TWO MECHANISMS FOR SEGREGATING MIXTURES OF BROWNIAN PARTICLES

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Dedication

To

Feleke Getachew Mekonnen

and

Sr. Degefech H/Yesus Sorsa

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Abstract

We present two mechanisms for segregating mixtures of Brownian particles. In the first model, we used a W-potential, which is piece-wise linear, with non-homogeneous temperature background to separate mixtures of two types of Brownian particles that differ in their diffusion constants. We found closed form expression for the dynamics of the separation as a function of the parameters characterizing the model. For a given set of model parameter, we explored how the separation evolves with time and found it to take a maximum value at a finite time. We are specifically interested in how the barrier height affects the process of segregation and found that the best separation between the particles occurs at infinite potentials which corresponds to waiting for infinite times. As such we optimized the segregation and found the barrier height that gives us the optimized separation. In the second model, we used a periodic sawtooth potential, created by a uniform gravitational field, to separate mixtures of two types of Brownian particles. With the application of a small load and a non-homogeneous temperature background, we have shown that it is possible to separate two types of Brownian particles that have different masses by making them move in opposite directions.

Contents

Chapter 1

INTRODUCTION

Noise is unavoidable for any system in thermal contact with its surrounding. In technological devices, it is typical to incorporate mechanisms for reducing noise to an absolute minimum. An alternative approach is emerging these decades, however, in which attempts are made to harness noise for useful purposes.

Fluctuation-driven transport uses noise to accomplish mass transport without macroscopic forces or gradients. An important insight is that, in some cases, thermal noise can assist directed motion by providing a mechanism for overcoming energy barriers. In those cases, one speaks of "Brownian Motors" [1].

However, recent work has focused on the possibility of an energy source other than thermal gradient to power a microscopic motor. If energy is supplied by external fluctuations or a non-equilibrium chemical reaction, Brownian motion can be biased provided the medium is anisotropic, even in an isothermal system [2].

Brownian motors or "ratchets" consist of Brownian particles moving in asymmetric potentials and subject to non-equilibrium backgrounds, like external fluctuations or temperature gradients [3]. In general, the essential ingredients for the directed motion of a Brownian particle can be listed as follows:

i)Thermal noise to cause Brownian motion. More generally, random forces (of thermal, non-thermal, or even deterministic origin) should play a prominent role.

ii)Symmetry breaking (asymmetry) arising from the structure of the medium in which the particle diffuses.

iii)Spatial periodicity.

iv)All acting forces have to vanish after averaging over space, time, and statistical ensemble.

v)Breaking detailed balance symmetry.

Using ratchets for separating mixtures of Brownian particles that differ in diffusion constant, mass, diameter, etc. has attracted many researchers in the field. Among the earliest works is by A. Ajdari, et al [4] where Brownian particles are subjected to a spatially asymmetric periodic potential that is switched on and off as a function of time. When the potential is switched on, the Brownian particles are driven to the minimum of the spatially periodic potential, whereas the Brownian particles can diffuse freely when the spatial potential is switched off. This gives rise to a net directional motion in one-dimension, and the rectifying mechanism of the Brownian ratchet can be used to separate Brownian particles that have different diffusion constants.This method of separating Brownian Particles has also been done experimentally and the result of the experiment agree with theoretical calculations [5].

There is an analysis which shows that making the potential on and off can also be used to separate Brownian particles even in the presence of a small load. The smaller particles feel only a small force due to gravity while there is enough Brownian motion which can be biased by the ratchet to cause motion uphill. The larger particles, on the other hand, experience less Brownian motion and feel a greater force due to gravity and so move downhill [2].

It is also reported that a 3-state fluctuating potential, $V_+(x)$, $V_0(x)$ and $V_-(x)$, can also be used for separating mixtures with different damping constants [6]. By choosing the flipping rate between these potentials appropriately, one can separate small particles in opposite directions, as the Brownian motion can be biased in different directions.

An experimental realization has also been reported where a geometrical ratchet can be used as a molecular sieve to separate mixtures of membrane-associated molecules that differ in electrophoretic mobility and diffusion constant [7].

In this thesis, we present two mechanisms for segregating mixtures of non-interacting Brownian particles. The first mechanism makes use of a bistable potential while the second mechanism uses a periodic sawtooth (ratchet) potential.

In the first model, in stead of taking the periodically repeating potential, we simply take a bistable potential. We then put the two types of particles, having different diffusion constants, mixed up, in the left well. We create a non-homogeneous temperature background. The temperature varies spatially along the potential. We then let the particles flow by the thermal kick they get from the background, count the number of particles that are coming to the right well and stop the flow when the difference between the number of particles of the two types is maximum. We have calculated the time to get the best separation between the particles. We have also calculated numerically the barrier height that gives us the optimum, rather than the best, separation between the particles.

In the second model, we use the periodically repeating sawtooth potential to segregate mixtures of Brownian particles that differ in their mass. We apply a small external load and create a non-homogeneous temperature background on the ratchet potential, created by a uniform gravitational field. Since the two Brownian particles have different masses, the potential they experience is also different. Due to this, the two particles will have different currents. Under appropriate choice of the masses, and hence the potentials, we show that we can have a situation in which one particle moves in the positive direction while the other particle moves in the negative direction. So using this mechanism, one can succeed in separating the mixtures in opposite directions.

The rest of our work is organized as follows. In chapter 2, we look at the dynamics of a particle in a double well potential. We derive expressions for the mean first passage time and the escape rate for a particle in a double well potential. The expression for the time evolution of the number of particles in a double well potential is also given. In chapter 3, we give both the analytical and numerical results for the first model. We apply the results obtained in chapter 2 to our specific model and solve for the mean first passage time and the escape rates for both types of particles. Using the expression for the time evolution of the number of particles, we calculate the number of particles at any time for each type of particle in each well. We also find expressions for the maximum separation between the particles and the time required to get the maximum separation. Finally, we calculate the barrier height that gives us the optimum separation between the particles. For comparison, we discuss the homogeneous temperature case. In chapter 4, we present our second model. We derive the expression for the steady state current of a particle moving on a tilted ratchet potential with non-homogeneous temperature background. Next we apply this to the second model and look how we can segregate the mixtures. The last chapter is devoted to summary and concluding remarks.

Chapter 2

DYNAMICS OF A BROWNIAN PARTICLE IN A BISTABLE POTENTIAL

Our goal is to separate mixtures of ideal Brownian particles. Our model can be explained as follows. We have a double well potential, with non-homogeneous temperature background, in which two types of non-interacting Brownian particles, say A and B, with different diffusion constants are originally found in mixtures in the left well while the right well is empty. As a result of the temperature gradient, a flow of particles will be induced from the left to the right well. Since the two particles have different diffusion constants, their rate of escape to the right well will be different. This gives rise to a different number of particles of type A and B in the right well as the process proceeds. We want to know the time when the difference in the number of particles of the two types is maximum. This is the time we need to stop the process to get the best segregation of the mixtures.

To do this, first we have to look at the dynamics of a Brownian particle in a double well potential. We calculate the mean first passage time (MFPT) for a particle to move from one well to the other, and hence the escape rates. This is done in the next sections. We also study how the number of particles vary with time in each well.

2.1 Particle in a Double Well Potential

Consider a double well potential like the one shown in Fig 2.1. Consider a Brownian particle moving in such a potential. The Langevin equation governing the motion of such a particle is given by

$$m\frac{d^2x}{dt^2} \;=\; -\gamma\frac{dx}{dt} \;-\; V'(x) \;+\; \sqrt{2k_BT(x)\gamma}\,\xi(t), \tag{2.1}$$

where x describes the position of the particle at time t, m is the mass of the particle, γ is the damping (friction) coefficient due to the fluid in which the particle is moving, k_B is the Boltzmann constant, $T(x)$ is the position-dependent temperature, $V'(x)$ is the force derivable from some potential $V(x)$ and the prime denotes differentiation with respect to x, $\xi(t)$ is a Gaussian white noise satisfying

$$< \xi(t) > \;=\; 0, \tag{2.2}$$

and

$$< \xi(t)\xi(t') > \;=\; A\delta(t-t'), \tag{2.3}$$

where A is a constant which is equal to $\sqrt{2k_BT(x)\gamma}$ for a Gaussian white noise.

For heavy damping (γ very large), the above equation reduces to

$$dx \;=\; -\frac{1}{\gamma}V'(x)dt \;+\; \sqrt{\frac{2k_BT(x)}{\gamma}}\,dW(t) \tag{2.4}$$

where $dW(t) \;=\; \xi(t)dt$. The Fokker-Planck equation (FPE) corresponding to this Langevin

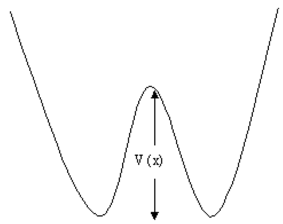

Figure 2.1: Double well potential

equation is

$$\partial_t p(x,t) \;=\; \frac{1}{\gamma}\,\partial_x[V'(x)p(x,t)] \;+\; \frac{k_B}{\gamma}\,\partial_x^2[T(x)p(x,t)], \tag{2.5}$$

where $p(x,t)$ is the probability density of finding the particle at position x at time t and γ is taken to be the same through out the medium.

