

# LATTICE MODEL OF BROWNIAN MOTOR

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By

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*"Thanks be unto God for his  
unspeakable gift"*

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## *Abstract*

Now a days science focuses on small size machine such as Brownian motors due to the need to use energy at small scale. Thus it is important to develop model for studying their working principles. One famous model is Feynman's ratchet and pawl system. We developed a discrete lattice model for this system.

The model is Brownian particles moving in a sawtooth potential with or with out external load and trap potential in one dimensional discrete lattice and the lattice is periodically coupled to two (hot and cold) heat reservoirs. We found explicit expressions for current, drift velocity, efficiency and coefficient of performance as a function of the parameters characterizing the model. The parameters are trap potential, ratchet barrier, the strength of noise of the hot reservoir and the external load. From detailed analysis of the expressions we are able to observe that

- trap potential affects the current. Current decreases as the strength of trap depth increases. Trap is obstacle for both directions of motion.
- the noise and the load are the sources of current and
- the ratchet barrier is responsible for rectification of the noise.

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# Chapter 1

## Introduction

Even though macroscopic as well as microscopic heat engines work on the same thermodynamic principles, wide-ranging studies have been done in improving the performance of the macroscopic heat engines [1]. At present study of microscopic heat engines has received a considerable attention [2]. This is because of the trend in miniaturization and the need to use energy resources available at microscopic scales. To understand the working of molecular motors, in principle, simplified models are desired which are amenable to explicit calculations. To this regard researchers design different models.

Feynman's 'ratchet and pawl' system [3] which is magnified and easy to understand, is a well known example of model of Brownian motors. The idea is beautifully simple: set up a ratchet and pawl so that a wheel turns in only one direction and attach that wheel to windmill whose vanes are surrounded by gas at finite temperature. This is illustrated in Fig 1.1. Every so often an accumulation of collision of the gas molecules against the vanes will cause the wheel to rotate by one notch in the allowed direction but presumably never in the forbidden direction. Such rectification of the thermal noise could be harnessed to perform useful work (such as lifting a flea against gravity) in direct violation of the second law of thermodynamics.

Of course, in order for statistical fluctuations to cause rotation at perceptible

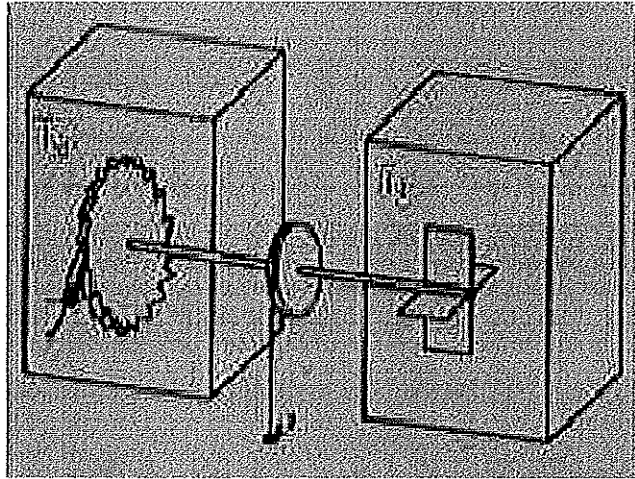


Figure 1.1: Feynman's ratchet and pawl machine.

rate, the ratchet and the pawl must be microscopic, and this points towards the solution of the paradox. If thermal motion of the gas molecules are sufficient to cause the wheel to rotate a notch, then the thermal pawl itself will occasionally cause it to disengage from the ratchet, at which point the ratchet could move in the 'forbidden' direction. Feynman compared the rate of the two processes - rotation in the allowed and forbidden directions - and found them to be equal when the system is maintained at the single temperature. Thus no net rotation arises, and second law of thermodynamics is saved.

Since the failure of the ratchet and pawl system to perform work arises from thermal fluctuations of the pawl, the natural solution to the problem is to reduce

these fluctuation by externally cooling the heat bath of the pawl to a temperature below that of the vanes' heat bath. In this case the device indeed operates as designed, but this is no longer to constitute violation of the second law: the ratchet and pawl is now efficiently a microscopic heat engine, capitalizing on a temperature difference to extract useful work from thermal motions.

While the ratchet and pawl was introduced in Feynman's lectures primarily for pedagogical purpose, recent years have shown a renewed interest in this system [4] due to the fact that analogous mechanisms have been proposed as simple models of motor proteins. Now we want to develop a model of Feynman's microscopic heat engine. Our model is discrete, but it captures an essential feature of the original model: a periodic but asymmetric interaction potential between the ratchet and the pawl (corresponding to the sawtooth shape for the ratchet teeth).

Note that a particle (or more generally reaction coordinate), evolving from sufficiently deep potential energy to another behaves much as if it is hopping from one site to another on a discrete lattice [5].

Our model briefly is as follows. Consider a particle that moves on a one dimensional lattice. Each lattice point acts as a trap to the particle. The particle moves from one lattice point to the next due to the thermal kick it gets from the background lattice medium. The lattice medium is taken to be thermally inhomogeneous since the lattice points are coupled periodically to hot and cold heat reservoirs. The trap potential which the particle experiences at each point is assumed to be strong enough to cause the particle spend a major part of its time at lattice sites compared to the time spent in moving between sites. This kind of motion of particle is Markovian in nature where all past memories are washed out except the immediate past. We say such a movement to be hopping from one site to the next.

However in the previous study [6], the the trap potential is neglected and it has no contribution to the dynamics of the particle. But this is not in reality.

The aim of this work is to find exact expressions for current and efficiency of lattice model of Feynman's microscopic heat engine and to discuss them with respect to the parameters which specify the model.

The work is organized as follows. In Chapter 2, we will present the basic physics of the Brownian motion and the dynamics of discrete lattice model of Brownian motor. In Chapter 3, we study the current of the model for different conditions. Thus we will derive the exact expression for the current as a function of trap potential, barrier height due to ratchet, external load and the temperature of the two reservoirs. In addition we will explore energetics of the model. In Chapter 4, we will discuss the results we get in Chapter 3. Finally Chapter 5 deals with the summary and conclusion.

