.48}$$

In the limit of $\kappa \rightarrow 0$, both $\langle y_1^2(t) \rangle = \langle x_1^2(t) \rangle = 0$. The final expression for the mean-square displacement along the x is given by

$$\begin{aligned}
\langle x^2(t) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa} \right) \left[\left(1 - e^{-2\kappa\bar{\Gamma}t} \right) \right. \\
&\quad + \left(\frac{\kappa\Delta\Gamma}{2} \right) \cos 2\theta_0 \left(\frac{e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma} - 4D_\theta} + \frac{e^{-2\kappa\bar{\Gamma}t} - e^{-(2\kappa\bar{\Gamma} + 4D_\theta)t}}{4D_\theta} \right) \\
&\quad \left. + \left(\frac{\kappa\Delta\Gamma}{2} \right)^2 \left(\frac{1}{4D_\theta^2} e^{-2\kappa\bar{\Gamma}t} (1 - e^{-4D_\theta t}) - \frac{t}{D_\theta} e^{-2\kappa\bar{\Gamma}t} \right) + \mathcal{O} \left(\frac{\kappa\Delta\Gamma}{2} \right)^3 \right]
\end{aligned} \tag{3.49}$$

and that along the y - direction is given by

$$\begin{aligned}
\langle y^2(t) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa} \right) \left[\left(1 - e^{-2\kappa\bar{\Gamma}t} \right) - \left(\frac{\kappa\Delta\Gamma}{2} \right) \cos 2\theta_0 \left(\frac{e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma} - 4D_\theta} + \frac{e^{-2\kappa\bar{\Gamma}t} - e^{-(2\kappa\bar{\Gamma} + 4D_\theta)t}}{4D_\theta} \right) \right. \\
&\quad \left. + \left(\frac{\kappa\Delta\Gamma}{2} \right)^2 \left(\frac{1}{4D_\theta^2} e^{-2\kappa\bar{\Gamma}t} (1 - e^{-4D_\theta t}) - \frac{t}{D_\theta} e^{-2\kappa\bar{\Gamma}t} \right) + \mathcal{O} \left(\frac{\kappa\Delta\Gamma}{2} \right)^3 \right]
\end{aligned} \tag{3.50}$$

3.3 Mean-square displacement for large rotational diffusion constant

In this section we present an alternate expression for mean-square displacement of an anisotropic particle which is valid for which rotational diffusion constant is large as compared to the inverse times scales $\kappa\bar{\Gamma}$ and $\kappa\Delta\Gamma$. In such a scenario, since the particle rotates faster, the mobility of the anisotropic particle is an average mobility over the rotational noise.

The general solution in this case from Eq.(3.2) we can write

$$\begin{aligned}
\mathbf{R}(t) &= e^{-\kappa \int_0^t \bar{\Gamma}[\theta(t')] dt'} \int_0^t \boldsymbol{\eta}(t') e^{\kappa \int_0^{t'} \bar{\Gamma}[\theta(t'')] dt''} dt' \\
&= \int_0^t \boldsymbol{\eta}(t') e^{-\kappa \int_t^{t'} \bar{\Gamma}[\theta(t'')] dt''} dt'
\end{aligned} \tag{3.51}$$

We start our analysis with Eq.(3.52), but we set $\mathbf{R}(0) = 0$. To proceed further, and in particular to look at the asymptotic limit of the correlations, we define the variable $u = (t - t')/t$. In terms of the new variable u , the solution for $\mathbf{R}(t)$ takes the form

$$\mathbf{R}(t) = t \int_0^1 du e^{-\kappa\bar{\Gamma}1tu} e^{-\frac{\kappa}{2}\Delta\Gamma \int_{t(1-u)}^t dt'' \overline{\mathcal{R}}[\theta(t'')]} \boldsymbol{\eta}[t(1-u)] \quad (3.52)$$

The equal-time correlation is then given by

$$\begin{aligned} \langle \mathbf{R}(t)\mathbf{R}(t) \rangle_{\eta} &= \int_0^1 du \int_0^1 du' e^{\kappa\bar{\Gamma}1tu} e^{-\kappa\bar{\Gamma}1tu'} e^{-\frac{\kappa}{2}\Delta\Gamma \int_{t(1-u)}^t dt'' \overline{\mathcal{R}}[\theta(t'')]} e^{-\frac{\kappa}{2}\Delta\Gamma \int_{t(1-u')}^t dt'' \overline{\mathcal{R}}[\theta(t'')]} \\ &\quad \langle \boldsymbol{\eta}[t(1-u)] \boldsymbol{\eta}[t(1-u')] \rangle_{\eta} \end{aligned} \quad (3.53)$$

The correlation of the thermal noise in the transformed variable is

$$\langle \boldsymbol{\eta}[t(1-u)] \boldsymbol{\eta}[t(1-u')] \rangle_{\eta} = \frac{2k_B T}{t} \overline{\overline{\Gamma}}[t(1-u)] \delta(u-u') \quad (3.54)$$

Substituting the noise correlation into Eq.(3.53) and integration over u' we get

$$\langle \mathbf{R}(t)\mathbf{R}(t) \rangle = 2k_B T t \int_0^1 du e^{-2\kappa\bar{\Gamma}1tu} e^{-\kappa\Delta\Gamma \int_{t(1-u)}^t dt'' \overline{\mathcal{R}}[\theta(t'')]} \times \left[\overline{\overline{\Gamma}}\mathbf{1} + \frac{\Delta\Gamma}{2} \overline{\overline{\mathcal{R}}}[\theta(t(1-u))] \right] \quad (3.55)$$

In the asymptotic limit, the integral is dominated by small values of u , the integral in the exponential from $t(1-u)$ to t is vanishingly small and can be set to zero. Further, we set $\overline{\overline{\mathcal{R}}}[\theta(t(1-u))] \approx \overline{\overline{\mathcal{R}}}[\theta(t)]$. Consequently, the correlation matrix averaged over the translational noise take the form

$$\langle \mathbf{R}(t)\mathbf{R}(t) \rangle = 2k_B T t \int_0^1 du e^{-2\kappa\bar{\Gamma}1tu} \left[\overline{\overline{\Gamma}}\mathbf{1} + \frac{\Delta\Gamma}{2} \overline{\overline{\mathcal{R}}}[\theta(t)] \right] \quad (3.56)$$

Now we have to perform the average over the rotational noise and the integral over u we arrive at

$$\langle \mathbf{R}(t)\mathbf{R}(t) \rangle_{\eta, \theta} = 2k_B T t \left(\frac{1 - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma}t} \right) \left(\overline{\overline{\Gamma}}\mathbf{1} + \frac{\Delta\Gamma}{2} \langle \overline{\overline{\mathcal{R}}}[\theta(t)] \rangle_{\theta} \right) \quad (3.57)$$

Simplifying the result and using Eq.(2.29) we arrive at

$$\langle \mathbf{R}(t)\mathbf{R}(t) \rangle_{\eta, \theta} = \frac{k_B T}{\kappa\bar{\Gamma}} \left(1 - e^{-2\kappa\bar{\Gamma}t} \right) \left(\overline{\overline{\Gamma}}\mathbf{1} + \frac{\Delta\Gamma}{2} \overline{\overline{\mathcal{R}}}(\theta_0) e^{-4D_{\theta}t} \right) \quad (3.58)$$

The mean-square displacement in the explicit form is given by

$$\langle \Delta x^2(t) \rangle_{\eta, \theta} = \frac{k_B T}{\kappa} \left(1 - e^{-2\kappa \bar{\Gamma} t} \right) \left(1 + \frac{\Delta \Gamma}{2\bar{\Gamma}} \cos 2\theta_0 e^{-4D\theta t} \right) \quad (3.59)$$

$$\langle \Delta y^2(t) \rangle_{\eta, \theta} = \frac{k_B T}{\kappa} \left(1 - e^{-2\kappa \bar{\Gamma} t} \right) \left(1 - \frac{\Delta \Gamma}{2\bar{\Gamma}} \cos 2\theta_0 e^{-4D\theta t} \right) \quad (3.60)$$

and

$$\langle \Delta x(t) \Delta y(t) \rangle_{\eta, \theta} = \frac{k_B T}{\kappa} \left(1 - e^{-2\kappa \bar{\Gamma} t} \right) \left(\frac{\Delta \Gamma}{2\bar{\Gamma}} \sin 2\theta_0 e^{-4D\theta t} \right) \quad (3.61)$$

Note that there is striking difference between the Eqs.(3.59) and (3.60) and that of Eqs.(3.50) and (3.52) with respect to the limit of $\kappa \rightarrow 0$. While the later expressions correctly reproduces the free diffusion of the anisotropic particle, the limit of $\kappa \rightarrow 0$ in Eq.(3.58) yields the correct asymptotic result by setting $e^{-4D\theta t} \rightarrow 0$:

$$\langle x^2(t) \rangle = \langle y^2(t) \rangle = 2k_B T \bar{\Gamma} t \quad (3.62)$$

and

$$\langle \Delta x(t) \Delta y(t) \rangle_{\eta, \theta} = 0 \quad (3.63)$$

The analytical expressions of Eqs.(3.50), (3.52), (3.59) and (3.60) are compared with the numerically mean-square displacements along the two directions in Figs.(3.1) and (3.2). The mean-square displacements are computed from the numerical integration of the equations of motion using an Euler discretization scheme with a time step of $\delta t = 0.001$.

3.4 Persistence Probability

We now turn our attention to the persistence probability of the harmonically trapped ellipsoid particle. As in the case of a free particle, we assume the anisotropy to be very small so that the deviation from the Gaussian nature of the stochastic variables can be ignored. We focus on the two time correlated function $\langle x(t_1)x(t_2) \rangle_{\eta, \theta}$. Using the perturbation series given in Eq.(3.4) we have up to order $\mathcal{O}(\kappa \Delta \Gamma / 2)$

$$\langle x(t_1)x(t_2) \rangle_{\eta, \theta} = \langle x_0(t_1)x_0(t_2) \rangle_{\eta, \theta} - \left(\frac{\kappa \Delta \Gamma}{2} \right) \left[\langle x_0(t_1)x_1(t_2) \rangle_{\eta, \theta} + \langle x_0(t_2)x_1(t_1) \rangle_{\eta, \theta} \right] \quad (3.64)$$

where $t_1 > t_2$. The correlation functions $\langle x_0(t_1)x_1(t_2) \rangle_{\eta, \theta}$ are equal only in the asymptotic limit, that is for t_1 and t_2 large. In this limit, the expression for the two time correlation

function takes the form

$$\langle x(t_1)x(t_2) \rangle_{\eta,\theta} = \langle x_0(t_1)x_0(t_2) \rangle_{\eta,\theta} - (\kappa\Delta\Gamma) \left[\langle x_0(t_1)x_1(t_2) \rangle_{\eta,\theta} \right] \quad (3.65)$$

The correlation functions $\langle x_0(t_1)x_0(t_2) \rangle_{\eta,\theta}$ and $\langle x_0(t_1)x_1(t_2) \rangle_{\eta,\theta}$ have been derived in Eq.(3.14) and Eq.(3.41) respectively. For completeness, we quote the main results here.

$$\begin{aligned} \langle x_0(t_1)x_0(t_2) \rangle_{\eta,\theta} &= \frac{k_B T}{\kappa} \left[e^{-\kappa\bar{\Gamma}|t_1-t_2|} - e^{-\kappa\bar{\Gamma}(t_1+t_2)} \right] \\ &+ \left(\frac{k_B T}{\kappa} \right) \kappa\Delta\Gamma \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_1} \left[\frac{e^{(\kappa\bar{\Gamma}-4D_\theta)t_2} - e^{-\kappa\bar{\Gamma}t_2}}{2\kappa\bar{\Gamma} - 4D_\theta} \right] \end{aligned} \quad (3.66)$$

$$\begin{aligned} \langle x_0(t_1)x_1(t_2) \rangle_{\eta,\theta} &= \left(\frac{k_B T}{\kappa} \right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_1} \left(\frac{e^{(\kappa\bar{\Gamma}-4D_\theta)t_2} - e^{-\kappa\bar{\Gamma}t_2}}{2\kappa\bar{\Gamma} - 4D_\theta} - \frac{e^{-\kappa\bar{\Gamma}t_2} - e^{(\kappa\bar{\Gamma}+4D_\theta)t_2}}{4D_\theta} \right) \\ &+ \left(\frac{k_B T}{\kappa} \right) \left(\frac{\Delta\Gamma}{2\bar{\Gamma}} \right) e^{-\kappa\bar{\Gamma}t_1} \left[\frac{e^{\kappa\bar{\Gamma}t_2} - e^{-\kappa\bar{\Gamma}t_2}}{(2\kappa\bar{\Gamma} + 4D_\theta)} - \frac{2\kappa\bar{\Gamma} e^{-\kappa\bar{\Gamma}t_2} - e^{-(2\kappa\bar{\Gamma}+4D_\theta)t_2}}{(4D_\theta)(\kappa\bar{\Gamma} + 4D_\theta)} \right] \end{aligned} \quad (3.67)$$

Note that in calculating the two line correlation function up to an order $\mathcal{O}(\kappa\Delta\Gamma)$, we will use only the first term appearing in Eq.(3.67). Looking at Eq.(3.65), Eqs.(3.66) and (3.67), it is clear that the first term contained in the parenthesis in Eq.(3.67) cancels with the term proportional to $\kappa\Delta\Gamma$ in Eq.(3.66). The final expression for $\langle x(t_1)x(t_2) \rangle_{\eta,\theta}$ reads,

$$\langle x(t_1)x(t_2) \rangle_{\eta,\theta} = \left(\frac{2k_B T}{\kappa} \right) e^{-\kappa\bar{\Gamma}t_1} \left[\sinh \kappa\bar{\Gamma}t_2 + \left(\frac{\kappa\Delta\Gamma}{2} \right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_2} \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta} \right) \right] \quad (3.68)$$

As before, defining the variable $X(T) = x(t)/\sqrt{\langle x^2 \rangle_{\eta,\theta}}$, the correlation function of $\langle X(T_1)X(T_2) \rangle_{\eta,\theta}$ is given by

$$\langle X(t_1)X(t_2) \rangle_{\eta,\theta} = \frac{e^{-\kappa\bar{\Gamma}t_1/2}}{e^{-\kappa\bar{\Gamma}t_2/2}} \left[\frac{\sinh \kappa\bar{\Gamma}t_2 + \left(\frac{\kappa\Delta\Gamma}{2} \right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_2} \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta} \right)}{\sinh \kappa\bar{\Gamma}t_1 + \left(\frac{\kappa\Delta\Gamma}{2} \right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_1} \left(\frac{1 - e^{-4D_\theta t_1}}{4D_\theta} \right)} \right]^{1/2} \quad (3.69)$$

Using the transformation $e^T = e^{\kappa\bar{\Gamma}t} \left[\sinh \kappa\bar{\Gamma}t + \frac{\kappa\Delta\Gamma}{2} \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t} \left(\frac{1 - e^{-4D_\theta t}}{4D_\theta} \right) \right]$ for a transformed effective time variable T , the correlation function $\langle X(T_1)X(T_2) \rangle_{\eta,\theta}$ becomes a stationary correlator : $\langle X(T_1)X(T_2) \rangle_{\eta,\theta} = e^{-(T_1-T_2)/2}$ and the corresponding persistence probability is given by

$$p(t) \sim \frac{\sqrt{\kappa} e^{-\kappa\bar{\Gamma}t/2}}{\left[\sinh \kappa\bar{\Gamma}t + \left(\frac{\kappa\Delta\Gamma}{2} \right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t} \left(\frac{1 - e^{-4D_\theta t}}{4D_\theta} \right) \right]^{1/2}} \quad (3.70)$$

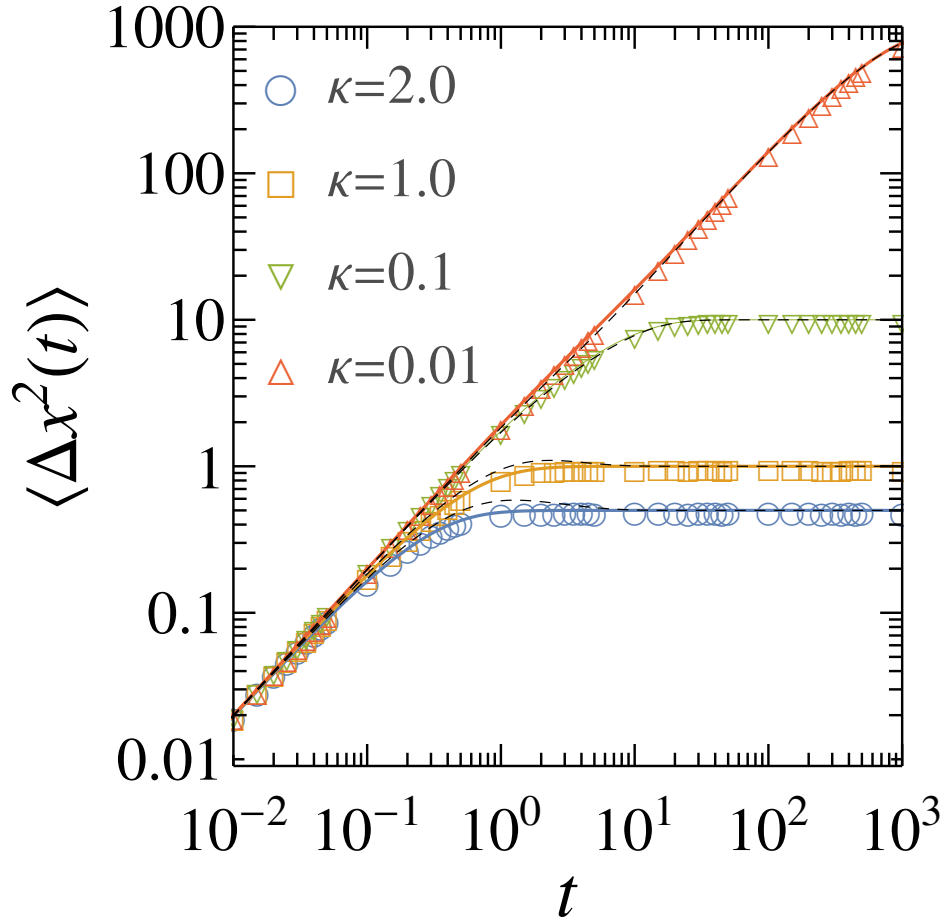


Figure 3.1 Plot of the mean-square displacement along the x direction of the harmonically trapped anisotropic particle for different choices of the stiffness of the harmonic potential, as indicated in the legend. The translational diffusivities and the rotational diffusion constant were kept fixed at $D_{\parallel} = 1$, $D_{\perp} = 0.5$, and $D_{\theta} = 0.1$ in all the cases. The initial orientation of the particles was also fixed at $\theta_0 = 0$. The solid lines are plots of Eq. (3.50), and the dashed lines are plots of Eq.(3.60) with the appropriate values of κ , D_{\parallel} , D_{\perp} , and D_{θ} .

In the limit of $\Delta\Gamma \rightarrow 0$ the equation correctly reproduces the persistence probability of an isotropic particle in the presence of a harmonic trap³⁶. The other limit of $\kappa \rightarrow 0$ reproduces the persistence probability of a free anisotropic particle derived in Eq.(2.45).

In Fig. 3.3, we show the comparison between the analytical expression of $p(t)$ given in Eq. (3.70) with the numerically obtained persistence probability. The numerical estimation of the persistence probability was done by discretizing the equations of motion in Eq. (3.2) with an integration time step of $\delta t = 0.001$. The fraction of trajectories that did not change sign up to time t gives the persistence probability $p(t)$. A total of 10^9 trajectories were used in determining $p(t)$.

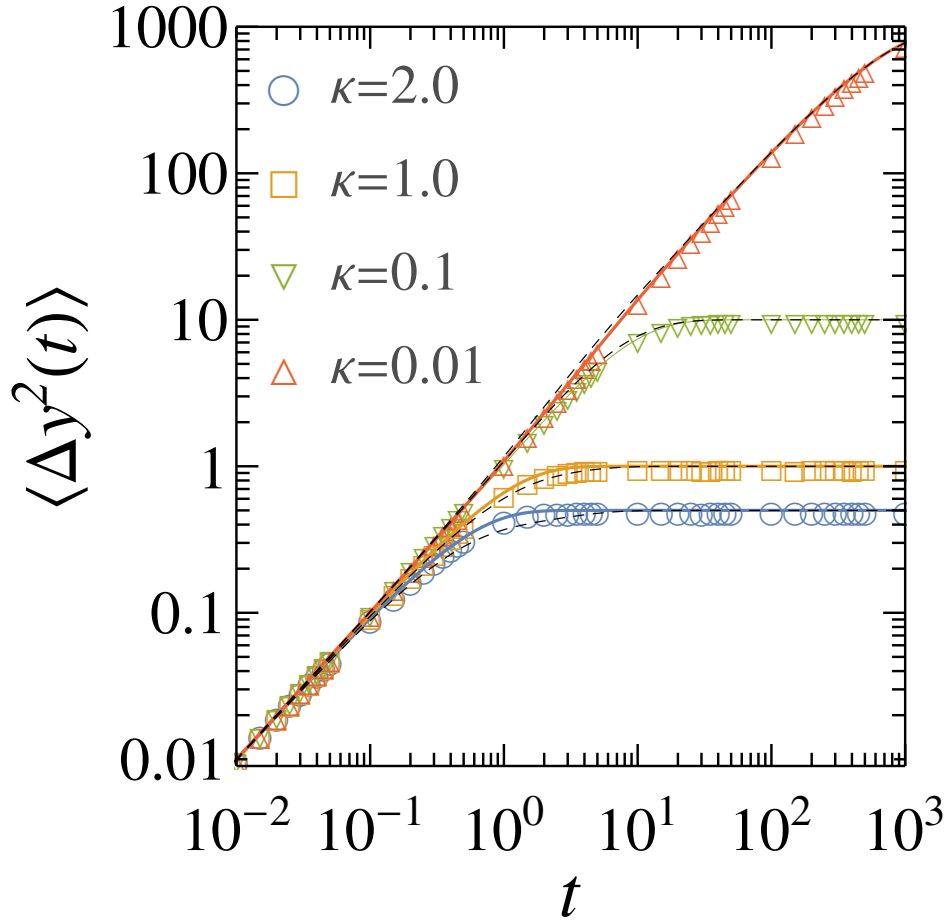


Figure 3.2 Plot of the mean-square displacement along the y direction of the harmonically trapped anisotropic particle for different choices of the stiffness of the harmonic potential, as indicated in the legend. The translational diffusivities and the rotational diffusion constant were kept fixed at $D_{\parallel} = 1$, $D_{\perp} = 0.5$, and $D_{\theta} = 0.1$ in all cases. The initial orientation of the particles was also fixed at $\theta_0 = 0$. The solid lines are plots of Eq. (3.52), and the dashed lines are plots of Eq. (3.58) with the appropriate values of κ , D_{\parallel} , D_{\perp} , and D_{θ} .

3.5 Conclusion

In summary, we have determined the persistence probability of an anisotropic particle in two spatial dimensions, in the presence as well as in the absence of a confining harmonic potential. The two-time correlation functions of the position of the particle have been calculated in both cases. In the case of a harmonically confined particle, a perturbative solution has been provided for the correlation functions. The persistence probability is computed from the two-time correlation function using suitable transformations in space and time. The determination of the rotational and the translational diffusion coefficients has been explicitly carried out for an anisotropic particle that undergoes free Brownian motion. Additionally, the analytical results have been confirmed by numerical

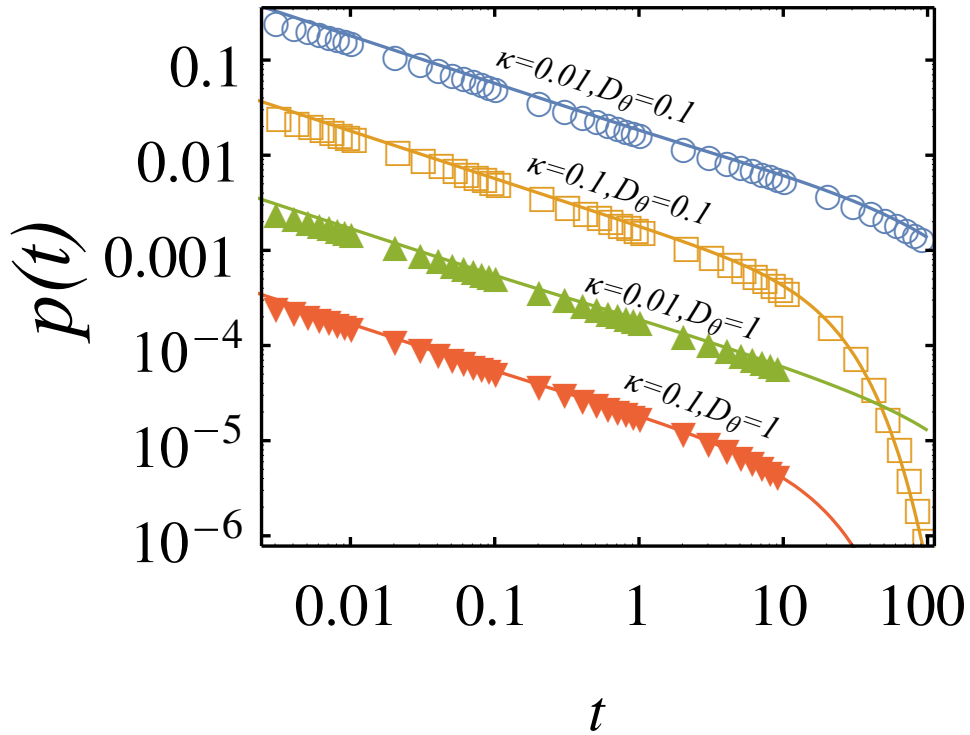


Figure 3.3 Plot of the survival probability $p(t)$ of a harmonically trapped anisotropic particle for different choices of the rotational diffusion constant and the stiffness of the potential, as indicated alongside each plot. The plots have been shifted for a better visibility. The solid lines are plots of Eq. (3.70) with the appropriate values of κ , D_{\parallel} , D_{\perp} and D_{θ} . While the rotational diffusion constant and the spring stiffness were varied, the translational diffusivities and the initial angle θ_0 were fixed at values $D_{\parallel} = 1$, $D_{\perp} = 0.5$ and $\theta_0 = 0$

simulation of the underlying stochastic dynamics.