For a Langevin equation of the form

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

the forward FPE is given by [8]

$$\partial_t p(x,t) \;=\; -\;\partial_x[A(x)\;p(x,t)] \;+\; \frac{1}{2}\partial_x^2[B(x)^2\;p(x,t)],$$

and the backward FPE is given by

$$\partial_t p(x,t) \;=\; A(x)\partial_x p(x,t) \;+\; \frac{1}{2}B(x)^2\;\partial_x^2 p(x,t).$$

We begin by calculating the Mean First Passage Time (MFPT) taken by the particle to move from one well to the other, and vice versa.

2.2 Calculation of Mean First Passage Time

We want to know how long a particle whose dynamics is governed by the FPE, Eq.(2.5), remains in a certain region of x. The solution of this problem can be achieved by using the backward FPE.

2.2.1 Two Absorbing Barriers

Let a particle be initially at position x at time t=0 in an interval (a,b).

$$a \leq x \leq b$$

We erect absorbing barriers at a and b so that the particle is removed when it reaches a or b. Then by mean first passage time we mean the average time taken by the particle to reach point a or b for the first time. Hence if it is still in the interval (a,b), it has never left the interval. Let G(x,t) be the probability of finding the particle still in the interval (a,b) at time t. Then,

$$G(x,t) \;=\; \int_a^b dx' p(x',t|x,0). \tag{2.6}$$

Note that $p(x',t|x,0)$ is the conditional probability that the particle is at x' at time t given that it was at x at time $t \;=\; 0$.

Let $\mathcal{P}(t)dt$ be the probability that the particle leaves the interval (a,b) between t and t+dt. This probability is the same as the probability of staying in the interval until time t, and then leaving the interval between t and t+dt, i.e.,

$$\mathcal{P}(t)dt \;=\; G(x,t)\int_a^b dx\ p(z,t+\Delta t|x,t), \tag{2.7}$$

where $z \notin (a,b)$. Eq.(2.7) can equally be expressed as

$$\mathcal{P}(t)dt \;=\; G(x,t)[1-\int_a^b dx' \int_a^b dx\ \ p(x',t+\Delta t|x,t)],$$

where the term with the double integral is the probability of staying in the interval up to t+dt, so that

$$\int_a^b dx\ p(z, t+\Delta t|x, t)\ +\ \int_a^b dx' \int_a^b dx\ p(x', t+\Delta t|x, t)\ =\ 1. \tag{2.8}$$

Hence,

$$\mathcal{P}(t)dt\ =\ G(x, t)\ -\ G(x, t+\Delta t)\ =\ -\,\partial_t G(x, t)dt. \tag{2.9}$$

Now, the mean first passage time is given by

$$< t >\ =\ \int_0^\infty dt\ t\ \mathcal{P}(t). \tag{2.10}$$

Using Eq.(2.9) and integrating Eq.(2.10) by parts, we get

$$< t >\ =\ t(x)\ =\ \int_0^\infty dt\ G(x, t). \tag{2.11}$$

Since the system is time homogeneous, Eq.(2.6) can be written as

$$G(x, t)\ =\ \int dx' p(x', 0|x, -t). \tag{2.12}$$

Differentiating this once with respect to time, we get

$$\partial_t G(x, t)\ =\ \int dx' \partial_t p(x', 0|x, -t). \tag{2.13}$$

From the backward FPE, we have

$$\partial_t p(x', 0|x, -t)\ =\ A(x)\partial_x p(x', 0|x, -t)\ +\ \frac{1}{2}B(x)\partial_x^2 p(x', 0|x, -t). \tag{2.14}$$

Eq.(2.13) then becomes

$$\partial_t G(x, t)\ =\ \int dx'[A(x)\partial_x p(x', 0|x, -t)\ +\ \frac{1}{2}B(x)\partial_x^2 p(x', 0|x, -t)],$$

so that,

$$\partial_t G(x, t)\ =\ A(x)\partial_x G(x, t) + \frac{1}{2}B(x)\partial_x^2 G(x, t). \tag{2.15}$$

Let us integrate Eq.(2.15) over dt in the interval $(0, \infty)$.

$$\begin{aligned}\int_0^\infty dt\ \partial_t G(x,t) &= \int_0^\infty dt\ [A(x)\partial_x G(x,t)] + \frac{1}{2}\int_0^\infty dt\ [B(x)\partial_x^2 G(x,t)],\\ G(x,\infty) - G(x,0) &= A(x)\partial_x \int_0^\infty dt\ G(x,t) + \frac{1}{2}B(x)\partial_x^2 \int_0^\infty dt\ G(x,t).\end{aligned} \tag{2.16}$$

At $t = \infty$, the particle will leave the interval and hence $G(x,\infty) = 0$. But at $t = 0$, we have

$$G(x,0) = \int dx' p(x', 0|x, 0) = \int dx' \delta(x' - x) = 1.$$

With this and Eq.(2.11), we can write Eq.(2.16) as

$$A(x)\partial_x t(x) + \frac{1}{2}B(x)\partial_x^2 t(x) = -1. \tag{2.17}$$

Eq.(2.17) is the ordinary differential equation for t(x) with the boundary condition,

$$t(a) = t(b) = 0, \tag{2.18}$$

where a and b are the absorbing boundaries. This is because if the particle is originally at a or b, it is removed from the system. To get the mean first passage time, we have to solve Eq.(2.17) which can be written as

$$\frac{d^2t(x)}{dx^2} + \frac{2A(x)}{B(x)}\frac{dt(x)}{dx} = -\frac{2}{B(x)}. \tag{2.19}$$

Let us define a function $f(x)$ as

$$f(x) = \partial_x t(x). \tag{2.20}$$

Then Eq.(2.19) can be written as

$$\frac{df(x)}{dx} + \frac{2A(x)}{B(x)}f(x) = -\frac{2}{B(x)}. \tag{2.21}$$

This is a non-homogeneous differential equation. Let us first find the solution of the homogeneous differential equation

$$\frac{df(x)}{dx} + \frac{2A(x)}{B(x)}f(x) = 0,$$

whose solution is given by

$$f(x) = \frac{f(a)}{\psi(x)}, \tag{2.22}$$

where

$$\psi(x) = e^{2\int_a^x dx' \frac{A(x')}{B(x')}}. \tag{2.23}$$

Eq.(2.22) is a solution to the homogeneous differential equation. For the non-homogeneous differential equation, Eq.(2.21), we assume a general equation of the form,

$$f(x) = \frac{F(x)}{\psi(x)}. \tag{2.24}$$

Inserting this in to Eq.(2.21), we find after some manipulation,

$$F(x) = F(a) - 2\int_a^x dx' \frac{\psi(x')}{B(x')}. \tag{2.25}$$

Eq.(2.24) then becomes,

$$f(x) = \frac{F(a)}{\psi(x)} - \frac{2}{\psi(x)}\int_a^x dx' \frac{\psi(x')}{B(x')}.$$

Using Eq.(2.20) we can write this as

$$\frac{dt(x)}{dx} = \frac{F(a)}{\psi(x)} - \frac{2}{\psi(x)}\int_a^x dx' \frac{\psi(x')}{B(x')}. \tag{2.26}$$

Integrating this once more with respect to x, we get

$$t(x) - t(a) = F(a)\int_a^x \frac{dy}{\psi(y)} - 2\int_a^x \frac{dy'}{\psi(y')}\int_a^{y'} dz \frac{\psi(z)}{B(z)}. \tag{2.27}$$

Applying the boundary condition given by Eq.(2.18), we get

$$F(a) = 2\frac{[\int_a^x \frac{dy'}{\psi(y')}\int_a^{y'} dz \frac{\psi(z)}{B(z)} + \int_x^b \frac{dy'}{\psi(y')}\int_a^{y'} dz \frac{\psi(z)}{B(z)}]}{\int_a^b \frac{dy}{\psi(y)}}. \tag{2.28}$$

Substituting Eq.(2.28) into (2.27),we get the mean first passage time for a particle between two absorbing barriers to be

$$t(x) = 2\frac{[\int_a^x \frac{dy}{\psi(y)}\int_x^b \frac{dy'}{\psi(y')}\int_a^{y'} dz \frac{\psi(z)}{B(z)} - \int_x^b \frac{dy}{\psi(y)}\int_a^x \frac{dy'}{\psi(y')}\int_a^{y'} dz \frac{\psi(z)}{B(z)}]}{\int_a^b \frac{dy}{\psi(y)}}. \tag{2.29}$$

We are interested in the case where one of the boundaries is absorbing while the other is reflecting. The MFPT in that case is shown in the next section.