## Chapter 2

# General characteristics of Brownian motion and discrete model of Brownian motor

### 2.1 Brownian motion

Look through a microscope at very still dirty water or curdled milk and you will see tiny particles in a state of constant rapid erratic motion. In 1827 a botanist named Robert Brown saw this movement in pollen grain dispersed in water. What he observed, to be precise, was that pollen, dropped into water, was disintegrated into a very large number of tiny particles of size a few  $\mu m$  and which were seen to be dancing ceaselessly. He thought first that the movements were a sign of life, and that the tiny particles were the fundamental constituents of living matter since pollen grain came from plants. He later found that inorganic materials did similar movements as well and speculated that all matter was made of these primitive molecules. People have realized quite soon that these tiny but visible particles were not molecules, just finely divided matter, and the focus shifted to what was causing that random motion. Many explanations were offered: perhaps the particles were carried around by flows produced by small temperature difference in the water; may be illuminating

the material was itself causing the movement; may be electrical or/and magnetic force and so forth. Experiments and speculations continued through 1880s. A particular careful set of experiments by Gouy showed that the fluctuations become more rapid if the viscosity is decreased and neither change in the intensity of light nor larger electromagnetic field affects the movement. He was thus convinced of the view that, the molecules of the liquid were moving around rapidly simply because the liquid had a temperature and the pollen grains were being kicked here and there by repeated collision with these molecules [7]. A satisfactory explanations was given by Einstien in 1905. He argued that small particles suspended in fluid should be agitated by collision with molecules. He constructed a detailed quantitative description of the motion of such particle. There were two major points in Einstien's quantitative formulation of Brownain motion:

1. The motion is caused by the exceedingly frequent impacts on the Brownian particle of the incessantly moving molecules of the the fluid in which it is suspended.
2. The motion of the molecules is so complicated that its effect on the Brownian particle can only be described probablistically in terms of exceedingly frequent statistically independent impact.

From these assumptions he developed a diffusion equation

$$\frac{\partial f(x, t)}{\partial t} = D \frac{\partial^2 f(x, t)}{\partial x^2}. \quad (2.1)$$

The solution of Eq.2.1 is  $f(x, t) = \frac{n \exp(-x^2/4Dt)}{\sqrt{4\pi t}}$ , where  $f(x, t)$  is the probability density of getting the particle at position  $x$  at time  $t$  and  $D$  is the diffusion constant and  $n$  is the total number of particles suspended in the fluid. He found that  $\sqrt{\bar{x}^2} = \sqrt{2Dt}$  where  $\bar{x}^2$  is the arithmetic mean of the square of the displacement in one dimension.

Sometime after Einstein's original derivation, Langevin [7] presented a new method which was quite different from Einstein's and according to him "infinitely more simpler". His reasoning was as follows:

From statistical mechanics, it is known that the mean kinetic energy of a Brownian particle in equilibrium has a value  $\langle \frac{mv^2}{2} \rangle = \frac{k_B T}{2}$  in one dimension, where  $k_B$  is Boltzman's constant and  $T$  is the absolute temperature. He hypothesized that the force on the particle due to the solvent can be split into two components:

1. A viscous drag force that always slows the motion induced by fluctuation which is given by  $-6\pi\eta a\dot{x}$  where  $\eta$  is the viscosity and  $a$  is the diameter of the particle, assumed spherical.
2. The fluctuating (noise) force  $\chi$  that changes direction and magnitude frequently compared to any other time scale of the system and averaged to zero over time.

So the motion of the particle in position is governed by Newton's second law  $m\frac{d^2x}{dt^2} = -\gamma\frac{dx}{dt} + \chi$ , for  $\gamma = 6\pi\eta a$ . From these he derived  $\langle x^2 \rangle - \langle x_0^2 \rangle = [k_B T / 3\pi\eta a]t$ . This is equivalent to Einstein's result provided that  $D = k_B T / 6\pi\eta a$ .

The two components of the force are not independent: the amplitude of the fluctuating force is governed by the viscosity of the solution. These and other studies have given a great advance for the studies of Brownian motion. In particular expressing the motion using Langevin equation helps us to study the motion with additional external driving forces.

The combined action of the external driving force and noise force has given rise to a new phenomenon, where the constructive role of the Brownian motion provides a rich scenario of far from equilibrium effects [8]. A more recent but increasingly popular example of the constructive role of fluctuation (intrinsic and external) is the noise assisted transport in periodic system, namely Brownian Motor.

## 2.2 Brownian motor

A nonequilibrium fluctuation combined with broken reflection symmetry (usually provided by a periodic but asymmetric potential) can cause directed motion even in the absence of any macroscopic biasing force. We mean by 'directed motion' quite literally the transport of particles, but the same idea applies to transport in some more abstract parameter space, such as a reaction coordinate [9]. A model system for nonequilibrium transport based on the rectification of Brownian motion is called Brownian motor. One example is flashing ratchet [10].

P.Reimann and P. Hanggi and others [11, 12, 13, 14, 15] defined a set of characteristics for Brownian Motors:

1. Thermal noise plays a central role in achieving transport. Without Brownian motion during off-phase (temperature  $T = 0$  or macroscopic object) no net current occurs. In this, the external potential rectifies thermal fluctuation (the hall mark of Brownian motion).
2. Symmetry is broken. In ratchets, spatial symmetry is broken through the use of a potential without inversion symmetry. Instead symmetry may also be broken by unbiased, but skewed external, time dependent force (dynamical symmetry breaking)[15] or due to spontaneous symmetry breaking [16].
3. Except for load force, all forces have to be averaged to zero (the average might be spatial, temporal and ensemble).
4. Detailed balance is broken (that is, the system is kept far from equilibrium, usually at the cost of sustained energy input).
5. Finally the use of periodicity (spatial or temporal) is typical for Brownian motors and is required for a clear definition of what constitutes 'transports' or 'works' in a Brownian system.



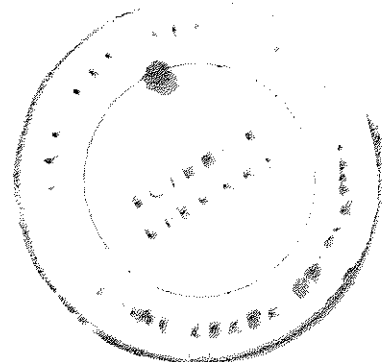
A magnified rectifier of noise (Brownian motor) is designed by Feynman. The device is nothing but an axle with vanes in one of its end and ratchet in the other that in principle can move in one direction [3]. If the vanes are surrounded by a gas at a given temperature, they will undergo a collision with the gas molecules and oscillate as a one dimensional rotor. However, due to the presence of the ratchet at the other end of the axle, in principle only fluctuations in one direction if they are strong enough could make ratchet lift the pawl and advance to the next notch. Feynman carried out the analysis of such an engine proving that, in order to obtain useful work out of thermal fluctuations the vanes must be within thermal bath of temperature  $T_1$  higher than the temperature  $T_2$  of the ratchet. In the next section we introduce the discrete model of Brownian motor.

## 2.3 Discrete lattice model of Brownian motor

Here the model is discrete, but it fulfils the basic characteristics of Feynman's model. The motion of the ratchet is represented by hopping of the Brownian particles from site to site. The sawtooth shape of the ratchet is mimicked by the sawtooth potential profile. There are two thermal baths at different temperatures. We will see this topic by splitting into two sub topics: the model without trap and the model with strong trap.

