Dynamics of Interacting Colloids

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Certificate of Examination

This is to certify that the dissertation titled "**Dynamics of interacting colloids**" submitted by Mr.Srikanth Subramanian (Reg No.MP12014) for the partial fulfillment MS degree 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 the report to be accepted.

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Dated:12-05-2015

Declaration

This work presented in the dissertation has been carried out by me under the guidance of Dr.Dipanjan Chakraborty at the Indian Institute of Science Education, Mohali.

This work has not been submitted in part or in full for a degree, or diploma or a fellowship to other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgment of collaborative research and discussions. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

Srikanth Subramanian

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

Dr.Dipanjan Chakraborty

(Supervisor)

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Abstract

Presented here are the results of analytical and numerical simulations for colloidal systems driven by ratcheting potential switching on and off stochastically. We observe the variation of the resultant directed current as a function of the ratcheting frequency. In the case of an interacting colloidal system, molecular dynamics [3] has revealed resonance of directed current with ratcheting frequency. The analytical tools necessary, the theoretical paradigm of non-equilibrium statistical mechanics and stochastic processes(relevant parts) are also discussed in detail.

Chapter 1

Introduction

This master thesis studies a system of repulsively interacting colloids under the influence of an external ratchet potential that turns 'on' and 'off' stochastically. Brownian particles under the influence of a flashing asymmetric potential experience a time averaged directed current. The Flashing ratchets have been extensively studied in the context of molecular motors[4], dynamics of colloidal dispersion[5], Ferro Fluids[6] and particle segregation[7]. Recent experiments with interacting paramagnetic 2-dimensional colloid in the presence of a 1-dimensional magnetic flashing ratchet showed variation of the local structure of the particles with change in frequency of ratcheting[8] and an enhancement of diffusion coefficient in the transverse direction[9]. Moreover, Laser trapping in colloids by coupling 2D interacting colloidal particles with 1D time independent, spatially periodic potential is known to give rise to several interesting mechanical properties and phase transitions[10].

The outline of this thesis is the following. In Chapter 1, we will introduce some basic dynamics of Brownian particles and their importance. The theoretical paradigm in which these Brownian particles are studied will also be expanded upon, which are the Langevin and the Fokker-Planck formulations. Furthermore, the mechanism of a ratcheting potential and its influence on the Brownian particle is discussed. We will understand how useful work can be extracted from ratcheting. We also present analytical and numerical results of the transport in ratchet systems in the Fokker-Planck regime in Chapter 2[11]. The analytical results for the net flux are worked in the asymptotic limits of the ratcheting frequency. In Chapter 3 we explore the system of interacting colloidal particles. Here we will employ the machinery developed in the previous chapters to describe the system. We will see that the interesting properties of the flashing ratchet system studied in Chapter 2 is preserved in addition to new emergent properties. The behavior of the space and time averaged directed current with respect to the ratcheting frequency in the asymptotic limits is observed to be identical to the case of a non-interacting ratchet system. But, the interesting dynamics happen in the intermediate frequencies, where the directed current shows resonance with ratcheting frequency and the resonance frequencies shows non-monotonic variation with densities. Dynamical phase transitions from modulated solid to modulated liquid phase and back to solid phase is observed with increase in frequency at suitable densities.

1.1 Brownian Motion and Langevin Equations

Here, we look at the dynamics of a mesoscopic system where the length scales are of the order of a few μm. Brownian motion in general describes some collective property of a system in many cases, not just of a single particle. Consider the motion of an particle in a fluid medium(viscosity η). Even though the motion appears random, it can obviously be described by Newton's equations. The generic equation for a particle under the influence of a damped force is,

$$m\frac{dv}{dt} = -\zeta v \tag{1.1}$$

This cannot explain the dynamics of the Brownian particle since the solution tells you that the velocity after a long time goes to zero. But, we know that the mean square velocity in thermal equilibrium is kT/m(k Boltzmann constant). So, the term that represents the random force should be added. Then eqn(1.1) becomes,

$$m\frac{dv}{dt} = -\zeta v + \Gamma(t) \tag{1.2}$$

where $\Gamma(t)$ represents the fluctuating force. This is called the *Langevin equation*.

1.1.1 Nature of Brownian Particle

In generic cases the fluctuating forces are expected to arise from random impacts of the Brownian particle with the surrounding medium. This force is supposed to vary rapidly over any observation time. The important first and second order moments of this force can be modeled as following,

$$\langle\Gamma(t)\rangle = 0, \langle\Gamma(t)\Gamma(t')\rangle = 2B\delta(t - t') \tag{1.3}$$

The second moment gives us the correlation in time of the "noise" force. A delta function indicates that the noise at one instant is independent of the noise at another. This is called a *Gaussian White noise*. B is the noise strength.

1.1.2 Fluctuation Dissipation Theorem

As we understand, there must exist a relation between the friction experienced by the Brownian particle and the random fluctuations on it. This is called the *Fluctuation Dissipation theorem* that relation friction coefficient to strength of the noise. As seen in section(1.1.1), the Langevin equation for a Brownian particle is,

$$m\frac{dv}{dt} = -\zeta v + \Gamma(t)$$

And moments of noise(Γ) is given eqn(1.3) Now solving the above first order inhomogeneous differential equation for an expression of velocity $v(t)$ we get,

$$v(t) = e^{\zeta t/m}v(0) + \frac{1}{m}\int_0^t dt' e^{-\zeta(t-t')/m}\Gamma(t') \tag{1.4}$$

To find the expression for root mean squared velocity, we square expression(A.1) and take averages,

$$v^2(t) = e^{-2\zeta t/m}v^2(0) + \frac{2}{m}v(0)e^{-\zeta t/m}\int_0^t dt' e^{-\zeta(t-t')/m}\Gamma(t') + \frac{1}{m^2}\int_0^t dt' e^{-\zeta(t-t')/m}\Gamma(t')\int_0^t dt'' e^{-\zeta(t-t'')/m}\Gamma(t'') \tag{1.5}$$

The first two terms go to zero as $t \to \infty$. The only contribution is from the third term. After averaging the noise correlation gives a delta term,

$$\langle v^2(t)\rangle = \frac{1}{m^2}\int_0^t dt' e^{-\zeta(t-t')/m}\int_0^t e^{-\zeta t''/m}2B\delta(t'-t'') \tag{1.6}$$

The delta function handles one time integration, the other is done normally.

$$\langle v^2(t)\rangle = \frac{2B}{m^2}\int_0^t dt' e^{-2\zeta(t-t')/m} \tag{1.7}$$

$$\langle v^2(t)\rangle = e^{-2\zeta t/m}v^2(0) + \frac{B}{\zeta m}(1 - e^{2\zeta t/m}) \tag{1.8}$$

Again as $t \to \infty$ we get,

$$\langle v^2(t)\rangle = \frac{B}{\zeta m} \tag{1.9}$$

But in thermal equilibrium value mean squared velocity must approach kT/m. So comparing with eqn(1.9) we get,

$$B = \zeta kT \tag{1.10}$$

This gives us the relation between the strength of the noise force and the coefficient of friction.

1.2 Fokker-Planck Equations

Fokker-Planck equations are a form of Liouville equation used in studying dynamical systems, with a noise term. Currently, there are no impositions on the noise term, apart from the requirement to be Markovian. Markovian noise is memory less,i.e the present value of the noise depends only on the previous instant and nothing else.

Assuming all constants are scaled let's write the eqn(1.2) in its primitive form(without constants):

$$\frac{d\mathbf{x}}{dt} = F(\mathbf{x}) + \Gamma(t) \tag{1.11}$$

$\mathbf{x}$ represents all independent phase variables, i.e $\mathbf{x} = [x_1, x_2, ...]$.