2.2.2 One Absorbing Barrier

Here we consider motion of a particle still in the interval (a,b) but when only either a or b is absorbing.

i) a reflecting and b absorbing

From the backward FPE, the boundary conditions are

$$\partial_x t(a) \;=\; 0, \tag{2.30}$$

and

$$t(b) \;=\; 0, \tag{2.31}$$

where Eq.(2.30) holds for a reflecting boundary, while Eq.(2.31) for an absorbing boundary. With this boundary conditions, let us consider Eq.(2.25)

$$F(x) \;=\; F(a) \;-\; 2\int_a^x dx' \frac{\psi(x')}{B(x')} \tag{2.25}$$

with

$$F(a) \;=\; f(a)\psi(a) \;=\; \partial_x t(a)\psi(a) \;=\; 0,$$

and hence

$$F(x) \;=\; -\; 2\int_a^x dx' \frac{\psi(x')}{B(x')}. \tag{2.32}$$

Eq.(2.24) then becomes

$$f(x) \;=\; -\; \frac{2}{\psi(x)} \int_a^x dx' \frac{\psi(x')}{B(x')}. \tag{2.33}$$

Using Eq.(2.20) and integrating, we will have

$$t(x) - t(a) = -2\int_a^x \frac{dy}{\psi(y)} \int_a^y dz \frac{\psi(z)}{B(z)}. \tag{2.34}$$

Applying the boundary conditions in Eq.(2.30) and (2.31), we get

$$t(a) = 2\int_a^b \frac{dy}{\psi(y)} \int_a^y dz \frac{\psi(z)}{B(z)}. \tag{2.35}$$

Substituting Eq.(2.35) into (2.34), we find

$$t(x) = 2\int_x^b \frac{dy}{\psi(y)} \int_a^y dz \frac{\psi(z)}{B(z)}. \tag{2.36}$$

ii) a absorbing and b reflecting

In this case the boundary conditions become

$$t(a) = 0, \tag{2.37}$$

and

$$\partial_x t(b) = 0. \tag{2.38}$$

With Eq.(2.37), Eq.(2.27) can be written as

$$t(x) = F(a)\int_a^x \frac{dy}{\psi(y)} - 2\int_a^x \frac{dy'}{\psi(y')} \int_a^{y'} dz \frac{\psi(z)}{B(z)}. \tag{2.39}$$

Differentiating this once with respect to x, we get

$$\partial_x t(x) = \frac{F(a)}{\psi(x)} - \frac{2}{\psi(x)} \int_a^x dz \frac{\psi(z)}{B(z)}. \tag{2.40}$$

Applying the boundary condition in Eq.(2.38), we will get

$$F(a) = 2\int_a^b dz \frac{\psi(z)}{B(z)} \tag{2.41}$$

With this Eq.(2.39) becomes

$$t(x) \;=\; 2\int_a^x \frac{dy}{\psi(y)}\int_y^b dz\frac{\psi(z)}{B(z)} \tag{2.42}$$

As described earlier, the main aim of this thesis is to segregate mixtures of Brownian particles. This is achieved by counting the number of particles of each type that reaches the right well. To do that we have to know the escape rates of each type of particle from one well to the other. The escape rates can easily be found from the MFPTs. It was proved that for an arbitrary time-homogeneous stochastic process, Kramer's flux-over-barrier (escape) rate is identical to the inverse of the associated mean first passage time [9]. Hence, getting the MFPT is equivalent to getting the escape rates. Once we get the escape rates we can proceed to see how the particles evolve in time from one well to the other.

2.3 Evolution in time of the number of particles

Consider a double well potential. Suppose initially there are N particles in the left well and no particles in the right well. The equations governing the number of particles in the left and right wells at any time t are

$$\frac{dn_L(t)}{dt} \;=\; -\;\lambda_1 n_L(t) \;+\; \lambda_2 n_R(t) \tag{2.43}$$

$$\frac{dn_R(t)}{dt} \;=\; \lambda_1 n_L(t) \;-\; \lambda_2 n_R(t), \tag{2.44}$$

where λ_1 is the escape rate from the left well to the right well, λ_2 is the escape rate from the right well to the left well and $n_{L(R)}(t)$ is the number of particles in the left (right) well at any time. To get the number of particles in the left and right wells at any time, we have to solve the coupled differential equations, Eqs.(2.43) and (2.44). To do that we assume a solution of the form

$$n_L(t) \;=\; Ae^{\omega t} \quad and \quad n_R(t) \;=\; Be^{\omega t}, \tag{2.45}$$

with initial conditions, $n_L(0) = N$ and $n_R(0) = 0$. Substituting Eq.(2.45) into Eqs.(2.43) and (2.44), and solving the resulting equations, we get $\omega = 0$ or $\omega = -(\lambda_1 + \lambda_2)$ so that

$$n_L(t) \;=\; A_1 \;+\; A_2 e^{-\lambda t} \tag{2.46}$$

$$n_R(t) \;=\; B_1 \;+\; B_2 e^{-\lambda t}, \tag{2.47}$$

where $\lambda = \lambda_1 + \lambda_2$. Since

$$\frac{dn_L(t)}{dt} \;=\; -\;\frac{dn_R(t)}{dt}, \tag{2.48}$$

and using the initial conditions, we finally arrive at the population in each well to be given by

$$n_L(t) \;=\; \frac{N}{\lambda}(\lambda_2 \;+\; \lambda_1 e^{-\lambda t}), \tag{2.49}$$

and

$$n_R(t) \;=\; \frac{N\lambda_1}{\lambda}(1 \;-\; e^{-\lambda t}). \tag{2.50}$$

In this chapter, we have calculated the MFPT for a particle in a double well potential. From the MFPT, one can write for the escape rate [9] as

$$\lambda_{1(2)} \;=\; \frac{1}{t_{1(2)}}, \tag{2.51}$$

where $\lambda_{1(2)}$ is the escape rate from the left (right) to the right (left) well and $t_{1(2)}$ is the corresponding MFPT. In this chapter, in addition to the MFPTs, We have shown how the number of particles evolve in time.

In the next chapter, we apply these results to our model. To be able to solve our problem analytically, we have taken a double well potential which is piecewise linear (W-potential) with a piecewise constant non-homogeneous temperature background. In addition to the expressions for the MFPTs, we will study the dependence of the process of segregation on the parameters characterizing our model.

Chapter 3

SEGREGATION OF BROWNIAN PARTICLES USING A BISTABLE POTENTIAL

Suppose we have an asymmetric W-potential like the one shown in Fig.(3.1) below. We have two types of non-interacting Brownian particles, say A and B, with different diffusion constants D_A and D_B mixed up in the left well. We create a non-homogeneous temperature background as shown. The particles are free to diffuse across the wells and we want to know the time to get an optimum separation of the mixtures.

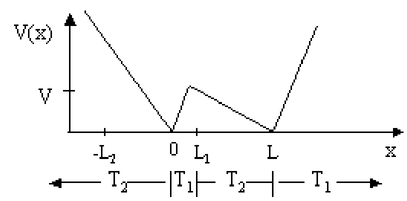

Figure 3.1: An asymmetric W-potential

The potential profile for this asymmetric potential is

$$V(x) = \begin{cases} -\frac{V_0}{L_2}x, & \text{if } x < 0; \\ \frac{V}{L_1}x, & \text{if } 0 \le x \le L_1, \\ -\frac{V}{L_2}\left(x - L\right), & \text{if } L_1 \le x \le L, \\ \frac{V_0}{L_1}\left(x - L\right), & \text{if } x \ge L_1, \end{cases}$$

Figure 3.1 is the double well potential considered in the last chapter except for the piecewise linear nature of the potential. So using Eq.(2.36) and (2.42), we can calculate the MFPT taken by a particle to move from $x = 0$ to $x = L$ and from $x = L$ to $x = 0$.

3.1 MFPT from $x = 0$ to $x = L$

In this case, we have a reflecting boundary to the left of $x = 0$ at $-\infty$ and the particle is considered to be absorbed when it reaches $x = L$. So we use Eq.(2.36) with the substitution that $x = 0$, $b = L$ and take the limit $a \to -\infty$. And with $A(x) = -\frac{V'(x)}{\gamma}$ and $B(x) = \frac{2k_BT(x)}{\gamma}$, Eq.(2.36) can be written as

$$t(0 \to L) = \frac{\gamma}{k_B} \int_0^L \frac{dx}{\psi(x)} \int_a^x dx' \frac{\psi(x')}{T(x')}, \tag{3.1}$$

where

$$\psi(x) = Exp\,[-\frac{1}{k_B} \int_a^x dx' \frac{V'(x')}{T(x')}]. \tag{3.2}$$

We can write Eq.(3.1) as

$$t(0 \to L) = \frac{\gamma}{k_B}[F_1 + F_2], \tag{3.3}$$

where

$$F_1 = \int_0^{L_1} \frac{dx}{\psi(x)} \int_a^x dx' \frac{\psi(x')}{T(x')}, \tag{3.4}$$

and

$$F_2 = \int_{L_1}^{L} \frac{dx}{\psi(x)} \int_a^x dx' \frac{\psi(x')}{T(x')}. \tag{3.5}$$

Integrating Eqs.(3.4) and (3.5), and taking the limit as $a \to -\infty$, we get

$$F_1 = \frac{k_BL_2}{V_0}\frac{k_BT_1L_1}{V}(e^{\frac{V}{k_BT_1}} - 1) + \frac{k_BL_1}{V}\frac{k_BT_1L_1}{V}(e^{\frac{V}{k_BT_1}} - 1) - \frac{k_BL_1^2}{V}, \tag{3.6}$$

and

$$F_2 = -\frac{k_BL_2}{V_0}\frac{k_BT_2L_2}{V}e^{\frac{V}{k_BT_1}}(e^{\frac{-V}{k_BT_2}} - 1) - \frac{k_BL_1}{V}\frac{k_BT_2L_2}{V}(e^{\frac{V}{k_BT_1}} - 1)(e^{\frac{-V}{k_BT_2}} - 1)$$
$$+ \frac{k_BL_2}{V}\frac{k_BT_2L_2}{V}(e^{\frac{-V}{k_BT_2}} - 1) + \frac{k_BL_2^2}{V}. \tag{3.7}$$