### 2.3.1 The model without trap potential

The model is taken as the modified version of the one considered by Jarzynski and Mazonka [18] in modelling Feynman's ratchet and pawl system. Consider a particle that moves by hopping in a one dimensional lattice of lattice spacing  $d$  and the motion is assisted by the thermal kick it gets from periodically placed hot and cold heat reservoirs along its path. The particle is also exposed to an external discrete



periodic asymmetric sawtooth potential which has the same period as the placement of the heat reservoirs.

Analogy between this model and Feynman's ratchet :

- The position of the particle corresponds to the angle variable  $\theta$  (orientation of the ratchet wheel). One period ( $3d$ ) of the profile for the lattice site is equivalent to one notch or teeth size ( $\Delta\theta$ ).
- The sawtooth potential is analogous to the sawtooth of the ratchet.

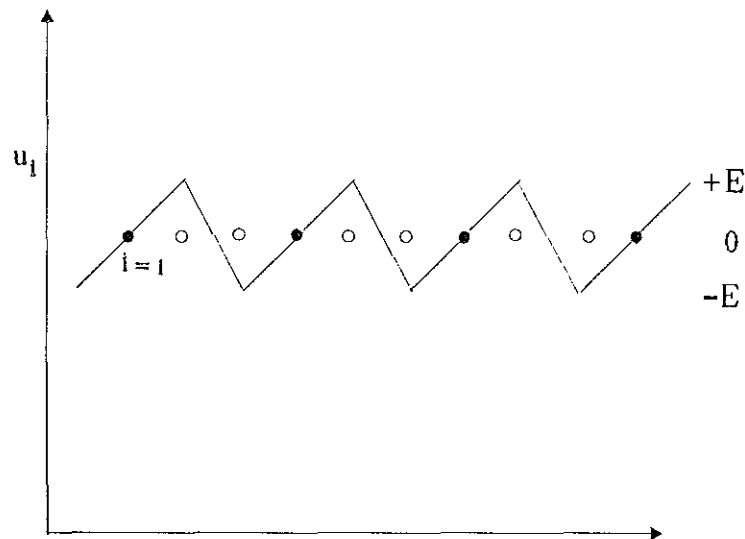


Figure 2.1: The plot of discrete sawtooth potential without external load. Sites with dark circles are coupled the hot reservoir ( $T_h$ ) while sites with open circles are coupled to the cold reservoir ( $T_c$ )

The discrete ratchet potential at site  $i$ , is given by

$$U_i = E[i(\text{mod})3 - 1],$$

where  $E$  is a positive constant having a unit of energy . The temperature profile is given by:

$$T_i = \begin{cases} T_h & \text{if } [i \pmod{3} - 1] = 0 \\ T_c & \text{otherwise} \end{cases}$$

where  $T_h$  and  $T_c$  are the temperatures of the hot and cold reservoirs, respectively. Fig.2.1 shows the model.

Since the jump of the particle from one site to the other is assisted by thermal kick, it can be assumed as a random process. So the jump probability per unit time is determined by the amount of energy it crosses and the temperature of the reservoir to which it is coupled [6].

We now describe more precisely the stochastic process governing the dynamics of the particle. We assume the process is a Poisson process occurring at rate  $\Gamma$ . That is during every infinitesimal time interval  $\delta t$  there is a probability  $\Gamma \delta t$  that the particle will attempt a jump to a neighboring site. An attempt is preceded by a decision (randomly with equal probability) of whether the jump is to the left or to the right, and followed by a decision of accepting or rejecting the jump. The probability of making decision to accept hopping is based on the Metropolis algorithm to satisfy detailed balance [17]: suppose a particle is to jump from site  $i$  to  $j$  and the barrier height between the sites is  $\Delta E = E_j - E_i$  and  $T_i$  is the temperature of at the site  $i$ . Then if  $\Delta E > 0$ , the jump will occur with probability  $\exp(-\Delta E/T_i)$ . The temperature is measured in a unit such that  $k_B$ (Boltzmann's constant) is taken unity. But if  $\Delta E \leq 0$  the jump will take place with probability one. So the probability per unit time of jumping from site  $i$  to  $i+1$  is given by  $(\Gamma/2)\min(1, \exp(-\Delta E/T_i))$ . We have introduced parameters which we view as "internal" to the system:  $d, E, \Gamma$ . These essentially set the relevant length ( $d$ ), energy ( $E$ ) and time ( $\Gamma^{-1}$ ) scales. The two remaining parameters are  $T_h$  and  $T_c$  which are viewed as "external".

To analyze the model we first note that it maps nicely onto the problem of spin-1

particle coupled to two heat reservoirs, denoting the spin  $s$  by  $(0, \pm 1)$ . The energy function of the particle of spin  $s$  is given by:

$$E(s) = Es. \quad (2.2)$$

The change of the spin  $s$  corresponds to the jump of particle from site to site. The changes of  $s$  from  $-1$  to  $0$ , from  $0$  to  $1$  or  $1$  to  $-1$  is the same as the flow of particles to the right and the reverse corresponds to the flow of particles to the left. Fig.2.2 shows the spin-1 system coupled to the two reservoirs.

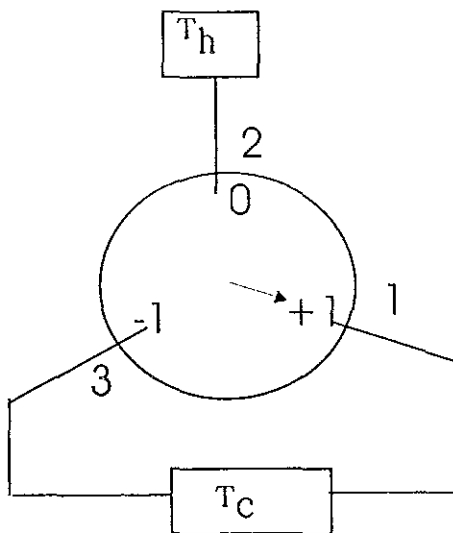


Figure 2.2: Our system maps onto that of a spin-1 coupled to two (hot and cold) heat reservoirs. The arrow can point in one of the three directions on the face of a cloke. The lines denote coupling between the spin and the heat reservoirs. The inner numbers indicate the spin but the outer represents the states of the system

Since the process is Markovian the dynamics of the particle is described by a master equation. Let the probability for the system to be found in the state  $n$  at time  $t$  be  $p_n(t)$ . The rate equation governing the evolution of the three states is:

$$dp_n(t)/dt = (\Gamma/2) \sum_{n' \neq n} w_{nn'} p_{n'}(t) - w_{n'n} p_n(t) \quad \text{for } n', n \in \{1, 2, 3\}, \quad (2.3)$$

where  $\frac{\Gamma}{2}w_{n'n}$  is the transition probability rate at which the system at state  $n'$  hops to a state  $n$ .