We can look for the probability distribution $p(\mathbf{x}, t)$ of the values of $\mathbf{x}$ at time t. We want the average of this probability distribution over the noise. This can be achieved by recognizing that $p(\mathbf{x}, t)$ is a conserved quantity

$$\int dx p(\mathbf{x}, t) = 1 \tag{1.12}$$

for all t. Like all conserved quantities in phase space we can expect a 'divergence of a flux' term balancing the time derivative of this quantity. The conservation law is

$$\frac{\partial p(\mathbf{x},t)}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \left(\frac{\partial \mathbf{x}}{\partial t} p(\mathbf{x},t) \right) = 0 \tag{1.13}$$

Replacing the time derivative of the phase variable using the right hand side of eqn.(1.2), we get

$$\frac{\partial p(\mathbf{x},t)}{\partial t} = -\frac{\partial}{\partial \mathbf{x}} \cdot \left(F(\mathbf{x}) p(\mathbf{x},t) + \Gamma(t) p(\mathbf{x},t) \right) \tag{1.14}$$

We have to derive a noise average solution of p. To simplify the equations, we write out a symbolic operator. For an arbitrary function ϕ, define :

$$L\phi \equiv \frac{\partial}{\partial \mathbf{x}} . (F(\mathbf{x})\phi) \tag{1.15}$$

L is analogous to the Liouville operator. Hence, the noise free equation can be written as,

$$\frac{\partial p}{\partial t} = -Lp \tag{1.16}$$

Formal solution for the initial value equation of above form,

$$p(\mathbf{x},t) = e^{-tL} p(\mathbf{x},0) \tag{1.17}$$

Adding the noise term to eqn(1.16), we get

$$\frac{\partial p(\mathbf{x},t)}{\partial t} = -Lp(\mathbf{x},t) - \frac{\partial}{\partial \mathbf{x}} \cdot \left(\Gamma(t) p(\mathbf{x},t) \right) \tag{1.18}$$

Integration over time leads to the equation,

$$p(\mathbf{x},t) = e^{-tL} p(\mathbf{x},0) - \int_0^t ds e^{-(t-s)L} \frac{\partial}{\partial \mathbf{x}} \cdot \left(\Gamma(s) p(\mathbf{x},s) \right) \tag{1.19}$$

We recall that $p(\mathbf{x},t)$ depends on the noise $\Gamma(t)$ for times smaller than $s(t < s)$, as these are Markovian processes. Substituting eqn(1.19), in eqn(1.18) we get,

$$\frac{\partial p(\mathbf{x},t)}{\partial t} = -Lp(\mathbf{x},t) - \frac{\partial}{\partial \mathbf{x}} . (\Gamma(t) p(\mathbf{x},0)) + \frac{\partial}{\partial \mathbf{x}} . \Gamma(t) \int_0^t ds e^{-(t-s)L} \frac{\partial}{\partial \mathbf{x}} . (\Gamma(s) p(\mathbf{x},s)) \tag{1.20}$$

Now, we average the equation over noise. The $p(x,0)$ is the initial distribution, hence is not affected by averaging and goes to zero. The second term has a $\Gamma(t)\Gamma(s)$ term. This introduces a $\delta(t-s)$, which removes the $e^{-(t-s)}$ factor in the integral. The *Fokker-Planck equation* for the noise-averaged distribution function $\langle p(\mathbf{x},t) \rangle$ is,

$$\frac{\partial}{\partial t} \langle p(\mathbf{x},t) \rangle = -\frac{\partial}{\partial \mathbf{x}} . F(\mathbf{x}) \langle p(\mathbf{x},t) \rangle + \frac{\partial}{\partial \mathbf{x}} . B . \frac{\partial}{\partial \mathbf{x}} \langle p(\mathbf{x},t) \rangle \tag{1.21}$$

The second term on the RHS of eqn(1.21) accounts for the average effects over noise. We will drop the ($\langle\rangle$) noise averaging symbols here on as we will deal with averaged distributions only.

1.3 The Flashing ratchets

The first reference to ratchets used in a context relevant to us, was made by the polish physicist Smoluchowski in his thought experiment about Brownian ratchet. It is now popular due to its feature in *Feynman Lectures in Physics*[12]. The Feynman-Smoluchowski ratchet and pawl consists of a paddle wheel and a ratchet and appears to extract useful work from *random fluctuations* in a system at **thermal equilibrium**. To understand more about the Feynman ratchet, refer to detailed calculations in [13] about the efficiency of such a ratchet.

Can useful work be obtained from random forces?

In the case of a dynamical system we expect thermal fluctuations inherent to the system to be random. In other words it is one of the sources of noise. In the present context a ratchet is an asymmetric periodic potential. The flashing ratchet switches between an asymmetric form and a zero potential(flat line). The ratchet systems have a defining feature, the cooperation of two opposing tendencies: diffusion which tends to spread and dissipate energy and transport which concentrates density at specific sites determined by the energy landscape.
Consider Brownian particles kept under the influence of an asymmetric periodic potential in space. The schematic[Fig 3] presented in the next page illustrates the operation of the ratchet and transport of particles due to it.The process of ratcheting of the particles is as follows:

1. When asymmetric potential ($V(x)$) is "On"[Fig 1] the particle density is maximum at the valleys. The blue particles are tagged to show drift.

2. When the potential is "Off"($V(x) = 0$) [Fig 2] there is no external force on the particles other than the drag. Hence, they undergo free diffusion spreading in all directions uniformly.

3. The potential is turned "On" again but now due to the potential landscape there are more particles that go down the side with the greater slope than the opposite. This results in a greater aggregation of tagged particles towards the right in [Fig 3] than towards the left. Let P_{right} be the probability for the particle to move right and P_{left} likewise. Now $P_{left} = \alpha L$, where α is the asymmetry parameter that determines the location of the peak in ratchet potential(L is the length of the period). This is proportional to the area under the green portion in the [Fig 3]. Similarly,$P_{right} = (1 - \alpha)L$ is proportional to the area under yellow. Since, $\alpha < 1/2$, $P_{right} > P_{left}$. Hence, net drift was created in the +ve x-direction just by taking the aid of random forces and an asymmetric external potential switching between two states.

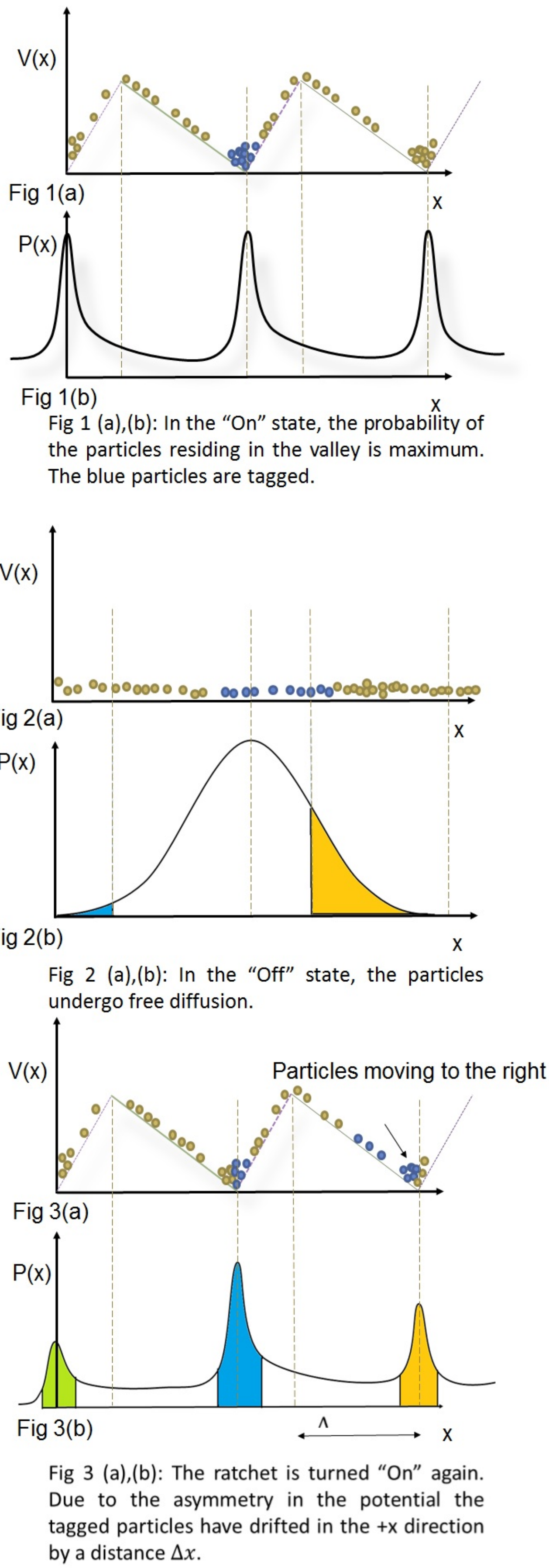

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Figure 1.1: Mechanism of Flashing Ratchets