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4

Persistence of Active asymmetric Brownian particle in two dimensions

We have studied the persistence probability $p(t)$ of an active Brownian particle with shape asymmetry in two dimensions. The persistence probability is defined as the probability of a stochastic variable that has not changed its sign in the fixed given time interval. We have investigated two cases- diffusion of a free active particle and that of the harmonically trapped particle. In our earlier work, *Ghosh et. al.* we had shown that $p(t)$ can be used to determine translational and the rotational diffusion constant of an asymmetric shape particle. The method has the advantage that the measurement of the rotational motion of the anisotropic particle is not required. In this chapter, we extend the study to an active anisotropic particle and show how the persistence probability of an anisotropic particle is modified in the presence of a propulsion velocity. Further, we validate our analytical expression against the measured persistence probability from the numerical simulations of single particle Langevin dynamics and test whether the method proposed in our earlier work can distinguish between an active and a passive anisotropic particle.

In recent years there has been a huge interest in research activities developed regarding the statistical description of systems far from equilibrium. Quite many numbers of classes in biological and physical systems which are referred to as active matter have been studied both theoretically¹⁻¹² and experimentally^{13,14}. The term "active" refers here to the motion of individual units to move actively by gaining kinetic energy from the environment. Examples of such systems spread from the dynamical behavior of individual units such as Brownian motors^{15,16}, motile cells^{17,18} macroscopic animals¹⁹⁻²³ or artificial self-propelled particles to large ensembles of interacting active particles and their large-scale collective dynamics. Active matter is a driven system where energy is provided directly, isotropically, and independently at the level of active particles- which under dissipation of the energy, generally achieves a systematic movement. In simple Brownian motion, energy is supplied to the particle by molecular agitation which leads to stochastic forces. We here generalized the idea of Brownian particles by including an additional energy source. Self-propulsion is the essential source of energy for most living systems, maintaining metabolism and performing movement. The aims of the active particle paradigm are: to bring the living systems into the ambit of condensed matter physics, and to study the emergent statistical and thermodynamic laws governing the system of intrinsically propelled particles.

Thus we study the active Brownian particle. Moreover, the shape deformation of the particles plays an important role in nonequilibrium transport processes. Han and co-workers experimentally studied the Brownian motion of isolated ellipsoidal particles in two dimensions and quantified the crossover from the short-time anisotropic to long-time isotropic diffusion²⁴. At the same time, our previous work was to find the persistence probability of such two-dimensional ellipsoidal Brownian particle²⁵. Now we are aiming to study the effect of activity on the system, and how the persistence probability changes thereafter. It is pertinent to mention here that the first passage properties of an active Brownian particle was investigated by Basu *et. al.*²⁶

This chapter has been organized in the following way: in section 4.2, the basic system has been described for the free active particle and the mean squared displacement, and the persistence are studied. In section 4.3, the active particle has been taken in harmonic confinement. The dynamics of the particle have been studied and along with that, we studied the persistence probability verifying it numerically. Section 4.4 concludes the chapter.

4.2

Asymmetric Free Active Brownian Particle in two dimensions

We have considered an asymmetric self propelled with velocity v_0 in two dimensions with mobilities Γ_{\parallel} and Γ_{\perp} along the longer and the shorter axes of the particle respectively. We have fixed the body frame x - and y - directions as the long and the short axis, respectively. The particle has a single rotational mobility Γ_{θ} . The particle is immersed in a bath of temperature T so that the translational diffusion coefficients along the two directions are given by $D_{\parallel} = k_B T \Gamma_{\parallel}$ and $D_{\perp} = k_B T \Gamma_{\perp}$, and the rotational diffusion constant is $D_{\theta} = k_B T \Gamma_{\theta}$. At a given time t the particle can be described by the position vector of its center of mass $\mathbf{r}(t)$ and the angle $\theta(t)$ between the x - axis of the lab-frame and the long axis of the particle. In this frame the self-propulsion speed, which is taken along the long axis of the rod, is given by, $v_0 \hat{n}(t)$, where $\hat{n}(t) \equiv (\cos \theta(t), \sin \theta(t))$ is a unit vector along the long axis of the particle. In the body frame, the equations of motion for the center of mass of the particle take the form

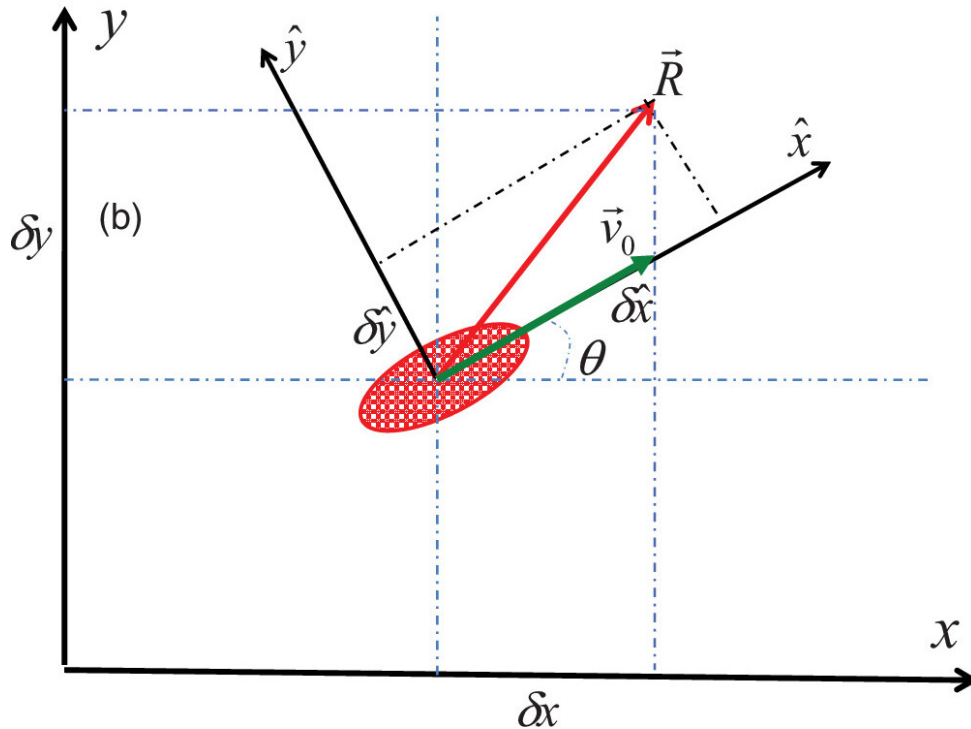


Figure 4.1 Representation of an ellipsoid in the $x - y$ lab frame and the $\hat{x} - \hat{y}$ body frame. The angle between two frames is θ . The displacement \mathbf{R} can be decomposed as $(\delta \hat{x}, \delta \hat{y})$ or $(\delta x, \delta y)$.

$$\begin{aligned}
\Gamma_1^{-1} \frac{\partial \tilde{x}}{\partial t} &= F_x \cos \theta(t) + F_y \sin \theta(t) + \tilde{\xi}_x(t) + \frac{v_0}{\Gamma_1} \\
\Gamma_2^{-1} \frac{\partial \tilde{y}}{\partial t} &= F_y \cos \theta(t) - F_x \sin \theta(t) + \tilde{\xi}_y(t) \\
\Gamma_3^{-1} \frac{\partial \theta(t)}{\partial t} &= \tau + \tilde{\xi}_\theta(t)
\end{aligned} \tag{4.1}$$

Here F_x and F_y are the forces acting on the particle along the x and y axes (in the lab frame) respectively, and τ is the torque acting on the particle. The correlation of the thermal fluctuations in the body frame are given by

$$\begin{aligned}
\langle \tilde{\xi}_i \rangle &= 0 \\
\langle \tilde{\xi}_i(t) \tilde{\xi}_j(t') \rangle &= \frac{2k_B T}{\Gamma_i} \delta_{ij} \delta(t - t')
\end{aligned} \tag{4.2}$$

In the lab frame, the displacements are related to the body frame as

$$\begin{aligned}
\delta x &= \cos \theta \delta \tilde{x} - \sin \theta \delta \tilde{y} \\
\delta y &= \sin \theta \delta \tilde{x} + \cos \theta \delta \tilde{y}
\end{aligned} \tag{4.3}$$

Replacing the values of Eq. (4.3) in Eq. (4.1) we get the equations in lab frame in the Ito convention²⁷⁻³⁰ as,

$$\begin{aligned}
\frac{\partial x}{\partial t} &= v_0 \cos \theta(t) + F_x \left[\bar{\Gamma} + \frac{\Delta \Gamma}{2} \cos 2\theta(t) \right] + \frac{\Delta \Gamma}{2} F_y \sin 2\theta(t) + \xi_x(t) \\
\frac{\partial y}{\partial t} &= v_0 \sin \theta(t) + F_y \left[\bar{\Gamma} - \frac{\Delta \Gamma}{2} \cos 2\theta(t) \right] + \frac{\Delta \Gamma}{2} F_x \sin 2\theta(t) + \xi_y(t) \\
\frac{\partial \theta(t)}{\partial t} &= \Gamma_3 \tau + \xi_\theta(t)
\end{aligned} \tag{4.4}$$

Using Eq.(4.1) , the corresponding Langevin equation in the lab frame is given by,

$$\frac{\partial x_i}{\partial t} = -\Gamma_{ij} \frac{\partial U}{\partial x_j} + \xi_i \tag{4.5}$$

where $U(r)$ is the external potential, and the thermal fluctuations from Eq.(4.3) can be written as

$$\begin{aligned}
\langle \xi_\theta(t) \xi_\theta(t') \rangle &= 2D_\theta \delta(t - t') \\
\langle \xi_i(t) \xi_j(t') \rangle_{\theta(t)}^{\xi_1, \xi_2} &= 2k_B T \Gamma_{ij} \delta(t - t')
\end{aligned} \tag{4.6}$$

and

$$\Gamma_{ij} = \bar{\Gamma} \delta_{ij} + \frac{\Delta \Gamma}{2} \begin{pmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{pmatrix} \tag{4.7}$$

Here $\bar{\Gamma} = (\Gamma_{\parallel} + \Gamma_{\perp})/2$ and $\Delta\Gamma = (\Gamma_{\parallel} - \Gamma_{\perp})$, and mobility tensor can be written as $\Gamma_{ij} = \bar{\Gamma}\delta_{ij} + \frac{\Delta\Gamma}{2}\Delta\mathcal{R}_{ij}[\theta(t)]$, when the form of $\Delta\mathcal{R}$ is written as

$$\Delta\mathcal{R} = \begin{pmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{pmatrix}$$

The model investigated in the work of Basu *et. al.*²⁶ is different than the one that is presented here. They consider an active Brownian particle without the thermal fluctuations and an explicit shape asymmetry. The dynamics is mapped to that of a Brownian particle with an effective noise that is not only bounded by the propulsion velocity but the two time correlation function of the noise decays exponentially. Consequently, in Eq. (4.4) the second and the third terms are not present.

4.2.1 Mean Square Displacement of the free active particle

We first take the case of free active ellipsoidal particle setting the external potential zero, the equation of motion takes the form

$$x_i(t) = v_0 \int_0^t \cos \theta(t') dt' + \int_0^t \xi_i(t') dt' \quad (4.8)$$

The mean $\langle \Delta x(t) \rangle$, where $\Delta x = x(t) - x(0)$ takes

$$\langle \Delta x(t) \rangle = v_0 \int_0^t \langle \cos \theta(t') \rangle dt' = v_0 \cos \theta_0 \left(\frac{1 - e^{-D\theta t}}{D\theta} \right). \quad (4.9)$$

The mean square displacement of the particle is calculated from Eq. (4.8)

$$\langle \Delta x_i^2 \rangle_{\xi_\theta} = v_0^2 \int_0^t \langle \cos \theta(t') \cos \theta(t'') \rangle dt' dt'' + \int_0^t \langle \xi_i(t') \xi_i(t'') \rangle dt' dt'' \quad (4.10)$$

To solve the above integral, we separately solve the two integrals I_1, I_2 which are shown below respectively from Eq. (4.11) to Eq. (4.16).

$$\begin{aligned} I_1 &= \int_0^t \langle \cos \theta(t') \cos \theta(t'') \rangle dt' dt'' \\ &= \frac{1}{2} \int_0^t dt' \int_0^t dt'' \langle [\cos(\theta(t') + \theta(t'')) + \cos(\theta(t') - \theta(t''))] \rangle \\ &= \frac{1}{2} \cos 2\theta_0 \int_0^t e^{-D\theta[t'+t''+2\min(t',t'')]} dt' dt'' + \frac{1}{2} \int_0^t e^{-D\theta[t'+t''-2\min(t',t'')]} dt' dt'' \end{aligned} \quad (4.11)$$

Integral I_1 is having two separate integrals and solving these two separately

$$\begin{aligned}
I' &= \int_0^t e^{-D_\theta[t'+t''+2\min(t',t'')]} dt' dt'' \\
&= \int_0^t dt' \int_0^{t'} dt'' e^{-D_\theta(t'+3t'')} + \int_0^t dt'' \int_0^{t''} dt' e^{-D_\theta(3t'+t'')} \\
&= \int_0^t e^{-D_\theta t'} dt' \int_0^{t'} e^{-3D_\theta t''} dt'' + \int_0^t e^{-D_\theta t''} dt'' \int_0^{t''} e^{-3D_\theta t'} dt' \\
&= \frac{1}{6D_\theta^2} (3 - 4e^{-D_\theta t} + e^{-4D_\theta t})
\end{aligned} \tag{4.12}$$

and

$$\begin{aligned}
I'' &= \int_0^t dt' \int_0^t dt'' e^{-D_\theta[t'+t''-2\min(t',t'')]} \\
&= \int_0^t dt' \int_0^{t'} dt'' e^{-D_\theta(t'-t'')} + \int_0^t dt'' \int_0^{t''} dt' e^{-D_\theta(t''-t')} \\
&= \int_0^t e^{-D_\theta t'} dt' \int_0^{t'} e^{D_\theta t''} dt'' + \int_0^t e^{-D_\theta t''} dt'' \int_0^{t''} e^{D_\theta t'} dt' \\
&= \frac{2}{D_\theta^2} (D_\theta t + e^{-D_\theta t} - 1)
\end{aligned} \tag{4.13}$$

So values of Eq.(4.12) and Eq.(4.13) is added to get I_1 as

$$I_1 = \frac{\cos 2\theta_0}{12D_\theta^2} (3 - 4e^{-D_\theta t} + e^{-4D_\theta t}) + \frac{1}{D_\theta^2} (D_\theta t + e^{-D_\theta t} - 1) \tag{4.14}$$

Now the second integral I_2 of Eq.(4.10) is calculated as

$$\begin{aligned}
I_2 &= \int_0^t dt' \int_0^t dt'' \langle \xi_i(t') \xi_i(t'') \rangle \\
&= 2k_B T \int_0^t dt' \int_0^t dt'' \langle \Gamma_{ii}[\theta(t')] \rangle_{\xi_\theta} \delta(t-t'') \\
&= 2k_B T \int_0^t dt' \langle \Gamma_{ii}[\theta(t')] \rangle_{\xi_\theta}
\end{aligned} \tag{4.15}$$

Using the explicit form of Γ_{xx} from Eq.(4.7) the mean-square displacement along the x -direction becomes

$$I_2 = 2k_B T \left[\bar{\Gamma} t + \Delta \Gamma \cos 2\theta_0 \left(\frac{1 - e^{-4D_\theta t}}{4D_\theta} \right) \right] \tag{4.16}$$

The final form of Mean-squared displacement is

$$\begin{aligned} \langle \Delta x^2(t) \rangle &= 2k_B T \left[\bar{\Gamma} t + \Delta \Gamma \cos 2\theta_0 \left(\frac{1 - e^{-4D_\theta t}}{4D_\theta} \right) \right] \\ &+ \frac{v_0^2 \cos 2\theta_0}{12D_\theta^2} (3 - 4e^{-D_\theta t} + e^{-4D_\theta t}) + \frac{v_0^2}{D_\theta^2} (D_\theta t + e^{-D_\theta t} - 1) \end{aligned} \quad (4.17)$$

and for y-direction

$$\begin{aligned} \langle \Delta y^2(t) \rangle &= 2k_B T \left[\bar{\Gamma} t - \Delta \Gamma \cos 2\theta_0 \left(\frac{1 - e^{-4D_\theta t}}{4D_\theta} \right) \right] \\ &- \frac{v_0^2 \cos 2\theta_0}{12D_\theta^2} (3 - 4e^{-D_\theta t} + e^{-4D_\theta t}) + \frac{v_0^2}{D_\theta^2} (D_\theta t + e^{-D_\theta t} - 1) \end{aligned} \quad (4.18)$$

In the absence of an active propulsion velocity, the position of the particle in the lab frame is a non-Gaussian stochastic variable. The non-Gaussian parameter is defined as,

$$\phi(t, \theta_0) = \frac{\langle [\Delta x(t) - \langle \Delta x(t) \rangle]^4 \rangle - 3(\langle [\Delta x(t) - \langle \Delta x(t) \rangle]^2 \rangle)^2}{3(\langle [\Delta x(t) - \langle \Delta x(t) \rangle]^2 \rangle)^2} \quad (4.19)$$

Defining $\tau_\theta = 1/2D_\theta$ and $\tau_n(t) = (1 - e^{-nD_\theta t})/nD_\theta$, the expressions in Eq. (4.9) and Eq. (4.17) take the form

$$\langle \Delta x(t) \rangle = v_0 \cos \theta_0 \tau_1(t) \quad (4.20)$$

and

$$\langle \Delta x(t)^2 \rangle = 2\bar{D}t + \Delta D \tau_4 \cos 2\theta_0 + 2\tau_\theta v_0^2 \left((t - \tau_1) + \frac{1}{3}(\tau_1 - \tau_4) \cos 2\theta_0 \right) \quad (4.21)$$

Further, defining $C_{\theta_0}^4(t) = \langle [\Delta x(t) - \langle \Delta x(t) \rangle]^4 \rangle - 3(\langle [\Delta x(t) - \langle \Delta x(t) \rangle]^2 \rangle)^2$, the non-Gaussian parameter is written as,

$$\phi(t, \theta_0) = \frac{C_{\theta_0}^4(t)}{3(\langle \Delta x(t)^2 \rangle)^2} \quad (4.22)$$

Since we evaluate the persistence probability keeping the initial angle θ_0 fixed, specifically $\theta_0 = 0$, we estimate the non-Gaussian parameter at $\theta_0 = 0$. Further, we will also consider a weak asymmetry and weak propulsion velocity so that we evaluate $\phi(t, \theta_0 = 0)$ only up to the order of v_0^2 . The expression for $C_{\theta_0=0}^4(t)$ takes the form

$$\begin{aligned}
C_{\theta_0=0}^4(t) = & \Delta D^2 \left[\frac{3}{2} t \tau_\theta - 3 \tau_4^2(t) - \frac{1}{2} \tau_\theta \tau_{16}(t) - \tau_4(t) \tau_\theta \right. \\
& \left. + v_0^2 \left(12 \Delta D \tau_1(t) \tau_4(t) \left[1 + \frac{16}{36} \tau_\theta \right] + t \left[24 \bar{D} \tau_1^2(t) + \frac{32}{3} \bar{D} \tau_1(t) \tau_\theta - 8 \Delta D \tau_4(t) \tau_\theta \right] - 16 \bar{D} \tau_\theta^2 \right) \right]
\end{aligned} \tag{4.23}$$

The expression for $\langle \Delta x^2(t) \rangle$ up to the order of v_0^2 has the

$$\begin{aligned}
3 \langle \Delta x^2(t) \rangle = & 12 \bar{D}^2 t^2 + 12 \bar{D} \Delta D t \tau_4(t) + 3 \Delta D \tau_4^2 \\
& + v_0^2 \left[\left(-6 \Delta D \tau_1^2(t) \tau_4(t) - 8 \Delta D \tau_\theta \tau_1(t) \tau_4(t) - 4 \Delta D \tau_\theta \tau_4^2(t) \right) \right. \\
& \left. + t \left(-12 \bar{D} \tau_1^2(t) - 16 \bar{D} \tau_1(t) \tau_\theta - 8 \bar{D} \tau_4(t) \tau_\theta + 12 \Delta D \tau_4(t) \tau_\theta \right) + 24 \bar{D} \tau_\theta t^2 \right]
\end{aligned} \tag{4.24}$$

Clearly from Eq. (4.23) and Eq. (4.24), the non-Gaussian parameter depends on the ratio $\Delta D^2/\bar{D}^2$ and v_0^2/\bar{D}^2 . In the limit of weak asymmetry and small propulsion velocity, the non-Gaussian parameter remains small. Further, we note that as $t \rightarrow \infty$ the ratio $\phi(t,0)$ decays as t^{-1} so that the non-Gaussian parameter vanishes. A comparison of $\phi(t,0)$ for an anisotropic particle with weak asymmetry is shown in Fig. 4.2 for two distinct cases -that of a passive anisotropic particle (dashed line) and that of an active anisotropic particle (dotted line). The time-dependent $\phi(t,0)$ exhibits a non-monotonic behaviour with a peak at $D_\theta t \approx 1$. Furthermore, we note that $\phi(t,0)$ of an active anisotropic particle vanishes quickly compared to a passive anisotropic particle for identical values of translational and rotational diffusivities. The higher order moments for $\Delta x(t)$ can also be calculated from Eq.(4.8). The linearity of the equation dictates that moments $\langle \Delta x^{2n} \rangle$ with $n > 2$ would contain terms proportional to v_0^{2n} and $\Delta \Gamma^n$ and would be vanishingly small for weak anisotropy and a small propulsion velocity.