Using Eqs.(3.6) and (3.7) in Eq.(3.3), we find the MFPT from $x = 0$ to $x = L$ to be

$$t(0 \to L) = \frac{\gamma}{V}[k_BT_1L_1(\frac{L_2}{V_0} + \frac{L_1}{V})(e^{\frac{V}{k_BT_1}} - 1) - k_BT_2L_2^2(\frac{e^{\frac{V}{k_BT_1}}}{V_0} - \frac{1}{V})(e^{\frac{-V}{k_BT_2}} - 1)$$
$$- \frac{k_BT_2L_1L_2}{V}(e^{\frac{V}{k_BT_1}} - 1)(e^{\frac{-V}{k_BT_2}} - 1) - (L_1^2 - L_2^2)]. \tag{3.8}$$

3.2 MFPT from $x = L$ to $x = 0$

Here we have a reflecting boundary to the right of $x = L$ at $x = \infty$ and the particle is considered to be absorbed when it reaches $x = 0$. So we use Eq.(2.42) with the substitution that $a = 0$, $x = L$ and take the limit $b \to \infty$. And with $A(x) = -\frac{V'(x)}{\gamma}$and $B(x) = \frac{2k_B T(x)}{\gamma}$, Eq.(2.42) can be written as

$$t(L \to 0) = \frac{\gamma}{k_B} \int_0^L \frac{dx}{\psi(x)} \int_x^b dx' \frac{\psi(x')}{T(x')},$$

which can be written as

$$t(L \to 0) = \frac{\gamma}{k_B} \int_L^0 \frac{dx}{\psi(x)} \int_b^x dx' \frac{\psi(x')}{T(x')}, \tag{3.9}$$

where $\psi(x)$ is given by Eq.(3.2). We can write Eq.(3.9) as

$$t(L \to 0) = \frac{\gamma}{k_B}[G_1 + G_2], \tag{3.10}$$

where

$$G_1 = \int_L^{L_1} \frac{dx}{\psi(x)} \int_b^x dx' \frac{\psi(x')}{T(x')}, \tag{3.11}$$

and

$$G_2 = \int_{L_1}^0 \frac{dx}{\psi(x)} \int_b^x dx' \frac{\psi(x')}{T(x')}. \tag{3.12}$$

Integrating Eqs.(3.11) and (3.12), and taking the limit as $b \to \infty$, we get

$$G_1 = \frac{k_B L_1}{V_0} \frac{k_B T_2 L_2}{V} (e^{\frac{V}{k_B T_2}} - 1) + \frac{k_B L_2}{V} \frac{k_B T_2 L_2}{V} (e^{\frac{V}{k_B T_2}} - 1) - \frac{k_B L_2^2}{V}, \tag{3.13}$$

and

$$G_2 = -\frac{k_B L_1}{V_0} \frac{k_B T_1 L_1}{V} e^{\frac{V}{k_B T_2}} (e^{\frac{-V}{k_B T_1}} - 1) - \frac{k_B L_2}{V} \frac{k_B T_1 L_1}{V} (e^{\frac{-V}{k_B T_1}} - 1)(e^{\frac{V}{k_B T_2}} - 1)$$
$$+ \frac{k_B L_1}{V} \frac{k_B T_1 L_1}{V} (e^{\frac{-V}{k_B T_1}} - 1) + \frac{k_B L_1^2}{V}. \tag{3.14}$$

Using Eq.(3.13) and (3.14) into Eq.(3.10), we get the MFPT from $x = L$ to $x = 0$ to be

$$t(L \to 0) = \frac{\gamma}{V}[k_B T_2 L_2 (\frac{L_1}{V_0} + \frac{L_2}{V})(e^{\frac{V}{k_B T_2}} - 1) - k_B T_1 L_1^2 (\frac{e^{\frac{V}{k_B T_2}}}{V_0} - \frac{1}{V})(e^{\frac{-V}{k_B T_1}} - 1) - \frac{k_B T_1 L_1 L_2}{V}(e^{\frac{-V}{k_B T_1}} - 1)(e^{\frac{V}{k_B T_2}} - 1) + (L_1^2 - L_2^2)]. \quad (3.15)$$

Consider the situation of Fig.(3.1). Let the hot region be at a temperature T_1 and the cold region be at a temperature T_2 such that

$$T_1 = (1 + \alpha)T_2$$

where α is some non-negative number, and let $u = \frac{V}{k_B T_2}$, $u_0 = \frac{V_0}{k_B T_2}$, and $\beta = \frac{L_2}{L_1}$. With this, the MFPTs given by Eqs.(3.8) and (3.15) can be written as

$$t(0 \to L) = \frac{\gamma}{u}\frac{L_1^2}{k_B T_2}[(1 + \alpha)(\frac{\beta}{u_0} + \frac{1}{u})(e^{\frac{u}{1+\alpha}} - 1) - \beta^2(\frac{e^{\frac{u}{1+\alpha}}}{u_0} - \frac{1}{u})(e^{-u} - 1) - \frac{\beta}{u}(e^{\frac{u}{1+\alpha}} - 1)(e^{-u} - 1) - (1 - \beta^2)], \quad (3.16)$$

and

$$t(L \to 0) = \frac{\gamma}{u}\frac{L_1^2}{k_B T_2}[\beta(\frac{1}{u_0} + \frac{\beta}{u})(e^{u} - 1) - (1 + \alpha)(\frac{e^{u}}{u_0} - \frac{1}{u})(e^{-\frac{u}{1+\alpha}} - 1) - \frac{\beta}{u}(1 + \alpha)(e^{-\frac{u}{1+\alpha}} - 1)(e^{u} - 1) + (1 - \beta^2)]. \quad (3.17)$$

We have two types of particles mixed up in the left well. The two particles have diffusion constants D_A and D_B such that

$$D_{A(B)}(x) = \frac{k_B T(x)}{\gamma_{A(B)}}.$$

Since $T(x)$ varies in the same interval for both particles, the difference in the diffusion constants is as a result of the damping coefficients on the particles.

Using Eqs.(2.51), (2.52), (3.16) and (3.17), we will find the escape rates for particles of type A and type B to be

$$\lambda_{1A} = \frac{u}{\gamma_A g}, \quad (3.18)$$

$$\lambda_{2A} = \frac{u}{\gamma_A h}, \tag{3.19}$$

$$\lambda_{1B} = \frac{u}{\gamma_B g}, \tag{3.20}$$

$$\lambda_{2B} = \frac{u}{\gamma_B h}, \tag{3.21}$$

where

$$g = \frac{L_1^2}{k_B T_2} [(1 + \alpha)(\frac{\beta}{u_0} + \frac{1}{u})(e^{\frac{u}{1+\alpha}} - 1) - \beta^2(\frac{e^{\frac{u}{1+\alpha}}}{u_0} - \frac{1}{u})(e^{-u} - 1)$$
$$- \frac{\beta}{u}(e^{\frac{u}{1+\alpha}} - 1)(e^{-u} - 1) - (1 - \beta^2)], \tag{3.22}$$

and

$$h = \frac{L_1^2}{k_B T_2} [\beta(\frac{1}{u_0} + \frac{\beta}{u})(e^{u} - 1) - (1 + \alpha)(\frac{e^{u}}{u_0} - \frac{1}{u})(e^{-\frac{u}{1+\alpha}} - 1)$$
$$- \frac{\beta}{u}(1 + \alpha)(e^{-\frac{u}{1+\alpha}} - 1)(e^{u} - 1) + (1 - \beta^2)]. \tag{3.23}$$

Using Eqs.(2.49) and (2.50), the number of particles of type A and B in the left and right wells at any time is given by

$$n_{LA}(t) = \frac{N_A}{\lambda_A}(\lambda_{2A} + \lambda_{1A} e^{-\lambda_A t}), \tag{3.24}$$

$$n_{RA}(t) = \frac{N_A \lambda_{1A}}{\lambda_A}(1 - e^{-\lambda_A t}), \tag{3.25}$$

$$n_{LB}(t) = \frac{N_B}{\lambda_B}(\lambda_{2B} + \lambda_{1B} e^{-\lambda_B t}), \tag{3.26}$$

$$n_{RB}(t) = \frac{N_B \lambda_{1B}}{\lambda_B}(1 - e^{-\lambda_B t}), \tag{3.27}$$

where $\lambda_A = \lambda_{1A} + \lambda_{2A}$ and $\lambda_B = \lambda_{1B} + \lambda_{2B}$.