Chapter 2

Two State Systems : A Fokker-Planck Treatment

In this Chapter we work on a couple of examples of two state systems. This will help us understand the important role played by Fokker-Planck equations in the understanding of a wide array of systems. The two state ratchet is of importance as the results emerging from its analysis will help us understand the system of interacting colloids better. Ratchet systems are ubiquitous in literature. Several reviews articles have been dedicated to their descriptions or implementations [14]-[16].

2.1 Dichotomic Noise Process

Consider a case of switching between two Stochastic diffusion processes, i.e in terms of dichotomous noise $\Gamma_i(t) = \pm 1$ where $i = +, -$.
The stochastic differential equations have the form[11],

$$\dot{x} = f(x) + \Gamma_+(t) \tag{2.1a}$$

$$\dot{x} = f(x) + \Gamma_-(t) \tag{2.1b}$$

The Fokker-Planck equations of for a process like eqn(2.1a) and eqn(2.1b) can be written as [11]:

$$\frac{\partial}{\partial t}p_+(x,t) = -\frac{\partial}{\partial x}f(x)p_+(x,t) + D_1\frac{\partial^2}{\partial x^2}p_+(x,t) - \nu[p_+(x,t) - p_-(x,t)] \tag{2.2a}$$

$$\frac{\partial}{\partial t}p_-(x,t) = -\frac{\partial}{\partial x}f(x)p_-(x,t) + D_2\frac{\partial^2}{\partial x^2}p_-(x,t) - \nu[p_-(x,t) - p_-(x,t)] \tag{2.2b}$$

where $p_+(x,t) = p_+(x,\xi = +1,t)$ and $p_-(x,t) = p_-(x,\xi = -1,t)$. D_1 and D_2 are the diffusion coefficient corresponding to each state of the noise.Also $f(x) = \frac{-dV(x)}{dx}$, where $V(x)$ is some potential. From the above eqns(2.2a) and (2.2b) we can construct a continuity equation of the form of eqn(1.13) by adding them:

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}f(x)p(x,t) + D_1\frac{\partial^2}{\partial x^2}p_+(x,t) + D_2\frac{\partial^2}{\partial x^2}p_-(x,t) \tag{2.3}$$

From the above equation one can obtain the expression for the current J(x,t). In the stationary state the current J is obtained from the following eqns:

$$J = -(D_1 - D_2)p'_+(x) - D_2p'(x) + f(x)p(x) \tag{2.4a}$$

$$D_1p''_+(x) - [f(x)p(x)]' - 2\nu p_+(x) + \nu p(x) = 0 \tag{2.4b}$$

where $p_+(x)$ and $p_-(x)$ are the long time (stationary) limits of $p_+(x,t)$ and $p_-(x,t)$. We get eqn(2.4b) when we take the left hand side of eqn(2.2a) to 0. The primes are differentiation with respect to x.

Asymptotic Limits

Analytically what we can look at is the asymptotic limits of the above equation and check the form of J(steady state current).

1. **Large frequency (ν) limit**: We expand $p(x)$,$p_+(x)$ and J as a power series in ν^{-1}. $p_+(x) = \sum_{n=0}^{\infty}\nu^{-n}p_{n+}(x)$, $p(x) = \sum_{n=0}^{\infty}\nu^{-n}p_n(x)$ and $J = \sum_{n=0}^{\infty}\nu^{-n}J_n$. The leading order term when the above forms are substituted in eqn(2.4a):

$$J_0 = -(D_1 - D_2)p'_{0+} - D_2p'_0(x) + f(x)p_0(x)$$

Put, $J_0 = 0$,

$$-(D_1 - D_2)p'_{0+}(x) - D_2p'_0(x) + f(x)p_0(x) = 0 \tag{2.5a}$$

$$-2p_{+0}(x) + p_0(x) = 0 \tag{2.5b}$$

from eqn(2.5b) for the 1st order terms we get,

$$p_{0+}(x) = \frac{p_0(x)}{2} \tag{2.6}$$

Substituting eqn(2.6) in eqn(2.5a),

$$-(D_1 - D_2)\frac{p'_{0+}(x)}{2} - D_2p'_0(x) + f(x)p_0(x) = 0 \tag{2.7}$$

$$p'_0(x) = -\frac{2f(x)}{D_1 + D_2}p_0(x)$$

$$p_0(x) = \frac{e^{-2V(x)/D_1+D_2}}{\int_0^L e^{-2V(x)/D_1+D_2} dx} \tag{2.8}$$

Define,

$$U(x) = e^{-2V(x)/D_1+D_2} \tag{2.9}$$

Then eqn(2.8),

$$p_0(x) = \frac{U(x)}{\int_0^L U(x)dx}$$

Now from eqn(2.4a) for the 2nd order equation,

$$-(D_1 - D_2)p'_{1+}(x) - D_2 p'_1(x) + f(x)p_1(x) = J_1 \tag{2.10a}$$

$$D_1 p''_{0+}(x) - [f(x)p_{0+}(x)]' - 2p_{1+} + p_1(x) = 0 \tag{2.10b}$$

eliminating for $p'_{1+}(x)$ from eqn(2.10b) in substituting in eqn(2.16a),

$$-(D_1 - D_2)\frac{1}{2}[D_1 p''_{0+}(x) - [f(x)p_{0+}(x)]'' + p'_1(x)] - D_2 p'_1(x) + f(x)p_1(x) = J_1 \tag{2.11}$$

using eqn(2.6) we get,

$$-(D_1 - D_2)[D_1 p''_0(x) - [f(x)p_0(x)]'' + \frac{p'_1(x)}{2}] - D_2 p'_1(x) + f(x)p_1(x) = J_1 \tag{2.12}$$

Multiply and divide by U^{-1} on the both sides and integrate over the period,

$$-(D_1-D_2)\frac{\int_0^L \left\langle \boxed{D_1 p'''_0(x) - [f(x)p_0(x)]''} + \frac{p'_1(x)}{2} - D_2 p'_1(x) + f(x)p_1(x) \right\rangle U^{-1}(x)dx}{\int_0^L U^{-1}(x)dx} = J_1 \frac{\int_0^L U^{-1}(x)dx}{\int_0^L U^{-1}(x)dx} \tag{2.13}$$

Consider the numerator with the boxed terms as term (b) and the rest as term (a) on the Left hand side of eqn(2.13).