4.2.2 Persistence of the free particle

We now turn our attention to the persistence probability of a free asymmetrical active Brownian particle. Setting the external potential zero, the formal solution to the equation of motion becomes

$$x_i(t) = x_i(0) + \int_0^t \xi_i(t') dt' + v_0 \int_0^t \cos \theta(t') dt' \tag{4.25}$$

To calculate the persistence probability, we start from Eq. (4.25) and choose initial condition $x_i(0) = 0$. The calculation of two-time correlation function $\langle x(t_1)x(t_2) \rangle_{\xi_\theta}$ can

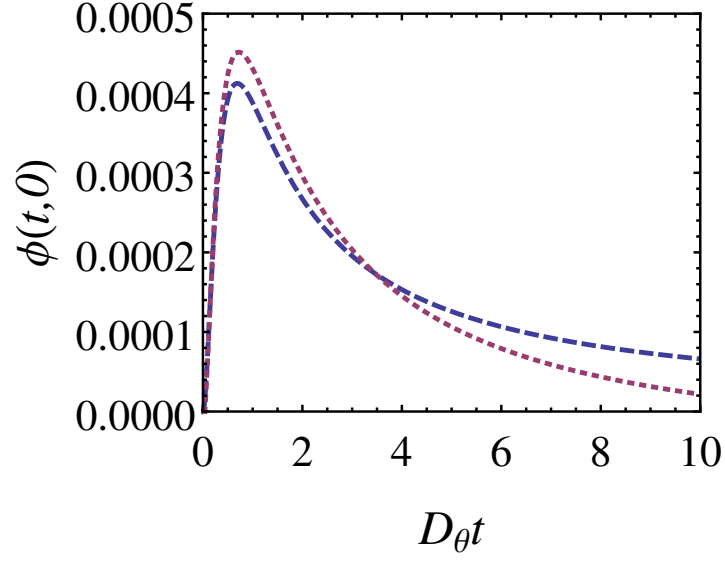


Figure 4.2 Plot of the non-Gaussian parameter $\phi(t, 0)$ for different choices of propulsion velocity v_0 of the anisotropic particle: $v_0 = 0$ (dotted line); $v_0 = 0.01$ (dashed line). The translational diffusivities were fixed at $D_{\parallel} = 1$, $D_{\perp} = 0.9$. The rotational diffusivity and the initial angle θ_0 were fixed at $D_{\theta} = 1$ and $\theta_0 = 0$, respectively.

be achieved by

$$\langle x(t_1)x(t_2) \rangle_{\xi_{\theta}} = v_0^2 \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \langle \cos \theta(t'_1) \cos \theta(t'_2) \rangle + \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \langle \xi_1(t'_1) \xi_2(t'_2) \rangle \quad (4.26)$$

We can separate Eq.(4.26) into two separate integrals as I_3 and I_4 , and calculate them individually

$$\begin{aligned} I_3 &= v_0^2 \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \langle \cos \theta(t'_1) \cos \theta(t'_2) \rangle \\ &= \frac{v_0^2}{2} \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \cos 2\theta_0 e^{-D_{\theta}[t'_1+t'_2+2\min(t'_1,t'_2)]} + \frac{v_0^2}{2} \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 e^{-D_{\theta}[t'_1+t'_2-2\min(t'_1,t'_2)]} \end{aligned} \quad (4.27)$$

for $t'_1 < t'_2$

$$\begin{aligned} t'_1 + t'_2 \pm 2t'_1 &= 3t'_1 + t'_2 \\ &= -t'_1 + t'_2 \end{aligned}$$

for $t'_1 > t'_2$

$$\begin{aligned} t'_1 + t'_2 \pm 2t'_2 &= t'_1 + 3t'_2 \\ &= t'_1 - t'_2 \end{aligned}$$

Lets take the two integrals of Eq.(4.27) as I'_3 and I''_3 . The integral Eq.(4.27) can be calculated in general terms like,

$$I_3 = \int_0^{t_2} dt'_2 \int_0^{t'_2} e^{-D_\theta(\alpha t'_1 + \beta t'_2)} + \int_0^{t'_2} dt' \int_{t'_2}^{t_1} dt'_1 e^{-D_\theta(\beta t'_1 + \alpha t'_2)}$$

$$= \frac{1 - e^{-\beta D_\theta t_2}}{\alpha \beta D_\theta^2} - \frac{1 - e^{-(\alpha + \beta) D_\theta t_2}}{\alpha(\alpha + \beta) D_\theta^2} + \frac{1 - e^{-(\alpha + \beta) D_\theta t_2}}{\beta(\alpha + \beta) D_\theta^2} - e^{-\beta D_\theta t_1} \frac{1 - e^{-\alpha D_\theta t_2}}{\alpha \beta D_\theta^2}$$

for integral I'_3 , $(\alpha, \beta) \equiv (3, 1)$

$$I'_3 = \frac{1 - e^{-D_\theta t_2}}{6D_\theta^2} + \frac{1 - e^{-4D_\theta t_2}}{12D_\theta^2} - e^{-D_\theta t_1} \frac{1 - e^{-3D_\theta t_2}}{6D_\theta^2}$$

and for integral I''_3 , $(\alpha, \beta) \equiv (-1, 1)$

$$I''_3 = -\frac{1 - e^{-D_\theta t_2}}{2D_\theta^2} + \frac{t_2}{D_\theta} - e^{-D_\theta t_1} \frac{1 - e^{D_\theta t_2}}{D_\theta^2}$$

So final form of I_3 becomes

$$I_3 = v_0^2 \left[\cos 2\theta_0 \left(\frac{1 - e^{-D_\theta t_2}}{6D_\theta^2} + \frac{1 - e^{-4D_\theta t_2}}{12D_\theta^2} - e^{-D_\theta t_1} \frac{1 - e^{-3D_\theta t_2}}{6D_\theta^2} \right) - \frac{1 - e^{-D_\theta t_2}}{2D_\theta^2} + \frac{t_2}{D_\theta} - e^{-D_\theta t_1} \frac{1 - e^{D_\theta t_2}}{D_\theta^2} \right] \quad (4.28)$$

The second integral I_4 of Eq. (4.26) is solved as

$$I_4 = \int_0^{t_1} dt'_1 \int_0^{t'_1} dt'_2 \langle \xi_x(t'_1) \xi_x(t'_2) \rangle$$

$$= 2k_B T \bar{\Gamma} t_2 \left[1 + \frac{\Delta \Gamma}{\bar{\Gamma}} \cos 2\theta_0 \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta t_2} \right) \right] \quad (4.29)$$

Considering $t_1 > t_2$, the whole integral has been solved. We have solved the integral considering combination of two integrals I_3 and I_4 , solving them separately in Eq. (4.27) to Eq. (4.29). We find

$$\langle x(t_1) x(t_2) \rangle = 2k_B T \bar{\Gamma} t_2 \left[1 + \frac{\Delta \Gamma}{\bar{\Gamma}} \cos 2\theta_0 \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta t_2} \right) \right] + v_0^2 \left[\cos 2\theta_0 \left(\frac{1 - e^{-D_\theta t_2}}{6D_\theta^2} + \frac{1 - e^{-4D_\theta t_2}}{12D_\theta^2} - e^{-D_\theta t_1} \frac{1 - e^{-3D_\theta t_2}}{6D_\theta^2} \right) - \frac{1 - e^{-D_\theta t_2}}{2D_\theta^2} + \frac{t_2}{D_\theta} - e^{-D_\theta t_1} \frac{1 - e^{D_\theta t_2}}{D_\theta^2} \right] \quad (4.30)$$

We now set the initial angle $\theta_0 = 0$. The diffusion coefficients \bar{D} and ΔD are renormalized by the active velocity. Furthermore, we note that the last term in Eq. (4.30) contains a stationary component which survives in the long time limit of t_1 and t_2 large but $(t_1 - t_2)$ finite. This, of course, makes the conversion of this non-stationary correlator to a stationary one slightly problematic. In order to transform the non-stationary correlation into a stationary correlator, we make the approximation $t_1 \gg t_2$ so that both the terms $2v_0^2 \tau_\theta \tau_3(t) e^{-D_\theta t_1}$ and the last term $v_0^2 e^{-D_\theta t_1} (1 - e^{D_\theta t_2}) / D_\theta^2$ in Eq. (4.30). Dropping the second term in Eq. (4.30) is strictly valid only when $t_1 \gg t_2$. It should be pointed out that both the terms are proportional to v_0^2 and for small v_0 the effect of these two terms are not significant as demonstrated later from the numerical estimation of the persistence probability $p(t)$. Nevertheless, even with this approximation, we want to figure out how well the analytical expression for $p(t)$ compares with the numerical results.

Active Brownian particle dynamics is not zero centric stochastic process as the average of the position variable $\langle x(t) \rangle$ has non-zero value unlike simple Brownian particle. So we need to transform the stochastic process as zero centric stochastic process by subtracting $\langle x(t_1) \rangle \langle x(t_2) \rangle$ from the above value of Eq.(4.30).

$$\langle x(t_1) \rangle \langle x(t_2) \rangle = \frac{v_0^2 \cos^2 \theta_0}{D_\theta^2} (1 - e^{-D_\theta t_1} - e^{-D_\theta t_2} + e^{-D_\theta(t_1+t_2)}) \quad (4.31)$$

Now for $\theta_0 = 0$, we subtract Eq.(4.31) from Eq.(4.30) and approximating $(t_1 - t_2)$ very small and t_1, t_2 are very large we get,

$$\langle x(t_1)x(t_2) \rangle_{\theta_0=0} = 2D_{eff}t_2 \left[1 + \frac{1}{2D_{eff}} \left(\Delta D + \frac{v_0^2}{3D_\theta} \right) \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta t_2} \right) - \frac{2v_0^2}{3D_\theta D_{eff}} \left(\frac{1 - e^{-D_\theta t_2}}{D_\theta t_2} \right) \right] \quad (4.32)$$

Here, $D_{eff} = \bar{D} + \frac{v_0^2}{2D_\theta}$

We use the transformation in the spatial coordinate³¹ $\tilde{X}(t) = x(t) / \sqrt{\langle x^2(t) \rangle_{\xi_\theta}}$. The two-time correlation function of the rescaled variable $\langle \tilde{X}(t_1) \tilde{X}(t_2) \rangle_{\xi_\theta}$ becomes,

$$\langle \bar{X}(t_1)\bar{X}(t_2) \rangle = (t_2/t_1)^{1/2} \left[2D_{\text{eff}} + \Delta D_{\text{eff}} \left(\frac{1 - e^{-4D_{\theta}t_2}}{4D_{\theta}t_2} \right) - \frac{4v_0^2}{3D_{\theta}} \left(\frac{1 - e^{-D_{\theta}t_2}}{D_{\theta}t_2} \right) \right]^{1/2} \left[2D_{\text{eff}} + \Delta D_{\text{eff}} \left(\frac{1 - e^{-4D_{\theta}t_1}}{4D_{\theta}t_1} \right) - \frac{4v_0^2}{3D_{\theta}} \left(\frac{1 - e^{-D_{\theta}t_1}}{D_{\theta}t_1} \right) \right]^{-1/2} \quad (4.33)$$

where the effective diffusivity is given by $D_{\text{eff}} = \bar{D} + v_0^2/2D_{\theta}$ and $\Delta D_{\text{eff}} = \Delta D + v_0^2/3D_{\theta}$. We now define the transformation in time as

$$e^T = 2D_{\text{eff}} \left[1 + \frac{\Delta D_{\text{eff}}}{2D_{\text{eff}}} \left(\frac{1 - e^{-4D_{\theta}t}}{4D_{\theta}t} \right) - \frac{4v_0^2}{3D_{\theta}D_{\text{eff}}} \left(\frac{1 - e^{-D_{\theta}t}}{D_{\theta}t} \right) \right] \quad (4.34)$$

Using this transformation in time the two-time correlation function $\langle \bar{X}(T_1)\bar{X}(T_2) \rangle$ from Eq. (4.33) takes the simple form of $\langle \bar{X}(t_1)\bar{X}(t_2) \rangle = e^{-(T_1-T_2)/2}$. Since the stationary correlation function now decays exponentially for all times, following Slepian³², the asymptotic form of the persistence probability is found as

$$P(T) = e^{-\lambda T} \quad (4.35)$$

Transforming back to real-time t , we get the persistence probability for the free particle as

$$p(t, \theta_0 = 0) = \frac{1}{\sqrt{2D_{\text{eff}}t}} \left[1 + \frac{\Delta D_{\text{eff}}}{2D_{\text{eff}}} \left(\frac{1 - e^{-4D_{\theta}t}}{4D_{\theta}t} \right) - \frac{4v_0^2}{3D_{\theta}D_{\text{eff}}} \left(\frac{1 - e^{-D_{\theta}t}}{D_{\theta}t} \right) \right]^{-1/2} \quad (4.36)$$

Rearranging the above expression, we get

$$t^{1/2}p(t, \theta_0 = 0) = \frac{1}{\sqrt{2D_{\text{eff}}}} \left[1 + \left(\frac{\Delta D_{\text{eff}}}{2D_{\text{eff}}} \right) \left(\frac{1 - e^{-4D_{\theta}t}}{4D_{\theta}t} \right) - \frac{4v_0^2}{3D_{\theta}D_{\text{eff}}} \left(\frac{1 - e^{-D_{\theta}t}}{D_{\theta}t} \right) \right]^{-1/2} \quad (4.37)$$

For simple brownian particle where propulsion velocity $v_0 = 0$, we get

$$t^{1/2}p(t) = \frac{1}{\sqrt{2\bar{D} \left[1 + \frac{\Delta D}{2\bar{D}} \left(\frac{1 - e^{-4D_{\theta}t}}{4D_{\theta}t} \right) \right]}} \quad (4.38)$$

This expression is exactly same as for ellipsoidal Brownian particle in two-dimensions²⁵. In order to validate the expression for the persistence probability we performed numer-

ical simulations of Eq. (4.4). The initial condition was chosen from a Gaussian distribution with a very small width, so the sign of $\mathbf{r}(0)$ is clearly defined. The trajectories were evolved in time with an integration time-step of $\delta t = 0.001$. At every instant, the survival of the particle trajectory was checked by looking at the sign of $\mathbf{r}(t)$. Fraction of trajectories for which the position did not change its sign up to time t gave the survival probability $p(t)$. A total of 10^9 trajectories were used in estimating the survival probability. A comparison of the measured $p(t)$ with that of the predictions of Eq. (4.37) is shown Figs. 4.3 and 4.4. Both the figures compare the persistence probability for weakly asymmetric particles. We observe that while the asymmetry of the particle is picked up as expected from our earlier work²⁵, for small propulsion velocity $t^{1/2}p(t)$ is unable to pick up the activity of the particle. In the case when the activity of the particle is comparatively large, the $t^{1/2}p(t)$ indeed picks up the activity of the particle. When compared with the analytical expression of Eq. (4.37), for the small propulsion velocity, the expression compares quite well with the simulation results with the overall constant as the only fit parameter (the dotted lines in the figures). When the data is fitted to Eq. (4.37) with the overall constant fixed and \bar{D} and ΔD as fit parameters, it yields the correct values of \bar{D} and ΔD . However, for comparatively larger values of v_0 , when the expression is plotted against the numerical data with the overall constant as the only fit parameter, the data matches only asymptotically with the analytical expression. On the other hand, when the data is fitted with Eq. (4.37) with \bar{D} and ΔD as fit parameters, the fit yields a slightly lower value of \bar{D} and a slightly higher value of ΔD . For example, in the case of $\bar{D} = 0.975$ and $\Delta D = 0.05$ (Fig. 4.3 open triangles), we obtain from the fit a value of $\bar{D} \approx 0.96$ and $\Delta D \approx 0.08$. In the case of $\bar{D} = 0.95$ and $\Delta D = 0.1$ (Fig. 4.4 open triangles), we obtain from the fit a value of $\bar{D} \approx 0.93$ and $\Delta D \approx 0.14$.

Before we conclude this section, for completeness we also present the results for the persistence probability for the stochastic variable $y(t)$, the y -coordinate of the active anisotropic particle in the lab frame. Two-time correlation along the y -direction is given by,

$$\langle y(t_1)y(t_2) \rangle_{\xi, \theta} = v_0^2 \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \langle \sin \theta(t'_1) \sin \theta(t'_2) \rangle + \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \langle \xi_1(t'_1) \xi_2(t'_2) \rangle \quad (4.39)$$

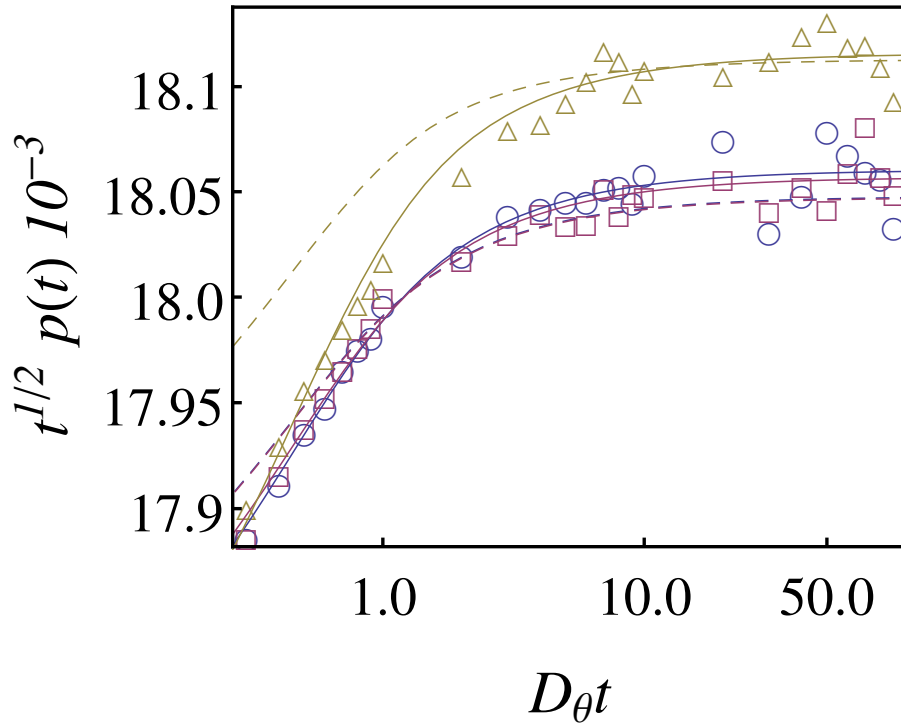


Figure 4.3 Plot of $t^{1/2} p(t)$ for different choices of propulsion velocity v_0 of the anisotropic particle: $v_0 = 0$ (open circles); $v_0 = 0.01$ (open square) and $v_0 = 0.1$ (open triangles). The translational diffusivities were fixed at $D_{\parallel} = 1$, $D_{\perp} = 0.95$. The rotational diffusivity and the initial angle θ_0 were fixed at $D_{\theta} = 1$ and $\theta_0 = 0$, respectively. The dashed lines are the plot of Eq. (4.37) whereas the solid lines are fit to the data using Eq. (4.37) with D_{eff} and ΔD as fit parameters.

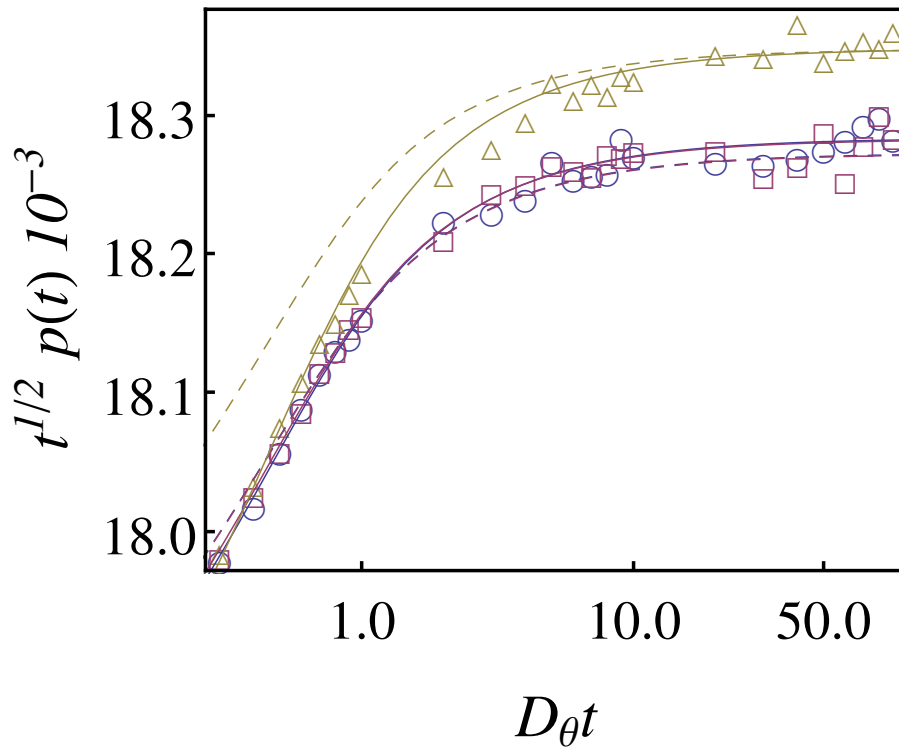


Figure 4.4 Plot of $t^{1/2} p(t)$ for different choices of propulsion velocity v_0 of the anisotropic particle: $v_0 = 0$ (open circles); $v_0 = 0.01$ (open square) and $v_0 = 0.1$ (open triangles). The translational diffusivities were fixed at $D_{\parallel} = 1$, $D_{\perp} = 0.90$. The rotational diffusivity and the initial angle were fixed at $D_{\theta} = 1$ and $\theta_0 = 0$, respectively. The dashed lines are the plot of Eq. (4.37) whereas the solid lines are fit to the data using Eq. (4.37) with D_{eff} and ΔD as fit parameters.

From the above Eq.(4.39) we can show the first integral as,

$$\begin{aligned}
& v_0^2 \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \langle \sin \theta(t'_1) \sin \theta(t'_2) \rangle \\
&= \frac{v_0^2}{2} \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 e^{-D_\theta[t'_1+t'_2-2\min(t'_1,t'_2)]} - \frac{v_0^2}{2} \cos 2\theta_0 \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 e^{-D_\theta[t'_1+t'_2+2\min(t'_1,t'_2)]} \\
&= v_0^2 \left[\frac{1 - e^{-D_\theta t_2}}{2D_\theta^2} + \frac{t_2}{D_\theta} - e^{-D_\theta t_1} \frac{1 - e^{-D_\theta t_2}}{D_\theta^2} - \cos 2\theta_0 \left(\frac{1 - e^{-D_\theta t_2}}{6D_\theta^2} + \frac{1 - e^{-4D_\theta t_2}}{12D_\theta^2} - e^{-D_\theta t_1} \frac{1 - e^{-3D_\theta t_2}}{6D_\theta^2} \right) \right]
\end{aligned} \tag{4.40}$$

The two-time correlation along y-direction can be found from Eq.(4.39) and Eq.(4.40).

$$\begin{aligned}
\langle y(t_1)y(t_2) \rangle_{\xi,\theta} &= 2k_B T \bar{\Gamma} t_2 \left[1 + \frac{\Delta \Gamma}{2\bar{\Gamma}} \cos 2\theta_0 \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta t_2} \right) \right] + v_0^2 \left[\frac{1 - e^{-D_\theta t_2}}{2D_\theta^2} + \frac{t_2}{D_\theta} + e^{-D_\theta(t_1-t_2)} \frac{1 - e^{-D_\theta t_2}}{D_\theta^2} \right. \\
&\quad \left. - \cos 2\theta_0 \left(\frac{1 - e^{-D_\theta t_2}}{6D_\theta^2} + \frac{1 - e^{-4D_\theta t_2}}{12D_\theta^2} - e^{-D_\theta t_1} \frac{1 - e^{-3D_\theta t_2}}{6D_\theta^2} \right) \right]
\end{aligned} \tag{4.41}$$

Setting $\theta_0 = 0$ and neglecting the terms $e^{-D_\theta(t_1-t_2)} \frac{1 - e^{-D_\theta t_2}}{D_\theta^2}$ and $e^{-D_\theta t_1} \frac{1 - e^{-3D_\theta t_2}}{6D_\theta^2}$ in the above expression for $\langle y(t_1)y(t_2) \rangle_{\xi,\theta}$ we get

$$\langle y(t_1)y(t_2) \rangle_{\xi,\theta} = \left(2k_B T \bar{\Gamma} + v_0^2/2D_\theta \right) t_2 + \left(\Delta D - \frac{v_0^2}{3D_\theta} \right) \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta t_2} \right) + \frac{v_0^2}{3D_\theta} \left(\frac{1 - e^{-D_\theta t_2}}{D_\theta} \right). \tag{4.42}$$

Note that along the y-direction the difference in diffusivities is renormalised to $\Delta D - v_0^2/3D_\theta$ as opposed to $\Delta D + v_0^2/3D_\theta$ along the x-direction and the term $v_0^2 \tau_1(t_2)/3D_\theta$ has an opposite sign when compared to Eq. (4.31). We now use the transformation $Y(t) = y(t)/\sqrt{\langle y^2(t) \rangle}$ and the two time correlation function takes the form

$$\begin{aligned}
\langle \bar{Y}(t_1)\bar{Y}(t_2) \rangle &= (t_2/t_1)^{1/2} \left[2D_{\text{eff}} + \Delta D'_{\text{eff}} \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta t_2} \right) + \frac{v_0^2}{6D_\theta} \left(\frac{1 - e^{-D_\theta t_2}}{D_\theta t_2} \right) \right]^{1/2} \\
&\quad \left[2D_{\text{eff}} + \Delta D'_{\text{eff}} \left(\frac{1 - e^{-4D_\theta t_1}}{4D_\theta t_1} \right) + \frac{v_0^2}{6D_\theta} \left(\frac{1 - e^{-D_\theta t_1}}{D_\theta t_1} \right) \right]^{-1/2}
\end{aligned} \tag{4.43}$$

As before, using the transformation in time

$$e^T = \sqrt{2D_{\text{eff}} t \left[1 + \frac{\Delta D'_{\text{eff}}}{2D_{\text{eff}}} \left(\frac{1 - e^{-4D_\theta t}}{4D_\theta t} \right) + \frac{v_0^2}{6D_\theta D_{\text{eff}}} \left(\frac{1 - e^{-D_\theta t}}{D_\theta t} \right) \right]} \tag{4.44}$$

we transform the correlator in Eq. (4.42) to a stationary correlation function of the form $e^{-(T_1-T_2)}$ and the persistence probability along the y -direction takes the form

$$p(t, \theta_0 = 0) = \frac{1}{\sqrt{2D_{\text{eff}}t}} \left[1 + \frac{\Delta D'_{\text{eff}}}{2D_{\text{eff}}} \left(\frac{1 - e^{-4D_{\theta}t}}{4D_{\theta}t} \right) + \frac{v_0^2}{6D_{\theta}D_{\text{eff}}} \left(\frac{1 - e^{-D_{\theta}t}}{D_{\theta}t} \right) \right]^{-1/2} \quad (4.45)$$

4.3 Harmonically Trapped Asymmetric Particle

For the experimental purposes harmonical trapping is always an important method. In this section we will discuss the effect of harmonic trapping on the particle when the harmonic potential is taken as isotropic potential having no preferred directional alignment. The potential is taken as $U(x, y) = \kappa(x^2 + y^2)/2$, and this corresponds to the Langevin equation from Eq.(4.4)

$$\begin{aligned} \frac{\partial x}{\partial t} &= -\kappa x \left(\bar{\Gamma} + \frac{\Delta\Gamma}{2} \cos 2\theta(t) \right) - \kappa y \frac{\Delta\Gamma}{2} \sin 2\theta(t) + v_0 \cos \theta(t) + \xi_1(t) \\ \frac{\partial y}{\partial t} &= -\kappa x \frac{\Delta\Gamma}{2} \sin 2\theta(t) - \kappa y \left(\bar{\Gamma} - \frac{\Delta\Gamma}{2} \cos 2\theta(t) \right) + v_0 \sin \theta(t) + \xi_2(t) \\ \frac{\partial \theta}{\partial t} &= \Gamma_3 \tau + \xi_3(t) \end{aligned} \quad (4.46)$$

Correlation of the thermal noise follows the Eq. (4.6).

