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# ENTROPY-DRIVEN INSIGHTS INTO NON-EQUILIBRIUM SYSTEMS AND DAMPED STOCHASTIC PROCESSES

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## ABSTRACT
*In this paper a study on Brownian motion been made and further extended to the Ornstein-Uhlenbeck Process. For the Ornstein-Uhlenbeck Process we reviewed the Langevin equations and then the non-equilibrium Fokker-Planck equations. The Langevin equation is then used for a one-dimensional model. Following this we define the generated entropy and the produced entropy of the Ornstein-Uhlenbeck Process and thus we have calculated the entropy. In conclusion, we have performed a sample calculation of the entropy trend for the Ornstein-Uhlenbeck.*

## INTRODUCTION
In this section we will describe Brownian motion and Ornstein-Uhlenbeck Stochastic Process separately.

### 1.1 BROWNIAN MOTION
Brownian motion is a understood to be an extremely important phenomenon which can describe systems in nature with a high degree of accuracy [41]. A trivial example of Brownian motion is particles suspended in a liquid in thermal equilibrium and free to move around. Such particles or systems appear to be random and not correlated when observed under a magnifying device. There are many ways of expressing the Brownian motion dynamics. One such way is to express it in terms of Langevin equations [42, 43]. Studies of Brownian motion have been applied to a variety of fields in physics and interdisciplinary fields as well. Fields such as mathematics, statistics, and chemistry are some of the fields where the Brownian motion has answered lots of questions. Apart from the studies of Brownian motion, there have been numerous studies of Brownian motion subjected to electric fields, magnetic fields, charged particles, colloidal mixtures and many more [44].

Brownian motion has also been studied in equilibrium and non-equilibrium systems [45]. It is widely known that a system under equilibrium is well understood in terms of its thermodynamic properties. Systems under non-equilibrium are still far from being understood and they reveal more details and as we keep studying them. Brownian motion has also been widely used to understand various physical and chemical properties of the medium [46]. This also includes the particles which are suspended in the medium, the interaction of the particles among themselves, the medium interactions with the particles and ways in which the particle dynamics affects the dynamics of the medium. These are some questions which have been widely studied and there is a fair consensus. There has been an increase interest in the theoretical approaches to understand Brownian motion and the experimental approaches to understand Brownian motion. Some studies based on theoretical research involves focusing on some aspects such as,

- Studying the individual particle dynamics in the medium
- Understanding the interactions between 2 or more particles in the medium
- Applying many body physics approach to investigate the overall structure of the Brownian motion
- Studying the concepts of self-similarity in particles [47]
- Understanding if there is a criticality in the dynamics [48]
- Applying the chaos theory principles to explain particle dynamics.
- An interaction between particles and the medium bio-molecules as Brownian particles [49]

There have also been numerous studies involving experimental Brownian motion. Some of these give us an insight into how the Brownian motion can be applied in applications. Needless to mention some such studies-

- Studying light scattering using Brownian motion dynamics [50]
- Explaining optical properties of Brownian motion [51]
- Temperature dependence on the dynamics of the particles and/or the medium [52]
- Study the hydrodynamics of resonances [53]
- Explaining and applying granular motion involving friction to other similar systems [54]

The studies mentioned above are some of the widely researched areas related to Brownian motion and their connection with other fields and systems.

### 1.2 MEAN-REVERTING STOCHASTIC PROCESS

The Mean-Reverting stochastic or Ornstein-Uhlenbeck Process is a stochastic process which is widely used in physical sciences. The original Ornstein-Uhlenbeck Process was studying the Brownian motion under friction and resistance and explaining how the dynamics of the Brownian motion differs between systems having no friction from a system having friction. Ornstein-Uhlenbeck Process is also used widely in evolutionary biology [55]. The Ornstein-Uhlenbeck Process is a Gaussian process which is described by all the paths being continuous. It is also a Markov process and is stationary with the condition that the initial state has a stationary distribution. The Ornstein-Uhlenbeck Process has also been studied in a large spectrum of ways. Some of these studies are theoretical and computational and some are experimental. Some of the theoretical aspects in which Ornstein-Uhlenbeck Process is studied are,

- Understanding perturbation theory of an Ornstein-Uhlenbeck Process [57]
- Applying Ornstein-Uhlenbeck Process in finance studies [58]
- Studying likelihood theories in mathematics and statistics based on Ornstein-Uhlenbeck Process [28]

Similarly, there are multiple experimental studies and applications. Some of these studies are,

- Designing optimal conditions for processes which follow Ornstein-Uhlenbeck dynamics [58]
- Using Ornstein–Uhlenbeck process to analyze single-cell expression [59]

These are some applications of Ornstein-Uhlenbeck Process in theoretical or experimental studies.