(a)

$$\int_0^L [-(D_1 - D_2)\frac{p'_1(x)}{2} - D_2 p'_1(x) + f(x)p_1(x)]U^{-1}(x)dx$$

Integrating the first 2 terms of the above expression by parts:

$$= \int_0^L [-(D_1 - D_2)p_1(x)\frac{f(x)}{D_1 + D_2} - 2D_2 p_1(x)\frac{f(x)}{D_1 + D_2} + f(x)p_1(x)]U^{-1}(x)dx$$

$$= \int_0^L [-(\frac{D_1 + D_2}{D_1 + D_2})p_1(x)f(x) + p_1(x)f(x)]U^{-1}(x)dx$$

$$= 0$$

Now consider the boxed terms:

(b)

$$-(D_1 - D_2)\int_0^L \left\langle D_1 p_0'''(x) - [f(x)p_0(x)]'' \right\rangle U^{-1}(x)dx$$

$$= -(D_1 - D_2)\int_0^L \left\langle \frac{8D_1 f^3(x)}{(D_1+D_2)^3} p_0(x) - f(x)p_0''(x) - \boxed{2f'(x)p_0'(x) - f''(x)p_0(x)} \right\rangle U^{-1}(x)dx$$

Consider the boxed terms first,

$$(D_1 - D_2)\int_0^L \left\langle 2f'(x)p_0'(x) + f''(x)p_0(x) \right\rangle U^{-1}(x)dx$$

integrating by parts the boxed term,

$$= (D_1 - D_2)\int_0^L \left\langle 2f'(x)p_0'(x) - f'(x)p_0'(x) + \frac{2f'(x)f(x)}{D_1+D_2} \right\rangle U^{-1}(x)dx$$

$$= (D_1 - D_2)\int_0^L \left\langle f'(x)p_0'(x) + \frac{2f'(x)f(x)}{D_1+D_2} \right\rangle U^{-1}(x)dx$$

$$= (D_1 - D_2)\int_0^L \left\langle \frac{2f'(x)f(x)}{D_1+D_2} \right\rangle U^{-1}(x)dx$$

$$= 0$$

Now, consider the remaining terms,

$$= -(D_1 - D_2)\int_0^L \left\langle \frac{8D_1 f^3(x)}{(D_1+D_2)^3} p_0(x) - \frac{4f^3(x)}{(D_1+D_2)^2} p_0(x) \right\rangle U^{-1}(x)dx$$

$$= -(D_1 - D_2)\int_0^L \left\langle \frac{8D_1 f^3(x)p_0(x) - 4f^3(x)p_0(x)(D_1+D_2)}{(D_1+D_2^3)} \right\rangle U^{-1}(x)dx$$

$$J_1 = \frac{(D_1 - D_2)^2}{(D_1+D_2)^3} \frac{\int_0^L f^3(x)dx}{\int_0^L e^{2V(x)/D_1+D_2} \int_0^L e^{-2V(x)/D_1+D_2}} \tag{2.14}$$

Revisiting the expression of stationary current J:

$$J \sim \nu^{-1}\mathbf{x}\frac{(D_1 - D_2)^2}{(D_1+D_2)^3} \frac{\int_0^L f^3(x)dx}{\int_0^L e^{2V(x)/D_1+D_2}dx \int_0^L e^{-2V(x)/D_1+D_2}dx} + O(\nu^{-2}) \tag{2.15}$$

2. **Small frequency limit**:

For small frequencies the probabilities $p_+(x)$, $p_-(x)$ and current J are expanded in linear powers of ν. $p_+(x) = \sum_{n=0}^{\infty} \nu^n p_{n+}(x)$, $p_-(x) = \sum_{n=0}^{\infty} \nu^n p_{n-}(x)$ and $J = \sum_{n=0}^{\infty} \nu^n J_n$. The 1st order contribution to flux in eqn(2.4a) is zero. The second order terms in current are,

$$J_1 = -D_1 p_{1+}'(x) - D_2 p_{1-}'(x) + f(x)p_{1+}(x) + f(x)p_{1-}(x) \tag{2.16}$$

The normalization conditions on the probabilities are:

$$\int_0^L p_+(x) = \int_0^L p_-(x) = 1/2; \int_0^L p(x) = 1 \tag{2.17}$$

First order terms of eqn(2.10b) for small frequencies gives,

$$D_1 p''_{0+}(x) - [f(x)p_{0+}(x)]' = 0 \tag{2.18a}$$

$$D_2 p''_{0-}(x) - [f(x)p_{0-}(x)]' = 0 \tag{2.18b}$$

So the expression for $p_{0+}(x)$ and $p_{0-}(x)$ becomes,

$$p_{0+}(x) = \frac{e^{-V(x)/D_1}}{2\int_0^L e^{-V(x)/D_1}dx}; p_{0-}(x) = \frac{e^{-V(x)/D_2}}{2\int_0^L e^{-V(x)/D_2}dx} \tag{2.19}$$

Consider the eqn(2.4b) for 2nd order terms,

$$D_1 p''_{1+}(x) - [f(x)p_{1+}]' - p_{0+}(x) + p_{0-} = 0 \tag{2.20a}$$

$$D_2 p''_{1-}(x) - [f(x)p_{1-}]' - p_{0-}(x) + p_{0+} = 0 \tag{2.20b}$$

Integrating the above equations from 0 to x,

$$D_1 p'_{1+}(x) - [f(x)p_{1+}] - \int_0^x p_{0+}(x) + \int_0^x p_{0-} = 0 \tag{2.21a}$$

$$D_2 p'_{1-}(x) - [f(x)p_{1-}] - \int_0^x p_{0-}(x) + \int_0^x p_{0+} = 0 \tag{2.21b}$$

Define,

$$P_+(x) = \int_0^x p_{0+}(y)dy; P_-(x) = \int_0^x p_{0-}(y)dy$$

Multiply and divide eqn(2.21a) by $e^{V(x)/D_1}$ and eqn(2.21b) by $e^{V(x)}/D_2$ and integrate over the period,

$$\langle D_1 p'_{1+}(x)\rangle_1 - \langle [f(x)p_{1+}]\rangle_1 - \langle P_+(x)\rangle_1 + \langle P_-(x)\rangle_1 = 0 \tag{2.22a}$$

$$\langle D_2 p'_{1-}(x)\rangle_2 - \langle [f(x)p_{1-}]\rangle_2 - \langle P_-(x)\rangle_2 + \langle P_+(x)\rangle_2 = 0 \tag{2.22b}$$

where for any function $K(x)$,

$$\langle K(x)\rangle_i = \frac{\int_0^L K(x)e^{V(x)/D_i}}{\int_0^L e^{V(x)/D_i}}$$

i=1,2

Using the above expressions in eqns(2.22) we get,

$$J_1 = \langle P_+(x)\rangle_1 + \langle P_-(x)\rangle_2 - \langle P_-(x)\rangle_1 - \langle P_+(x)\rangle_2 \tag{2.23}$$

The expression for current is,

$$J \sim \nu \left[\langle P_+(x) \rangle_1 + \langle P_-(x) \rangle_2 - \langle P_-(x) \rangle_1 - \langle P_+(x) \rangle_2 \right] + O(\nu^2) \tag{2.24}$$

2.2 Two State Ratchet

Consider the case when the system switches between two states, from an asymmetric potential to zero potential. The diffusion constants is same for both states now. So $D_1 = D_2 = D$. The potentials are $f_1(x) = f(x)$ and $f_2(x) = 0$. The Fokker-Planck equations the following process are:

$$\frac{\partial}{\partial t} p_+(x,t) = -\frac{\partial}{\partial x} f(x) p_+(x,t) + D \frac{\partial^2}{\partial x^2} p_+(x,t) - \nu[p_+(x,t) - p_-(x,t)] \tag{2.25a}$$

$$\frac{\partial}{\partial t} p_-(x,t) = D \frac{\partial^2}{\partial x^2} p_-(x,t) - \nu[p_-(x,t) - p_+(x,t)] \tag{2.25b}$$