$$dp_1(t)/dt = \Gamma/2 (-[w_{21} + w_{31}] p_1(t) + w_{12} p_2(t) + w_{13} p_3(t)) \quad (2.4)$$

$$dp_2(t)/dt = \Gamma/2 (w_{21}p_1(t) - [w_{12} + w_{32}]p_2(t) + w_{23}p_3(t)) \quad (2.5)$$

and

$$dp_3(t)/dt = \Gamma/2 (w_{31}p_1(t) + w_{32}p_2(t) - [w_{13} + w_{23}]p_3(t)). \quad (2.6)$$

We can write these equations using matrix equation as

$$\frac{d\vec{p}(t)}{dt} = \frac{\Gamma}{2}\mathbf{R}\vec{p}, \quad (2.7)$$

where

$$\mathbf{R} = \begin{pmatrix} -(w_{21} + w_{31}) & w_{12} & w_{13} \\ w_{21} & -(w_{12} + w_{32}) & w_{23} \\ w_{31} & w_{32} & -(w_{13} + w_{23}) \end{pmatrix},$$

and  $\vec{p}$  is a column matrix given by

$$\vec{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}.$$

The entries of  $\mathbf{R}$  are given from Metropolis algorithm as

$$\left. \begin{aligned} w_{12} &= \exp(-E/T_h) \\ w_{21} &= 1 \\ w_{13} &= \exp(-2E/T_c) \\ w_{31} &= 1 \\ w_{23} &= \exp(-E/T_c) \\ w_{32} &= 1 \end{aligned} \right\}. \quad (2.8)$$

Let  $\exp(-E/T_h) = \mu$  and  $\exp(-E/T_c) = \nu$ , then the matrix  $\mathbf{R}$  will be given by

$$\mathbf{R} = \begin{pmatrix} -2 & \mu & \nu^2 \\ 1 & -(\mu + 1) & \nu \\ 1 & 1 & (\nu + \nu^2) \end{pmatrix}. \quad (2.9)$$

For steady state the derivative of the probability vector with time will be zero, i.e.,  $\frac{d\vec{p}(t)}{dt} = 0$ . This means the distribution probability is a null eigen vector of  $\frac{\Gamma\mathbf{R}}{2}$  i.e.,  $\frac{\Gamma\mathbf{R}\vec{p}}{2} = 0$  and we can solve for the normalized components of  $\vec{p}$ . For the general matrix equation  $\mathbf{A}\vec{x} = 0$  where the matrix  $\mathbf{A}$  is given by

$$\mathbf{A} = \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix},$$

and the column matrix  $\vec{x}$  by

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix},$$

we will have the simultaneous equation

$$a_1x_1 + a_2x_2 + a_3x_3 = 0, \quad (2.10)$$

$$b_1x_1 + b_2x_2 + b_3x_3 = 0, \quad (2.11)$$

$$c_1x_1 + c_2x_2 + c_3x_3 = 0, \quad (2.12)$$

and from normalization condition we have

$$x_1 + x_2 + x_3 = 1. \quad (2.13)$$

We can convert the four equations into two by eliminating the second term. From Eq.(2.11),  $x_2 = -[b_1x_1 + b_3x_3]/b_2$  inserting it in to Eq.(2.10) and from Eq.(2.13),  $x_2 = 1 - x_1 - x_3$  inserting it in to Eq.(2.12) the resulting equations will be

$$[a_1b_2 - a_2b_1]x_1 + [a_3b_2 - a_2b_3]x_3 = 0 \quad (2.14)$$

and

$$(c_1 - c_2)x_1 + c_2 + (c_3 - c_2)x_3 = 0. \quad (2.15)$$

From these

$$x_1 = -c_2[a_2b_3 - a_3b_2]/y, \quad (2.16)$$

$$x_2 = c_2[a_2b_3 - a_3b_2] + c_3[a_1b_2 - a_2b_1]/y, \quad (2.17)$$

$$x_3 = -c_2[a_1b_2 - a_2b_1]/y, \quad (2.18)$$

where

$$y = (c_1 - c_2)[a_2b_3 - a_3b_2] + (c_3 - c_2)[a_1b_2 - a_2b_1]. \quad (2.19)$$

For this model

$$a_2b_3 - a_3b_2 = \mu\nu + \nu^2(1 + \mu)$$

$$a_1b_2 - a_2b_1 = \mu + 2$$

and  $y = -(2 + \mu)[1 + \nu + \nu^2]$ , the solution will be

$$x_1 = p_1 = \frac{\mu\nu + \nu^2(1 + \mu)}{(2 + \mu)(1 + \nu + \nu^2)} \quad (2.20)$$

$$x_2 = p_2 = \frac{\nu(2 + \nu)}{(2 + \mu)(1 + \nu + \nu^2)} \quad (2.21)$$

$$x_3 = p_3 = \frac{1}{1 + \nu + \nu^2}. \quad (2.22)$$

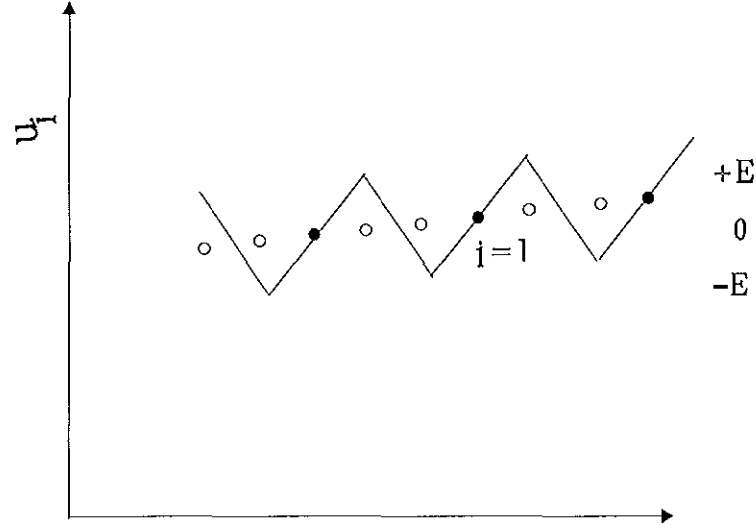


Figure 2.3: The plot of discrete sawtooth potential with external load. Sites with dark circles are coupled the hot reservoir ( $T_h$ ) while sites with open circles are coupled to the cold reservoir ( $T_c$ )

Now let us consider the case in which the model is biased by an external load. The potential profile will be modified as  $u_i = u_i + ifd$  as shown in Fig.2.3. The dynamics of the particle will have the same form as we have seen in the previous case except the modification for the expression of transition probability per unit time (entries of  $\mathbf{R}$ ). Accordingly the entries of  $\mathbf{R}$  will be given by

$$\left. \begin{aligned} w_{12} &= \exp(-(E + fd)/T_h) \\ w_{21} &= 1 \\ w_{13} &= \exp(-(2E + fd)/T_c) \\ w_{31} &= 1 \\ w_{23} &= \exp(-(E + fd)/T_c) \\ w_{32} &= 1 \end{aligned} \right\} \quad (2.23)$$