In the following sections the authors have studied the Ornstein-Uhlenbeck Process for a damping and expressed the Langevin equations for the process. Finally we have calculated the Fokker-Planck equations and the entropy for the system under consideration.

## 2 GENERALIZED FOKKER-PLANCK DYNAMICS

Let us start by taking a set of n particles which are interacting with each other. The interacting particles are evolving with time and can be described by the Langevin equations given by [12, 13, 34, 35] $\frac{dx_i}{dt} = f_i(x) + r_i(t)$

(2.1)

where $f_i(\boldsymbol{x})$ and $x_i$ is the force acting and the coordinate respectively on the i$^{th}$ particle, $\mathbf{x} = \{x_i\}$, $r_i$ , stochastic variable, is the noise defined mathematically such that

$$< r_i(t) >= 0 \qquad (2.2)$$

$$< r_i(t) r_j(t') = 2\, D_i \delta_{ij} \delta(t - t') \qquad (2.3)$$

$P$ ($\mathbf{x}$, $t$) is the probability distribution evolves with time described by associated Fokker-Planck equations [14, 34, 35]. Also, $D_i \geq 0$, constants different for each particle. Probability distribution is

$$\frac{\partial P(x,t)}{\partial t} = -\sum \frac{\partial}{\partial x_i}[f_i(\boldsymbol{x})P(x,t)] + \sum D_i \frac{\partial^2}{\partial x^2} P(\boldsymbol{x},t) \qquad (2.4)$$

Generally the Fokker-Planck equation is as a continuity equation, expressed as, $\frac{\partial P(x,t)}{\partial t} = -\sum \frac{\partial}{\partial x_i} J_i(x,t)$ (2.5)

$$J_i(x,t) = \left[f_i(\boldsymbol{x}) - D_i \frac{\partial}{\partial x_i}\right] P(\boldsymbol{x},t) \qquad (2.6)$$

where $J_i$ is the $i^{th}$ component of the probability current. The condition of irreversibility of the system can be expressed as $D_i \neq D_j\ ,i \neq j$ or $D_i = D_j = D\ ,i \neq j$

but $\frac{\partial f_j}{\partial x_j} \neq \frac{\partial f_i}{\partial x_j}$ (2.7)

We need to solve Fokker-Planck equation for a region of space spanned by the set of variables $x_i$ and subject to initial boundary conditions. For thermodynamics equilibrium, Fokker-Planck and associated Langevin equation describe a system given by $\frac{\partial f_j}{\partial x_j} = \frac{\partial f_i}{\partial x_j}$

and $D_i = D_j$ (2.8)

## 3 LANGEVIN EQUATION FOR A 1-D BROWNIAN MOTION

For a free particle in a fluid, one-dimensional Brownian motion is $\frac{dx(t)}{dt} = v(t)$ (3.1)

and $m\frac{dv(t)}{dt} + \gamma v(t) = \eta(t)$ (3.2)

where $m$ is mass and $\gamma$ is the dissipation. $\eta(t)$ is the random force due to the fluctuation in the density of the surrounding medium.

The Gaussian white noise with zero mean and covariance in the Langevin equation is given as, $< \eta(t)\eta(s) >= \delta(t-s)$ (3.3)

For the Ornstein-Uhlenbeck velocity v($t$), eqn. (3.2) is generally known as the Langevin equation.