4.3.1 Perturbative expansion

Looking at Eq.(4.46), we note in the absence of any asymmetry the equations reduce to that of an isotropic particle and the correction due to the shape asymmetry comes in the combination of $\kappa\Delta\Gamma/2$. Furthermore, the equations of motion in Eq.(4.46) are coupled and consequently are non-Markovian in nature. Since we are interested in the persistence probability, the non-Markovian nature of the process plays a significant role in determining $p(t)$. Fortunately, the coupling is proportional to the difference in the mobilities $\Delta\Gamma$ and therefore vanishes in the limit of weak anisotropy of $\Delta\Gamma \rightarrow 0$. In this problem, we will assume weak asymmetry. Let us define the vector space $\mathbf{R} \equiv (x, y)^T$, and the equation takes the general form as

$$\dot{\mathbf{R}} = -\kappa \left[\bar{\Gamma} \mathbf{1} + \frac{\Delta\Gamma}{2} \bar{\mathcal{R}}(t) \right] \mathbf{R}(t) + v_0 \hat{\mathbf{n}} + \xi(t) \quad (4.47)$$

To solve this equation we take the perturbative expansion

$$\mathbf{R}(t) = \mathbf{R}_0(t) - \left(\frac{\kappa\Delta\Gamma}{2}\right)\mathbf{R}_1(t) + \left(\frac{\kappa\Delta\Gamma}{2}\right)^2\mathbf{R}_2(t) + \mathcal{O}\left(\frac{\kappa\Delta\Gamma}{2}\right)^3 \quad (4.48)$$

Substituting Eq. (4.48) in Eq. (4.47) and equalizing both sides we get the equations for $\mathbf{R}_0(t)$ and $\mathbf{R}_1(t)$ as

$$\begin{aligned} \dot{\mathbf{R}}_0(t) &= -\kappa\bar{\Gamma}\mathbf{R}_0(t) + v_0\hat{\mathbf{n}}(t) + \xi(t) \\ \dot{\mathbf{R}}_1(t) &= -\kappa\bar{\Gamma}\mathbf{R}_1(t) + \bar{\mathcal{H}}(t)\mathbf{R}_0(t) \\ \dot{\mathbf{R}}_2(t) &= -\kappa\bar{\Gamma}\mathbf{R}_2(t) + \bar{\mathcal{H}}(t)\mathbf{R}_1(t) \end{aligned} \quad (4.49)$$

The solutions for Eq. (4.49) defining the initial condition $\mathbf{R}(0) = 0$, becomes

$$\begin{aligned} \mathbf{R}_0(t) &= \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} [\xi(t') + v_0\hat{\mathbf{n}}(t')] \\ \mathbf{R}_1(t) &= \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \bar{\mathcal{H}}(t')\mathbf{R}_0(t') \\ \mathbf{R}_2(t) &= \int_0^t dt' e^{-\kappa\bar{\Gamma}(t-t')} \bar{\mathcal{H}}(t')\mathbf{R}_1(t') \end{aligned} \quad (4.50)$$

The explicit form of the correlation matrix $R_i(t)R_j(t)$ in the equal time, is given by

$$\begin{aligned} \langle R_i(t)R_j(t) \rangle_{\xi,\theta} &= \langle R_{0,i}(t)R_{0,j}(t) \rangle_{\xi,\theta} - \left(\frac{\kappa\Delta\Gamma}{2}\right)\langle R_{0,i}(t)R_{1,j}(t) \rangle_{\xi,\theta} + \left(\frac{\kappa\Delta\Gamma}{2}\right)^2 \left[\langle R_{1,i}(t)R_{1,j}(t) \rangle_{\xi,\theta} \right. \\ &\quad \left. + 2\langle R_{0,i}(t)R_{2,j}(t) \rangle_{\xi,\theta} \right] + \mathcal{O}\left(\frac{\kappa\Delta\Gamma}{2}\right)^3 \end{aligned} \quad (4.51)$$

Here we have considered the fact that $\langle R_{0,i}R_{1,j} \rangle = \langle R_{0,j}R_{1,i} \rangle$. We now start to calculate the different terms of the correlation matrix. The correlation matrix for $\mathbf{R}_0(t)$ is given as averaging over the translational and the rotational noise.

4.3.2 Calculation of $\langle \mathbf{R}_{0,i}(t)\mathbf{R}_{0,j}(t) \rangle$

$$\begin{aligned} \langle R_{0,i}(t)R_{0,j}(t) \rangle &= \int_0^t dt' \int_0^t dt'' e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t-t'')} \langle \xi(t')\xi(t'') \rangle \\ &\quad + \int_0^t dt' \int_0^t dt'' e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t-t'')} v_0^2 \langle \hat{\mathbf{n}}(t')\hat{\mathbf{n}}(t'') \rangle \end{aligned} \quad (4.52)$$

Full calculation is done below and the result along the x -direction is found.

There are two integrals, lets say I_5 and I_6 respectively. Lets calculate these two

separately

$$\begin{aligned}
I_5 &= \int_0^t dt' \int_0^t dt'' e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t-t'')} \langle \xi(t') \xi(t'') \rangle \\
&= \int_0^t dt' \int_0^t dt'' e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t-t'')} \left[\bar{\Gamma} \mathbf{1} + \frac{\Delta\Gamma}{2} \bar{\mathcal{R}}(t') \right] \delta(t' - t'') \\
&= 2k_B T e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' e^{2\kappa\bar{\Gamma}t'} \left[\bar{\Gamma} \mathbf{1} + \frac{\Delta\Gamma}{2} \langle \bar{\mathcal{R}}(t') \rangle \right] \\
&= \frac{k_B T}{\kappa} \mathbf{1} (1 - e^{-2\kappa\bar{\Gamma}t}) + 2k_B T e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' e^{2\kappa\bar{\Gamma}t'} \frac{\Delta\Gamma}{2} \bar{\mathcal{R}}(\theta_0) e^{-4D_\theta t'} \\
&= \frac{k_B T}{\kappa} \mathbf{1} (1 - e^{-2\kappa\bar{\Gamma}t}) + \Delta D \bar{\mathcal{R}}(\theta_0) e^{-2\kappa\bar{\Gamma}t} \left(\frac{e^{(2\kappa\bar{\Gamma}-4D_\theta)t} - 1}{2\kappa\bar{\Gamma} - 4D_\theta} \right)
\end{aligned} \tag{4.53}$$

For x -direction

$$I_5 = \frac{k_B T}{\kappa} (1 - e^{-2\kappa\bar{\Gamma}t}) + \Delta D \cos 2\theta_0 \left(\frac{e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma} - 4D_\theta} \right) \tag{4.54}$$

$$\begin{aligned}
I_6 &= \int_0^t dt' \int_0^t dt'' e^{-\kappa\bar{\Gamma}(t-t')} e^{-\kappa\bar{\Gamma}(t-t'')} v_0^2 \langle \hat{\mathbf{n}}(t') \hat{\mathbf{n}}(t'') \rangle \\
&= v_0^2 e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^t dt'' e^{\kappa\bar{\Gamma}(t'+t'')} \langle \cos \theta(t') \cos \theta(t'') \rangle \\
&= \frac{v_0^2}{2} e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^t dt'' e^{\kappa\bar{\Gamma}(t'+t'')} \left[\cos 2\theta_0 e^{-D_\theta[t'+t''+2\min(t',t'')]} + e^{-D_\theta[t'+t''-2\min(t',t'')]} \right]
\end{aligned} \tag{4.55}$$

Lets solve the integrals separately

$$\begin{aligned}
I'_5 &= \frac{v_0^2}{2} e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^t dt'' e^{\kappa\bar{\Gamma}(t'+t'')} \cos 2\theta_0 e^{-D_\theta[t'+t''+2\min(t',t'')]} \\
&= \frac{v_0^2 \cos 2\theta_0}{2} e^{-2\kappa\bar{\Gamma}t} \left[\int_0^t dt' \int_0^{t'} dt'' e^{\kappa\bar{\Gamma}(t'+t'')} e^{-D_\theta(t'+3t'')} + \int_0^t dt' \int_{t'}^t dt'' e^{\kappa\bar{\Gamma}(t'+t'')} e^{-D_\theta(3t'+t'')} \right] \\
&= \frac{v_0^2 \cos 2\theta_0}{2} e^{-2\kappa\bar{\Gamma}t} \left[\int_0^t e^{(\kappa\bar{\Gamma}-D_\theta)t'} dt' \int_0^{t'} e^{(\kappa\bar{\Gamma}-3D_\theta)t''} dt'' + \int_0^t e^{(\kappa\bar{\Gamma}-3D_\theta)t'} dt' \int_{t'}^t e^{(\kappa\bar{\Gamma}-D_\theta)t''} dt'' \right] \\
&= \frac{v_0^2 \cos 2\theta_0}{2} \left[\frac{2D_\theta (e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t})}{(2\kappa\bar{\Gamma} - 4D_\theta)(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} - D_\theta)} + \frac{e^{-4D_\theta t} - 2e^{-(\kappa\bar{\Gamma}+D_\theta)t} + e^{-2\kappa\bar{\Gamma}t}}{(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} - 3D_\theta)} \right]
\end{aligned} \tag{4.56}$$

$$\begin{aligned}
I_6'' &= \frac{v_0^2}{2} e^{-2\kappa\bar{\Gamma}t} \int_0^t dt' \int_0^t dt'' e^{-D_\theta[t'+t''-2\min(t',t'')]} \\
&= \frac{v_0^2}{2} e^{-2\kappa\bar{\Gamma}t} \left[\int_0^t dt' \int_0^{t'} dt'' e^{\kappa\bar{\Gamma}(t'+t'')} e^{-D_\theta(t'-t'')} + \int_0^t dt' \int_{t'}^t dt'' e^{\kappa\bar{\Gamma}(t'+t'')} e^{-D_\theta(t''-t')} \right] \\
&= \frac{v_0^2}{2} e^{-2\kappa\bar{\Gamma}t} \left[\int_0^t e^{(\kappa\bar{\Gamma}-D_\theta)t'} dt' \int_0^{t'} e^{(\kappa\bar{\Gamma}+D_\theta)t''} dt'' + \int_0^t e^{(\kappa\bar{\Gamma}+D_\theta)t'} dt' \int_{t'}^t e^{(\kappa\bar{\Gamma}-D_\theta)t''} dt'' \right] \\
&= \frac{v_0^2}{2} \left[\frac{1 - 2e^{-(\kappa\bar{\Gamma}+D_\theta)t} + e^{-2\kappa\bar{\Gamma}t}}{(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)} - \frac{D_\theta(1 - e^{-2\kappa\bar{\Gamma}t})}{\kappa\bar{\Gamma}(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)} \right]
\end{aligned} \tag{4.57}$$

$$\begin{aligned}
\langle x_0^2(t) \rangle &= \frac{k_B T}{\kappa} (1 - e^{-2\kappa\bar{\Gamma}t}) + \Delta D \cos 2\theta_0 \left(\frac{e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t}}{2\kappa\bar{\Gamma} - 4D_\theta} \right) \\
&+ \frac{v_0^2 \cos 2\theta_0}{2} \left[\frac{2D_\theta(e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t})}{(2\kappa\bar{\Gamma} - 4D_\theta)(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} - D_\theta)} + \frac{e^{-4D_\theta t} - 2e^{-(\kappa\bar{\Gamma}+D_\theta)t} + e^{-2\kappa\bar{\Gamma}t}}{(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} - 3D_\theta)} \right] \\
&+ \frac{v_0^2}{2} \left[\frac{1 - 2e^{-(\kappa\bar{\Gamma}+D_\theta)t} + e^{-2\kappa\bar{\Gamma}t}}{(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)} - \frac{D_\theta(1 - e^{-2\kappa\bar{\Gamma}t})}{\kappa\bar{\Gamma}(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)} \right]
\end{aligned} \tag{4.58}$$

In the limit of $\kappa \rightarrow 0$, Eq. (4.58) reproduces Eq. (4.17) which is the correct result of free diffusion of an anisotropic particle.

4.3.3 Calculation of $\langle \mathbf{R}_{0,i}(t_1) \mathbf{R}_{0,j}(t_2) \rangle$

$$\begin{aligned}
\langle \mathbf{R}_{0,i}(t_1) \mathbf{R}_{0,j}(t_2) \rangle &= \int_0^{t_1} dt' \int_0^{t_2} dt'' e^{-\kappa\bar{\Gamma}(t_1-t')} e^{-\kappa\bar{\Gamma}(t_2-t'')} \langle \xi(t'_1) \xi(t'_2) \rangle \\
&+ v_0^2 \int_0^{t_1} dt' \int_0^{t_2} dt'' e^{-\kappa\bar{\Gamma}(t_1-t')} e^{-\kappa\bar{\Gamma}(t_2-t'')} \langle \hat{\mathbf{n}}(t'_1) \hat{\mathbf{n}}(t'_2) \rangle
\end{aligned} \tag{4.59}$$

It can be calculated as two separately I_7 and I_8 integrals

$$\begin{aligned}
I_7 &= \int_0^{t_1} dt' \int_0^{t_2} dt'' e^{-\kappa\bar{\Gamma}(t_1-t')} e^{-\kappa\bar{\Gamma}(t_2-t'')} \langle \xi(t'_1) \xi(t'_2) \rangle \\
&= 2k_B T e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 e^{\kappa\bar{\Gamma}(t'_1+t'_2)} \left[\bar{\Gamma} \delta_{ij} + \Delta \Gamma \langle \mathcal{R}_{ij}(t'_1) \rangle \right] \delta(t'_1 - t'_2) \\
&= 2k_B T e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{\min(t_1, t_2)} e^{2\kappa\bar{\Gamma}t'_1} dt'_1 + 2k_B T \Delta \Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{\min(t_1, t_2)} e^{2\kappa\bar{\Gamma}t'_1} \langle \mathcal{R}_{ij}(t'_1) \rangle dt'_1 \\
&= \frac{k_B T}{\kappa} \left[e^{-\kappa\bar{\Gamma}(t_1-t_2)} - e^{-\kappa\bar{\Gamma}(t_1+t_2)} \right] + \frac{2k_B T}{\kappa} (\kappa \Delta \Gamma) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{\min(t_1, t_2)} e^{(2\kappa\bar{\Gamma}-4D_\theta)t'_1} dt'_1 \\
&= \frac{k_B T}{\kappa} \left[e^{-\kappa\bar{\Gamma}(t_1-t_2)} - e^{-\kappa\bar{\Gamma}(t_1+t_2)} \right] + \frac{2k_B T}{\kappa} (\kappa \Delta \Gamma) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}(t_1+t_2)} \left[\frac{e^{(2\kappa\bar{\Gamma}-4D_\theta)t_2} - 1}{2\kappa\bar{\Gamma} - 4D_\theta} \right] \\
&= \frac{k_B T}{\kappa} e^{-\kappa\bar{\Gamma}t_1} \left[e^{\kappa\bar{\Gamma}t_2} - e^{-\kappa\bar{\Gamma}t_2} \right] + \frac{2k_B T}{\kappa} (\kappa \Delta \Gamma) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_1} \left[\frac{e^{(\kappa\bar{\Gamma}-4D_\theta)t_2} - e^{-\kappa\bar{\Gamma}t_2}}{2\kappa\bar{\Gamma} - 4D_\theta} \right]
\end{aligned} \tag{4.60}$$

$$\begin{aligned}
I_8 &= \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 e^{-\kappa\bar{\Gamma}(t_1-t'_1)} e^{-\kappa\bar{\Gamma}(t_2-t'_2)} v_0^2 \langle \hat{\mathbf{n}}(t'_1) \hat{\mathbf{n}}(t'_2) \rangle \\
&= v_0^2 e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 e^{\kappa\bar{\Gamma}(t'_1+t'_2)} \langle \cos \theta(t'_1) \cos \theta(t'_2) \rangle \\
&= \frac{v_0^2}{2} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 e^{\kappa\bar{\Gamma}(t'_1+t'_2)} \left[\cos 2\theta_0 e^{-D_\theta[t'_1+t'_2+2\min(t'_1,t'_2)]} + e^{-D_\theta[t'_1+t'_2-2\min(t'_1,t'_2)]} \right]
\end{aligned} \tag{4.61}$$

Lets calculate integrals separately

$$\begin{aligned}
I'_8 &= \frac{v_0^2 \cos 2\theta_0}{2} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 e^{\kappa\bar{\Gamma}(t'_1+t'_2)} e^{-D_\theta[t'_1+t'_2+2\min(t'_1,t'_2)]} \\
&= \frac{v_0^2 \cos 2\theta_0}{2} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \left[\int_0^{t_2} dt'_2 \int_0^{t'_2} dt'_1 e^{\kappa\bar{\Gamma}(t'_1+t'_2)} e^{-D_\theta(3t'_1+t'_2)} + \int_0^{t_2} dt'_2 \int_{t'_2}^{t_1} dt'_1 e^{\kappa\bar{\Gamma}(t'_1+t'_2)} e^{-D_\theta(t'_1+3t'_2)} \right] \\
&= \frac{v_0^2 \cos 2\theta_0}{2} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \left[\int_0^{t_2} e^{(\kappa\bar{\Gamma}-D_\theta)t'_2} dt'_2 \int_0^{t'_2} e^{(\kappa\bar{\Gamma}-3D_\theta)t'_1} dt'_1 + \int_0^{t_2} e^{(\kappa\bar{\Gamma}-3D_\theta)t'_2} dt'_2 \int_{t'_2}^{t_1} e^{(\kappa\bar{\Gamma}-D_\theta)t'_1} dt'_1 \right] \\
&= \frac{v_0^2 \cos 2\theta_0}{2} \left[\frac{2D_\theta(e^{-\kappa\bar{\Gamma}t_1} e^{(\kappa\bar{\Gamma}-4D_\theta)t_2} - e^{-\kappa\bar{\Gamma}(t_1+t_2)})}{(2\kappa\bar{\Gamma}-4D_\theta)(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}-3D_\theta)} \right. \\
&\quad \left. + \frac{e^{-D_\theta t_1} e^{-3D_\theta t_2} - e^{-\kappa\bar{\Gamma}t_2} e^{-D_\theta t_1} - e^{-\kappa\bar{\Gamma}t_1} e^{-D_\theta t_2} + e^{-\kappa\bar{\Gamma}(t_1+t_2)}}{(\kappa\bar{\Gamma}-3D_\theta)(\kappa\bar{\Gamma}-D_\theta)} \right]
\end{aligned} \tag{4.62}$$

$$\begin{aligned}
I''_8 &= \frac{v_0^2}{2} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 e^{\kappa\bar{\Gamma}(t'_1+t'_2)} e^{-D_\theta[t'_1+t'_2-2\min(t'_1,t'_2)]} \\
&= \frac{v_0^2}{2} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \left[\int_0^{t_2} dt'_1 \int_0^{t'_1} dt'_2 e^{\kappa\bar{\Gamma}(t'_1+t'_2)} e^{-D_\theta(t'_2-t'_1)} + \int_0^{t_2} dt'_2 \int_{t'_2}^{t_1} dt'_1 e^{\kappa\bar{\Gamma}(t'_1+t'_2)} e^{-D_\theta(t'_1-t'_2)} \right] \\
&= \frac{v_0^2}{2} \left[\frac{2D_\theta(e^{-\kappa\bar{\Gamma}(t_1+t_2)} - e^{-\kappa\bar{\Gamma}(t_1-t_2)})}{2\kappa\bar{\Gamma}(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}+D_\theta)} + \frac{e^{-D_\theta t_1} e^{D_\theta t_2} - e^{-D_\theta t_1} e^{-\kappa\bar{\Gamma}t_2} - e^{-\kappa\bar{\Gamma}t_1} e^{-D_\theta t_2} + e^{-\kappa\bar{\Gamma}(t_1+t_2)}}{(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}+D_\theta)} \right]
\end{aligned} \tag{4.63}$$

$$\begin{aligned}
\langle x_0(t_1)x_0(t_2) \rangle &= \frac{k_B T}{\kappa} e^{-\kappa\bar{\Gamma}t_1} \left[e^{\kappa\bar{\Gamma}t_2} - e^{-\kappa\bar{\Gamma}t_2} \right] + \frac{2k_B T}{\kappa} (\kappa\Delta\Gamma) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_1} \left[\frac{e^{(\kappa\bar{\Gamma}-4D_\theta)t_2} - e^{-\kappa\bar{\Gamma}t_2}}{2\kappa\bar{\Gamma}-4D_\theta} \right] \\
&+ \frac{v_0^2 \cos 2\theta_0}{2} \left[\frac{e^{-D_\theta t_1} e^{-3D_\theta t_2} - e^{-\kappa\bar{\Gamma}t_2} e^{-D_\theta t_1} - e^{-\kappa\bar{\Gamma}t_1} e^{-D_\theta t_2} + e^{-\kappa\bar{\Gamma}(t_1+t_2)}}{(\kappa\bar{\Gamma}-3D_\theta)(\kappa\bar{\Gamma}-D_\theta)} \right. \\
&+ \frac{2D_\theta(e^{-\kappa\bar{\Gamma}t_1} e^{(\kappa\bar{\Gamma}-4D_\theta)t_2} - e^{-\kappa\bar{\Gamma}(t_1+t_2)})}{(2\kappa\bar{\Gamma}-4D_\theta)(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}-3D_\theta)} \left. \right] + \frac{v_0^2}{2} \left[\frac{e^{-D_\theta t_1} e^{D_\theta t_2} - e^{-D_\theta t_1} e^{-\kappa\bar{\Gamma}t_2} - e^{-\kappa\bar{\Gamma}t_1} e^{-D_\theta t_2} + e^{-\kappa\bar{\Gamma}(t_1+t_2)}}{(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}+D_\theta)} \right. \\
&+ \left. \frac{2D_\theta(e^{-\kappa\bar{\Gamma}(t_1+t_2)} - e^{-\kappa\bar{\Gamma}(t_1-t_2)})}{2\kappa\bar{\Gamma}(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}+D_\theta)} \right]
\end{aligned} \tag{4.64}$$

As the active particle dynamics is not zero centric stochastic process, we need to transform the process to zero centric by subtracting $\langle R_0(t_1) \rangle \langle R_0(t_2) \rangle$ from Eq.(4.64). Taking for only x -direction, we get

$$\langle x_0(t_1) \rangle \langle x_0(t_2) \rangle = v_0^2 \cos^2 \theta_0 \frac{e^{-D_\theta(t_1+t_2)} - e^{-D_\theta t_1} e^{-\kappa \bar{\Gamma} t_2} - e^{-D_\theta t_2} e^{-\kappa \bar{\Gamma} t_1} + e^{-\kappa \bar{\Gamma}(t_1+t_2)}}{(\kappa \bar{\Gamma} - D_\theta)^2} \quad (4.65)$$

In Eq(4.65), we neglect the first two terms consisting $e^{-D_\theta(t_1+t_2)}$ and $e^{-D_\theta t_1} e^{-\kappa \bar{\Gamma} t_2}$ and subtract rest of the term from Eq.(4.64) getting transformed two-time correlation as,

$$\langle x_0(t_1) x_0(t_2) \rangle_{trans} = \langle x_0(t_1) x_0(t_2) \rangle - \langle x_0(t_1) \rangle \langle x_0(t_2) \rangle \quad (4.66)$$