Let  $\exp(-fd/T_h) = \epsilon_1$ ,  $\exp(-fd/T_c) = \epsilon_2$ , i.e,  $\mu \rightarrow \mu\epsilon_1$ ,  $\nu \rightarrow \nu\epsilon_2$  and  $\nu^2 \rightarrow \nu^2\epsilon_2$ . Then the matrix  $\mathbf{R}$  will back



$$R = \begin{pmatrix} -2 & \mu\epsilon_1 & \nu^2\epsilon_2 \\ 1 & -(\mu\epsilon_1 + 1) & \nu\epsilon_2 \\ 1 & 1 & (\nu\epsilon_2 + \nu^2\epsilon_2) \end{pmatrix}. \quad (2.24)$$

By the same technique as in the previous one for steady state the normalized components of probability distribution of the biased model will be given by

$$p_1 = \frac{\mu\epsilon_1\nu\epsilon_2 + \nu^2\epsilon_2(1 + \mu\epsilon_2)}{(2 + \mu\epsilon_2)(1 + \nu\epsilon_2 + \nu^2\epsilon_2)}, \quad (2.25)$$

$$p_2 = \frac{2\nu\epsilon_2 + \nu^2\epsilon_2}{(2 + \mu\epsilon_2)(1 + \nu\epsilon_2 + \nu^2\epsilon_2)} \quad (2.26)$$

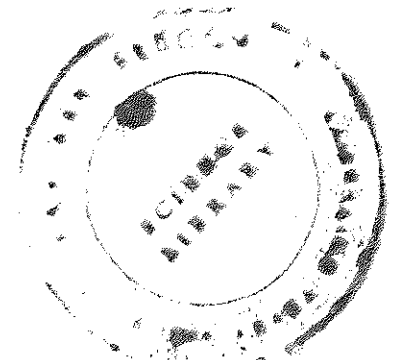
and

$$p_3 = \frac{1}{1 + \nu\epsilon_2 + \nu^2\epsilon_2}. \quad (2.27)$$

### 2.3.2 The model with strong trap potential

We study such a discrete lattice model in the presence of uniformly distributed traps and non-homogenous temperature background. Consider a particle that moves by hopping on a one dimensional lattice, with spacing  $d$  and trap potential  $\Phi$ . The motion of particle is assisted by the thermal kick it gets from the heat reservoirs which are coupled to the lattice sites periodically. The period of the ratchet potential and the position of the reservoirs are taken to be the same which is equivalent to three lattices. So in one cycle the particle hops three lattice sites either to the left or to the right. This corresponds to the particle crossing one sawtooth potential. The potential profile of the system is shown in Fig.2.4.

The concepts (rate of jump attempt, choosing direction probability and Metropolis algorithm) we used in pervious cases to determine the jump probability per unit time



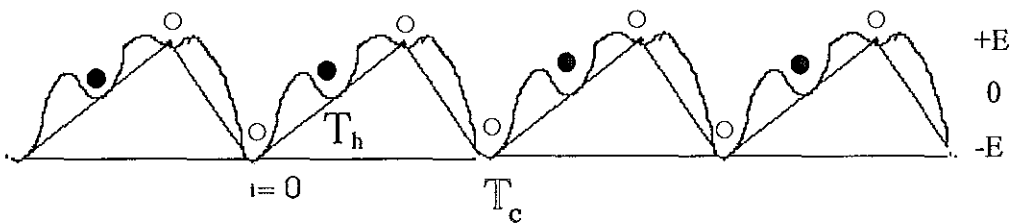
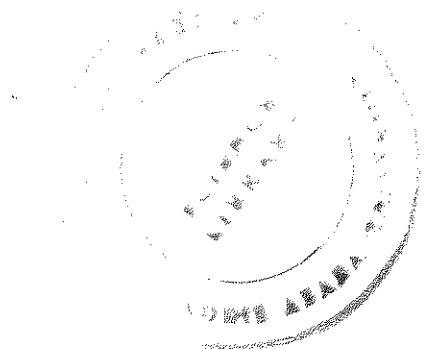


Figure 2.4: The plot of discrete sawtooth potential with trap but without external load. Sites with dark circles are coupled the hot reservoir ( $T_h$ ) while sites with open circles are coupled to the cold reservoir ( $T_c$ )

can be applied here except the change in the values of the barrier height that the particle crosses when it jumps from site to site. It can be also mapped into spin -1 particle of spin  $s = 0, \pm 1$ .

The trap is taken to lie approximately at the middle of two adjacent sites and  $\Phi > E$ . The state change of spin  $s$  corresponds to the particle jump. If the spin  $s$  changes from 0 to 1, 1 to -1 and -1 to 1 then this amounts to the particle jumping to right and in the case of reverse direction to the left. The following table shows the possible changes of state and the corresponding energy barrier height to be crossed.



state changes	barriers height
$2 \rightarrow 1$	$\Phi + \frac{E}{2}$
$1 \rightarrow 2$	$\Phi - \frac{E}{2}$
$1 \rightarrow 3$	$\Phi - E$
$3 \rightarrow 1$	$\Phi + E$
$3 \rightarrow 2$	$\Phi + \frac{E}{2}$
$2 \rightarrow 3$	$\Phi - \frac{E}{2}$

The dynamics of the particle is then described by stochastic jumps among the three states. The process is Markovian and we can describe the evolution of the states with rate equation as in the previous section. The entries for  $\mathbf{R}$  are given from Metropolis algorithm by

$$\left. \begin{aligned} w_{12} &= \exp(-(\Phi + E/2)/T_h) \\ w_{21} &= \exp(-(\Phi - E/2)/T_c) \\ w_{13} &= \exp(-(\Phi + E)/T_c) \\ w_{31} &= \exp(-(\Phi - E)/T_c) \\ w_{23} &= \exp(-(\Phi + E/2)/T_c) \\ w_{32} &= \exp(-(\Phi - E/2)/T_h) \end{aligned} \right\}. \quad (2.28)$$

Let  $\exp(-\Phi/T_h) = \delta_1$ ,  $\exp(-E/2T_h) = \mu$ ,  $\exp(-\Phi/T_c) = \delta_2$ , and  $\exp(-E/2T_c) = \nu$ . Then the matrix  $\mathbf{R}$  will be

$$\mathbf{R} = \begin{pmatrix} -(\delta_2/\nu + \delta_2/\nu^2) & \delta_1\mu & \delta_2\nu^2 \\ \delta_2/\nu & -(\delta_1\mu + \delta_1/\mu) & \delta_2\nu \\ \delta_2/\nu^2 & \delta_1/\mu & -(\delta_2\nu + \delta_2\nu^2) \end{pmatrix}. \quad (2.29)$$