Adding eqn(2.25a) and eqn(2.25b) we get,

$$\frac{\partial}{\partial t} p(x,t) = -\frac{\partial}{\partial x} f(x) p_+(x,t) + D \frac{\partial^2}{\partial x^2} p(x,t) \tag{2.26a}$$

$$-Dp'(x) + f(x) p_+(x) = J \tag{2.26b}$$

Put left hand side of eqn(2.25a) to zero,

$$Dp''_+(x) - [f(x)p(x)]' - 2\nu p_+(x) + \nu p(x) = 0 \tag{2.27}$$

1. **Large frequency limit**: The probabilities $p_+(x), p(x)$ and current J are expanded in a series of ν^{-1} like in section (2.1). First order terms are,

$$-2p_{0+}(x) + p_{0+}(x) = 0$$

$$p_{0+}(x) = \frac{p_0(x)}{2} \tag{2.28}$$

First order terms in eqn(2.26b) with J_0 are,

$$-2Dp'_{0+}(x) + f(x) p_0(x) = 0$$

$$p_{0+}(x) = \frac{e^{-V(x)/2D}}{\int_0^L e^{-V(x)/2D}} \tag{2.29}$$

Define,

$$U(x) = e^{-V(x)/2D} \tag{2.30}$$

So eqn(2.29) now looks like,

$$p_{0+}(x) = \frac{U(x)}{2 \int_0^L U(x) dx}$$

$p_{0+}(x)$ is normalized to 1/2 and $p_0(x)$ to 1. The second order terms of eqn(2.27),

$$p_{1+} = \frac{1}{2}\left[Dp_{0+}(x) - (f(x)p_{0+})' + p_1(x)\right]$$

Substituting the above expression for $p_{1+}(x)$ in second order terms of eqn(2.26b)

$$\frac{f(x)}{2}\left[Dp_{0+}(x) - (f(x)p_{0+})' + p_1(x)\right] - Dp_1' = J_1 \tag{2.31}$$

Using eqn(2.28) the above eqn(2.31) becomes,

$$f(x)\left[Dp_0'' - (f(x)p_0(x))' + \frac{p_1(x)}{2}\right] - Dp_1'(x) = J_1$$

Multiply and divide the above equation by $U^{-1}(x)$ and integrate over the period,

$$\frac{\int_0^L \left\langle f(x)\left\{Dp_{0+}''(x) - [f(x)p_0(x)]' + \frac{p_1(x)}{2}\right\} - Dp_1'(x)\right\rangle U^{-1}(x)dx}{\int_0^L U^{-1}(x)dx} = J_1 \frac{\int_0^L U^{-1}(x)}{\int_0^L U^{-1}(x)} \tag{2.32}$$

Consider the numerator of Left hand side of eqn(2.32),

$$\int_0^L \left\langle \boxed{f(x)D_1p_{0+}''(x) - f(x)[f(x)p_0(x)]'} + f(x)\frac{p_1(x)}{2} - Dp_1'(x)\right\rangle U^{-1}(x)dx$$

Call the boxed terms as (a) and the rest (b)

(a)

$$\int_0^L \left\langle f(x)Dp_{0+}''(x) - f(x)[f(x)p_0(x)]'\right\rangle U^{-1}(x)dx$$

substituting the expression for $p_0(x)$ in the above integral,

$$= \int_0^L \left\langle -\frac{1}{4D}f^3(x)p_0(x) - f^2(x)p_0'(x) - f(x)f'(x)p_0(x)\right\rangle U^{-1}(x)dx$$

$$= \int_0^L \left\langle -\frac{1}{4D}f^3(x)p_0(x)U^{-1}(x) + \frac{1}{2D}f^3(x)p_0(x)U^{-1}(x) - f(x)f'(x)p_0(x)U^{-1}(x)\right\rangle dx$$

$$= \int_0^L \left\langle \frac{1}{4D}f^3(x) - f(x)f'(x)\right\rangle dx$$

$$= \int_0^L \frac{1}{4D}f^3(x)dx \tag{2.33}$$

(b)

$$\int_0^L \left\langle \frac{1}{2}f(x)p_1(x) - Dp_1'(x) \right\rangle U^{-1}(x)dx$$

Integrating by parts the second term,

$$= \int_0^L \left\langle \frac{1}{2}f(x)p_1(x) - D\frac{f(x)}{2}p_1(x) \right\rangle U^{-1}(x)dx$$

$$= 0$$

Revisiting the expression for current eqn(2.26b) and using eqn(2.33) we have similar expression as in section (2.1)

$$J \sim \nu^{-1}\mathbf{x}\frac{1}{D}\frac{\int_0^L f^3(x)dx}{\int_0^L e^{V(x)/2D dx}\int_0^L e^{-V(x)/2D}dx} + O(\nu^2) \tag{2.34}$$

From the above expression for directed current we can see that if we have reflection-symmetric potential then the integral over the period of $f^3(x)$ vanishes.

2. **Small Frequency limit**:

For small frequencies the probabilities $p_+(x)$, $p_-(x)$ and current J are expanded in linear powers of ν. $p_+(x) = \sum_{n=0}^{\infty}\nu^n p_{n+}(x)$, $p_-(x) = \sum_{n=0}^{\infty}\nu^n p_{n-}(x)$ and $J = \sum_{n=0}^{\infty}\nu^n J_n$. The 1st order contribution to flux in eqn(2.4a) is zero. The second order terms in current are,

$$-Dp_{1+}'(x) - Dp_{1-}'(x) + f(x)p_{1+}(x) = J_1 \tag{2.35}$$

From eqn(2.27), the 2nd order terms in stationary state are,

$$Dp_{1+}''(x) - [f(x)p_{1+}(x)]' - p_{0+}(x) + p_{0-}(x) = 0 \tag{2.36a}$$

$$Dp_{1-}''(x) - p_{0-}(x) + p_{0+}(x) = 0 \tag{2.36b}$$

Integrating the above equations from 0 to x and borrowing expressions from section,

$$Dp_{1+}'(x) - f(x)p_{1+}(x) - P_+(x) + P_-(x) = 0 \tag{2.37a}$$

$$Dp_{1-}'(x) - P_-(x) + P_+(x) = 0 \tag{2.37b}$$

Multiplying and dividing eqn(2.37a) by $e^{V(x)/D}$ and integrating over the period we get,

$$\langle Dp_{1+}'(x)\rangle - \langle f(x)p_{1+}(x)\rangle - \langle P_+(x)\rangle + \langle P_-(x)\rangle = 0$$

From the above expression and eqn(2.37b) the expression for second order current becomes,

$$J_1 = \langle P_+(x) \rangle - \langle P_-(x) \rangle + P_-(x) - P_+(x) \tag{2.38}$$

where for any function $K(x)$,

$$\langle K(x) \rangle = \frac{\int_0^L K(x) e^{V(x)/D}}{\int_0^L e^{V(x)/D}}$$

The current is,

$$J \sim \nu \left[\langle P_+(x) \rangle - \langle P_-(x) \rangle + P_-(x) - P_+(x) \right] + O(\nu^2) \tag{2.39}$$

2.3 Numerical Scheme

As we have seen the analytical results show us the partial story of the behavior directed current with changing ratcheting frequency. The numerical scheme[1] used here generates finite difference form of the Fokker-Planck [eqn(1.21)] which can be seen as a discrete Markov chain(Memory less processes). The equations have been discretized on a lattice as a jump process in the following manner. Consider a particle residing on the n^{th} site,

$$\frac{dP_n}{dt} = -(B_{n-1/2} + F_{n+1/2})P_n + F_{n-1/2}P_{n-1/2} + B_{n+1/2}P_{n+1/2} \tag{2.40}$$

$$(F_{n-1/2}P_{n-1} - B_{n-1/2}P_n) - (F_{n+1/2}P_n - B_{n+1/2}P_{n+1}) = J_{n-1/2} - J_{n+1/2}$$

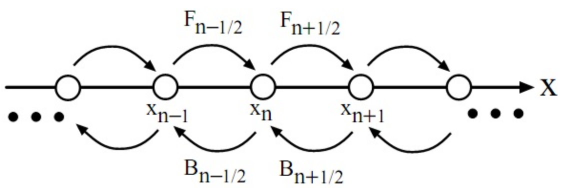

Figure 2.1: Spatial discretization schematic [1]

P_n is the probability of finding the particle at site n at time t. $x_n = x_0 + n\Delta x$, where Δx is the step size.