4.3.4 Calculation of $\langle \mathbf{R}_{0,i}(t_1) \mathbf{R}_{1,j}(t_2) \rangle$

$$\begin{aligned} \langle \mathbf{R}_{0,i}(t_1) \mathbf{R}_{1,j}(t_2) \rangle &= \left\langle \mathbf{R}_{0,i}(t_1) \int_0^{t_2} dt'_2 e^{-\kappa \bar{\Gamma}(t_2-t'_2)} \sum \mathcal{R}_{jk}(t'_2) \mathbf{R}_{0,k}(t'_2) \right\rangle \\ &= \int_0^{t_2} dt'_2 e^{-\kappa \bar{\Gamma}(t_2-t'_2)} \sum \mathcal{R}_{jk}(t'_2) \langle \mathbf{R}_{0,i}(t_1) \mathbf{R}_{0,k}(t'_2) \rangle \\ &= \int_0^{t_2} dt'_2 e^{-\kappa \bar{\Gamma}(t_2-t'_2)} \sum \mathcal{R}_{jk}(t'_2) \int_0^{t_1} dt'_1 \int_0^{t'_2} dt''_2 e^{-\kappa \bar{\Gamma}(t_1-t'_1)} e^{-\kappa \bar{\Gamma}(t'_2-t''_2)} \left[\langle \xi_i(t'_1) \xi_k(t''_2) \rangle + v_0^2 \langle \hat{\mathbf{n}}_i(t'_1) \hat{\mathbf{n}}_k(t''_2) \rangle \right] \end{aligned} \quad (4.67)$$

Lets calculate the integrals separately

$$\begin{aligned}
I_9 &= \int_0^{t_2} dt'_2 e^{-\kappa\bar{\Gamma}(t_2-t'_2)} \sum \mathcal{R}_{jk}(t'_2) \int_0^{t_1} dt'_1 \int_0^{t'_2} dt''_2 e^{-\kappa\bar{\Gamma}(t_1-t'_1)} e^{-\kappa\bar{\Gamma}(t'_2-t''_2)} \langle \xi(t'_1) \xi(t''_2) \rangle \\
&= \int_0^{t_2} dt'_2 e^{-\kappa\bar{\Gamma}(t_2-t'_2)} \left\langle \sum \mathcal{R}_{jk}(t'_2) \left[\frac{k_B T}{\kappa} \delta_{ij} (e^{-\kappa\bar{\Gamma}(t_1-t'_2)}) \right. \right. \\
&\quad \left. \left. + 2k_B T \Delta e^{-\kappa\bar{\Gamma}(t_1+t'_2)} \int_0^{\min(t_1, t'_2)} dt'' e^{2\kappa\bar{\Gamma}t''} \mathcal{R}_{ik}(t'') \right] \right\rangle \\
&= \frac{k_B T}{\kappa} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 e^{\kappa\bar{\Gamma}t'_2} \langle \mathcal{R}_{ji}(t'_2) \rangle (e^{\kappa\bar{\Gamma}t'_2} - e^{-\kappa\bar{\Gamma}t'_2}) \\
&\quad + 2k_B T \Delta \Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{\min(t_1, t'_2)} e^{2\kappa\bar{\Gamma}t''} \sum \langle \mathcal{R}_{jk}(t'_2) \mathcal{R}_{ik}(t'') \rangle \\
&= \frac{k_B T}{\kappa} e^{-\kappa\bar{\Gamma}(t_1+t_2)} \mathcal{R}_{ji}(\theta_0) \int_0^{t_2} dt'_2 e^{-4D_\theta t'_2} (e^{2\kappa\bar{\Gamma}t'_2} - 1) \\
&\quad + 2k_B T \Delta \Gamma e^{-\kappa\bar{\Gamma}(t_1+t_2)} \int_0^{t_2} dt'_2 \int_0^{t'_2} dt'' e^{2\kappa\bar{\Gamma}t''} e^{-4D_\theta(t'_2+t''-2\min(t'_2, t''))} \\
&= \left(\frac{k_B T}{\kappa} \right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma}t_1} \left(\frac{e^{(\kappa\bar{\Gamma}-4D_\theta)t_2} - e^{-\kappa\bar{\Gamma}t_2}}{2\kappa\bar{\Gamma}-4D_\theta} - \frac{e^{-\kappa\bar{\Gamma}t_2} - e^{-(4D_\theta+\kappa\bar{\Gamma})t_2}}{4D_\theta} \right) \\
&\quad + \left(\frac{k_B T}{\kappa} \right) \left(\frac{\Delta \Gamma}{\bar{\Gamma}} \right) e^{-\kappa\bar{\Gamma}t_1} \left[\frac{e^{\kappa\bar{\Gamma}t_2} - e^{-\kappa\bar{\Gamma}t_2}}{2\kappa\bar{\Gamma}+4D_\theta} - \frac{2\kappa\bar{\Gamma} e^{-\kappa\bar{\Gamma}t_2} - e^{-(2\kappa\bar{\Gamma}+4D_\theta)t_2}}{4D_\theta (\kappa\bar{\Gamma}+4D_\theta)} \right] \\
I_{10} &= \int_0^{t_2} dt'_2 e^{-\kappa\bar{\Gamma}(t_2-t'_2)} \sum \mathcal{R}_{jk}(t'_2) \int_0^{t_1} dt'_1 \int_0^{t'_2} dt''_2 e^{-\kappa\bar{\Gamma}(t_1-t'_1)} e^{-\kappa\bar{\Gamma}(t'_2-t''_2)} v_0^2 \langle \hat{\mathbf{n}}_i(t'_1) \hat{\mathbf{n}}_k(t''_2) \rangle
\end{aligned} \tag{4.68}$$

For x -direction Eq.(4.69) transforms as

$$\begin{aligned}
I_{10} &= \int_0^{t_2} dt'_2 e^{-\kappa\bar{\Gamma}(t_2-t'_2)} \int_0^{t_1} dt'_1 \int_0^{t'_2} dt''_2 e^{-\kappa\bar{\Gamma}(t_1-t'_1)} e^{-\kappa\bar{\Gamma}(t'_2-t''_2)} v_0^2 [\langle \cos 2\theta(t'_2) \cos \theta(t'_1) \cos \theta(t''_2) \rangle \\
&\quad + \langle \sin 2\theta(t'_2) \cos \theta(t'_1) \cos \theta(t''_2) \rangle]
\end{aligned} \tag{4.70}$$

We can write

$$\begin{aligned}
\cos 2\theta_1 \cos \theta_2 \cos \theta_3 &= \frac{1}{4} [\cos(2\theta_1 - \theta_2 - \theta_3) + \cos(2\theta_1 + \theta_2 - \theta_3) \\
&\quad + \cos(2\theta_1 - \theta_2 + \theta_3) + \cos(2\theta_1 + \theta_2 + \theta_3)] \\
\sin 2\theta_1 \cos \theta_2 \cos \theta_3 &= \frac{1}{4} [\sin(2\theta_1 - \theta_2 - \theta_3) + \sin(2\theta_1 + \theta_2 + \theta_3) \\
&\quad + \sin(2\theta_1 - \theta_2 + \theta_3) + \sin(2\theta_1 + \theta_2 + \theta_3)]
\end{aligned} \tag{4.71}$$

$$\begin{aligned}
\langle \cos(2\theta_1 - \theta_2 - \theta_3) \rangle &= e^{-D_\theta(4t'_2+t'_1+t''_2-4\min(t'_2,t'_1)-4\min(t'_2,t''_2)+2\min(t'_1,t''_2))} \\
\langle \cos(2\theta_1 + \theta_2 - \theta_3) \rangle &= \cos 2\theta_0 e^{-D_\theta(4t'_2+t'_1+t''_2+4\min(t'_2,t'_1)-4\min(t'_2,t''_2)-2\min(t'_1,t''_2))} \\
\langle \cos(2\theta_1 - \theta_2 + \theta_3) \rangle &= \cos 2\theta_0 e^{-D_\theta(4t'_2+t'_1+t''_2-4\min(t'_2,t'_1)+4\min(t'_2,t''_2)-2\min(t'_1,t''_2))} \\
\langle \cos(2\theta_1 + \theta_2 + \theta_3) \rangle &= \cos 4\theta_0 e^{-D_\theta(4t'_2+t'_1+t''_2+4\min(t'_2,t'_1)+4\min(t'_2,t''_2)+2\min(t'_1,t''_2))} \\
\langle \sin(2\theta_1 - \theta_2 - \theta_3) \rangle &= e^{-D_\theta(4t'_2+t'_1+t''_2-4\min(t'_2,t'_1)-4\min(t'_2,t''_2)+2\min(t'_1,t''_2))} \\
\langle \sin(2\theta_1 + \theta_2 - \theta_3) \rangle &= \sin 2\theta_0 e^{-D_\theta(4t'_2+t'_1+t''_2+4\min(t'_2,t'_1)-4\min(t'_2,t''_2)-2\min(t'_1,t''_2))} \\
\langle \sin(2\theta_1 - \theta_2 + \theta_3) \rangle &= \sin 2\theta_0 e^{-D_\theta(4t'_2+t'_1+t''_2-4\min(t'_2,t'_1)+4\min(t'_2,t''_2)-2\min(t'_1,t''_2))} \\
\langle \sin(2\theta_1 + \theta_2 + \theta_3) \rangle &= \sin 4\theta_0 e^{-D_\theta(4t'_2+t'_1+t''_2+4\min(t'_2,t'_1)+4\min(t'_2,t''_2)+2\min(t'_1,t''_2))}
\end{aligned} \tag{4.72}$$

Let us calculate Eq.(4.70) by using Eq.(4.72), at first we take the first term (a) $\langle \cos(2\theta_1 - \theta_2 - \theta_3) \rangle$ and calculate separately

$$\frac{v_0^2 e^{-\kappa\bar{\Gamma}(t_1+t_2)}}{4} \int_0^{t_2} dt'_2 \int_0^{t'_1} dt'_1 \int_0^{t'_2} dt''_2 e^{\kappa\bar{\Gamma}t'_1} e^{\kappa\bar{\Gamma}t''_2} e^{-D_\theta(4t'_2+t'_1+t''_2-4\min(t'_2,t'_1)-4\min(t'_2,t''_2)+2\min(t'_1,t''_2))} \tag{4.73}$$

Here in the above integral always $t'_2 > t''_2$ and in the first case let us take $t'_1 > t'_2$ we get

Case(1), $t'_1 > t'_2$

$$\begin{aligned}
&\frac{v_0^2 e^{-\kappa\bar{\Gamma}(t_1+t_2)}}{4} \int_0^{t_2} dt'_2 \int_{t'_2}^{t'_1} dt'_1 \int_0^{t'_2} dt''_2 e^{\kappa\bar{\Gamma}t'_1} e^{\kappa\bar{\Gamma}t''_2} e^{-4D_\theta t'_2} e^{-D_\theta t'_1} e^{-D_\theta t''_2} e^{4D_\theta t'_2} e^{4D_\theta t''_2} e^{-2D_\theta t'_2} \\
&= \frac{v_0^2 e^{-D_\theta t_1} (e^{D_\theta t_2} - e^{-\kappa\bar{\Gamma}t_2})}{4(\kappa\bar{\Gamma} + D_\theta)^2 (\kappa\bar{\Gamma} - D_\theta)} - \frac{v_0^2 e^{-\kappa\bar{\Gamma}t_1} (e^{\kappa\bar{\Gamma}t_2} - e^{-\kappa\bar{\Gamma}t_2})}{8\kappa\bar{\Gamma}(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)} \\
&+ \frac{v_0^2 e^{-\kappa\bar{\Gamma}t_1} (e^{-D_\theta t_2} - e^{-\kappa\bar{\Gamma}t_2})}{4(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)^2} - \frac{t_2 v_0^2 e^{-\kappa\bar{\Gamma}t_2} e^{-D_\theta t_1}}{4(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)}
\end{aligned} \tag{4.74}$$

Case(2), $t'_1 < t'_2$

$$\begin{aligned}
&\frac{v_0^2 e^{-\kappa\bar{\Gamma}(t_1+t_2)}}{4} \left[\int_0^{t_2} dt'_2 \int_0^{t'_2} dt'_1 \int_0^{t'_1} dt''_2 e^{\kappa\bar{\Gamma}t'_1} e^{\kappa\bar{\Gamma}t''_2} e^{-4D_\theta t'_2} e^{3D_\theta t'_1} e^{3D_\theta t''_2} e^{-2D_\theta t'_2} \right. \\
&\left. + \int_0^{t_2} dt'_2 \int_0^{t'_2} dt'_1 \int_{t'_1}^{t'_2} dt''_2 e^{\kappa\bar{\Gamma}t'_1} e^{\kappa\bar{\Gamma}t''_2} e^{-4D_\theta t'_2} e^{3D_\theta t'_1} e^{3D_\theta t''_2} e^{-2D_\theta t'_1} \right] \\
&= \frac{v_0^2 e^{-\kappa\bar{\Gamma}t_1}}{8(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} + 2D_\theta)} \left[\frac{\sinh \kappa\bar{\Gamma}t_2}{\kappa\bar{\Gamma}} - \frac{e^{-\kappa\bar{\Gamma}t_2} - e^{-(\kappa\bar{\Gamma}+4D_\theta)t_2}}{4D_\theta} \right] \\
&- \frac{v_0^2 e^{-\kappa\bar{\Gamma}t_1}}{4(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} + 3D_\theta)} \left[\frac{e^{-D_\theta t_2} - e^{-\kappa\bar{\Gamma}t_2}}{\kappa\bar{\Gamma} - D_\theta} - \frac{e^{-\kappa\bar{\Gamma}t_2} - e^{-(\kappa\bar{\Gamma}+4D_\theta)t_2}}{4D_\theta} \right] \\
&+ \frac{v_0^2 e^{-\kappa\bar{\Gamma}t_1}}{4(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} + 3D_\theta)} \left[\frac{\sinh \kappa\bar{\Gamma}t_2}{\kappa\bar{\Gamma}} - \frac{e^{-D_\theta t_2} - e^{-\kappa\bar{\Gamma}t_2}}{\kappa\bar{\Gamma} - D_\theta} \right] \\
&- \frac{v_0^2 e^{-\kappa\bar{\Gamma}t_1}}{8(\kappa\bar{\Gamma} + 2D_\theta)(\kappa\bar{\Gamma} + 3D_\theta)} \left[\frac{\sinh \kappa\bar{\Gamma}t_2}{\kappa\bar{\Gamma}} - \frac{e^{-\kappa\bar{\Gamma}t_2} - e^{-(\kappa\bar{\Gamma}+4D_\theta)t_2}}{4D_\theta} \right]
\end{aligned} \tag{4.75}$$

Adding Eq.(4.74) and Eq.(4.75) terms we get the term Eq.(4.73) as,

$$I_a = \frac{v_0^2 e^{-D_\theta t_1} (e^{D_\theta t_2} - e^{-\kappa \bar{\Gamma} t_2})}{4(\kappa \bar{\Gamma} + D_\theta)^2 (\kappa \bar{\Gamma} - D_\theta)} + \frac{t_2 v_0^2 e^{-\kappa \bar{\Gamma} t_2} e^{-D_\theta t_1}}{4(\kappa \bar{\Gamma} + D_\theta)(\kappa \bar{\Gamma} - D_\theta)} - \frac{3v_0^2 D_\theta e^{-\kappa \bar{\Gamma} t_1} \sinh \kappa \bar{\Gamma} t_2}{4\kappa \bar{\Gamma} (\kappa \bar{\Gamma} + D_\theta)(\kappa \bar{\Gamma} - D_\theta)(\kappa \bar{\Gamma} + 2D_\theta)}$$

$$- \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1} (e^{-\kappa \bar{\Gamma} t_2} - e^{-(\kappa \bar{\Gamma} + 4D_\theta)t_2})}{16(\kappa \bar{\Gamma} + 2D_\theta)(\kappa \bar{\Gamma} + D_\theta)(\kappa \bar{\Gamma} + 3D_\theta)} - \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1} (\kappa \bar{\Gamma} - 5D_\theta)(e^{-D_\theta t_2} - e^{-\kappa \bar{\Gamma} t_2})}{4(\kappa \bar{\Gamma} + D_\theta)(\kappa \bar{\Gamma} + 3D_\theta)(\kappa \bar{\Gamma} - D_\theta)^2}$$
(4.76)

The way first term has been calculated similarly other terms are calculated to find the exact expression of Eq.(4.70). The results of Integrals due to terms (b), (c), and (d) are as follows

$$I_b = \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1}}{8\kappa \bar{\Gamma} (\kappa \bar{\Gamma} + 5D_\theta)} \left[\frac{e^{(\kappa \bar{\Gamma} - 4D_\theta)t_2} - e^{-\kappa \bar{\Gamma} t_2}}{2\kappa \bar{\Gamma} - 4D_\theta} - \frac{e^{-\kappa \bar{\Gamma} t_2} - e^{-(\kappa \bar{\Gamma} + 4D_\theta)t_2}}{4D_\theta} \right] - \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1}}{4(\kappa \bar{\Gamma} + 5D_\theta)(\kappa \bar{\Gamma} - 5D_\theta)}$$

$$\left[\frac{e^{-9D_\theta t_2} - e^{-\kappa \bar{\Gamma} t_2}}{\kappa \bar{\Gamma} - 9D_\theta} - \frac{e^{-\kappa \bar{\Gamma} t_2} - e^{-(\kappa \bar{\Gamma} + 4D_\theta)t_2}}{4D_\theta} \right] + \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1}}{4(\kappa \bar{\Gamma} + 3D_\theta)(\kappa \bar{\Gamma} - 3D_\theta)} \left[\frac{e^{(\kappa \bar{\Gamma} - 4D_\theta)t_2} - e^{-\kappa \bar{\Gamma} t_2}}{2\kappa \bar{\Gamma} - 4D_\theta} \right.$$

$$\left. + \frac{e^{-\kappa \bar{\Gamma} t_2} - e^{-D_\theta t_2}}{\kappa \bar{\Gamma} - D_\theta} \right] - \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1}}{8\kappa \bar{\Gamma} (\kappa \bar{\Gamma} + 3D_\theta)} \left[\frac{e^{(\kappa \bar{\Gamma} - 4D_\theta)t_2} - e^{-\kappa \bar{\Gamma} t_2}}{2\kappa \bar{\Gamma} - 4D_\theta} - \frac{e^{-\kappa \bar{\Gamma} t_2} - e^{-(\kappa \bar{\Gamma} + 4D_\theta)t_2}}{4D_\theta} \right]$$

$$+ \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1}}{4(\kappa \bar{\Gamma} - D_\theta)(\kappa \bar{\Gamma} + 5D_\theta)} \left[\frac{e^{-9D_\theta t_2} - e^{-\kappa \bar{\Gamma} t_2}}{\kappa \bar{\Gamma} - 9D_\theta} - \frac{e^{(\kappa \bar{\Gamma} - 4D_\theta)t_2} - e^{-\kappa \bar{\Gamma} t_2}}{2\kappa \bar{\Gamma} - 4D_\theta} \right]$$

$$+ \frac{v_0^2 e^{-D_\theta t_1}}{4(\kappa \bar{\Gamma} - D_\theta)(\kappa \bar{\Gamma} + 5D_\theta)} \left[\frac{e^{-3D_\theta t_2} - e^{-\kappa \bar{\Gamma} t_2}}{\kappa \bar{\Gamma} - 3D_\theta} - \frac{e^{-\kappa \bar{\Gamma} t_2} - e^{-(\kappa \bar{\Gamma} + 8D_\theta)t_2}}{8D_\theta} \right]$$
(4.77)

$$I_c = \frac{v_0^2 e^{-D_\theta t_1}}{4(\kappa \bar{\Gamma} - D_\theta)(\kappa \bar{\Gamma} - 3D_\theta)} \left[\frac{e^{-3D_\theta t_2} - e^{-\kappa \bar{\Gamma} t_2}}{(\kappa \bar{\Gamma} - 3D_\theta)} - t_2 e^{-\kappa \bar{\Gamma} t_2} \right] + \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1}}{4(\kappa \bar{\Gamma} - D_\theta)(\kappa \bar{\Gamma} - 3D_\theta)}$$

$$\left[\frac{e^{-D_\theta t_2} - e^{-\kappa \bar{\Gamma} t_2}}{\kappa \bar{\Gamma} - D_\theta} - \frac{e^{(\kappa \bar{\Gamma} - 4D_\theta)t_2} - e^{-\kappa \bar{\Gamma} t_2}}{\kappa \bar{\Gamma} - 2D_\theta} \right] + \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1}}{4(\kappa \bar{\Gamma} + 5D_\theta)(\kappa \bar{\Gamma} - 5D_\theta)} \left[\frac{e^{-4D_\theta t_2} - e^{-\kappa \bar{\Gamma} t_2}}{\kappa \bar{\Gamma} - 4D_\theta} \right.$$

$$\left. - \frac{e^{-9D_\theta t_2} - e^{-\kappa \bar{\Gamma} t_2}}{\kappa \bar{\Gamma} - 9D_\theta} \right] + \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1}}{16\kappa \bar{\Gamma} (\kappa \bar{\Gamma} - 3D_\theta)} \left[\frac{e^{(\kappa \bar{\Gamma} - 4D_\theta)t_2} - e^{-\kappa \bar{\Gamma} t_2}}{\kappa \bar{\Gamma} - 2D_\theta} - \frac{e^{-\kappa \bar{\Gamma} t_2} - e^{-(\kappa \bar{\Gamma} + 4D_\theta)t_2}}{2D_\theta} \right]$$

$$+ \frac{v_0^2 e^{-\kappa \bar{\Gamma} t_1}}{4(\kappa \bar{\Gamma} - 3D_\theta)(\kappa \bar{\Gamma} + 3D_\theta)} \left[\frac{e^{-\kappa \bar{\Gamma} t_2} - e^{-(\kappa \bar{\Gamma} + 4D_\theta)t_2}}{4D_\theta} - \frac{e^{-D_\theta t_2} - e^{-\kappa \bar{\Gamma} t_2}}{\kappa \bar{\Gamma} - D_\theta} \right]$$
(4.78)

$$\begin{aligned}
I_d = & \frac{v_0^2 e^{-D_\theta t_1}}{4(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} - 7D_\theta)} \left[\frac{e^{-15D_\theta t_2} - e^{-\kappa\bar{\Gamma} t_2}}{\kappa\bar{\Gamma} - 15D_\theta} - \frac{e^{-\kappa\bar{\Gamma} t_2} - e^{-(\kappa\bar{\Gamma} + 8D_\theta)t_2}}{8D_\theta} \right] + \frac{v_0^2 e^{-\kappa\bar{\Gamma} t_1}}{4(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} - 7D_\theta)} \\
& \left[\frac{e^{-9D_\theta t_2} - e^{-\kappa\bar{\Gamma} t_2}}{\kappa\bar{\Gamma} - 9D_\theta} - \frac{e^{(\kappa\bar{\Gamma} - 16D_\theta)t_2} - e^{-\kappa\bar{\Gamma} t_2}}{2(\kappa\bar{\Gamma} - 8D_\theta)} \right] + \frac{v_0^2 e^{-\kappa\bar{\Gamma} t_1}}{8(\kappa\bar{\Gamma} - 7D_\theta)(\kappa\bar{\Gamma} - 6D_\theta)} \left[\frac{e^{(\kappa\bar{\Gamma} - 16D_\theta)t_2} - e^{-\kappa\bar{\Gamma} t_2}}{2\kappa\bar{\Gamma} - 16D_\theta} \right. \\
& \left. - \frac{e^{-\kappa\bar{\Gamma} t_2} - e^{-(\kappa\bar{\Gamma} + 4D_\theta)t_2}}{4D_\theta} \right] + \frac{v_0^2 e^{-\kappa\bar{\Gamma} t_1}}{4(\kappa\bar{\Gamma} - 5D_\theta)(\kappa\bar{\Gamma} - 7D_\theta)} \left[\frac{e^{-\kappa\bar{\Gamma} t_2} - e^{-(\kappa\bar{\Gamma} + 4D_\theta)t_2}}{4D_\theta} - \frac{e^{-9D_\theta t_2} - e^{-\kappa\bar{\Gamma} t_2}}{\kappa\bar{\Gamma} - 9D_\theta} \right] \\
& + \frac{v_0^2 e^{-\kappa\bar{\Gamma} t_1}}{4(\kappa\bar{\Gamma} - 5D_\theta)(\kappa\bar{\Gamma} - 7D_\theta)} \left[\frac{e^{(\kappa\bar{\Gamma} - 16D_\theta)t_2} - e^{-\kappa\bar{\Gamma} t_2}}{2\kappa\bar{\Gamma} - 16D_\theta} - \frac{e^{-9D_\theta t_2} - e^{-\kappa\bar{\Gamma} t_2}}{\kappa\bar{\Gamma} - 9D_\theta} \right] \\
& + \frac{v_0^2 e^{-\kappa\bar{\Gamma} t_1}}{8(\kappa\bar{\Gamma} - 5D_\theta)(\kappa\bar{\Gamma} - 6D_\theta)} \left[\frac{e^{-\kappa\bar{\Gamma} t_2} - e^{-(\kappa\bar{\Gamma} + 4D_\theta)t_2}}{4D_\theta} - \frac{e^{(\kappa\bar{\Gamma} - 16D_\theta)t_2} - e^{-\kappa\bar{\Gamma} t_2}}{2\kappa\bar{\Gamma} - 16D_\theta} \right]
\end{aligned} \tag{4.79}$$

Integral values to due term (e) will be same of (a) similarly others. Terms due to (f), (g), (h) of Eq.(4.72) will be zero for the initial orientational angle $\theta_0 = 0$. Now for the simplification we are taking only the term associated with $\sinh \kappa\bar{\Gamma} t_2$ of Eq.(4.76). Similarly another same term of $\sinh \kappa\bar{\Gamma} t_2$ will arise due to the contribution of (e) of Eq.(4.72).