3.3 Result and Discussions

The particles are free to flow from one well to the other by the thermal kick they get from the background with their respective escape rates. Initially, there are N_A particles of type

A and N_B particles of type B mixed up in the left well and the right well is empty. We want to separate the mixtures and hence we are interested in the number of particles in the right well. In order to have a good separation, we have to stop the flow when

$$\Delta = n_{RA} - n_{RB} \tag{3.28}$$

is maximum, assuming $D_A > D_B$ or $\gamma_A < \gamma_B$.

$$\Delta(u,t,r_i) = \frac{h}{(g + h)}[N_A(1 - e^{-\lambda_A t}) - N_B(1 - e^{-\lambda_B t})], \tag{3.29}$$

where r_i stands for the parameters like α, β,and γ and noting that

$$\frac{\lambda_{1A}}{\lambda_A} = \frac{\lambda_{1B}}{\lambda_B} = \frac{h}{(g + h)},$$

Eq.(3.29) can also be written as

$$\Delta(u,t,r_i) = \frac{h}{(g + h)}[(N_A - N_B) + N_B e^{[-\frac{u}{\gamma_B}\frac{h + g}{gh} t]} - N_A e^{[-\frac{u}{\gamma_A}\frac{h + g}{gh} t]}]. \tag{3.30}$$

We have to stop the flow when Δ, given by Eq.(3.30) is maximum. This occurs for

$$\partial_t \Delta(u,t,r_i) = 0. \tag{3.31}$$

With this we find the time, t_m, to get the maximum separation between the particles to be

$$t_m = \frac{\gamma_A\gamma_B}{\gamma_B - \gamma_A}\frac{Log\frac{\gamma_B}{N_B} - Log\frac{\gamma_A}{N_A}}{u(\frac{h + g}{gh})}. \tag{3.32}$$

Rearranging Eq.(3.32), we get

$$(\frac{h + g}{gh})ut_m = \frac{\gamma_A\gamma_B}{\gamma_B - \gamma_A}(Log\frac{\gamma_B}{N_B} - Log\frac{\gamma_A}{N_A}). \tag{3.33}$$

Using Eq.(3.33) into Eq.(3.30), we will get the maximum separation between the particles to be,

$$\Delta_m = \frac{h}{(g + h)}[(N_A - N_B) + N_B\, exp[-\frac{\gamma_A}{\gamma_B - \gamma_A}(Log\frac{\gamma_B}{N_B} - Log\frac{\gamma_A}{N_A})] - N_A\, exp[-\frac{\gamma_B}{\gamma_B - \gamma_A}(Log\frac{\gamma_B}{N_B} - Log\frac{\gamma_A}{N_A})]]. \tag{3.34}$$

Let us now consider the case of high and low barrier limits.

3.3.1 High Barrier Limit $(u >> 1)$

Here we take the limit $u >> 1$ in Eq.(3.34) above. Let us define a function $f(\gamma_{A,B}, N_{A,B})$ such that

$$f(\gamma_{A,B}, N_{A,B}) = (N_A - N_B) + N_B\, exp[-\frac{\gamma_A}{\gamma_B - \gamma_A}(Log\frac{\gamma_B}{N_B} - Log\frac{\gamma_A}{N_A})]$$
$$- N_A\, exp[-\frac{\gamma_B}{\gamma_B - \gamma_A}(Log\frac{\gamma_B}{N_B} - Log\frac{\gamma_A}{N_A})]. \quad (3.35)$$

This function is independent of u. So we can write Eq.(3.34) as

$$\Delta_m = \frac{h}{(g + h)}f(\gamma_{A,B}, N_{A,B}). \quad (3.36)$$

The dependence of Δ_m on u is thus through g and h as can be seen from Eqs.(3.22) and (3.23). So for u very large we will have $e^u >> 1$ and $e^{-u} << 1$ and hence we ignore 1 compared to e^u and e^{-u} compared to 1. With this Eqs.(3.22) and (3.23) can be written as

$$g = \frac{L_1^2}{k_B T_2}\,[(1 + \alpha)(\frac{\beta}{u_0} + \frac{1}{u}) + \frac{\beta^2}{u_0} + \frac{\beta}{u}]e^{\frac{u}{(1 + \alpha)}}, \quad (3.37)$$

and

$$h = \frac{L_1^2}{k_B T_2}\,[(1 + \alpha)(\frac{1}{u_0} + \frac{\beta}{u}) + \frac{\beta}{u_0} + \frac{\beta^2}{u}]e^u. \quad (3.38)$$

With this Eq.(3.36) becomes

$$\Delta_m = \frac{1}{(1 + \frac{\frac{1}{u_0}(\beta^2 + (1 + \alpha)\beta) + \frac{1}{u}(1 + \alpha + \beta)}{\frac{1}{u_0}(1 + \alpha + \beta) + \frac{1}{u}(\beta^2 + (1 + \alpha)\beta)})\, e^{-\frac{\alpha u}{1 + \alpha}}}f(\gamma_{A,B}, N_{A,B}). \quad (3.39)$$

For u_0 and u very large, Eq.(3.39) can be approximated as

$$\Delta_m = f(\gamma_{A,B}, N_{A,B}). \quad (3.40)$$

3.3.2 Low Barrier Limit$(u << 1)$

Here we take the limit $u << 1$ in Eq.(3.36). Clearly $f(\gamma_{A,B}, N_{A,B})$ is independent of u. For u very small, we can expand the exponential terms. Let us expand g and h, given by

Eqs.(3.22) and (3.23), in powers of u and take terms of order u only. With this we will have,

$$g = \frac{uL_1^2}{k_B T_2}[\frac{\beta(\beta + 1)}{u_0} + \frac{(1 + \beta^2(1 + \alpha) + \beta)}{1 + \alpha}], \tag{3.41}$$

and

$$h = \frac{uL_1^2}{k_B T_2}[\frac{(1 + \beta)}{u_0} + \frac{(1 + \beta^2(1 + \alpha) + \beta(1 + \alpha))}{1 + \alpha}]. \tag{3.42}$$

Eq.(3.36) can then be written as

$$\Delta_m = \frac{\frac{(1 + \beta)}{u_0} + \frac{(1 + \beta^2(1 + \alpha) + \beta(1 + \alpha))}{1 + \alpha}}{\frac{(\beta + 1)^2}{u_0} + \frac{(2 + 2\beta^2(1 + \alpha) + \beta(2 + \alpha))}{(1 + \alpha)}} f(\gamma_{A,B}, N_{A,B}), \tag{3.43}$$

which for u_0 large reduces to

$$\Delta_m = \frac{(1 + \beta^2(1 + \alpha) + \beta(1 + \alpha))}{(2 + 2\beta^2(1 + \alpha) + \beta(2 + \alpha))} f(\gamma_{A,B}, N_{A,B}) \qquad (3.44).$$

This means that Δ_m will roughly be equal to $\frac{1}{2} f(\gamma_{A,B}, N_{A,B})$.

3.4 Numerical Results

As we have shown earlier, we have calculated analytically $\Delta(u, t, r_i)$, the difference in the number of particles of the two types. As our interest is to separate the mixtures, we have to stop the flow when Δ is maximum. We have also calculated analytically the time $t_m(u, r_i)$ to get the maximum separation and also the value of the maximum separation $\Delta_m(u, r_i)$. We are specifically interested in how the barrier height u affects both Δ and t.

We now study the effect numerically. We have plotted below Δ as a function of t for various values of the barrier height u. We begin with $N_A = N_B$ initially, i.e., initially we have equal number of particles of type A and B mixed up in the left box.

The plot of Δ versus t is shown in Fig.(3.2) - (3.4) for $\beta = 3$, $\alpha = 1$, $u_0 = 10$, $N_A = N_B = 100$, and $\gamma_B = 2\gamma_A$. In these figures D stands for Δ. We have plotted Δ

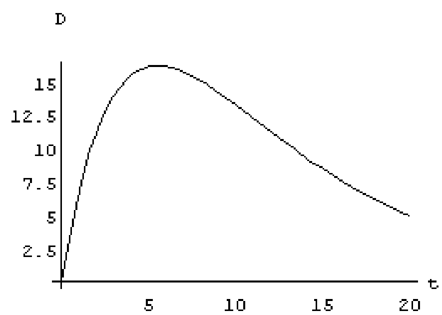

Figure 3.2: Plot of Δ versus t for $u = 1$

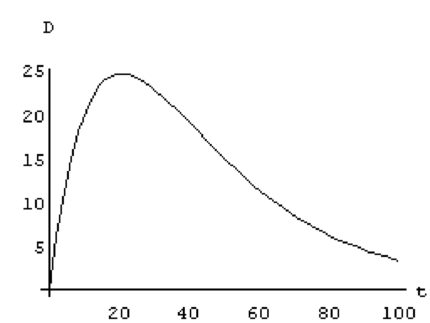

Figure 3.3: Plot of Δ versus t for $u = 8$

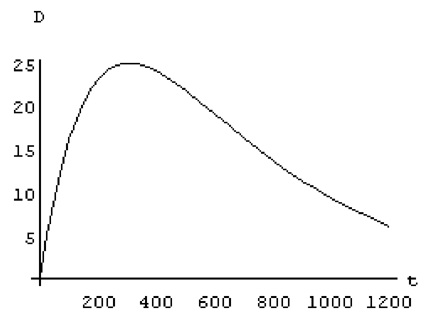

Figure 3.4: Plot of Δ versus t for $u = 15$

versus t from $u = 1$, $u = 8$ and $u = 15$. All the plots show us that Δ has a maximum at some value of t as expected. As we increase u, both the maximum value of Δ and the time at which this maximum occurs increase.