The terms $B_{n-1/2}$ and $B_{n+1/2}$ refer to backward fluxes from sites x_n and x_{n+1}, respectively and F_n's the forward fluxes .The terms have been arranged in order to show the net *forward*$(J_{n+1/2})$ and *backward* $(J_{n-1/2})$ fluxes from the site x_n. Eqn(2.40) can be written in a concise manner as,

$$\frac{d\mathbf{P}}{dt} = \mathbf{LP} \tag{2.41}$$

where L is tridiagonal NXN matrix with entries,

$$L_{n,n} = -(F_{n+1/2} + B_{n-1/2}) \tag{2.42a}$$

$$L_{n,n-1} = B_{n-1/2} \tag{2.42b}$$

$$L_{n,n+1} = F_{n+1/2} \tag{2.42c}$$

The quantity $P_n(t)$ is the probability of finding the motor site x_n at time t.

$$P_n(t) \approx \int_{x_{n-\Delta x/2}}^{x_n+\Delta x/2} p(x_n, t)dx \approx p(x_{n,}, t)\Delta x \tag{2.43}$$

as x_n represents the interval $(x_{n-1/2}, x_{n+1/2})$. The probability flux is zero at thermodynamic equilibrium. That is,

$$J_{n+1/2} = F_{n+1/2}p_{eq}(x_n)\Delta x - B_{n+1/2}p_{eq}(x_{n+1})\Delta x = 0 \tag{2.44}$$

for all n.This places a constraint on the jump rates. Similar constraints can be obtained by keeping $J_{n-1/2} = 0$.

The equilibrium solution of eqn(1.21) can be simply verified to be the Boltzmann distribution by equating the RHS to zero

$$p_{eq} \propto \exp(-V(x)) \tag{2.45}$$

Now from eqn(2.42) we can see that

$$\frac{F_{n+1/2}}{B_{n+1/2}} = \frac{p_{eq}(x_{n+1})}{p_{eq}(x_n)} = \exp(-\Delta V_{n+1/2}) \tag{2.46}$$

where

$$\Delta V_{n+1/2} \equiv V(x_{n+1}) - V_(x_n) \tag{2.47}$$

The expression for the jump rates are:

$$F_{n+1/2} = \frac{-D\Delta V_{n+1/2}}{(\Delta x)^2(\exp(-\Delta V_{n+1/2}) - 1)} \tag{2.48a}$$

$$B_{n+1/2} = \frac{D\Delta V_{n+1/2}}{(\Delta x)^2(\exp(\Delta V_{n+1/2}) - 1)} \tag{2.48b}$$

where D is the diffusion coefficient. This can be found by finding the local approximate solutions of the Fokker-Planck eqn(1.21). Knowing this we can recast eqn(1.21) in the form of eqn(2.40). Detailed derivation of eqn(2.48a,b) can be found in [1].

Two State Ratchet

Now we proceed to the Two State Ratchet system. We revisit eqn(2.25a,b):

$$\frac{\partial}{\partial t}p_+(x,t) = \frac{\partial}{\partial x}\frac{dV}{dx}p_+(x,t) + D\frac{\partial^2}{\partial x^2}p_+(x,t) - \nu[p_+(x,t) - p_-(x,t)]$$

$$\frac{\partial}{\partial t}p_-(x,t) = D\frac{\partial^2}{\partial x^2}p_-(x,t) - \nu[p_-(x,t) - p_+(x,t)]$$

The net flux at steady state goes to zero. The value of ν can be varied as a parameter. To solve eqns(2.21) and (2.22), we use boundary conditions $p_i(x + L, t) = p_i(x, t)$ where L is the period. We now have to solve it on a grid, say of N points, each with a co-ordinate in x. We choose a grid here such that $x_n = (n - 1/2)L/N$. Unlike eqn(2.40) here we have two equations describing the system, hence the matrix will be $2NX2N$ dimensional(call it **M**)

$$\frac{d\mathbf{P}}{dt} = \mathbf{MP} \tag{2.49}$$

The form of the matrix can be identified by looking at eqns(2.25a) and (2.25b):

$$\mathbf{M} = \begin{pmatrix} L^{(+)} - K & K \\ K & L^{(-)} - K \end{pmatrix} \tag{2.50}$$

where the $L^{(i)}$'s$(i = +, -)$ are $N \times N$ matrices evaluated using $V(x)$ and have the same form as defined in eqns(2.48a,b). But, **L** requires additional boundary conditions to make sure that entries still make sense at the ends as evaluation of $V(x)$ at the boundaries causes problems.

$$L^{(i)}_{N,1} = B^{(i)}_{1/2} \tag{2.51}$$

$$L^{(i)}_{1,N} = F^{(i)}_{N+1/2} \tag{2.52}$$

K are just $N \times N$ diagonal matrices with values of the ratcheting frequency. We take potentials of the form:

$$V(x) = sin(\frac{2\pi}{L}x) + 0.2sin(\frac{4\pi}{L}x) \tag{2.53}$$

The potential $\phi_1(x)$ has the first three terms of the fourier expansion of saw-tooth potential of period L and amplitude A. Now we have the full description of the algorithm, all we have to do is simulate it and analyze the behavior.

2.4 Simulation Results

Simulations were performed on a lattice size of $N = 100$, with periodic Length L=8. The time step $\Delta t = 7.1\text{x}10^{-9}$ and step size in space $\Delta x = 0.08$. The initial conditions for probabilities was $P_{N/4} = 1$.

The variation of scaled dimensionless directed current J with ratcheting frequency ν is shown in [Fig 2.2].

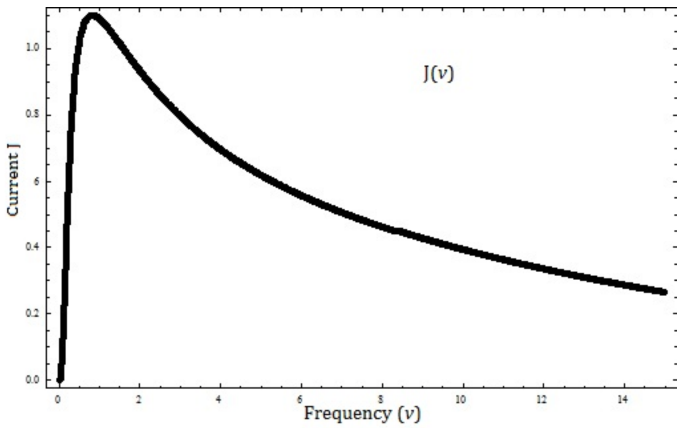

Figure 2.2: Scaled dimensionless probability current J vs Switching frequency ν

Asymptotic Nature:

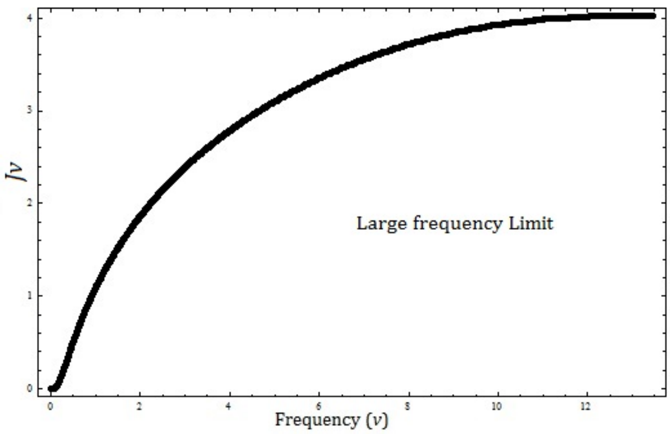

Figure 2.3: Product $J * \nu$ vs Switching frequency ν

We observe a saturation of the current with ν^{-1} at very large frequencies.