To make this two-time correlation as zero centric stochastic process we need to subtract the term $\langle R_0(t_1) \rangle \langle R_1(t_2) \rangle$ from Eq.(4.67). But for the simplicity of the calculation we have avoided this term. So, this two-time correlation term becomes,

$$\begin{aligned}
\langle x_0(t_1) x_1(t_2) \rangle = & \left(\frac{k_B T}{\kappa} \right) \cos 2\theta_0 e^{-\kappa\bar{\Gamma} t_1} \left(\frac{e^{(\kappa\bar{\Gamma} - 4D_\theta)t_2} - e^{-\kappa\bar{\Gamma} t_2}}{2\kappa\bar{\Gamma} - 4D_\theta} - \frac{e^{-\kappa\bar{\Gamma} t_2} - e^{-(4D_\theta + \kappa\bar{\Gamma})t_2}}{4D_\theta} \right) \\
& + \left(\frac{k_B T}{\kappa} \right) \left(\frac{\Delta\Gamma}{2\bar{\Gamma}} \right) e^{-\kappa\bar{\Gamma} t_1} \left[\frac{e^{\kappa\bar{\Gamma} t_2} - e^{-\kappa\bar{\Gamma} t_2}}{2\kappa\bar{\Gamma} + 4D_\theta} - \frac{2\kappa\bar{\Gamma} e^{-\kappa\bar{\Gamma} t_2} - e^{-(2\kappa\bar{\Gamma} + 4D_\theta)t_2}}{4D_\theta (\kappa\bar{\Gamma} + 4D_\theta)} \right] \\
& - \frac{3v_0^2 D_\theta e^{-\kappa\bar{\Gamma} t_1} \sinh \kappa\bar{\Gamma} t_2}{2\kappa\bar{\Gamma} (\kappa\bar{\Gamma} + D_\theta) (\kappa\bar{\Gamma} - D_\theta) (\kappa\bar{\Gamma} + 2D_\theta)}
\end{aligned} \tag{4.80}$$

Following Eq. (5.53), the mean-square displacement $\langle x^2(t) \rangle$ up to the first order correction is given by $\langle x^2(t) \rangle = \langle x_0^2(t) \rangle_{\xi, \theta} - (\kappa\Delta\Gamma) \langle x_0(t) x_1(t) \rangle_{\xi, \theta}$. From Eqs. (4.58) and (4.80) it is clear that the second term in Eq. (4.58) cancels with the first term in Eq. (4.80). Further, since we are interested in the expression for the mean square displacement up to the first order, the expression for $\langle x^2(t) \rangle$ becomes

$$\begin{aligned}
\langle x^2(t) \rangle = & \left(\frac{k_B T}{\kappa} \right) \left[(1 - e^{-2\kappa\bar{\Gamma}t}) + \kappa\Delta\Gamma \cos 2\theta_0 \left(\frac{e^{-2\kappa\bar{\Gamma}t} - e^{-(4D_\theta + 2\kappa\bar{\Gamma})t}}{4D_\theta} \right) \right. \\
& + \frac{v_0^2 \cos 2\theta_0}{2} \left[\frac{2D_\theta(e^{-4D_\theta t} - e^{-2\kappa\bar{\Gamma}t})}{(2\kappa\bar{\Gamma} - 4D_\theta)(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} - D_\theta)} + \frac{e^{-4D_\theta t} - 2e^{-(\kappa\bar{\Gamma} + D_\theta)t} + e^{-2\kappa\bar{\Gamma}t}}{(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} - 3D_\theta)} \right] \\
& + \frac{v_0^2}{2} \left[\frac{1 - 2e^{-(\kappa\bar{\Gamma} + D_\theta)t} + e^{-2\kappa\bar{\Gamma}t}}{(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)} - \frac{D_\theta(1 - e^{-2\kappa\bar{\Gamma}t})}{\kappa\bar{\Gamma}(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)} \right] \\
& \left. + \kappa\Delta\Gamma \frac{3v_0^2 D_\theta e^{-\kappa\bar{\Gamma}t} \sinh \kappa\bar{\Gamma}t}{2\kappa\bar{\Gamma}(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + 2D_\theta)} \right] \tag{4.81}
\end{aligned}$$

4.3.5 Persistence probability

We are going to calculate the persistence probability of the harmonically trapped active asymmetric Brownian particle. The two-time correlation function $\langle x(t_1)x(t_2) \rangle_{\xi, \theta}$ can be written in terms of perturbation series terms as

$$\langle x(t_1)x(t_2) \rangle_{\xi, \theta} = \langle x_0(t_1)x_0(t_2) \rangle_{\xi, \theta} - \frac{(\kappa\Delta\Gamma)}{2} [\langle x_0(t_1)x_1(t_2) \rangle_{\xi, \theta} + \langle x_1(t_1)x_0(t_2) \rangle_{\xi, \theta}] \tag{4.82}$$

where $t_1 > t_2$. The correlation functions $\langle x_0(t_1)x_1(t_2) \rangle_{\xi, \theta}$ and $\langle x_1(t_1)x_0(t_2) \rangle_{\xi, \theta}$ are equal in asymptotic limit, that is, for t_1 and t_2 large. In the limit, the expression for the two-time correlation function takes the form

$$\langle x(t_1)x(t_2) \rangle_{\xi, \theta} = \langle x_0(t_1)x_0(t_2) \rangle_{\xi, \theta} - (\kappa\Delta\Gamma) \langle x_0(t_1)x_1(t_2) \rangle_{\xi, \theta} \tag{4.83}$$

For initial angle $\theta_0 = 0$ all the terms of both $\langle x_0(t_1)x_0(t_2) \rangle$ and $\langle x_0(t_1)x_1(t_2) \rangle$ survive. But for the simplicity of the calculation we will neglect several terms. From Eq.(4.64) we neglect the first term of the third part and the terms $e^{-D_\theta t_1} e^{-3D_\theta t_2}$ and $e^{-\kappa\bar{\Gamma} t_2} e^{-D_\theta t_1}$ from the third part, and similarly from the fourth part we neglect the terms containing $e^{-D_\theta t_1} e^{D_\theta t_2}$ and $e^{-\kappa\bar{\Gamma} t_2} e^{-D_\theta t_1}$. Again we have taken consideration of the transformed two-time correlation terms defined in Eq.(4.65) and Eq.(4.66). And from the Eq.(4.80) only first part and the first term of the second part and the third part have been taken, and

other terms are neglected. Thus the correlation becomes,

$$\begin{aligned}
& \langle x(t_1)x(t_2) \rangle_{\theta_0=0} \\
&= e^{-\kappa\bar{\Gamma}t_1} \left[\left(\frac{2k_B T}{\kappa} - \frac{v_0^2 D_\theta}{\kappa\bar{\Gamma}(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)} + \frac{\Delta\Gamma}{2\bar{\Gamma}} \frac{3v_0^2 D_\theta}{(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + 2D_\theta)} \right) \sinh \kappa\bar{\Gamma}t_2 \right. \\
& \left. + \frac{4D_\theta^2 v_0^2 (e^{-\kappa\bar{\Gamma}t_2} - e^{-D_\theta t_2})}{(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)^2} + (\Delta D) \frac{1 - e^{-4D_\theta t_2}}{4D_\theta} \right]
\end{aligned} \tag{4.84}$$

After a little algebra, the two-time correlation function for the x -coordinate of the position vector,

$$\begin{aligned}
\langle x(t_1)x(t_2) \rangle_{\theta_0=0} &= e^{-\kappa\bar{\Gamma}t_1} \left[\left(\frac{2k_B T}{\kappa'} \right) \sinh \kappa\bar{\Gamma}t_2 + \frac{4D_\theta^2 v_0^2 (e^{-\kappa\bar{\Gamma}t_2} - e^{-D_\theta t_2})}{(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)^2} \right. \\
& \left. + \left(\frac{2k_B T}{\kappa} \right) \left(\frac{\kappa\Delta\Gamma}{2} \right) e^{-\kappa\bar{\Gamma}t_2} \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta} \right) \right]
\end{aligned} \tag{4.85}$$

where the effective trap constant κ' is defined as $\kappa'^{-1} = \kappa^{-1} \left[1 - \frac{v_0^2 D_\theta}{\bar{D}(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)} + \frac{\kappa\Delta\Gamma}{2} \frac{3v_0^2 D_\theta}{2\bar{D}(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + 2D_\theta)} \right]$

As before, we define the variable $X(t) = x(t)/\sqrt{\langle x^2 \rangle_{\xi, \theta}}$ and the correlation function of $\langle X(t_1)X(t_2) \rangle_{\xi, \theta}$ is found,

$$\begin{aligned}
& \langle X(t_1)X(t_2) \rangle_{\xi, \theta} = \\
& \frac{e^{-\kappa\bar{\Gamma}t_1/2}}{e^{-\kappa\bar{\Gamma}t_2/2}} \left[\left(\frac{2k_B T}{\kappa'} \right) \sinh \kappa\bar{\Gamma}t_1 + \frac{4D_\theta^2 v_0^2 (e^{-\kappa\bar{\Gamma}t_1} - e^{-D_\theta t_1})}{(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)^2} + \left(\frac{2k_B T}{\kappa} \right) \left(\frac{\kappa\Delta\Gamma}{2} \right) e^{-\kappa\bar{\Gamma}t_1} \left(\frac{1 - e^{-4D_\theta t_1}}{4D_\theta} \right) \right]^{1/2} \\
& \left[\left(\frac{2k_B T}{\kappa'} \right) \sinh \kappa\bar{\Gamma}t_2 + \frac{4D_\theta^2 v_0^2 (e^{-\kappa\bar{\Gamma}t_2} - e^{-D_\theta t_2})}{(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)^2} + \left(\frac{2k_B T}{\kappa} \right) \left(\frac{\kappa\Delta\Gamma}{2} \right) e^{-\kappa\bar{\Gamma}t_2} \left(\frac{1 - e^{-4D_\theta t_2}}{4D_\theta} \right) \right]
\end{aligned} \tag{4.86}$$

Using the time transformation for an imaginary time variable T , such that

$$\begin{aligned}
e^T &= e^{-\kappa\bar{\Gamma}t} \left[\left(\frac{2k_B T}{\kappa} - \frac{v_0^2 D_\theta}{\kappa\bar{\Gamma}(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)} + \frac{\Delta\Gamma}{2\bar{\Gamma}} \frac{3v_0^2 D_\theta}{(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + 2D_\theta)} \right) \sinh \kappa\bar{\Gamma}t \right. \\
& \left. + \frac{4D_\theta^2 v_0^2 (e^{-\kappa\bar{\Gamma}t} - e^{-D_\theta t})}{(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)^2} + (\Delta D) \frac{1 - e^{-4D_\theta t}}{4D_\theta} \right]
\end{aligned} \tag{4.87}$$

The two time correlation function in Eq. (4.86) transforms into a stationary correla-

tor of the form $C(T_1 - T_2) = e^{-(T_1 - T_2)/2}$ and the persistence probability in the asymptotic limit in the imaginary variable T is given by $p(T) \sim e^{-T/2}$. Transforming back into real-time, the persistence probability becomes

$$p(t, \theta_0 = 0) = e^{-\kappa\bar{\Gamma}t/2} \left[\left(\frac{2k_B T}{\kappa'} \right) \sinh \kappa\bar{\Gamma}t + \frac{4D_\theta^2 v_0^2 (e^{-\kappa\bar{\Gamma}t} - e^{-D_\theta t})}{(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} - D_\theta)^2} + \left(\frac{2k_B T}{\kappa} \right) \left(\frac{\kappa\Delta\Gamma}{2} \right) e^{-\kappa\bar{\Gamma}t} \frac{1 - e^{-4D_\theta t}}{4D_\theta} \right]^{-1/2} \quad (4.88)$$

In the limit of $v_0 \rightarrow 0$, the equation correctly reproduces the result for a passive anisotropic particle.²⁵ In order to validate the equation, we performed numerical simulations of Eq. (4.46) with the initial condition chosen from a Gaussian distribution with a very small width, so that the sign of $\mathbf{r}(0)$ is well defined. The trajectories were evolved in time with an integration time step of $\delta t = 0.001$. The persistence probability was determined from the fraction of trajectories for which $x(t)$ did not change its sign. A comparison of the measured persistence probability is shown in Fig. 4.5 for two values κ . There is an excellent agreement of the measured survival probability with the analytical expression given in Eq. (4.88).

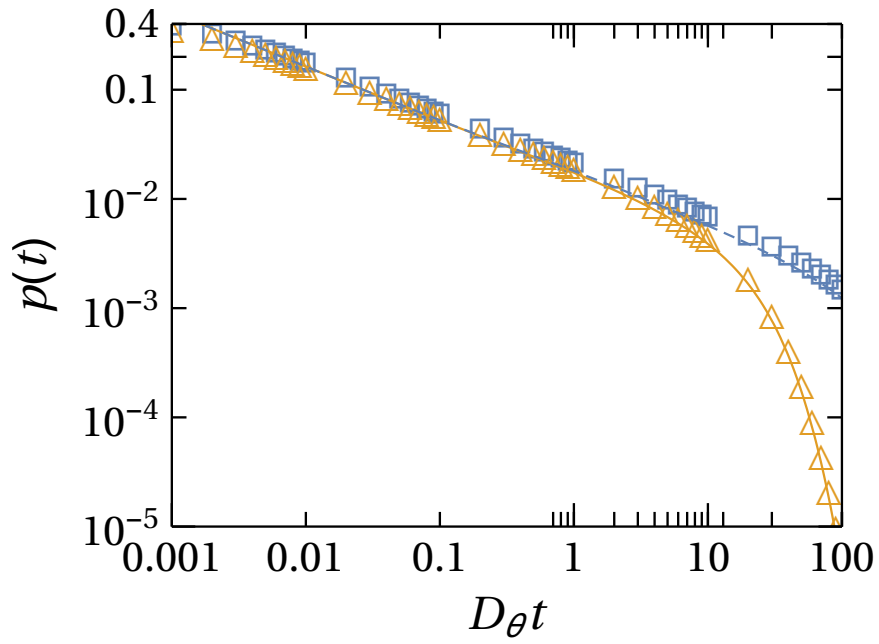


Figure 4.5 Plot of $p(t)$ for different choices of stiffness of the potential κ of the harmonically trapped anisotropic particle (blue square for $\kappa = 0.01$ and orange triangle for $\kappa = 0.10$) for self-propelled velocity $v_0 = 0.05$: the colours representing different stiffness of the potential are written above the plot. The rotational diffusion constant and initial angle θ_0 were fixed at $D_\theta = 1$ and $\theta_0 = 0$, translational diffusivities are fixed as $D_{\parallel} = 1$, $D_{\perp} = 0.5$. The blue dashed line is the plot of Eq.(4.88) for $\kappa = 0.01$ and the orange solid line is the plot of Eq.(4.88) for $\kappa = 0.10$ with the appropriate values of D_{\parallel} , D_{\perp} , and D_θ .

In brief, we have calculated the persistence probability along the x -axis of an active anisotropic particle in two dimensions in the absence of any potential and in the presence of a harmonic potential. Two-time correlation function has been calculated in the both cases. In the case of the harmonic trapping, we have used a perturbative solution for calculating the correlation functions. The persistence probability has been calculated with suitable space and time transformations. We have calculated persistence probability both analytically and numerically. We discussed single particle properties by the orientational and translational correlation functions presenting some analytical results for this model. We have shown how the addition of the self-propelled velocity for active Brownian particle changes the dynamics and the persistence of the system than the passive Brownian particle.

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5

Persistence of surface growth with finite size effect in KPZ interface

Surface growth is a common phenomenon in many processes of fundamental interest and applied fields, occurring over a broad range of length scales with atomistic growth models that range from a few nanometers to biological systems (such as the growth of tumors) that range to a few millimeters. Such deposition processes are inherently spatially extended systems that are stochastic in nature. Theoretical modeling of such systems is usually done using stochastic coarse-grained growth equations- the dynamical evolution of the surface height is governed by either a linear or a nonlinear Langevin equation, depending on the underlying microscopic dynamics. In this chapter, we look at the persistence probability $p(t)$ of stochastic models of surface growth which is restricted by finite system size. We look at two particular models of surface growth - the linear Edwards-Wilkinson model and the non-linear Kardar-Parisi-Zhang model. The purpose of this chapter is to present analytical results for the persistence $p(t)$ for finite-size system.

5.1 Introduction

Here we start the systematic study of the different growth processes and the corresponding universality classes¹⁻⁶. In the growth process, there are two simplest growth models, random deposition model(RD) and ballistic deposition model(BD)⁷. The simplest model RD allows us to determine the scaling components exactly, and to construct a continuum growth equation that leads to the same scaling exponents. A comparatively complicated model is BD model. RD model is described as: From a randomly taken site over the surface, a particle falls vertically until it reaches the top of the column under it, upon where it is deposited. Thus we choose a column randomly and increase its height $h(t)$ by one. The most important difference between RD and BD model is that the RD interface is uncorrelated. On the other hand in BD model, the particles are capable of sticking to the edge of the neighboring columns leading to lateral growth, allowing the spread of correlations along the surface.

The dynamic scaling behavior of stochastic growth equations is characterized by several universality classes. Every choice of universality class is characterized by a set of scaling exponents depending upon the dimensionality of the problem. The exponents are denoted as α , β , and z , when α represents the roughness exponent exploring the dependence of the amplitude of height fluctuations in the steady state regime ($t \gg L^z$) on the sample size L , β denotes the growth exponent describing the initial power-law growth of the interface width in the transient regime ($1 \ll t \ll L^z$), and z represents the dynamical exponent related to the system size dependence of the time when the interface width attains saturation. We use the single-valued function $h(\mathbf{r}, t)$ representing the height of the growing sample at position \mathbf{r} and deposition time t . The interfacial height fluctuations are denoted by the root-mean-squared height deviation which is the interface width, that is a function of the substrate size L and deposition time t :

$$W(L, t) = \langle [h(\mathbf{r}, t) - \bar{h}(t)]^2 \rangle^{1/2} \quad (5.1)$$

here $\bar{h}(t)$ = average sample thickness. $W(L, t) \propto t^\beta$ for $t \ll L^z$ and $W(L, t) \propto L^\alpha$ for $t \gg L^z$, L^z being the equilibration time of the interface when its stationary roughness is fully developed.

In RD model, every column grows independently as there is no correlation between the columns. The probability that the column grows independently is $p = 1/L$, where L is the system size. The probability that the column has height h after the deposition of

N particles is,

$$P(h, N) = \binom{N}{h} p^h (1-p)^{N-h}$$

Average height grows linearly with time $\langle h \rangle = \sum_{h=1}^N h P(h, n) = Np = N/L = t$. Similarly the second moment is straight forwardly calculated as $\langle h^2 \rangle = Np(1-p) + N^2 p^2$. The width of the interface is given $w^2(t) = \langle (h - \langle h \rangle)^2 \rangle = \langle h^2 \rangle - \langle h \rangle^2 = \frac{N}{L} (1 - \frac{1}{L})$. So we conclude as $w(t) \sim t^{1/2}$. So $\beta = \frac{1}{2}$. The differential equation representing the RD model is

$$\frac{\partial h(x, t)}{\partial t} = F + \eta(x, t)$$

F is the average number of particles arriving at site x . $\eta(x, t)$ is the random fluctuation whose average is zero and the second moment is $\langle \eta(x, t) \eta(x', t') \rangle = 2D \delta(x - x') \delta(t - t')$.

General solution

$$h(x, t) = Ft + \int_0^t dt' \eta(x, t')$$

From this relation, we can also derive $w^2(t) = 2Dt$. Thus we obtain the same exponent $\beta = 1/2$.

Let us generalize the growth equation with a form

$$\frac{\partial h(x, t)}{\partial t} = G(h, x, t) + \eta(x, t)$$

Here $G(h, x, t)$ is a general term that depends on the interface height, position, and time. To find the growth equation, we list some basic symmetries

- Invariance under translation in time.
- Translation invariance along the growth direction. This means that the equation is constructed from the combination of $\nabla h, \nabla^2 h, \dots, \nabla^n h$.
- Translational invariance in the direction perpendicular to the growth direction.
- Rotation and inversion symmetry about the growth direction.
- Up/down symmetry for h , that means the interface fluctuations are similar w.r.t the mean interface height.

Considering all these conditions we may construct a general growth equation as,

$$\frac{\partial h(x, t)}{\partial t} = (\nabla^2 h) + (\nabla^4 h) + \dots + (\nabla^{2n} h) + (\nabla^2 h)(\nabla h)^2 + \dots + (\nabla^{2k} h)(\nabla h)^{2j} + \eta(x, t)$$

The simplest equation describing the fluctuations of the equilibrium interface is Edward-Wilkinson(EW) equation, taking the form

$$\frac{\partial h(x,t)}{\partial t} = \nu \nabla^2 h + \eta(x,t) \quad (5.2)$$

here ν is surface tension, and $\nu \nabla^2 h$ term influences to smoothen the interface. The scaling exponents for EW equation is $\alpha = \frac{2-d}{2}$, $\beta = \frac{2-d}{4}$, and $z = 2$

Now the rather complicated form of describing a growth equation is the KPZ equation, which is obtained using physical principles which motivate the addition of nonlinear terms to the linear theory and symmetry principles as we use for the EW case. We include lateral growth in the equation. Growth happens locally normal to the interface generating the nonlinear term $(\nabla h)^2$. Adding this term to the EW equation we get the KPZ equation as follows

$$\frac{\partial h(x,t)}{\partial t} = \nu \nabla^2 h + \lambda (\nabla h)^2 + \eta(x,t) \quad (5.3)$$

The first term smoothen the interface with diffusivity $\nu > 0$, and the second term is the slope-dependent growth velocity of strength λ , $\lambda > 0$ for convenience. From this equation we can easily say that the interface growth governed by the KPZ equation has nonzero velocity even in the absence of an external driving force. The scaling exponents in this case are $\alpha = (2-d)/3$, $\beta = (2-d)/(4+d)$. For $d = 1$, $\alpha = 1/3$ and $\beta = 1/5$.

In this chapter, we look at the persistence probability $p(t)$ of stochastic models of surface growth which is restricted by a finite system size. We look at two particular models of surface growth - the linear Edwards-Wilkinson model (EW) and the non-linear Kardar-Parisi-Zhang model (KPZ). The phenomenon of persistence in the continuum version of these two models has been well studied and the persistence exponents are also known.^{8,9} For instance, the steady-state persistence exponents for both these models are related to the growth exponent β as $\theta = 1 - \beta$,^{8,9} even though the KPZ equation is a non-linear equation. Numerically obtained values of the steady state persistence exponent for the one-dimensional KPZ equation were found to be $\theta \approx 0.66$, close to the predicted value of $2/3$,⁹ whereas for the EW model the exponent was found to be ≈ 0.74 , close to the predicted value of $3/4$. While these results are for continuum equations of surface growth, expressions for the persistence probability in spatially discrete surface growth models with finite-size effects are not well-known. Our aim is to investigate the persistence probability for discrete models of surface growth equations with a finite-size. In an infinite spatially extended system, the boundary conditions do not play

a significant role. The scenario changes when the system size is finite and it is expected that the well-known algebraic decay of $p(t)$ is lost.

The rest of the chapter is organized as follows: in Section 5.2 we present a brief introduction to the models of surface growth. In Section 5.3 we present our work on the persistence probabilities for the Edwards-Wilkinson model of surface growth on a finite one-dimensional lattice (Section 5.3.1) and for the Kardar-Parisi-Zhang model of surface growth on a finite one-dimensional lattice (Section 5.3.2).