To look at how Δ_m and t_m vary as we vary u, we have plotted them as a function of u as shown in Fig.(3.5) and (3.6). In these figures D_m stands for Δ_m. As we increase the barrier height u, Δ_m goes increasing which, however, saturates for large values of u while t_m increases exponentially. So increasing the barrier height to very large values has very little or negligible advantage in separating the mixtures.

As we have shown above, keeping the potential very small gives a small value of Δ_m although the process takes place in short time. Keeping the potential very large gives us the best separation, but that is at the expense of waiting for a very long time. We want a reasonably good separation while, at the same time, not wait for an infinitely long time. How can we get an optimum separation in a finite time?

Let us define a function Ω such that

$$\Omega \;=\; \frac{\Delta_m}{t_m}. \tag{3.45}$$

This function is the ratio of the maximum separation between the particles to the time to get the maximum separation. It is a function which describes the rate of maximum segregation between the particles. We have plotted Ω as a function of u as shown in Fig.(3.7), where W stands for Ω. The graph has a maximum at a finite value of u. We take the value of u at which Ω is a maximum to be the appropriate value of the barrier height to get the optimized separation.

From the plot of Ω versus u, we found that Ω is maximum for $u = 2.56727$. With this value for the barrier height u and using Eqs.(3.32) and (3.34), we get the time to get the maximum separation to be

$$t_m \;=\; 6.1810, \tag{3.46}$$

and the maximum separation between the particles to be

$$\Delta_m \;=\; 20.184875, \tag{3.47}$$

for $N_A = N_B = 100$.

Let us compare the values of t_m and Δ_m with their value at the barrier height which gives us the best separation, i.e., u very large. As $u \to \infty$, $t_m \to \infty$ too, and

$$\Delta_m \to 25.$$

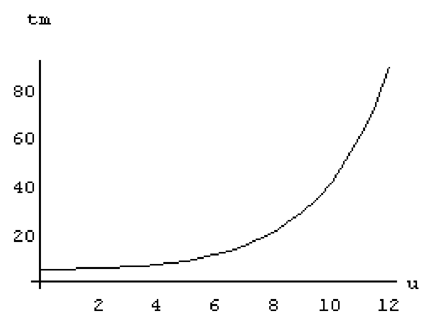

Figure 3.5: Plot of t_m versus u

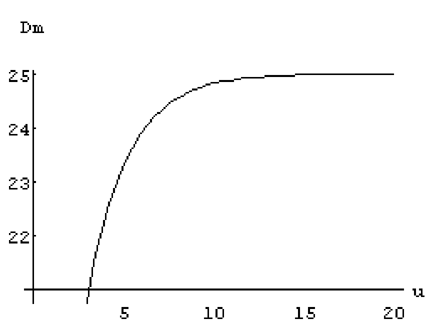

Figure 3.6: Plot of Δ_m versus u

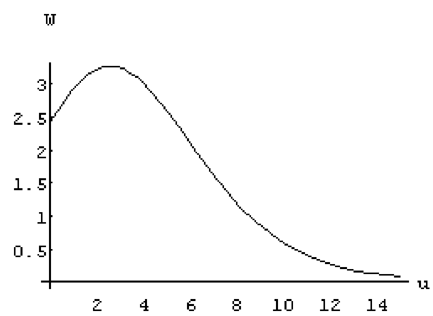

Figure 3.7: Plot of Ω versus u

Using $u = 2.56727$, we are able to get a Δ_m which is almost 80 percent of what we will get if we use u very large. In addition, our optimal barrier height gives us this separation in a very short time as compared to the time taken to get the best separation.

With a look at the plot of Ω versus t, we have seen that we get an optimized separation at $t = 6.1810$. So we have to stop the flow at this time and go to the next step.The next step is to shift the W-potential one step further or collect the particles in the two wells separately, put the particles that were in the right well to the left well and repeat the segregation process again. We should again find the time to get the maximum separation and the maximum separation between the particles.

To do this we have to first find the number of particles of each type in the right well at t_m. Using the value of t_m given in Eq.(3.46) and substituting it into Eqs.(3.25) and (3.27), we get,

$$n_{RA}(t_{m1}) = 60.554625$$

$$n_{RB}(t_{m1}) = 40.36975$$

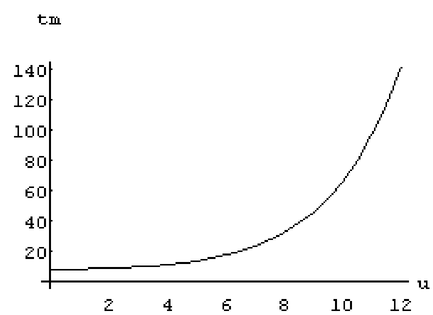

Figure 3.8: Plot of t_m versus u

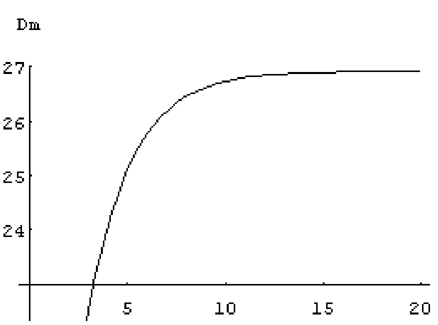

Figure 3.9: Plot of Δ_m versus u

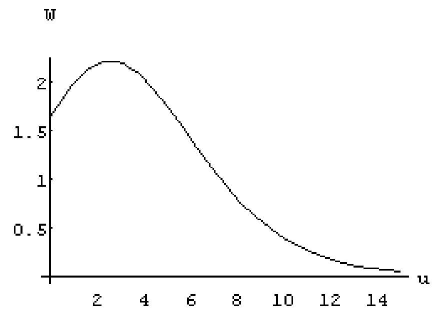

Figure 3.10: Plot of Ω versus u

These are the number of particles of type A and B in the left box for the next process. With this values for N_A and N_B, we have again plotted Ω versus u and the maximum occurs at the same value of u as in the first case.

The values of t_m and Δ_m are,

$$t_m = 9.80$$

$$\Delta_m = 21.72957$$

So for the second phase we have to stop the flow at the time we obtained above. The plots for t_m, Δ_m and Ω_m as a function of u are shown in Fig.(3.8)-(3.10). With this value of t_m and Eqs.(3.25) and (3.27), the number of particles of type A and B in the right well will be

$$n_{RA}(t_{m2}) = 43.45913,$$

and

$$n_{RB}(t_{m2}) \;=\; 21.72957.$$

These are the number of particles of the two types in the left well for the third phase of the process. By doing this repeatedly one can finally succeed in segregating the mixtures to a degree one is interested in. However, one can't get a pure separation unless one does the process infinite times.

3.5 The Homogeneous Temperature Case

To see the effect of having non-homogeneous temperature background, we have done the first phase of the separation process for the case of homogeneous temperature. We simply put $\alpha \;=\; 0$ in the expressions for t_m, Δ_m and Ω and plot them as a function of u.

As can be seen from Fig.(3.11)-(3.13), the time to get the maximum separation increases exponentially rapidly. So one has to wait for very long time to get the the maximum separation. Unlike the the non-homogeneous case, Δ_m has a maximum at some value of u and then decreases. This means that increasing the barrier height above some critical value will not help in getting the best separation. However, the plot of Ω versus u still exhibits a maximum.

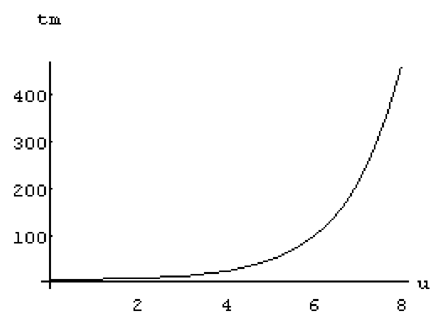

Figure 3.11: Plot of t_m versus u

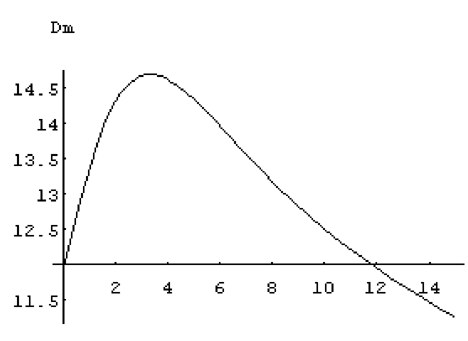

Figure 3.12: Plot of Δ_m versus u

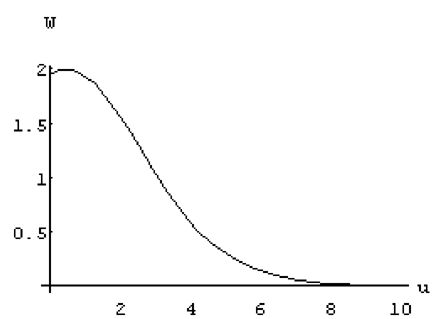

Figure 3.13: Plot of Ω versus u

Chapter 4

SEGREGATION OF BROWNIAN PARTICLES USING RATCHET POTENTIAL

In this chapter, we present another mechanism for segregating mixtures of Brownian particles that have different masses. We consider a ratchet potential that is tilted, by applying a small load, and exposed to a non-homogeneous temperature background. The ratchet potential is created by a uniform gravitational field. Due to the difference in their masses, the two particles look at different barrier height of the ratchet potential and hence the particles drift along the potential with different currents. We will make use of this fact to segregate the mixtures in such a way that one particle moves up the hill, while the other moves down the hill.