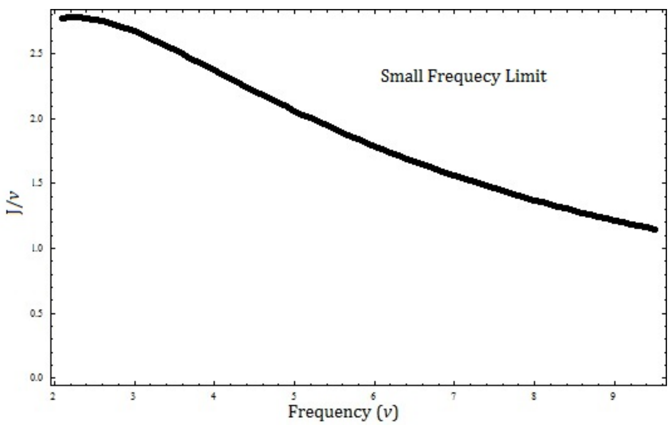

Figure 2.4: Product $J\nu$ vs Switching frequency ν

At small frequencies we observe a linear relation of the current with ν.
Hence, we observe that the numerical simulations of the directed current concur with the analytical results in the asymptotic limits of the ratcheting frequency.

Chapter 3

Interacting Colloids

We consider a system of two-dimensional repulsively interacting colloids, which are driven by a one-dimensional varying asymmetric potential turning on and off stochastically. This situation is similar to what we have dealt with in the previous chapter, but the interacting term complicates the solution and also gives rise to new effects which are observed in real colloidal systems. Experiments on confined colloids (say, between two glass plates) subject to a laser with spatially periodic 1D potential commensurate to the mean particle separation, have observed the remarkable phenomena of Laser Induced Freezing and melting with increase in the strength of the potential. It is found that at a particular wave vector of the incident laser (which corresponds to where the liquid structure develops its first peak) there emerges a triangular lattice with two-dimensional symmetry. Beyond a certain external field intensity of the external field the colloid becomes a crystal. The higher field strengths, the crystal structure becomes unstable and gives rise to re-entrant melting[2].

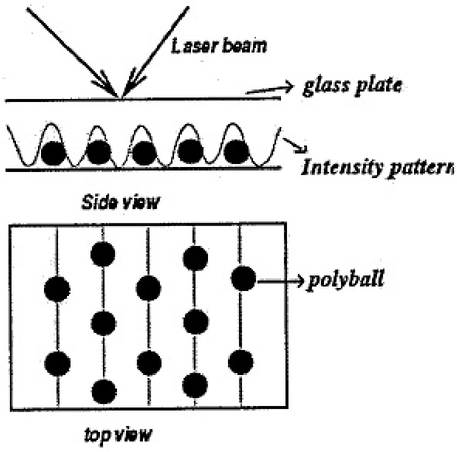

Figure 3.1: Laser Induced Freezing[2]

3.1 Model

Considered here as a model colloid, is a system of purely repulsively interacting particles interacting via a soft-core potential

$$\beta U(r) = \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r_c}\right)^{12} \tag{3.1}$$

with cut off distance $r = r_c$ beyond which $\beta U(r) = 0$. Here $\beta = 1/k_B T$ sets the energy scale and σ sets the length scale. The 1-D ratchet is along the y-direction with the following form:

$$U_{ext}(y,t) = V_0(t)\left[\sin(\frac{2\pi y}{L}) + \alpha \sin(\frac{4\pi y}{L})\right] \tag{3.2}$$

where $V_0(t)$ switches between 0 and U_0 with a frequency ν.

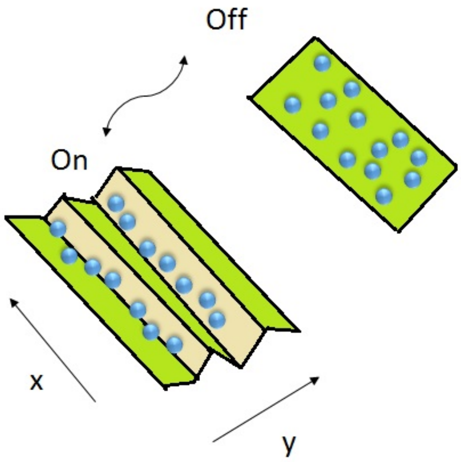

Figure 3.2: Schematic of a 2D colloid under the influence of an 1D asymmetric ratchet along y-direction, switching between 'on' and 'off' states.

Molecular Dynamics done by [3] using setting the parameter $\alpha = 0.2$ and $\beta U_0 = 1$. A leap frog algorithm (to solve equations of the type of Newton's equation) was used with periodic length of the ratcheting potential set commensurate to the lattice separation along the y-direction, $L = a_y$. For a triangular lattice, the plane separation $a_y = \sqrt{3}a/2$ and the density $\rho = 2/\sqrt{3}a^2$.

At very high and very low ratcheting frequencies the variation the directed current with frequency observed is similar to chapter(2). At high frequencies, much larger than the internal relaxation time of the particles, the system experiences and effective periodic potential. At low frequencies, there is observed a slow transition between modulated liquid and solid phase. In the intermediate frequencies, the directed current due to the ratchet show resonance with the frequency and varies non-monotonically with density.

3.2 Transport

Let us denote the 'on' and 'off' states of the ratchet as $'+'$ and $'-'$ which is characterized by N-particle probabilities densities $P_+(\mathbf{r}_1,\mathbf{r}_2...,\mathbf{r}_N)$ and $P_-(\mathbf{r}_1,\mathbf{r}_2...,\mathbf{r}_N)$ respectively. $U(\mathbf{r}-\mathbf{r'})$ denotes the interaction between particles.

For a system of a N particles the canonical ensemble(N,V,T),

$Z_N = \int ... \int e^{-\beta U_N} d\mathbf{r}_1 d\mathbf{r}_2 ... d\mathbf{r}_N$ is the configurational integral taken over all possible configurations of particle positions. For finding a particle in a configuration with particle 1 in position r_1, 2 in position r_2 we have,

$p^*(\mathbf{r}_1,\mathbf{r}_2 ...,\mathbf{r}_N) d\mathbf{r}_1 \ d\mathbf{r}_2 ... d\mathbf{r}_N = \frac{e^{-\beta U}}{Z_N} d\mathbf{r}_1 \ d\mathbf{r}_2 ... d\mathbf{r}_N$

One can obtain the reduced probability as in our case if we fix only 1 particle and the remaining N-1 particles have no constraint. We can integrate the above expression over the remaining coordinates,

$p^*(\mathbf{r}_1,\mathbf{r}_2 ...,\mathbf{r}_N) = \int ... \int \frac{e^{-\beta U}}{Z_N} d\mathbf{r}_2 ... d\mathbf{r}_N$

Here he particles being identical, the N-1 particles can occupy any of the coordinates. So the local density for a single particle becomes,

$p_i = \frac{N!}{(N-1)!} \int P_i(\mathbf{r}_1,\mathbf{r}_2 ...,\mathbf{r}_N) d\mathbf{r}_2 ... d\mathbf{r}_N = N \int P_i(\mathbf{r}_1,\mathbf{r}_2 ...,\mathbf{r}_N) d\mathbf{r}_2 ... d\mathbf{r}_N$

where $i = +, -$

The joint density distribution follows from arguments similar to above expression,

$\pi_i = N(N-1) \int P_i d\mathbf{r}_3 ... d\mathbf{r}_N = p_i \rho_0 g_i(\mathbf{r}\text{-}\mathbf{r}')$

$g_i(\mathbf{r}\text{-}\mathbf{r}')$ is the radial distribution function or the density-density correlation in the i the state, ρ_0 is the mean density. The ratcheting dynamics can be explained by the following equations [4]:

$$\frac{\partial}{\partial t} p_+(x,y,t) + \nabla . J_+ - \nu[p_+(x,y,t) - p_-(x,y,t)] = 0 \quad (3.3a)$$

$$\frac{\partial}{\partial t} p_-(x,y,t) + \nabla . J_- - \nu[p_-(x,y,t) - p_+(x,y,t)] = 0 \quad (3.3b)$$

where $J_i = -D\nabla p_i(x,y,t) + a\frac{D}{k_b T} p_i(x,y,t) F_i$.