5.2 Dynamic Scaling and Stochastic Growth Models

Since it is convenient to write the evolution equations in terms of the deviation of the height from its spatial average value, $h(\mathbf{r}, t) - \bar{h}(t)$, from now on we will denote by $\bar{h}(\mathbf{r}, t)$ the interface height fluctuation measured from the average height. Using different scaling exponents (α, β, z) we get,

(a) The Edward-Wilkinson (EW) second-order linear equation: $(\alpha = \frac{1}{2}, \beta = \frac{1}{4}, z = 2)$

$$\frac{\partial h(\mathbf{r}, t)}{\partial t} = v\nabla^2 h(\mathbf{r}, t) + \eta(\mathbf{r}, t) \quad (5.4)$$

(b) The KPZ second-order nonlinear equation: $(\alpha = \frac{1}{2}, \beta = \frac{1}{3}, z = \frac{3}{2})$

$$\frac{\partial h(\mathbf{r}, t)}{\partial t} = v\nabla^2 h(\mathbf{r}, t) + \lambda |\nabla h(\mathbf{r}, t)|^2 + \eta(\mathbf{r}, t) \quad (5.5)$$

(c) The Mullins-Herring (MH) fourth-order linear equation: $(\alpha = \frac{3}{2}, \beta = \frac{3}{8}, z = 4(1, \frac{1}{4}, 4))$

$$\frac{\partial h(\mathbf{r}, t)}{\partial t} = -v\nabla^4 h(\mathbf{r}, t) + \eta(\mathbf{r}, t) \quad (5.6)$$

(d) The MBE fourth-order nonlinear equation: $(\alpha = \frac{2}{3}, \beta = \frac{1}{5}, z = \frac{10}{3})$

$$\frac{\partial h(\mathbf{r}, t)}{\partial t} = -v\nabla^4 h(\mathbf{r}, t) + \lambda \nabla^2 |(\nabla h(\mathbf{r}, t))|^2 + \eta(\mathbf{r}, t) \quad (5.7)$$

The term $\eta(\mathbf{r}, t)$ represents the noise term. We assume that the noise has Gaussian

distribution with zero mean and correlator:

$$\langle \eta(\mathbf{r}_1, t_1) \eta(\mathbf{r}_2, t_2) \rangle = D \delta^d(\mathbf{r}_1 - \mathbf{r}_2) \delta(t_1 - t_2) \quad (5.8)$$

5.3 Calculation of Persistence

In this section, we present our calculations for the determination of the persistence probability of the local height fluctuation in two models of surface growth. In both the models, we consider the system to be bounded by a finite system size with a prescribed boundary condition. Our first step is to consider the linear stochastic model of growth described by the Edwards-Wilkinson model, discretized on a one-dimensional lattice. Consequent to this, we look at the non-linear Kardar-Parisi-Zhang model of surface growth.

5.3.1 Persistence for Edward-Wilkinson system on a finite lattice

We consider the Edwards-Wilkinson model of surface growth on a one-dimensional lattice with a finite domain size extending from $-L$ to L . The finite domain is discretized into a one-dimensional lattice with $2N$ points, such that $Na = L$, where the lattice spacing is defined as a . At each lattice point the height profile is denoted as $h_n(t)$. The continuum stochastic model of surface growth given in Eq. (5.4) in one dimension reads as

$$\frac{\partial h(x, t)}{\partial t} = v \frac{\partial^2 h}{\partial x^2} + \eta(x, t) \quad (5.9)$$

Where ξ is the Gaussian stochastic noise. The correlations of the ξ are given by

$$\begin{aligned} \langle \eta(x, t) \rangle &= 0 \\ \langle \eta(x, t) \eta(x', t') \rangle &= 2D \delta(t - t') \delta(x - x') \end{aligned} \quad (5.10)$$

The boundary condition is chosen to be $\left. \frac{\partial h}{\partial x} \right|_{\pm L} = 0$. The discretized form of Eq. (5.9) on a one dimensional lattice takes the form

$$\frac{\partial h_n(t)}{\partial t} = \frac{v}{a^2} [h_{n+1}(t) + h_{n-1}(t) - 2h_n] + \frac{\eta_n}{\sqrt{a}} \quad (5.11)$$

Note the \sqrt{a} in the Eq.(5.11) comes from the spatial delta correlation of the noise in the continuum equation. The formal solution to Eq. (5.11) together with the boundary

condition for h_n is given by

$$h_n(t) = X_0 + 2 \sum_p X_p \cos k_p n \quad (5.12)$$

where X_p are the Fourier modes for $p \neq 0$ and X_0 is the $p = 0$ mode. The boundary condition dictates that $\sin k_p N = 0$ and therefore we get $k_p = p\pi/N$, so that the formal solution takes the form

$$h_n(t) = X_0 + 2 \sum_p X_p \cos \frac{p\pi n}{N} \quad (5.13)$$

Substituting Eq. (5.13) in Eq. (5.11), we get for X_p

$$\sum_p \dot{X}_p \cos \left(\frac{p\pi n}{N} \right) = -\frac{2\nu}{a^2} \sum_p X_p \left[1 - \cos \left(\frac{p\pi}{N} \right) \right] \cos \left(\frac{p\pi n}{N} \right) + \frac{\eta_n}{2\sqrt{a}} \quad (5.14)$$

We multiply throughout Eq. (5.14) with $\cos(q\pi n/N)$ and carry out a sum over n . The left hand side of Eq. (5.14) gives

$$\sum_p \sum_n \dot{X}_p \cos \left(\frac{p\pi n}{N} \right) \cos \left(\frac{q\pi n}{N} \right) = \sum_p \dot{X}_p \frac{1}{a} \int_{-L}^L dx \cos \left(\frac{p\pi x}{L} \right) \cos \left(\frac{q\pi x}{L} \right) = \frac{L}{a} \sum_p \dot{X}_p \delta_{p,q} = \frac{L}{a} \dot{X}_q \quad (5.15)$$

Similarly, the first term on the right hand side of Eq. (5.14) becomes

$$\begin{aligned} -\sum_p \sum_n k_p X_p \cos \left(\frac{p\pi n}{N} \right) \cos \left(\frac{q\pi n}{N} \right) &= -\sum_p k_p X_p \frac{1}{a} \int_{-L}^L dx \cos \left(\frac{p\pi x}{L} \right) \cos \left(\frac{q\pi x}{L} \right) \\ &= -\frac{L}{a} \sum_p X_p \delta_{p,q} = -\frac{L}{a} k_q X_q \end{aligned} \quad (5.16)$$

Where $k_p = \frac{2\nu}{a^2} (1 - \cos \frac{p\pi}{N})$. For large enough N , we approximate k_p as $k_p = \frac{\nu p^2 \pi^2}{L^2}$, where we have used the fact that $Na = L$. The equation for the time evolution of X_p follows the stochastic differential equation

$$\frac{\partial X_p}{\partial t} = -k_p X_p + \eta_p \quad (5.17)$$

where the stochastic noise η_p is given by

$$\eta_p(t) = \frac{\sqrt{a}}{2L} \sum_n \eta_n \cos \left(\frac{p\pi n}{N} \right) \quad (5.18)$$

The statistical correlations of η_p follows from η_n . The first moment of η_p is zero. The

second moment is given by

$$\begin{aligned}
\langle \eta_p(t) \eta_q(t') \rangle &= \frac{a}{4L^2} \sum_{n,m} \langle \eta_n(t) \eta_m(t') \rangle \cos\left(\frac{p\pi n}{N}\right) \cos\left(\frac{q\pi m}{N}\right) \\
&= \frac{2Da}{4L^2} \delta(t-t') \sum_n \cos\left(\frac{p\pi n}{N}\right) \cos\left(\frac{q\pi n}{N}\right) \\
&= \frac{2Da}{4L^2} \delta(t-t') \frac{L}{a} \delta_{p,q} = \frac{D}{2L} \delta_{p,q} \delta(t-t')
\end{aligned} \tag{5.19}$$

The noise correlations for $p = 0$ mode also follows from Eq. (5.18). While the first moment remains zero due to the Gaussian nature of η_n , the second moment is given by

$$\begin{aligned}
\langle \eta_0(t) \eta_0(t') \rangle &= \frac{a}{4L^2} \sum_{n,m} \langle \eta_n(t) \eta_m(t') \rangle = \frac{2Da}{4L^2} \delta(t-t') \sum_{n,m} \delta_{n,m} \\
&= \frac{2Da}{4L^2} \delta(t-t') \sum_n = \frac{D}{L} \delta(t-t')
\end{aligned} \tag{5.20}$$

In deriving the last line of Eq. (5.20), we have used the fact that $\sum_n = 2N$ and $Na = L$. With the noise correlation at hand, we now proceed to calculate the two-time correlation functions. The solution for X_p , for $p \neq 0$, is given by

$$X_p(t) = \int_0^t dt' e^{-k_p(t-t')} \eta_p(t') \tag{5.21}$$

and for $p = 0$, X_0 obeys the simple random walk equation

$$X_0(t) = \int_0^t dt' \eta_0(t') \tag{5.22}$$

With $t_1 > t_2$, the two-time correlation function for $\langle X_p(t_1) X_q(t_2) \rangle$ take the form

$$\langle X_p(t_1) X_q(t_2) \rangle = \begin{cases} \frac{D}{L} t_2 & \text{for } p = q = 0 \\ \frac{D}{2L} \delta_{p,q} \left(\frac{v\pi^2 p^2}{L^2} + \frac{v\pi^2 q^2}{L^2} \right)^{-1} \times \\ \left[e^{-\frac{v\pi^2}{L^2}(t_1-t_2)} - e^{-\frac{v\pi^2 p^2}{L^2} t_1} e^{-\frac{v\pi^2 q^2}{L^2} t_2} \right] & \\ \text{for } p \neq q \neq 0 \end{cases} \tag{5.23}$$

We now want to determine the persistence probability in such a system. For this, we choose the height profile at $n = 0$ as the stochastic variable, corresponding to $x = 0$ in

the continuum limit. Putting $n = 0$ in the formal solution Eq. (5.13), we get

$$h_0(t) = X_0 + 2 \sum_p X_p \quad (5.24)$$

The two-time correlation function $\langle h_0(t_1)h_0(t_2) \rangle$ is given by

$$\langle h_0(t_1)h_0(t_2) \rangle = \langle X_0(t_1)X_0(t_2) \rangle + 4 \sum_{p,q} \langle X_p(t_1)X_q(t_2) \rangle \quad (5.25)$$

Substituting the two-time correlation functions derived in Eq. (5.23), and noting that the delta function in Eq. (5.23) for $p \neq q \neq 0$ is removed by the sum over q in Eq. (5.25) we get

$$\langle h_0(t_1)h_0(t_2) \rangle = \frac{D}{L}t_2 + \frac{2D}{L} \sum_{p=1}^{\infty} \left(\frac{2v\pi^2 p^2}{L^2} \right)^{-1} \times \left[e^{-\frac{v\pi^2 p^2}{L^2}(t_1-t_2)} - e^{-\frac{v\pi^2 p^2}{L^2}(t_1+t_2)} \right] \quad (5.26)$$

With this expression in hand, we first consider the limit of $L \rightarrow \infty$. To this end we use the Euler-Maclaurin formula for the sum over the Fourier modes.

$$\begin{aligned} & \sum_{p=1}^{\infty} \left(\frac{2v\pi^2 p^2}{L^2} \right)^{-1} \left[e^{-\frac{v\pi^2 p^2}{L^2}(t_1-t_2)} - e^{-\frac{v\pi^2 p^2}{L^2}(t_1+t_2)} \right] \\ &= \frac{L}{2\pi} \int_0^{\infty} \frac{e^{-vk^2(t_1-t_2)} - e^{-vk^2(t_1+t_2)}}{vk^2} - \frac{1}{2}f(0) \end{aligned} \quad (5.27)$$

where $f(k) = \frac{e^{-vk^2(t_1-t_2)} - e^{-vk^2(t_1+t_2)}}{2vk^2}$. Therefore, in this limit of $L \rightarrow \infty$, the sum is rewritten as

$$\sum_{p=1}^{\infty} \frac{e^{-k_p(t_1-t_2)} - e^{-k_p(t_1+t_2)}}{2k_p} = \int_0^{\infty} \frac{e^{-vk^2(t_1-t_2)} - e^{-vk^2(t_1+t_2)}}{2k_p} dk - \frac{1}{2}[f(0) + f(\infty)] \quad (5.28)$$

Where $f(k_p) = \frac{e^{-k_p(t_1-t_2)} - e^{-k_p(t_1+t_2)}}{2k_p}$. In the limit of $k \rightarrow 0$ we get $f(0) = t_2/2$ so that the expression in Eq. (5.26) become

$$\begin{aligned} \langle h_0(t_1)h_0(t_2) \rangle &= \frac{D}{L}t_2 + \frac{2D}{2\pi} \int_0^{\infty} dk \left[\frac{e^{-vk^2(t_1-t_2)} - e^{-vk^2(t_1+t_2)}}{vk^2} \right] - \frac{D}{L}t_2 \\ &= D \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[\frac{e^{-vk^2(t_1-t_2)} - e^{-vk^2(t_1+t_2)}}{vk^2} \right] \end{aligned} \quad (5.29)$$

The final form of the two-time correlation function in Eq. (5.29) is the well known result for the one dimensional Edwards-Wilkinson model of surface growth in the continuum

limit.^{8,10} Denoting $C(t_1, t_2) \equiv \langle h_0(t_1)h_0(t_2) \rangle$ we get

$$C(t_1, t_2) = \frac{D}{v} [(t_1 + t_2)^{1/2} - (t_1 - t_2)^{1/2}] \quad (5.30)$$

We now define the normalised variable $H(t) = h_0(t)/\sqrt{\langle h_0^2(t) \rangle}$ and the two-time correlation function of $H(t)$, $A(t_1, t_2) \equiv \langle H(t_1)H(t_2) \rangle = C(t_1, t_2)/\sqrt{C(t_1, t_1)C(t_2, t_2)}$ is given by

$$\begin{aligned} A(t_1, t_2) &= \frac{C(t_1, t_2)}{\sqrt{C(t_1, t_1)C(t_2, t_2)}} \\ &= \left[\frac{1}{2} \left(\sqrt{\frac{t_1}{t_2}} + \sqrt{\frac{t_2}{t_1}} \right) \right]^{1/2} - \left[\frac{1}{2} \left(\sqrt{\frac{t_1}{t_2}} - \sqrt{\frac{t_2}{t_1}} \right) \right]^{1/2} \end{aligned} \quad (5.31)$$

The non-stationary correlation function in Eq. (5.31) is transformed into a stationary correlator using the transformation $T = \ln t$, so that we get

$$A(T_1, T_2) = A(T_1 - T_2) = f_0(T) = [\cosh T/2]^{1/2} - [\sinh T/2]^{1/2} \quad (5.32)$$

In the opposite limit of $L \rightarrow 0$, only the first term in Eq. (5.26) survives and the correlation function for the normalised variable $H(t) = h_0(t)/\sqrt{\langle h_0^2(t) \rangle}$ is given by

$$\langle H(t_1)H(t_2) \rangle = \sqrt{\frac{t_2}{t_1}} \quad (5.33)$$

This is the result for a simple random walk and the non-stationary correlation function is converted to a stationary correlator using the transformation $T = \ln t$. In the imaginary time T , the two-time correlation function becomes stationary: $\langle H(T_1)H(T_2) \rangle = e^{-(T_1 - T_2)/2}$ and the persistence probability is that of a simple random walker $p(t) \sim t^{-1/2}$.

We now study the case when L is finite. Thus, L is kept fixed while t is varied.

To this end, in the expression for the two-time correlation function in Eq. (5.26) we keep the long wavelength mode π/L corresponding to $p = 1$. The two-time correlation function becomes

$$\langle h_0(t_1)h_0(t_2) \rangle = \frac{D}{L} \left[t_2 + \frac{2L^2}{v\pi^2} e^{-\frac{v\pi^2}{L^2}t_1} \sinh \frac{v\pi^2}{L^2}t_2 \right] \quad (5.34)$$

The first limiting case we note is that of $v \rightarrow 0$ when each lattice site is independent of its neighboring site and evolves according to a simple random walk model. In this case, we note that the correlation function in Eq. (5.34) becomes that of a simple random walker and consequently we expect the persistence probability to be $p(t) \sim t^{-1/2}$. In order to proceed further, we note that the non-stationary correlation function in Eq. (5.34) in

its exact form can not be transformed to a stationary correlator without any further approximation. When t_1 and t_2 are such that $v\pi^2 t/L^2 \gg 1$, the first term in Eq. (5.34) dominates and consequently the persistence probability is that of a random walker: $p(t) \sim t^{-1/2}$. In the opposite limit of $v\pi^2 t/L^2 \ll 1$ we approximate the correlator in Eq. (5.34) as:

$$\begin{aligned}\langle h_0(t_1)h_0(t_2) \rangle &= \frac{D}{L}t_2 \left[1 + 2 \left(1 - \frac{v\pi^2}{L^2}t_1 \right) \frac{\sinh \frac{v\pi^2}{L^2}t_2}{\frac{v\pi^2}{L^2}t_2} \right] \\ &= \frac{D}{L}t_2 \left[1 + 2 \left(1 - \frac{v\pi^2}{L^2}t_1 \right) \right] \\ &= \frac{3D}{L}t_2 \left[1 - \frac{2}{3} \frac{v\pi^2}{L^2}t_1 \right]\end{aligned}\tag{5.35}$$

We can now convert this to a stationary correlation function – first using the transformations $H(t) = h_0(t)/\sqrt{\langle h_0^2(t) \rangle}$ so that

$$\langle H(t_1)H(t_2) \rangle = \sqrt{\frac{t_2}{t_1}} \left[\frac{1 - (2/3) \frac{v\pi^2 t_1}{L^2}}{1 - (2/3) \frac{v\pi^2 t_2}{L^2}} \right]\tag{5.36}$$

The transformation to a time T is given by

$$e^{T/2} = \frac{t^{1/2}}{\left(1 - \frac{2}{3} \frac{v\pi^2 t}{L^2} \right)^{1/2}}\tag{5.37}$$

so that $\langle H(T_1)H(T_2) \rangle = e^{-(T_1-T_2)/2}$, and following Slepian¹¹, the persistence probability in real-time is given by

$$p(t) \sim \frac{1}{\sqrt{t}} \left(1 - \frac{2}{3} \frac{v\pi^2 t}{L^2} \right)^{1/2}\tag{5.38}$$

For term in the bracket in Eq. (5.38) can be exponentiated to get an alternate form for $p(t)$:

$$p(t) \sim \frac{1}{\sqrt{t}} e^{-\frac{1}{3} \frac{v\pi^2 t}{L^2}}\tag{5.39}$$

5.3.2 Persistence in KPZ growth at finite size limit

We now focus on the discretized Kardar-Parisi-Zhang model of surface growth. The continuum model in Eq. (5.5) in one-dimension take the form

$$\frac{\partial h_n}{\partial t} = v \frac{\partial^2 h_n}{\partial x^2} + \lambda \left(\frac{\partial h_n}{\partial x} \right)^2 + \eta_n \quad (5.40)$$

The boundary conditions remain the same as in the preceding section, that is, $\left. \frac{\partial h}{\partial t} \right|_{\pm L} = 0$. As before, we spatially discretize the equation on a one-dimensional lattice with a lattice spacing a :

$$\frac{\partial h_n}{\partial t} = \frac{v}{a^2} [h_{n+1} + h_{n-1} - 2h_n] + \lambda \left(\frac{h_{n+1} - h_{n-1}}{2a} \right)^2 + \frac{\eta_n}{\sqrt{a}} \quad (5.41)$$

Here λ is the non-linear coupling parameter. We choose a weak λ for two reasons- first a perturbative expansion around $\lambda = 0$ can be done and the solution to Eq. (5.41) can be constructed using the perturbative solution. Secondly, the choice of a weak λ is dictated by the requirement of $h(x, t)$ to be a Gaussian process. In the Edwards-Wilkinson model since $h(x, t)$ is linear, the process remains a Gaussian stochastic process. However, this is not true for the KPZ equation since it contains a nonlinear term.

We consider the perturbative expansion

$$h_n = h_n^0 + \lambda h_n^1 + \lambda^2 h_n^2 + \mathcal{O}(\lambda^3) \quad (5.42)$$

Substituting Eq. (5.42) in Eq. (5.41) and comparing the left hand and the right side to the powers of λ we get for h_n^0

$$\frac{\partial h_n^0}{\partial t} = \frac{v}{a^2} [h_{n+1}^0 + h_{n-1}^0 - 2h_n^0] + \frac{\eta_n}{\sqrt{a}} \quad (5.43)$$

and for h_n^1 as

$$\frac{\partial h_n^1}{\partial t} = \frac{v}{a^2} [h_{n+1}^1 + h_{n-1}^1 - 2h_n^1] + \left(\frac{h_{n+1}^0 - h_{n-1}^0}{2a} \right)^2 \quad (5.44)$$

To proceed further, we note that the solution given in Eq. (5.42), must obey the boundary condition at each order of λ . Specifically, one has $\left. \frac{\partial h_n^0}{\partial t} \right|_{\pm L} = 0$, $\left. \frac{\partial h_n^1}{\partial t} \right|_{\pm L} = 0$ and so on. Consequently, we write the solution as

$$\begin{aligned}
h_n^0 &= X_0^0 + 2 \sum_p X_p^0 \cos \frac{p\pi n}{N} \\
h_n^1 &= 2 \sum_p X_p^1 \cos \frac{p\pi n}{N} \\
h_n^2 &= 2 \sum_p X_p^2 \cos \frac{p\pi n}{N}
\end{aligned} \tag{5.45}$$

As before, we will be interested in the two-time correlation for h_0 . Using Eq. (5.45), the two-time correlation function $\langle h_0(t_1)h_0(t_2) \rangle$ takes the form

$$\begin{aligned}
\langle h_0(t_1)h_0(t_2) \rangle &= \langle h_0^0(t_1)h_0^0(t_2) \rangle + \lambda^2 \langle h_0^1(t_1)h_0^1(t_2) \rangle \\
&= \langle X_0^0(t_1)X_0^0(t_2) \rangle + 4 \sum_{p,q} \langle X_p^0(t_1)X_q^0(t_2) \rangle + 4\lambda^2 \sum_{p,q} \langle X_p^1(t_1)X_q^1(t_2) \rangle
\end{aligned} \tag{5.46}$$

In writing Eq. (5.46), we have ignored the term $\langle h_0^0(t_1)h_0^2(t_2) \rangle$ and $\langle h_0^2(t_1)h_0^0(t_2) \rangle$ in the order λ^2 term since they contain higher order exponential decays. The equation for the zeroth order h_n^0 obeys the same differential equation as that of the discrete Edwards-Wilkinson model (see Eq. (5.11)) and therefore the solution for h_n^0 is known. Consequently, the two-time correlation function $\langle X_p^0(t_1)X_q^0(t_2) \rangle$ follows from Eq. (5.23). We focus on the solution of h_n^1 . Substituting the expression of h_n^1 in terms of X_p^1 from Eq.(5.45), we get

$$\begin{aligned}
\frac{\partial}{\partial t} \left[2 \sum_p X_p^1 \cos \frac{p\pi n}{N} \right] &= \frac{v}{a^2} \left[2 \sum_p X_p^1 \left(\cos \frac{p\pi(n+1)}{N} \right. \right. \\
&\left. \left. + \cos \frac{p\pi(n-1)}{N} - 2 \cos \frac{p\pi n}{N} \right) \right] + \frac{1}{4a^2} \left[\sum_p X_p^0 \cos \frac{p\pi(n+1)}{N} - \sum_p X_p^0 \cos \frac{p\pi(n-1)}{N} \right]^2
\end{aligned} \tag{5.47}$$

This equation can be simplified to

$$\begin{aligned}
\sum_p \frac{\partial X_p^1}{\partial t} \cos \frac{p\pi n}{N} &= -\frac{2v}{a^2} \sum_p X_p^1 \cos \frac{p\pi n}{N} \left(1 - \cos \frac{p\pi}{N} \right) \\
&\quad + \frac{1}{2a^2} \sum_p X_p^0 X_q^0 \sin \frac{p\pi n}{N} \sin \frac{p\pi}{N} \sin \frac{q\pi n}{N} \sin \frac{q\pi}{N}
\end{aligned} \tag{5.48}$$

Multiplying both sides with the factor $\cos \frac{k\pi n}{N}$ and summing over n , we get

$$\begin{aligned} \sum_p \sum_n \frac{\partial X_p^1}{\partial t} \cos \frac{p\pi n}{N} \cos \frac{k\pi n}{N} &= -\frac{2v}{a^2} \sum_p \sum_n X_p^1 \cos \frac{p\pi n}{N} \cos \frac{k\pi n}{N} \left(1 - \cos \frac{p\pi}{N}\right) \\ &+ \frac{1}{2a^2} \sum_p \sum_n X_p^0 X_q^0 \sin \frac{p\pi n}{N} \sin \frac{q\pi n}{N} \cos \frac{k\pi n}{N} \sin \frac{p\pi}{N} \sin \frac{q\pi}{N} \end{aligned} \quad (5.49)$$