For steady state the derivative of the probability vector with time will be zero which implies that  $\mathbf{R}\vec{p} = 0$ . We can find the normalized components of  $\vec{p}$  just using the technique we applied in the previous case. So

$$-c_2[a_2b_3 - a_3b_2] = -\delta_1^2\delta_2k_2/\mu^2, \quad (2.30)$$

$$c_1[a_2b_3 - a_3b_2] + c_3[a_1b_2 - a_2b_1] = (\delta_2^2\delta_1/\mu\nu^2)[k_2 - (\nu^2 + \nu)k_1], \quad (2.31)$$

and

$$-c_2[a_1b_2 - a_2b_1] = -\delta_1^2\delta_2k_1/\mu^2\nu^2 \quad (2.32)$$

where  $k_2 = \mu^2\nu + \nu^2(\mu + 1)$ , and  $k_1 = \mu^2 + \nu + 1$ . With these  $y$  becomes

$$y = (\delta_1\delta_2/\mu^2\nu^2)\{\delta_2\mu(k_2 - (\nu^2 + \nu)k_1) - \delta_1(\nu^2k_2 + k_1)\}. \quad (2.33)$$

Finally the normalized components of the steady state probability vector  $\vec{p}_s$  turned out to be

$$x_1 = p_1 = -k_2\nu^2\delta_1/(m_1\delta_2 - \delta_1m_2), \quad (2.34)$$

$$x_2 = p_2 = \delta_2m_1/(m_1\delta_2 - m_2\delta_1), \quad (2.35)$$

$$x_3 = p_3 = -k_1\delta_1/(m_1\delta_2 - \delta_1m_2), \quad (2.36)$$

where  $m_1 = \mu k_2 - \nu\mu(\nu + 1)k_1$  and  $m_2 = \nu^2k_2 + k_1$ .

What if the model is biased by a constant nonzero external field? The potential of each sites and the barrier between the sites would be affected. Accordingly the potential profile of the model is modified as shown in Fig.2.5. Similar to the previous model,  $f$  is a constant force and if  $f < 0$  the right ward motion is supported so that rate for the right transition will be aggravated, while for  $f > 0$  left transition rate will be improved. There is competition between the force and the temperature

inhomogeneity for  $f > 0$ , when the load is dominant the net current will be to the left. However for the if the inhomogeneity of temperature is high enough current is to the right.

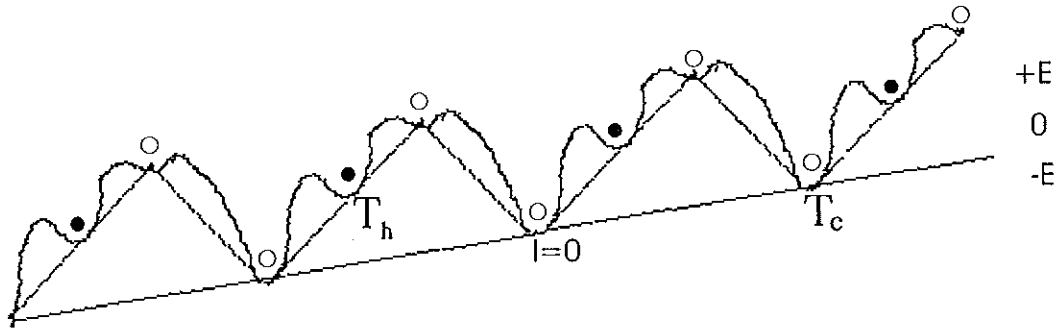


Figure 2.5: The plot of discrete sawtooth potential with trap and external load. sites with dark circles are coupled the hot reservoir ( $T_h$ ) while sites with open circles are coupled to the cold reservoir ( $T_c$ )

We only see for  $f > 0$  because this is more interesting than the  $f < 0$  case. Since the periodicity of the lattice is not affected by the constant biasing field, as in the previous case we can study the system only in a single period by mapping it on to spin-1 system of  $s \in \{0, \pm 1\}$ . We will have three changes of states and their inverse processes i.e 2 to 1, 1 to 3, 3 to 2 and the reverse (2 to 3, 3 to 1, 1 to 3). The corresponding barrier height will be changed. The barrier height that the particle has to cross when there is no load is modified as follows.

<u>state changes</u>	<u>barriers hight</u>
$2 \rightarrow 1$	$\Phi + \frac{E}{2} + \frac{fd}{2}$
$1 \rightarrow 2$	$\Phi - \frac{E}{2} - \frac{fd}{2}$
$1 \rightarrow 3$	$\Phi - E + \frac{fd}{2}$
$3 \rightarrow 1$	$\Phi + E - \frac{fd}{2}$
$3 \rightarrow 2$	$\Phi + \frac{E}{2} + \frac{fd}{2}$
$2 \rightarrow 3$	$\Phi - \frac{E}{2} - \frac{fd}{2}$

The dynamics is the same as the one we did previously for the case when there is no load except for change in the expression for the hoping rates due to the change in barrier. Each matrix element  $R_{ij}$  is piecewise continuous analytic function of  $f$ . Let us assume that  $\Phi > E$  and  $\Phi > E/2 + fd/2$  which implies that  $f < (2\Phi - E)/d$ . For this range of  $\Phi$  and load ( $f$ ), the matrix  $R$ :

$$\mathbf{R} = \begin{pmatrix} -(\delta_2/\nu\epsilon_2 + \delta_2\epsilon_2/\nu^2) & \delta_1\mu\epsilon_1 & \delta_2\nu^2/\epsilon_2 \\ \delta_2/\nu\epsilon_2 & -(\delta_1\mu\epsilon_1 + \delta_1/\mu\epsilon_1) & \delta_2\nu\epsilon_2 \\ \delta_2\epsilon_2/\nu^2 & \delta_1/\mu\epsilon_1 & -(\delta_2\nu\epsilon_2 + \delta_2\nu^2/\epsilon_2) \end{pmatrix}, \quad (2.37)$$

where  $\epsilon_1 = \exp(-fd/2T_h)$ ,  $\epsilon_2 = \exp(-fd/2T_c)$  and the other symbols are the same as in previous section.