If the Brownian motion is undergoing the properties of a damped harmonic oscillator driven by white noise, then we can write it as,

$$m\frac{d^2x(t)}{dt^2} + \gamma\frac{dx(t)}{dt} + \omega^2 x(t) = \eta(t) \qquad (3.4)$$

where $\omega$ is the intrinsic frequency of the oscillator. The damping force is given by $-\gamma v(t)$ and is viscous in nature. The term $\omega^2 x(t)$ represents the frequency motion of the oscillator. In the absence of the damping term, which is the second term on the R.H.S. in eqn. (3.4), the oscillator becomes a regular oscillator with noise. The inertial term in eqn. (3.4) is given by $m\frac{d^2x(t)}{dt^2}$. If the damping force is dominating the inertial term then the first term in eqn. (3.4) can be neglected. So under this approximation eqn. (3.4) takes the form,

$$\frac{dx(t)}{dt} = -\alpha x(t) + \kappa(t) \qquad (3.5)$$

Where $\alpha = \frac{\omega^2}{m\gamma}$ and $\kappa(t) = \frac{\eta(t)}{m\gamma}$ . Eqn. (3.5) is very similar to the Langevin equation and can be considered as the Langevin equation for a harmonic potential of $V(x) = \frac{\alpha x^2}{2}$ (3.6)

This harmonic potential can be understood as a diffusion process.

The solution of eqn.(3.5) is widely known as the Ornstein-Uhlenbeck process and interpreted to be associated with the quantum harmonic oscillator under various properties. As the system changes its dynamics, the solution of eqn.(3.5) also changes, giving various solutions for the Ornstein-Uhlenbeck process. The Ornstein-Uhlenbeck process for a stationary case is also known as oscillator process [36, 37].

So we can write eqn.(3.4), which is a stochastic equation for a damped oscillator as;

$$m(t)\frac{d^2x(t)}{dt^2}+\gamma(t)\frac{dx(t)}{dt}+\omega^2(t)\,x(t)=\eta(t) \qquad (3.7)$$

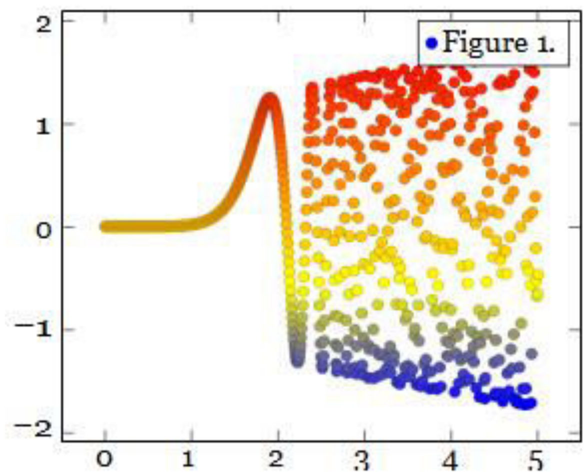
where $m(t)$, $\gamma(t)$, $\omega^2(t)$ are functions of time.

There are many cases for the above variables which have been studied by many authors [28, 39, 40]. This also, opens up a possibility that damping coefficient, frequency and the mass can behave as functions which fluctuate with time. In this article we will focus on the study Ornstein-Uhlenbeck process with random type of damping as shown in eqn. (3.5).

## 3.1 EXAMPLE OF LANGEVIN EQUATION BASED ON RANDOM POTENTIAL FUNCTION

In this section we will consider a function which is oscillatory initially but gets damped oscillatory and exhibits a random Brownian motion type dynamics. This is shown in Figure 1.

**Random Brownian motion type plot**




Considering an example, we take a sample function given by, $f(x)=\alpha x e^{\beta x^2}$ (3.8)

where $\alpha$ & $\beta$ are the coefficients.

Taking derivatives of $f(x)$ we get $\frac{df(x)}{dx}=\alpha e^{\beta x^2}+2\alpha\beta x^2 e^{\beta x^2}$ (3.9)

We will use this example to calculate entropy in the next sections.

## 4 FOKKER-PLANCK FORMALISM FOR ENTROPY PRODUCTION

The entropy production of an active operating system usually defined in terms of the Fokker-Planck equations. The rate of change of the entropy $S$ of a particular system expressed as [15] $\frac{dS}{dt}=\zeta-\Omega$ (4.1)

where Ω is the entropy flux can be thought of as flow from the system to the surroundings and $\zeta$ is entropy production output of active operating system because of the irreversible processes. Entropy is well defined quantity for the system in equilibrium and for the system in non-equilibrium state, entropy along with entropy production is not well defined. So here we tried a methodology to calculate entropy production for non-equilibrium systems. For ant time $t$, The Gibbs entropy of a is given by [14, 16–18, 26]

$$S(t)=-\int P(\boldsymbol{x},t)\,\ln[P(\boldsymbol{x},t)]\,d\boldsymbol{x} \qquad (4.2)$$

where $d\mathbf{x}=dx_1dx_2......dx_n$.