We first derive the current for a Brownian particle moving in such a potential and then show that such a particle can have both positive and negative currents depending on the barrier height of the ratchet potential it is experiencing. One can then choose the masses in such a way that the barrier height that the lighter particles experience produce a negative current while that the heavier particles experience produce a positive current.

4.1 Derivation of the current

Consider a Brownian particle that is moving in an asymmetric sawtooth potential, the so-called ratchet, with a small load and a piecewise constant non-homogeneous temperature background as shown in Fig.(4.1).

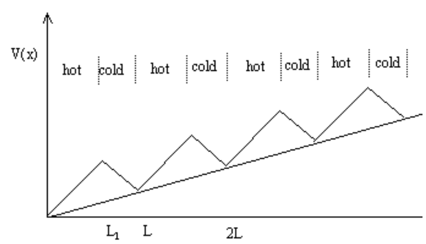

Figure 4.1: The model ratchet potential

The potential profile for the ratchet is given by

$$V_0(x) = \begin{cases} \frac{V_0}{L_1}x, & \text{if } 0 \leq x \leq L_1; \\ \frac{V_0}{L_2}\left(x - L\right), & \text{if } L_1 \leq x \leq L, \end{cases}$$

and this potential repeats itself periodically such that $V_0(x + L) = V_0(x)$. The potential due to the load varies linearly with position, i.e.,$V_L(x) = fx$. The temperature profile is

$$T(x) = \begin{cases} T_{hot} \;=\; T_1, & \text{if } 0 \leq x < L_1; \\ T_{cold} \;=\; T_2, & \text{if } L_1 \leq x < L, \end{cases}$$

and repeats itself periodically, $T(x + L) = T(x)$, like the potential. The Langevin equation governing the motion of a particle in such a profile is given by

$$m\frac{d^2x}{dt^2} \;=\; -\gamma\frac{dx}{dt} \;-\; V_0'(x) \;-\; V_L'(x) \;+\; \sqrt{2k_BT(x)\gamma}\,\xi(t), \tag{4.1}$$

where all the variables are as in chapter 2 with $V_0(x)$ corresponding to the ratchet potential and $V_L(x)$ is the potential due to the load. We can write this equation as

$$m\frac{d^2x}{dx^2} \;=\; -\gamma\frac{dx}{dt} \;-\; F(x) \;+\; \sqrt{2k_BT(x)\gamma}\,\xi(t), \tag{4.2}$$

where $F(x) = V_0'(x) + V_L'(x)$ and can be written as

$$F(x) = \begin{cases} \frac{fL_1 + V_0}{L_1}, & \text{if } 0 \leq x \leq L_1; \\ \frac{fL_2 - V_0}{L_2}, & \text{if } L_1 \leq x \leq L. \end{cases}$$

For heavy damping, Eq.(4.2) reduces to

$$dx \;=\; -\frac{1}{\gamma}F(x)dt \;+\; \sqrt{\frac{2k_BT(x)}{\gamma}}\,dW(t), \tag{4.3}$$

where $dW(t) = \xi(t)dt$.

The Fokker-Planck equation (FPE) corresponding to this Langevin equation is

$$\partial_t p(x,t) \;=\; \frac{1}{\gamma}\,\partial_x[F(x)p(x,t)] \;+\; \frac{k_B}{\gamma}\,\partial_x^2[T(x)p(x,t)], \tag{4.4}$$

where $p(x,t)$ is the probability density of finding the particle at position x at time t and γ is taken to be the same through out the medium. Eq(4.4) can be written as

$$\partial_t p(x,t) \;+\; \partial_x J(x,t) \;=\; 0, \tag{4.5}$$

where

$$J(x,t) \;=\; -\frac{1}{\gamma}\;[F(x)p(x,t)] \;-\; \frac{k_B}{\gamma}\;\partial_x[T(x)p(x,t)], \tag{4.6}$$

is the probability current density.

We are interested in the steady state current which is given by

$$\frac{-1}{\gamma}[F(x)p_{ss}(x)] \;-\; \frac{k_B}{\gamma}\;\partial_x[T(x)p_{ss}(x)] \;=\; const. \;=\; J. \tag{4.7}$$

where $p_{ss}(x)$ is the steady state probability distribution. Eq.(4.7) can be written as

$$\frac{d[T(x)p_{ss}(x)]}{dx} \;+\; \frac{F(x)}{k_B T(x)}[T(x)p_{ss}(x)] \;=\; -\frac{\gamma J}{k_B}. \tag{4.8}$$

Multiplying this by the integrating factor

$$\psi(x) \;=\; Exp[\frac{1}{k_B}\int_0^x dx'\frac{F(x')}{T(x')}], \tag{4.9}$$

and rearranging, we get

$$p_{ss}(x)T(x)\psi(x) \;-\; p_{ss}(0)T(0)\psi(0) \;=\; -\frac{\gamma J}{k_B}\int_0^x dx'\psi(x'). \tag{4.10}$$

The steady state probability distribution is periodic, i.e.,

$$p_{ss}(x \;+\; L) \;=\; p_{ss}(x), \tag{4.11}$$

and satisfies the normalization condition

$$\int_0^L dx\; p_{ss}(x) \;=\; 1. \tag{4.12}$$

Let us first apply Eq.(4.11) on Eq.(4.10),

$$p_{ss}(L) \;=\; p_{ss}(0) \;=\; p_0.$$

With this, Eq.(4.10) becomes

$$p_0 T_1 \;=\; -\frac{\gamma J}{k_B}\;\frac{\int_0^L dx\;\psi(x)}{[\psi(L) \;-\; 1]}. \tag{4.13}$$

Rearranging Eq(4.10), one finds

$$p_{ss}(x) \;=\; \frac{p_0 T_1}{T(x)\psi(x)} \;-\; \frac{\gamma J}{k_B}\,\frac{1}{T(x)\psi(x)}\int_0^x dx'\psi(x'). \tag{4.14}$$

Now using the normalization condition, Eq.(4.12), this becomes

$$p_0 T_1 \int_0^L \frac{dx}{T(x)\psi(x)} \;-\; \frac{\gamma J}{k_B}\int_0^L \frac{dx}{T(x)\psi(x)}\int_0^x dx'\psi(x') \;=\; 1 \tag{4.15}$$

Using Eq.(4.13) into Eq.(4.15) and rearranging terms, we find

$$J \;=\; -\,\frac{k_B}{\gamma}\,\frac{E}{GH \;+\; IE}, \tag{4.16}$$

where

$$E \;=\; \psi(L) \;-\; 1, \tag{4.17}$$

$$G \;=\; \int_0^L dx\;\psi(x), \tag{4.18}$$

$$H \;=\; \int_0^L \frac{dx}{T(x)\psi(x)}, \tag{4.19}$$

and

$$I \;=\; \int_0^L \frac{dx}{T(x)\psi(x)}\int_0^x dx'\psi(x'). \tag{4.20}$$

Integrating Eqs.(4.17) - (4.20), one will get

$$E \;=\; e^{[\frac{fL_1 \;+\; V_0}{k_B T_1} \;+\; \frac{fL_2 \;-\; V_0}{k_B T_2}]} \;-\; 1, \tag{4.21}$$

$$G \;=\; \frac{k_B T_1 L_1}{fL_1 \;+\; V_0}(e^{\frac{fL_1 \;+\; V_0}{k_B T_1}} \;-\; 1) \;+\; \frac{k_B T_2 L_2}{fL_2 \;-\; V_0}e^{\frac{fL_1 \;+\; V_0}{k_B T_1}}(e^{\frac{fL_2 \;-\; V_0}{k_B T_2}} \;-\; 1), \tag{4.22}$$

$$H \;=\; -\,\frac{k_B L_1}{fL_1 \;+\; V_0}(e^{-\frac{fL_1 \;+\; V_0}{k_B T_1}} \;-\; 1) \;-\; \frac{k_B L_2}{fL_2 \;-\; V_0}e^{-\frac{fL_1 \;+\; V_0}{k_B T_1}}(e^{-\frac{fL_2 \;-\; V_0}{k_B T_2}} \;-\; 1). \tag{4.23}$$

We can write Eq.(4.20) as the sum of two terms

$$I \;=\; I_1 \;+\; I_2, \tag{4.24}$$

where

$$I_1 = \int_0^{L_1} \frac{dx}{T(x)\psi(x)} \int_0^x dx'\psi(x'),$$

$$I_2 = \int_{L_1}^{L} \frac{dx}{T(x)\psi(x)} \int_0^x dx'\psi(x'),$$

which upon integration give

$$I_1 = \frac{k_B L_1^2}{fL_1 + V_0} + T_1(\frac{k_B L_1}{fL_1 + V_0})^2(e^{-\frac{fL_1 + V_0}{k_B T_1}} - 1), \tag{4.25a}$$

$$I_2 = \frac{k_B L_2^2}{fL_2 - V_0} + T_2(\frac{k_B L_2}{fL_2 - V_0})^2(e^{-\frac{fL_2 - V_0}{k_B T_2}} - 1)$$
$$+ \frac{k_B T_1 L_1}{fL_1 + V_0}\frac{k_B L_2}{fL_2 - V_0}(e^{-\frac{fL_1 + V_0}{k_B T_1}} - 1)(e^{-\frac{fL_2 - V_0}{k_B T_2}} - 1). \tag{4.25b}$$