Following the techniques as in the previous, we solve for steady state probability distributions. Here we can simply use Eqs.(2.16-19). By replacing the entries of matrix  $R$ , the solutions will be :

$$-c_2[a_2b_3 - a_3b_2] = -\delta_1^2\delta_2k_2/\mu^2\epsilon_1^2\epsilon_2, \quad (2.38)$$

$$c_1[a_2b_3 - a_3b_2] + c_3[a_1b_2 - a_2b_1] = [\delta_2^2\delta_1/\mu\epsilon_1\nu^2][\epsilon_2^2k_2 - (\nu^2 + \nu\epsilon_2^2)k_1], \quad (2.39)$$

and

$$-c_2[a_1b_2 - a_2b_1] = -\delta_1^2\delta_2k_1/\mu^2\epsilon_1^2\nu^2\epsilon_2, \quad (2.40)$$

where  $k_2 = \mu^2\epsilon_1^2\nu\epsilon_2^2 + \nu^2(\mu\epsilon_1^2 + 1)$  and  $k_1 = \epsilon_2^2(\mu^2\epsilon_1^2 + 1)\nu$  and

$$y = [\delta_1\delta_2/\mu^2\epsilon_1^2\nu^2\epsilon_2^2]\{\delta_2\mu\epsilon_1(\epsilon_2^2k_2 - (\nu^2 + \nu\epsilon_2^2)k_1) - \delta_1\epsilon_2(\nu^2k_2 + k_1)\}. \quad (2.41)$$

Finally

$$p_1 = -k_2\nu^2\delta_1/(m_1\delta_2 - \delta_1m_2), \quad (2.42)$$

$$p_2 = \delta_2m_1/(m_1\delta_2 - m_2\delta_1), \quad (2.43)$$

$$p_3 = -k_1\delta_1\epsilon_2/(m_1\delta_2 - \delta_1m_2), \quad (2.44)$$

where  $m_1 = \mu\epsilon_1\epsilon_2^2k_2 - \nu\mu\epsilon_1(\nu + \epsilon_2^2)k_1$  and  $m_2 = \nu^2\epsilon_2k_2 + \epsilon_2k_1$ .

## Chapter 3

# Current and energetics of lattice model of the Brownian motor

### 3.1 Current

In the previous studies it has been studied that asymmetric periodic ratchet potential is essential for unidirectional motion of particles [4]. But how does the strength of the ratchet potential affect the current? For example, electron in lattice is captured by trap potential (due to its interaction with the nucleus). What would be the effect of the trap on current? What could be the relation between the current and the external load when there is trap? We will see these points one by one .

The presence of hot and cold site along the lattice, and the ratchet potential leads to unidirectional motion for the particle at steady state. This is the same as unidirectional motion of the ratchet in Feynman's ratchet and pawl system. So the steady state current ( $J$ ) will be the difference between the current towards the right ( $J^+$ ) and towards to the left ( $J^-$ ) between any two states :  $J = J^+ - J^-$ .  $J^+$  is the current which is defined as the rate at which the spin is observed to change from state (+1) to state (-1) and  $J^-$  is the rate of the spin change in the reverse direction, i.e, from state (-1) to state (+1). This can be interpreted by imagining an observer placed at six o' clock on the clock face depicting spins in Fig. 2.2.  $J^+(J^-)$  is the rate which



the hand clock passes that observer in the clockwise (counterclockwise) direction. By "rate" we mean number of passes per unit time averaged over an infinitely long time. Of course we could just as well place our observer at any point, i.e, in the case of steady state current measured is independent of where the observer is placed or we can take any neighboring states (0 to +1, -1 to 0). Since the current represents the net average rate of clockwise revolution of spin (s) per unit time for ( $J^+ > J^-$ ) and each revolution corresponds to three steps of particle jump to the right, the net translational drift velocity will be  $v = 3dJ$ , where  $v$  denotes the average steady state velocity of the particle. Explicit expressions for  $J^+$  and  $J^-$  are give by :

$$J^+ = (\Gamma/2)R_{31}p_1, \quad (3.1)$$

and

$$J^- = (\Gamma/2)R_{13}p_3, \quad (3.2)$$

so that the net current  $J$  is

$$J = J^+ - J^-. \quad (3.3)$$

Using Eq.(3.1) and (3.2) in Eq.(3.3) one finds that

$$J = (\Gamma/2)[R_{31}p_1 - R_{13}p_3],$$

which can be written as

$$2J/\Gamma = j = [R_{31}p_1 - R_{13}p_3].$$

where  $j$  is the scaled dimensionless current.

The values of  $R_{31}$ ,  $R_{13}$ ,  $p_1$  and  $p_3$  are different for different conditions of the model. In our model we have the following cases.

1. When the model is not biased and the trap potential is neglected, the values of  $R_{31}$  and  $R_{13}$  are given from Eq.(2.9) and  $p_1$  and the values of  $p_3$  are given respectively from Eqs.(2.20) and (2.22). So the scaled current will be given by

$$j = \frac{\nu(\mu - \nu)}{(2 + \mu)(1 + \nu + \nu^2)}. \quad (3.4)$$

The drift velocity  $v$  of the particle then is given by

$$v = 3dJ = \frac{3\Gamma\nu(\mu - \nu)}{2(2 + \mu)(1 + \nu + \nu^2)}. \text{ Notice that the net current is to the right as long as } T_h > T_c, \text{ zero when } T_h = T_c \text{ and to the left for } T_h < T_c.$$

2. When the model is biased but the trap potential is neglected, the values of  $R_{31}$  and  $R_{13}$  are given from Eq.(2.24) and the values of  $p_1$  and  $p_3$  are given respectively from Eqs.(2.25) and (2.27). So the scaled current will be given by

$$j = \frac{\nu\epsilon_2\mu\epsilon_1 - \nu^2\epsilon_2}{(2 + \mu\epsilon_1)(1 + \nu\epsilon_2 + \nu^2\epsilon_2)}. \quad (3.5)$$

Here even for  $\mu = \nu$ ,  $j \neq 0$  which implies that force can cause current.

3. When the model is not biased but the trap potential is strong, the values of  $R_{31}$  and  $R_{13}$  are given from Eq.(2.29) and the values of  $p_1$  and  $p_3$  are given respectively from Eqs.(2.34) and (2.36). So the scaled current will be given by

$$j = (\nu^2 k_1 - k_2) / [m_1/\delta_1 - m_2/\delta_2]. \quad (3.6)$$

It can be written as  $j = z/x_3$  where  $z = \nu^2 k_1 - k_2$  and  $x_3 = m_1/\delta_1 - m_2/\delta_2$ .

4. When the model is biased and the trap potential is strong, the values of  $R_{31}$  and  $R_{13}$  are given from Eq.(2.37) and the values of  $p_1$  and  $p_3$  are given respectively from Eqs.(2.44) and (2.46). So the scaled current will be given by

$$j = (\nu^2 \epsilon_2 k_1 - \epsilon_2 k_2) / [m_1/\delta_1 - m_2/\delta_2]. \quad (3.7)$$

It can be written again as  $j = z/x_3$  where  $z = \nu^2 \epsilon_2 k_1 - \epsilon_2 k_2 x_3 = m_1/\delta_1 - m_2/\delta_2$ .

In the last two cases the expressions for current are not simple to see the effects of the the parameters. Thus we will discuss the properties of the net current as a function of the parameters by drawing the graphs in the next chapter.