with the help of eqn. (2.5), the derivative of the entropy is $\frac{d}{dt}S(t)=-\int[\ln P(\boldsymbol{x},t)+1]\sum\frac{\partial}{\partial x_i}J_i(\boldsymbol{x},t)\,d\boldsymbol{x}$ (4.3)

$$= -\int \sum J_i(\boldsymbol{x},t) \frac{\partial}{\partial x_i} \ln P(\boldsymbol{x},t)\, d\boldsymbol{x} \quad (4.4)$$

Using eqn. (2.6) $\frac{d}{dt} S(t) = -\int \sum \frac{1}{D_i} J_i(\boldsymbol{x},t) f_i(x)\, d\boldsymbol{x} + \int \sum \frac{[J_i(x,t)]^2}{D_i P(x,t)} d\boldsymbol{x}$ (4.5)

Comparing this with eqn. (3.1) we find $\Omega = \int \sum \frac{1}{D_i} J_i(\boldsymbol{x},t) f_i(x)\, d\boldsymbol{x}$ (4.6)

and $\zeta = \int \sum \frac{[J_i(x,t)]^2}{D_i P(x,t)} d\boldsymbol{x}$ (4.7)

Thus using eqn. (2.6), we can express (3.6) as $\Omega = \int \sum \left\{ \frac{1}{D_i} [f_i(x)]^2 + f_{ii}(x) \right\} P(\boldsymbol{x},t)\, d\boldsymbol{x}$ (4.8)

Where $f_{ii}(x) = \frac{\partial f_i(x)}{\partial x_i}$. Average over the probability distribution is $\Omega = < \sum \{ \frac{1}{D_i} [f_i(x)]^2 + f_{ii}(x) \} >$ (4.9)

There is multiple studies shows the total entropy production of a non-equilibrium process stating the total entropy production (*EP*), $\dot{S}_{tot}$ constituted by two parts adiabatic $\dot{S}_A$ and nonadiabatic $\dot{S}_{NA}$ contributions. These entropies individually for any system cannot be less than zero.

## 5 FOKKER-PLANCK EQUATIONS FOR ENTROPY GENERATION

We can think of Gibbs' formalism as a generalized form in a statistical inference theory for non-equilibrium systems, which deals with statistical and probabilistic physics of systems under equilibrium state [23]. Jayens et al used maximum entropy as the foundation to developed non-equilibrium statistical physics for the stationary state constraint. The approach involved maximizing the path. Thus the Shannon information entropy Is $S = -\sum_\gamma p_\gamma \ln p_\gamma$ (5.1)

with respect to $p_\gamma$ of the path $\gamma$ [22, 23, 38]. Under this approach, the entropy generation of open systems is associated with their information entropy through [19–21] $S_g = \kappa_B S = -\kappa_B \int p_\gamma(\boldsymbol{x},t) \ln[p_\gamma(\boldsymbol{x},t)] d\boldsymbol{x}$ (5.2)

with $p_\gamma = P_\gamma(\mathbf{x}, t)$. This can also be explained as the inability to predict the course that an ensemble system will take to transition from one state to another. The Guoy-Stodola theorem [22] gives $\overline{W} = T_0 S_g$ (5.3)

Where $\overline{W}$ is energy lost due to irreversibility within a system internally. Thus due to the irreversibility, the entropy generation can be linked to the power lost *P* as $S_g = \frac{1}{T_0} \int_0^\tau P\, dt$ (5.4)

where $T_0$ the surrounding temperature, considered to remain constant and τ is is the span of a physical process. Hence,

$$P = < \sum f_i(\boldsymbol{x}) \frac{dx_i}{dt} > \quad (5.5)$$

using the eqn. (2.1), we get $P = < \sum f_i(\boldsymbol{x})[f_i(\boldsymbol{x}) + \eta_i(t)] >$ (5.6)

and so $S_g$ can be expressed as $S_g = \frac{\tau}{T_0} < \sum([f_i(\boldsymbol{x})]^2 + D_i f_{ii}(\boldsymbol{x})) >$ (5.7)

where $f_{ii}(\boldsymbol{x}) = \frac{\partial f_i}{\partial x_i}$. Under mean value, we can express $S_g = \frac{\tau}{T_0} \int \sum([f_i(\boldsymbol{x})]^2 + D_i f_{ii}(\boldsymbol{x}))\, p_\gamma(\boldsymbol{x},t) d\boldsymbol{x}$ (5.8)

and hence $S_g = \frac{\tau}{T_0} \int \sum f_i(\boldsymbol{x}) J_i(\boldsymbol{x},t)\, d\boldsymbol{x}$ (5.9)