Let the hot and cold temperatures be such that

$$T_1 = (1 + \alpha)T_2,$$

and let us scale our parameters as follows: $\beta = \frac{L_2}{L_1}$, $u = \frac{V_0}{k_B T_2}$, $\ell = \frac{fL_1}{k_B T_2}$, $J_0 = \frac{\gamma L_1^2}{k_B T_2}J$. With this scaled variables the scaled current J_0 can be written as

$$J_0 = -\frac{E'}{G'H' + E'(I_1' + I_2')}, \tag{4.26}$$

where

$$E' = e^{[\frac{\ell + u}{1 + \alpha} + (\beta\ell - u)]} - 1, \tag{4.27}$$

$$G' = \frac{1 + \alpha}{\ell + u}(e^{\frac{\ell + u}{1 + \alpha}} - 1) + \frac{\beta}{\beta\ell - u} e^{\frac{\ell + u}{1 + \alpha}} (e^{\beta\ell - u} - 1), \tag{4.28}$$

$$H' = -\frac{1}{\ell + u}(e^{-\frac{\ell + u}{1 + \alpha}} - 1) - \frac{\beta}{\beta\ell - u} e^{-\frac{\ell + u}{1 + \alpha}} (e^{-(\beta\ell - u)} - 1), \tag{4.29}$$

$$I_1' = \frac{1}{\ell + u} + \frac{1 + \alpha}{\ell + u^2}(e^{-\frac{\ell + u}{1 + \alpha}} - 1), \tag{4.30}$$

and

$$I_2' = \frac{\beta^2}{\beta\ell - u} + (\frac{\beta}{\beta\ell - u})^2 (e^{-(\beta\ell - u)} - 1)$$

$$+ \frac{\beta(1 + \alpha)}{(\ell + u)(\beta\ell - u)} (e^{-\frac{\ell + u}{1 + \alpha}} - 1) (e^{-(\beta\ell - u)} - 1). \tag{4.31}$$

We have plotted the current as function of the load ℓ and the barrier height u in Fig.(4.2) for $\beta = \frac{1}{2}$ and $\alpha = 1$.

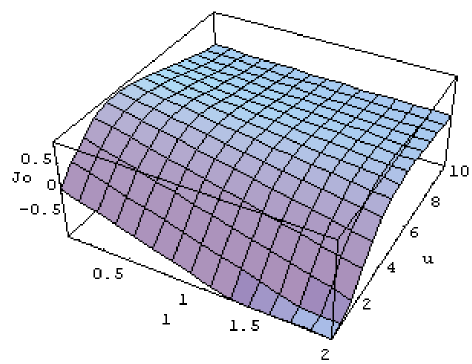

Figure 4.2: The 3D Plot of J as a function of ℓ and u

As one can see from the plot the current has both positive and negative values. That means under appropriate choice of the load and the barrier height, one can bias the motion of a Brownian particle either to the right or to the left. We are interested in the dependence of the current on the barrier height for a fixed choice of the load. The plot of J_0 versus u for $\ell = 1$, $\beta = \frac{1}{2}$ and $\alpha = 1$ is shown in Fig.(4.3). The plot shows that $J_0 = 0$ for a specific value of u. So depending on the value of u, one can generate both positive and negative currents.

In the next section, we will apply the expressions obtained above to our model and see how we can segregate mixtures of Brownian particles.

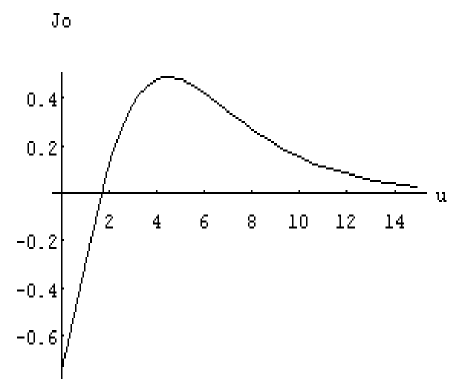

Figure 4.3: Plot of J versus u for $\ell = 1$

4.2 Mechanism for segregation

Consider the ratchet potential of Fig.(4.1) but this time with out the load. It is like we have a one-dimensional table, whose surface has a sawtooth nature. Imagine a Brownian particle trying to move on this surface. In order to move, the particle must get enough energy to overcome the barrier created by the gravitational field.

Consider two types of Brownian particles having different masses trying to move in such a microscopic table. In the presence of gravitational field, the heavier particles experience a larger barrier height than the lighter particle, as shown in Fig.(4.4).

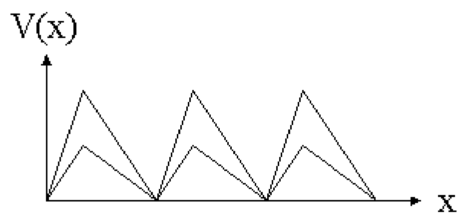

Figure 4.4: The potential for two particles with different masses

In our model we have two types of particles having different masses mixed up in one of the wells of a periodic sawtooth potential under a constant load. Since we consider the system in a gravitational field, the two types of particles experience different barrier heights. The lighter particles experience a barrier height, say u_1, which is less than the barrier height, say u_2, which the heavier particles experience. If we keep the other parameters fixed for both types of particles, then the expression for the steady state current in Eq.(4.26) holds true for both types of particles with the replacement of u by u_1 and u_2. It was shown in Fig.(4.3) that the current can be biased to the left or to the right by an appropriate choice of the barrier height. Let us choose u_1 and u_2 in such a way that the current for the lighter particles is in the negative direction while that for the heavier particles is in the positive direction. Then we can succeed in separating the mixtures such that the heavier particles move up the hill and be collected at the top, while the lighter particles move down the hill and be collected at the bottom.

Chapter 5

Summary and Conclusion

We considered two mechanisms for segregating mixtures of non-interacting Brownian particles. The first model uses a bistable potential with a non-homogeneous temperature background. The mixture contains two types of Brownian particles that have different diffusion constants. The particles are placed, mixed up, in the left well and allowed to diffuse to the right well by the thermal kick they get from the background. Since the particles have different diffusion constants, they arrive at the right well with different escape rates.

By making use of the difference in their escape rates, we have shown how one can have an optimum separation between the particles. We found closed form expressions for the MFPTs, escape rates, and the difference in the number of particles of the two types in the right well. We have also given analytic expressions for the maximum separation between the particles and the time to get this maximum separation. Since the time required to get the *best* separation needs infinite time, we have optimized our parameter with which one can succeed in getting 80 percent of the best separation in a finite time.

One can see our model this way. Consider a tiny tube in the shape of a ring. At one position positive charges are accumulated on the ring. At some other position negative

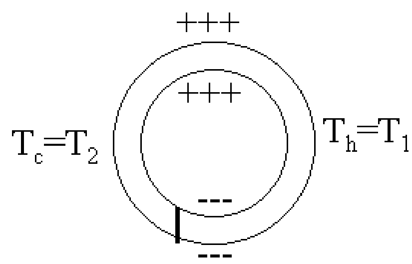

Figure 5.1: A circular ring as a double well potential

charges are accumulated and there is an impenetrable boundary near the negative charges. One portion of the ring is in contact with a hot heat reservoir at temperature T_1 while the other portion of the ring is in contact with a cold reservoir at temperature T_2 as shown in the figure below.

Imagine now that we put two types of particles with the same positive charge but different diffusion constants inside the tube at the location of the accumulated negative charges. We assume that the particles are ideal so that the force of interaction between them is negligible. A positively charged particle at this position gets it difficult to overcome the barrier which it experiences as a result of the accumulation of the positive charges on the ring. But if the thermal kick it gets from the background is sufficient, then the particle can definitely cross the barrier. Since the mixed particles carry the same amount of positive charge but differ in their diffusion constant, then these particles cross the barrier at different rates and can be accumulated on the other side of the impenetrable wall. Note that the asymmetry can also be created by varying the relative position of the accumulated charges. Then we can separate the mixtures using the method described in chapter 3.

In the second model, we made use of a periodic sawtooth potential that is tilted by applying a small load exposed to a non-homogeneous temperature background. With this model we have shown that we can separate two Brownian particles that have different masses in opposite direction by making use of a uniform gravitational field, which creates the ratchet potential.

In conclusion, we believe that experiments like the ones done by Fauchex and Libchaber [5] can be done to check the mechanisms we present in this thesis. Furthermore the mechanisms presented can have applications in various mining, food, and pharmaceutical industries.

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DECLARATION

I hereby declare that this thesis is my original work and has not been presented for a degree in any other University. All sources of material used for the thesis have been duly acknowledge.

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"Yaa rabi, galatnii kee hin badu atti....."