The term of L.H.S. of Eq.(5.49) can be expressed as

$$\sum_n \sum_p \dot{X}_p^1 \cos \frac{p\pi n}{N} \cos \frac{k\pi n}{N} = \sum_p \dot{X}_p^1 \frac{1}{a} \int_{-L}^{+L} dx \cos \frac{p\pi x}{L} \cos \frac{k\pi x}{L} = \frac{L}{a} \sum_p \dot{X}_p^1 \delta_{p,k} = \frac{L}{a} \dot{X}_k^1 \quad (5.50)$$

The first term of R.H.S. of Eq.(5.49) can be written as

$$\begin{aligned} -\sum_p \sum_n k_p X_p \cos \frac{p\pi n}{N} \cos \frac{k\pi n}{N} &= -\sum_p k_p X_p \frac{1}{a} \int_{-L}^{+L} dx \cos \frac{p\pi x}{L} \cos \frac{k\pi x}{L} = -\sum_p k_p X_p \frac{L}{a} \delta_{p,k} \\ &= -\frac{L}{a} k_k X_k \end{aligned} \quad (5.51)$$

The second term of R.H.S of Eq.(5.49) can be simplified as

$$\begin{aligned} &\frac{1}{2a^2} \sum_p \sum_n X_p^0 X_q^0 \sin \frac{p\pi n}{N} \sin \frac{q\pi n}{N} \cos \frac{k\pi n}{N} \sin \frac{p\pi}{N} \sin \frac{q\pi}{N} \\ &= \frac{1}{2a^2} \sum_p X_p^0 X_q^0 \sin \frac{p\pi}{N} \sin \frac{q\pi}{N} \frac{1}{a} \int_{-L}^{+L} dx \sin \frac{p\pi x}{L} \cos \frac{k\pi x}{L} \sin \frac{q\pi x}{L} \\ &= \frac{1}{2a^2} \sum_p X_p^0 X_q^0 \sin \frac{p\pi}{N} \sin \frac{q\pi}{N} \frac{L}{2a} (\delta_{p,q-k} + \delta_{p,q+k}) \\ &= \frac{L}{4a^3} \sum_p X_p^0 X_q^0 \sin \frac{p\pi}{N} \sin \frac{q\pi}{N} (\delta_{p,q-k} + \delta_{p,q+k}) \end{aligned} \quad (5.52)$$

Using the simplifications of Eq.(5.50), (5.51), (5.52) in Eq.(5.49) and we get

$$\begin{aligned} \frac{\partial X_p^1}{\partial t} &= -\frac{2v}{a^2} \left(1 - \cos \frac{p\pi}{N}\right) X_p^1 + \frac{1}{4a^2} \sum_p \sum_q X_p^0 X_q^0 \sin \frac{p\pi}{N} \sin \frac{q\pi}{N} [\delta_{p,q+k} + \delta_{p,q-k}] \\ &= -k_p X_p^1 + \frac{1}{4a^2} \sum_q X_{p+q}^0 X_q^0 \sin \frac{(q+p)\pi}{N} \sin \frac{q\pi}{N} + \frac{1}{4a^2} \sum_q X_{q-p}^0 X_q^0 \sin \frac{(q-p)\pi}{N} \sin \frac{q\pi}{N} \end{aligned} \quad (5.53)$$

The general solution is

$$X_p^1(t) = \frac{1}{4a^2} \sum \int_0^t dt' e^{-k_p(t-t')} \left[X_{p+q}^0(t') X_q^0(t') \sin \frac{(p+q)\pi}{N} \right. \\ \left. \sin \frac{q\pi}{N} + X_{q-p}^0(t') X_q^0(t') \sin \frac{(q-p)\pi}{N} \sin \frac{q\pi}{N} \right] \quad (5.54)$$

5.3.3 Calculation of $\langle X_p^1(t_1) X_p^1(t_2) \rangle$

$$\langle X_p^1(t_1) X_q^1(t_2) \rangle = \frac{1}{16a^4} \left[\int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \sum_{p_1, q_1} \langle X_{p+p_1}^0(t'_1) X_{p_1}^0(t'_1) X_{q+q_1}^0(t'_2) X_{q_1}^0(t'_2) \rangle \right. \\ e^{-k_p(t_1-t'_1)} e^{-k_q(t_2-t'_2)} \sin \frac{(p+p_1)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q+q_1)\pi}{N} \sin \frac{q_1\pi}{N} \\ + \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \sum_{p_1, q_1} \langle X_{p+p_1}^0(t'_1) X_{p_1}^0(t'_1) X_{q_1-q}^0(t'_2) X_{q_1}^0(t'_2) \rangle e^{-k_p(t_1-t'_1)} e^{-k_q(t_2-t'_2)} \\ \sin \frac{(p+p_1)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q_1-q)\pi}{N} \sin \frac{q_1\pi}{N} \\ + \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \sum_{p_1, q_1} \langle X_{p_1-p}^0(t'_1) X_{p_1}^0(t'_1) X_{q+q_1}^0(t'_2) X_{q_1}^0(t'_2) \rangle e^{-k_p(t_1-t'_1)} e^{-k_q(t_2-t'_2)} \\ \sin \frac{(p_1-p)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q+q_1)\pi}{N} \sin \frac{q_1\pi}{N} \\ + \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \sum_{p_1, q_1} \langle X_{p_1-p}^0(t'_1) X_{p_1}^0(t'_1) X_{q_1-q}^0(t'_2) X_{q_1}^0(t'_2) \rangle e^{-k_p(t_1-t'_1)} e^{-k_q(t_2-t'_2)} \\ \left. \sin \frac{(p_1-p)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q_1-q)\pi}{N} \sin \frac{q_1\pi}{N} \right] \quad (5.55)$$

First term of the correlation can be expanded as

$$\begin{aligned}
& \langle X_{p+p_1}^0(t'_1) X_{p_1}^0(t'_1) X_{q+q_1}^0(t'_2) X_{q_1}^0(t'_2) \rangle \sin \frac{(p+p_1)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q+q_1)\pi}{N} \sin \frac{q_1\pi}{N} \\
&= \left[\langle X_{p+p_1}^0(t'_1) X_{p_1}^0(t'_1) \rangle \langle X_{q+q_1}^0(t'_2) X_{q_1}^0(t'_2) \rangle + \langle X_{p+p_1}^0(t'_1) X_{q+q_1}^0(t'_2) \rangle \langle X_{p_1}^0(t'_1) X_{q_1}^0(t'_2) \rangle \right. \\
&+ \left. \langle X_{p+p_1}^0(t'_1) X_{q_1}^0(t'_2) \rangle \langle X_{p_1}^0(t'_1) X_{q+q_1}^0(t'_2) \rangle \right] \sin \frac{(p+p_1)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q+q_1)\pi}{N} \sin \frac{q_1\pi}{N} \\
&= \frac{D^2}{4L^2} \left[\sum_{p_1, q_1} \delta_{p+p_1, p_1} \frac{1 - e^{-k_{p+p_1} t'_1} e^{-k_{p_1} t'_1}}{k_{p+p_1} + k_{p_1}} \delta_{q+q_1, q_1} \frac{1 - e^{-k_{q+q_1} t'_2} e^{-k_{q_1} t'_2}}{k_{q+q_1} + k_{q_1}} \right. \\
&+ \sum_{p_1, q_1} \delta_{p+p_1, q+q_1} \frac{e^{-k_{p+p_1} |t'_1 - t'_2|} - e^{-k_{q+q_1} t'_2} e^{-k_{p+p_1} t'_1}}{k_{p+p_1} + k_{q+q_1}} \delta_{p_1, q_1} \frac{e^{-k_{p_1} |t'_1 - t'_2|} - e^{-k_{q_1} t'_2} e^{-k_{p_1} t'_1}}{k_{p_1} + k_{q_1}} \\
&+ \left. \sum_{p_1, q_1} \delta_{p+p_1, q_1} \frac{e^{-k_{p+p_1} |t'_1 - t'_2|} - e^{-k_{q_1} t'_2} e^{-k_{p+p_1} t'_1}}{k_{p+p_1} + k_{q_1}} \delta_{p_1, q+q_1} \frac{e^{-k_{p_1} |t'_1 - t'_2|} - e^{-k_{q+q_1} t'_2} e^{-k_{p_1} t'_1}}{k_{p_1} + k_{q+q_1}} \right] \\
&= \frac{D^2}{4L^2} \left[\sum_{p_1, q_1} \delta_{p,0} \delta_{q,0} \frac{1 - e^{-k_{p_1} t'_1} e^{-k_{p+p_1} t'_1}}{k_{p_1} + k_{p+p_1}} \frac{1 - e^{-k_{q_1} t'_2} e^{-k_{q+q_1} t'_2}}{k_{q_1} + k_{q+q_1}} \sin \frac{p_1\pi}{N} \sin \frac{(p+p_1)\pi}{N} \right. \\
&\sin \frac{q_1\pi}{N} \sin \frac{(q+q_1)\pi}{N} + \sum_{p_1} \delta_{p,q} \frac{e^{-k_{p+p_1} |t'_1 - t'_2|} - e^{-k_{p+p_1} t'_1} e^{-k_{q+p_1} t'_2}}{k_{p+p_1} + k_{q+p_1}} \frac{e^{-k_{p_1} |t'_1 - t'_2|} - e^{-k_{p_1} (t'_1 + t'_2)}}{2k_{p_1}} \\
&\sin \frac{(p+p_1)\pi}{N} \sin \frac{(q+p_1)\pi}{N} \sin^2 \frac{p_1\pi}{N} + \sum_{p_1} \delta_{p,-q} \frac{e^{-k_{p+p_1} |t'_1 - t'_2|} - e^{-k_{p+p_1} (t'_1 + t'_2)}}{2k_{p+p_1}} \\
&\left. \frac{e^{-k_{p_1} |t'_1 - t'_2|} - e^{-k_{p_1} t'_1} e^{-k_{p+q+p_1} t'_2}}{k_{p_1} + k_{p+q+p_1}} \sin^2 \frac{(p+p_1)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(p+q+p_1)\pi}{N} \right] \tag{5.56}
\end{aligned}$$

Before we carefully examine Eq. (5.56) term by term, we note that in the two-time correlation function in Eq. (5.46), the term in the order of λ^2 has a double sum over the Fourier modes denoted by p and q . Consequently, in the first term in Eq. (5.56), this double sum picks up the modes $p = 0$ and $q = 0$ and therefore, even for the choice of the lowest value of $p_1 = 1$, the first term corresponds to largest time scale $\tau_1^{-1} = v\pi^2/L^2$. In contrast, when we look at the second and the third term, the first term in the sum corresponds to $p = 1, p_1 = 1$ with $p + p_1 = 2$. Therefore, the lowest relaxation time scale that appears in these terms correspond to $\tau_4^{-1} = 4v\pi^2/L^2$. Consequently, in our final expression we ignore the two terms.

Looking at the three other terms in Eq. (5.55), the four-point correlation function

can be similarly decomposed as product of two-point correlation functions.

$$\begin{aligned}
& \sum_{p_1, q_1} \langle X_{p+p_1}^0(t'_1) X_{p_1}^0(t'_1) X_{q_1-q}^0(t'_2) X_{q_1}^0(t'_2) \rangle \sin \frac{(p+p_1)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q_1-q)\pi}{N} \sin \frac{q_1\pi}{N} \\
&= \sum_{p_1, q_1} [\langle X_{p+p_1}^0(t'_1) X_{p_1}^0(t'_1) \rangle \langle X_{q_1-q}^0(t'_2) X_{q_1}^0(t'_2) \rangle + \langle X_{p+p_1}^0(t'_1) X_{q_1-q}^0(t'_2) \rangle \langle X_{p_1}^0(t'_1) X_{q_1}^0(t'_2) \rangle] \quad (5.57) \\
&+ \langle X_{p+p_1}^0(t'_1) X_{q_1}^0(t'_2) \rangle \langle X_{p_1}^0(t'_1) X_{q_1-q}^0(t'_2) \rangle \sin \frac{(p+p_1)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q_1-q)\pi}{N} \sin \frac{q_1\pi}{N}
\end{aligned}$$

$$\begin{aligned}
& \sum_{p_1, q_1} \langle X_{p_1-p}^0(t'_1) X_{p_1}^0(t'_1) X_{q+q_1}^0(t'_2) X_{q_1}^0(t'_2) \rangle \sin \frac{(p_1-p)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q+q_1)\pi}{N} \sin \frac{q_1\pi}{N} \\
&= \sum_{p_1, q_1} [\langle X_{p_1-p}^0(t'_1) X_{p_1}^0(t'_1) \rangle \langle X_{q+q_1}^0(t'_2) X_{q_1}^0(t'_2) \rangle + \langle X_{p_1-p}^0(t'_1) X_{q+q_1}^0(t'_2) \rangle \langle X_{p_1}^0(t'_1) X_{q_1}^0(t'_2) \rangle] \quad (5.58) \\
&+ \langle X_{p_1-p}^0(t'_1) X_{q_1}^0(t'_2) \rangle \langle X_{p_1}^0(t'_1) X_{q+q_1}^0(t'_2) \rangle \sin \frac{(p_1-p)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q+q_1)\pi}{N} \sin \frac{q_1\pi}{N}
\end{aligned}$$

$$\begin{aligned}
& \sum_{p_1, q_1} \langle X_{p_1-p}^0(t'_1) X_{p_1}^0(t'_1) X_{q_1-q}^0(t'_2) X_{q_1}^0(t'_2) \rangle \sin \frac{(p_1-p)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q_1-q)\pi}{N} \sin \frac{q_1\pi}{N} \\
&= \sum_{p_1, q_1} [\langle X_{p_1-p}^0(t'_1) X_{p_1}^0(t'_1) \rangle \langle X_{q_1-q}^0(t'_2) X_{q_1}^0(t'_2) \rangle + \langle X_{p_1-p}^0(t'_1) X_{q_1-q}^0(t'_2) \rangle \langle X_{p_1}^0(t'_1) X_{q_1}^0(t'_2) \rangle] \quad (5.59) \\
&+ \langle X_{p_1-p}^0(t'_1) X_{q_1}^0(t'_2) \rangle \langle X_{p_1}^0(t'_1) X_{q_1-q}^0(t'_2) \rangle \sin \frac{(p_1-p)\pi}{N} \sin \frac{p_1\pi}{N} \sin \frac{(q_1-q)\pi}{N} \sin \frac{q_1\pi}{N}
\end{aligned}$$

The first terms in the all the three expression will have $\delta_{p,0}\delta_{q,0}$ and therefore we retain these terms in the final expression of $\langle X_p^1(t_1) X_q^1(t_2) \rangle$.

$$\begin{aligned}
\langle X_p^1(t_1) X_q^1(t_2) \rangle &= \frac{4D^2}{64L^2a^4} \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 e^{-k_p(t_1-t'_1)} e^{-k_q(t_2-t'_2)} \sum_{p_1, q_1} \frac{1 - e^{-2k_{p_1}t'_1}}{2k_{p_1}} \frac{1 - e^{-2k_{q_1}t'_2}}{2k_{q_1}} \\
&\quad \delta_{p,0}\delta_{q,0} \sin^2 \frac{p_1\pi}{N} \sin^2 \frac{q_1\pi}{N} \quad (5.60)
\end{aligned}$$

To break the summation, putting $p_1 = 1, q_1 = 1$, we get $\sin \frac{p_1\pi}{N} \sim \frac{p_1\pi}{N}$, for $N \rightarrow \infty$, simplify

delta functions as $p = 0, q = 0$ So Eq.(5.60) becomes

$$\begin{aligned}\langle X_p^1(t_1)X_q^1(t_2)\rangle &= \frac{D^2}{64L^2a^4} \int_0^{t_1} dt'_1 \int_0^{t_2} dt'_2 \left(\frac{L^2}{2v\pi^2}\right)^2 (1 - e^{-\frac{2v\pi^2 t'_1}{L^2}})(1 - e^{-\frac{2v\pi^2 t'_2}{L^2}}) \left(\frac{\pi^2 a^2}{L^2}\right)^2 \\ &= \frac{D^2}{64v^2L^2} \left[t_1 - \frac{L^2}{2v\pi^2}(1 - e^{-\frac{2v\pi^2 t_1}{L^2}})\right] \left[t_2 - \frac{L^2}{2v\pi^2}(1 - e^{-\frac{2v\pi^2 t_2}{L^2}})\right]\end{aligned}\quad (5.61)$$

5.3.4 Two-time correlation $\langle h_0(t_1)h_0(t_2)\rangle$

We have taken the initial condition $X_p^1(0) = 0$.

Using the general solution in Eq. (5.54) the detailed calculations of two-time correlation function in the order λ^2 has been presented in the Section(5.3.3). Combining Eqs.(5.23), (5.46) and (5.61), we get

$$\begin{aligned}\langle h_0(t_1)h_0(t_2)\rangle &= \frac{D}{L}t_2 + \frac{D}{L} \frac{L^2}{v\pi^2} \left[e^{-\frac{v\pi^2}{L^2}(t_1-t_2)} - e^{-\frac{v\pi^2}{L^2}(t_1+t_2)} \right] \\ &+ \frac{D^2}{L^2} \frac{\lambda^2}{16v^2} \left[t_1 - \frac{L^2}{2v\pi^2}(1 - e^{-\frac{2v\pi^2 t_1}{L^2}}) \right] \left[t_2 - \frac{L^2}{2v\pi^2}(1 - e^{-\frac{2v\pi^2 t_2}{L^2}}) \right]\end{aligned}\quad (5.62)$$

5.3.5 For finite t but $L \rightarrow 0$

In the finite t domain if $L \rightarrow 0$ the term related to L^2 can be neglected. Putting this condition in Eq.(5.62),

$$\begin{aligned}\langle h_0(t_1)h_0(t_2)\rangle_{L \rightarrow 0} &= \frac{D}{L}t_2 + \frac{D^2}{L^2} \frac{\lambda^2}{16v^2} t_1 t_2 \\ &= \frac{D}{L}t_2 \left[1 + \frac{D}{L} \frac{\lambda^2}{16v^2} t_1 \right]\end{aligned}\quad (5.63)$$

Let us take spatial transformation as $H(t) = \frac{h_0(t)}{\sqrt{\langle h_0^2(t)\rangle}}$ and we get

$$\begin{aligned}\langle H(t_1)H(t_2)\rangle &= \frac{\langle h_0(t_1)h_0(t_2)\rangle}{\sqrt{\langle h_0^2(t_1)\rangle \langle h_0^2(t_2)\rangle}} \\ &= \sqrt{\frac{\frac{D}{L}t_2}{\frac{D}{L}t_1}} \sqrt{\frac{1 + \frac{D}{L} \frac{\lambda^2}{16v^2} t_1}{1 + \frac{D}{L} \frac{\lambda^2}{16v^2} t_2}}\end{aligned}\quad (5.64)$$

Now time transformation may be taken as $e^T = \frac{t}{1 + \frac{D}{L} \frac{\lambda^2 t}{16v^2}}$.

After the time transformation we get, $\langle H(T_1)H(T_2) \rangle = e^{-(T_1-T_2)/2}$ Following Slepian¹¹, if the correlation function of a stochastic variable decays exponentially for all times $C(T) = e^{-\lambda T}$, then the persistence probability is given by

$$P(T) = \frac{2}{\pi} \sin^{-1}(e^{-\lambda T}) \quad (5.65)$$

Asymptotically, $P(T)$ takes the form $P(T) \sim e^{-\lambda T}$. Consequently, in real time the persistence probability is found as

$$p(t)_{L \rightarrow 0} \sim \sqrt{\frac{1}{\frac{D}{L}t} + \frac{\lambda^2}{16v^2}} \quad (5.66)$$

It is quite interesting that the expression of $p(t)$ in the asymptotic limit of $t \rightarrow \infty$ goes to a constant value of $\lambda^2/16v^2$. In principle, one can use this result to extract the ratio of λ/v , with the advantage being that the system size required to extract the information need not be very large.

5.4 Conclusion

We conclude that the results of the persistence in surface growth in finite lattice provide us with a valuable set of tools for investigating the dynamics of a non-equilibrium system. We have taken a lattice in finite domain size extending from $-L$ to $+L$. We have calculated the analytical expression of persistence for Edward-Wilkinson surface growth for the conditions $L \rightarrow 0$, $L \rightarrow \infty$ and for the finite value of L . Again we have calculated the persistence expression analytically for the KPZ surface growth process when $L \rightarrow 0$ and L is finite but large. In conclusion, we have investigated the persistence probability in the models of surface growth analytically strictly restricted by a finite domain.

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6

Summary and Outlook

We present a brief summary of the work done in this thesis. The summary of the work done and the significance of the work have been summarised briefly for a quick overview.

In this thesis, we have studied the phenomenon of persistence in a class of non-equilibrium systems. Persistence plays a very important role in describing a stochastic process in nature, specifically providing the non-stationary dynamics of the system. The phenomenon of persistence is typically quantified through the persistence probability $p(t)$ – the probability that a stochastic variable has not changed its sign up-to time t . For a wide range of non-equilibrium systems, this probability has been shown to decay as a power law with an exponent θ that depends on the non-trivial memory-dependent dynamics of such out-of-equilibrium systems.

In the course of this thesis, we have presented explicit results for the persistence probability of an anisotropic particle in two spatial dimensions, in presence, as well as in absence of a confining harmonic potential. The two-time correlation functions of the position of the particle have been calculated in both cases. In the case of a harmonically confined particle, a perturbative solution has been provided for the correlation functions. The persistence probability is computed from the two-time correlation function using suitable transformations in space and time. Further, we have demonstrated using numerical simulations, that the persistence probability can be an extremely useful tool in measuring the translational and the rotational diffusion coefficients of an asymmetric particle. The advantage of this method is that it does not require the measurement of the orientational degrees of freedom. As a corollary, our method also demonstrated that it can detect the shape asymmetry of the particle when the two translational diffusivities differed by 5%.

Additionally, the work on anisotropic Brownian particle has been extended for the case of an active anisotropic particle. From the analytic expression, it is clear that the propulsion velocity not only renormalizes the long-time diffusion coefficient, but also renormalizes the anisotropic part of the diffusion tensor. The analytic expression has been compared with numerical simulations and is in excellent agreement when the propulsion velocity is small. When compared to that of a passive anisotropic particle, we observed that the persistence probability can not detect propulsion velocities which are small even for those cases where the translational diffusivities differed by 5%. $p(t)$ however could distinguish between an active and a passive particle when the propulsion velocity was large. As before, we also provide an expression for $p(t)$, validated by numerical simulations, when such an active anisotropic particle is confined in an isotropic harmonic trap, a situation extremely relevant in experimental scenarios.

In our final work, we deviate from the single particle dynamics to that of coarse-grained models of surface growth in one dimension that are bounded by a finite domain. We took two models- one is the linear Edward-Wilkinson(EW) Model and building on

the results from the EW model, we studied the non-linear Kardar-Parisi-Zhang(KPZ) model. The phenomenon of persistence in the continuum version of these two models has been well studied and the persistence exponents are also known. But the expression for the persistence probability in spatially discrete surface growth models with finite size effect is not known. In an infinite spatially extended system, the boundary conditions do not play any significant role. The expression change when the system size is finite.

My future aim is to work on to study the entropy and work production in active systems. The most interesting part is the effect of active bath in the efficiency. We aim to model efficient engines, those have better application in energy harvesting techniques. Another interesting phenomena which I will work on stochastic resetting problems and fluctuations and entropy production associated with restart process.

Theoretical and experimental attempts have been made to understand the laws of thermodynamics and non-equilibrium fluctuation relations for active matter. Particularly, the dissipation of energy in active systems can be a useful tool to measure the violation of fluctuation dissipation theorem (FDT). We consider to investigate interesting problems related to the passive particle in an active bath. The entropy generation of such systems is an interesting study. Moreover the other interesting set of problems are investigating heat engines in active heat reservoirs. And entropy production due to stochastic resetting. More specifically saying, we will study entropy production, super diffusion properties of Brownian, colloidal particle, flexible and semi-flexible polymers in active bath. The effect of confinement in different potential like harmonic and time dependent potential and its effect on entropy production. Additionally we will study the shape effect of the particle in entropy production, specifically if the particle is asymmetric.

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List of Publications

The thesis is based on the following works:

1. Ghosh Anirban, and Dipanjan Chakraborty. "Persistence in Brownian motion of an ellipsoidal particle in two dimensions." *The Journal of Chemical Physics*, **152**, 174901 (2020) (Chapter-2, 3)
2. Ghosh Anirban, Mandal Sudipta, Chakraborty D., "Persistence of an asymmetric active Brownian particle in two dimensions", *The Journal of Chemical Physics*, **157**, 194905 (2022)(Chapter-4).
3. Ghosh Anirban, Chakraborty D., "Persistence of surface growth with finite size effect in Kardar- Parisi- Zhang interface", (*submitted*) Chapter- 5

The work which is not part of this thesis

1. Mandal Sudipta, Ghosh Anirban, Chakraborty D., "Directional transport dynamics of overdamped active ellipsoidal particle in two dimensions", (*Manuscript under preparation*)