## 6 A GENERALIZED MODEL FOR ENTROPIC ANALYSIS

As described earlier, the force term can be written, given in eqn. (3.8), as $f(x) = \alpha x e^{\beta x^2}$ (6.1)

where $\alpha$ is defined in section 3. Thus eqn. (4.9) is expressed as $\Omega = < \left\{ \frac{1}{D} \alpha^2 x^2 e^{2\beta x^2} - \alpha(1 + 2\beta x) e^{\beta x^2} \right\} >$ (6.2)

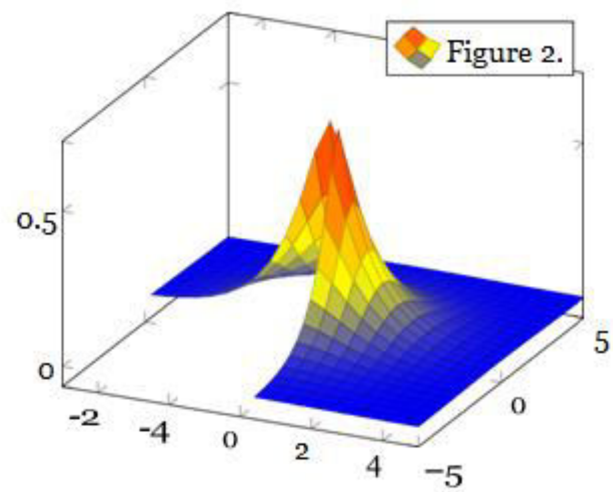
also, eqn. (2.6) can be written as
$$J(r,t) = \left[\alpha x e^{\beta x^2} - D\frac{\partial}{\partial r}\right]P(r,t) \quad (6.3)$$

and we can express eqn. (3.6) as
$$\zeta = \frac{1}{D}\int \frac{\left[\left[\alpha x e^{\beta x^2} - D\frac{\partial}{\partial r}\right]P(r,t)\right]^2}{P(r,t)}\,dr \quad (6.4)$$

And finally we can express eqn. (3.1) as
$$\frac{dS}{dt} = \frac{1}{D}\int \frac{\left[\left[\alpha x e^{\beta x^2} - D\frac{\partial}{\partial r}\right]P(r,t)\right]^2}{P(r,t)}\,dr - <\left\{\alpha^2 x^2 e^{2\beta x^2} - \alpha(1+2\beta x)e^{\beta x^2}\right\}> \quad (6.5)$$

Finally we can express eqn. (4.9), under entropy generation approach, as
$$S_g = \frac{\tau}{T_0}\int\left\{\alpha^2 x^2 e^{2\beta x^2} - \alpha(1+2\beta x)e^{\beta x^2}\right\}P(r,t)dr \quad (6.6)$$

**Trend in Increase in Entropy**




using the above analysis to see the entropic trend, we reached the result shown in the fig.2. Here we see that the entropy increase is very sharp and rapid as the random motion increases. This is very important because in models which are studied, the entropy increase is not as rapid as we have shown in our example shown in section (3.1). This clearly indicates that as the randomness in non-equilibrium system increases, the entropy increases even more sharply.

## 7 CONCLUSION

In this study we have shown the Langevin equations and the Fokker-Planck equations of a random motion and then extended it to Ornstein-Uhlenbeck Stochastic Process with damping. We took a simplified model to explain the entropy understanding and showed that the entropy increase is sharper than expected. The example under consideration in our study is a very simple model which was constructed to see the pattern of the entropy increase. This unexpected result of a sharp entropy increase could be due to the fact that there is a deeper physics dynamics occurring, rather than just a Ornstein-Uhlenbeck Stochastic Process with damping. Our future study is to understand this underlying reason as to why this unexpected sharp increase in entropy is observed.

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