$F_i = -\nabla V_i(\mathbf{r})$ - $\rho_0 \int dr' g_i(\mathbf{r}\text{-}\mathbf{r}') \nabla U(\mathbf{r} - \mathbf{r}')$.

for $i = +, -$. The force F_i is the mean force averaged over all configurations **2,...N** acting on a particle which at some fixed configuration. And a is a constant which takes the values $a = 0$ for non-interacting system and $a = 1$ for an interacting system.

Since the ratcheting potential acts along the y-direction, the current along it is $J_y = \mathbf{J}.\hat{\mathrm{y}}$ p The stationary state dynamics is given by the space and time-averaged particle in the y-direction(i.e the direction of ratcheting),

$$J_y = \frac{1}{\tau_m L_x L_y} \int^{\tau_m} dt \int^{L_x} dx \int^{L_y} dy j_y(x,y,t) \quad (3.4)$$

where the time is averaged over $\tau_m = nt$ $(t = 1/\nu)$, n denotes the number of switchings. L_x and L_y are the dimensions of the lattice.

From the MD simulation graphs of J(flux) vs Frequency ν the following interpolation formula was extracted for the form of the flux:

$$J_y = k\frac{\nu f}{\nu^2 + f^2}\rho v_0 \tag{3.5}$$

where k is some proportionality constant and ρv_0 has the dimensions of current with v_0 an intrinsic velocity. It can be seen that this corresponds to the behavior of the two state ratchet mentioned in the previous sections at high frequencies $J_y = \nu^{-1}$ and at low frequencies $J_y = \nu$. The aim is to reproduce this empirical form from other methods.

3.3 Non-Interacting case

Now in eqn(3.3a) and eqn(3.3b) put $a = 0$ in the expression for the mean force F_i. We also know that the external ratcheting potential is only a function of the y-direction. So we get,

$$F_+ = -\nabla V(y) \tag{3.6a}$$

$$F_- = 0 \tag{3.6b}$$

Now in eqns (3.3a) and (3.3b) let $p_+(x,y,t) = p_+(x,t)p_+(y,t)$ and $p_-(x,y,t) = p_-(x,t)p_-(y,t)$.

$$\frac{\partial}{\partial t}p_+(x,t)p_+(y,t) = D\nabla^2 p_+(x,t)p_+(y,t) + \nabla[\nabla V p_+(x,t)p_+(y,t)] + \nu[p_+(x,t)p_+(y,t) - p_-(x,t)p_-(y,t)] \tag{3.7a}$$

$$\frac{\partial}{\partial t}p_-(x,t)p_-(y,t) = D\nabla^2 p_-(x,t)p_-(y,t) + \nu[p_-(x,t)p_-(y,t) - p_+(x,t)p_+(y,t)] \tag{3.7b}$$

Now consider eqn(3.7a) and integrate it along the x-direction,

$$\int dx\left[p_+(y,t)\frac{\partial}{\partial t}p_+(x,t) + p_+(x,t)\frac{\partial}{\partial t}p_+(y,t)\right] = \int dx\Bigg[Dp_+(y,t)\frac{\partial^2}{\partial x^2}p_+(x,t) + Dp_+(x,t)\frac{\partial^2}{\partial y^2}p_+(y,t)$$
$$+p_+(x,t)\frac{\partial^2 V(y)}{\partial y^2}p_+(y,t) + p_+(x,t)\frac{\partial V(y)}{\partial y}\frac{\partial p_+(y,t)}{\partial y} + \nu[p_+(x,t)p_+(y,t) - p_-(x,t)p_-(y,t)]\Bigg] \tag{3.8}$$

We know the normalization conditions give us,

$$\int p_i(r,t)dr = 1 \tag{3.9}$$

where $i = +, -$ and $r = x, y$. Using this condition in eqn(3.8) we get,

$$\int dx\left[p_+(y,t)\frac{\partial}{\partial t}p_+(x,t) - Dp_+(y,t)\frac{\partial^2}{\partial x^2}p_+(x,t)\right] = -\frac{\partial}{\partial t}p_+(y,t) + D\frac{\partial^2}{\partial y^2}p_+(y,t) + \frac{\partial^2 V(y)}{\partial y^2}p_+(y,t)$$
$$+\frac{\partial V(y)}{\partial y}\frac{\partial p_+(y,t)}{\partial y} + \nu[p_+(y,t) - p_-(y,t)] \tag{3.10}$$

Now we integrate eqn(3.10) along the y-direction,

$$\int dy \int dx \left[p_+(y,t)\frac{\partial}{\partial t}p_+(x,t) - Dp_+(y,t)\frac{\partial^2}{\partial x^2}p_+(x,t)\right] = \int dy\Big[-\frac{\partial}{\partial t}p_+(y,t) + D\frac{\partial^2}{\partial y^2}p_+(y,t)$$
$$+\frac{\partial^2 V(y)}{\partial y^2}p_+(y,t) + \frac{\partial V(y)}{\partial y}\frac{\partial p_+(y,t)}{\partial y} + \nu[p_+(y,t) - p_-(y,t)]\Big]$$

Then we end up with,

$$\int dx \left[\frac{\partial}{\partial t}p_+(x,t) - D\frac{\partial^2}{\partial x^2}p_+(x,t)\right] + \int dy\Big[\frac{\partial}{\partial t}p_+(y,t) - D\frac{\partial^2}{\partial y^2}p_+(y,t) - \frac{\partial^2 V(y)}{\partial y^2}p_+(y,t)$$
$$-\frac{\partial V(y)}{\partial y}\frac{\partial p_+(y,t)}{\partial y}\Big] = 0 \tag{3.11}$$

The switching terms vanish with integration over the coordinates. Similarly if we integrate eqn(3.7b) along the x and y directions we end with following equation,

$$\int dx \left[\frac{\partial}{\partial t}p_-(x,t) - D\frac{\partial^2}{\partial x^2}p_-(x,t)\right] = \int dy \left[\frac{\partial}{\partial t}p_-(y,t) - D\frac{\partial^2}{\partial y^2}p_-(y,t)\right] \tag{3.12}$$

Now adding eqn(3.11) and eqn(3.12) and noting that $p_+(r,t) + p_-(r,t) = p(x,t)$.

$$\int dx \left[\frac{\partial}{\partial t}p(x,t) - D\frac{\partial^2}{\partial x^2}p(x,t)\right] + \int dy\left[\frac{\partial}{\partial t}p(y,t) - D\frac{\partial^2}{\partial y^2}p(y,t) - \frac{\partial^2 V(y)}{\partial y^2}p_+(y,t) - \frac{\partial V(y)}{\partial y}\frac{\partial p_+(y,t)}{\partial y}\right] = 0$$

The only way the above equation go to zero if terms under both integral signs go to zero. This give us

$$\frac{\partial}{\partial t}p(x,t) = D\frac{\partial^2}{\partial x^2}p(x,t) \tag{3.13a}$$
$$\frac{\partial}{\partial t}p(y,t) = D\frac{\partial^2}{\partial y^2}p(y,t) + \frac{\partial^2 V(y)}{\partial y^2}p_+(y,t) + \frac{\partial V(y)}{\partial y}\frac{\partial p_+(y,t)}{\partial y} \tag{3.13b}$$

Hence, we have simple diffusion along the x-direction. Direction motion is observed along the direction of ratcheting(y-direction). We can also see that in eqns(3.11) and (3.12) the equations should independently vanish. This tells us that the net drift along x-direction in both 'on' and 'off' states is zero and it is purely diffusive. Along, the y-direction in the 'off' state the process is purely diffusive.

3.4 Conclusions

The aim was partially achieved with the understanding of interacting systems from molecular dynamics simulations. The non-interacting case in 2-dimensions gives us results similar to what was observed in chapter 2. The Fokker-Planck equation presented above is clearly difficult to solve analytically in the interacting case. Numerical solutions seem to be possible. The challenge is to figure out the right form of the radial distribution function. This can be approximated from the Molecular

Dynamics simulations. The Fokker-Planck approach to the problem still remains interesting.

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