## 3.2 Energetics

### 3.2.1 Energetics of the unbiased system

As the particle climbs up and falls down the sawtooth potential there is a certain amount of energy transferred (carried) from the hot(cold) reservoir to the cold(hot) reservoir. We can compute the average rates at which heat is exchanged between the reservoirs. Whenever the particle hops from state 2 to 1, and 2 to 3 the particle absorbs an amount of energy  $\Phi + E/2$  and  $\Phi - E/2$ , respectively, from the hot reservoir to cross the barrier between the states. However to hop in the reverse direction the particle gives these amount of energy to the reservoir, since it falls from the higher energy to a lower one. But when it jumps from state 1 to 2 and state 3 to 2 it absorbs  $\Phi + E/2$  and  $\Phi - E/2$  amount of energy respectively from the cold reservoir and from 1 to 2 (upper of the energy profile)  $\Phi - E/2$ , 3 to 1 (lower of energy profile)  $\Phi + E$ . While in the reverse, i.e, 2 to 1, 1 to 3 (lower of the energy profile) and 3 to 1 (upper of the energy profile) the particle releases the indicated energy.

Let  $\dot{Q}_h$  be the net average rate heat given off by the hot reservoir, and  $\dot{Q}_c$  is the net average rate of heat taken by the cold reservoir. Then the rate of heat given off by the hot reservoir is given by

$$\begin{aligned} \dot{Q}_h = & (\Phi + E/2)(R_{12}p_2) - (\Phi + E/2)(R_{21}p_1) + (\Phi - E/2)(R_{32}p_2) \\ & - (\Phi - E/2)(R_{23}p_3). \end{aligned} \tag{3.8}$$

Rearranging Eq.(3.8)

$$\dot{Q}_h = \Phi\{R_{12}p_2 - R_{21}p_1 + R_{32}p_2 - R_{23}p_3\} + E/2\{R_{12}p_2 - R_{21}p_1 + R_{32}p_2 - R_{23}p_3\}. \quad (3.9)$$

On the other hand  $R_{12}p_2 - R_{21}p_1 = J$  and  $R_{32}p_2 - R_{23}p_3 = J$ . Hence

$$\dot{Q}_h = \Phi\{J - J\} + E/2\{J + J\} = EJ. \quad (3.10)$$

The rate of heat taken by the cold reservoir is given by

$$\dot{Q}_c = (\Phi - E/2)\{R_{12}p_2 - R_{21}p_1\} + (\Phi + E)\{R_{31}p_1 - R_{13}p_3\} + (\Phi + -E)\{R_{13}p_3 - R_{31}p_1\} + (\Phi + E/2)\{R_{32}p_2 - R_{23}p_3\} \quad (3.11)$$

Rearranging Eq.(3.11) we get

$$\begin{aligned} \dot{Q}_c = & \Phi\{\{R_{12}p_2 - R_{21}p_1\} + \{R_{31}p_1 - R_{13}p_3\} \\ & + \{R_{13}p_3 - R_{31}p_1\} + \{R_{32}p_2 - R_{23}p_3\}\} \\ & + (E/2)\{\{R_{21}p_1 - R_{12}p_2\} + 2\{R_{31}p_1 - R_{13}p_3\} \\ & + \{R_{32}p_2 - R_{23}p_3\}\}. \end{aligned} \quad (3.12)$$

Through the same algebra as in  $\dot{Q}_h$  above we get

$$\dot{Q}_c = EJ. \quad (3.13)$$

Eq.(3.10) and (3.13) shows that  $\dot{Q}_h = \dot{Q}_c$  which means the first law of thermodynamics holds true in absence of external load.

Another interesting quantity is the rate of entropy production of the system which is given by :  $\dot{s} = \dot{s}_h + \dot{s}_c$  where  $\dot{s}_h = -\dot{Q}_h/T_h$  and  $\dot{s}_c = \dot{Q}_c/T_c$

$$\dot{s} = (1/T_c - 1/T_h)\dot{Q}_{h \rightarrow c} = 2 \ln(\mu/\nu)J \quad (3.14)$$

This shows that entropy production is positive as long as  $T_h > T_c$ .

### 3.2.2 Energetics of biased system

In each hops the particle takes heat from one reservoir so as to cross the barrier. Some of this energy then will be used to do work on the environment and some will be given to the other reservoir. In the forward motion(2 to1, 1 to 3, 3 to 2) the work is against the field while in the reverse work is done on the system. The net average power per cycle is given by  $\dot{W} = fv$ . From conservation of energy  $\dot{W} = \dot{Q}_h - \dot{Q}_c = fv$ .

Since  $v$  is related to  $J$ , we can compute the average power and rates at which heat is exchanged between the reservoirs. Whenever the particle rotates from state 2 to 1 , 3 to 2 the particle absorbs  $\Phi + E/2 + fd/2$  and  $\Phi - E/2 - fd/2$  amount of energy respectively from the hot bath. When it is hopping in the reverse it releases these amount of energy since it falls from the higher to the lower. When it jumps from state 1 to 2, 3 to 2 it absorbs  $\Phi - E/2 - fd/2$  and  $\Phi + E/2 + fd/2$ , respectively, from the cold reservoir, from 1 to 3,(upper) the absorbed energy is  $\Phi - E + fd/2$  but in the case from 3 to 1 (lower ) is  $\Phi + E - fd/2$ . In the revers i.e 2 to 1, 2 to 3, 1 to 3 (lower) and 3 to 1 (upper) the system releases the indicated energy to the cold reservoir. After going through certain steps  $\dot{Q}_h = (E + fd)J$  and  $\dot{Q}_c = (E - 2fd)J$ . Hence  $\dot{Q}_h - \dot{Q}_c = (E + fd - E + 2fd)J = 3fdJ$  but  $3dJ = v$  so  $\dot{Q}_h - \dot{Q}_c = fv$ . Which is exactly  $\dot{W}$ . When  $f = 0$ ,  $\dot{Q}_h = \dot{Q}_c = 0$ .

The rate of entropy production per cycle  $\dot{s} = \dot{s}_c + \dot{s}_h$  where  $\dot{s}_h = -\dot{Q}_h/T_h = -[E + fd]J/T_h$  and  $\dot{s}_c = \dot{Q}_c/T_c = [E - 2fd]J/T_c$ . This implies

$$\dot{s} = [1/T_c - 1/T_h]EJ + [2/T_c - 1/T_h]fdJ.$$

It can be written as

$$\dot{s} = 2 \ln(\mu/\nu)J + (fdJ/E) \ln(\mu^2/\nu^4). \quad (3.15)$$

The rate of entropy production per cycle increased by  $(fdJ/E) \ln(\mu^2/\nu^4)$  due to the action of external load.

Efficiency:

If  $\dot{W} > 0$  the system works as heat engine. As any macroscopic motor, the efficiency of the Brownian motor is defined as the ratio of the out put power to the input power. In our model the input power is  $\dot{Q}_h$  and the out power is  $\dot{Q}_h - \dot{Q}_c$

$$\eta = \frac{\dot{Q}_h - \dot{Q}_c}{\dot{Q}_h} = \frac{3fd}{E + fd} \quad (3.16)$$

When  $\dot{W} < 0$  the model works as refrigerator. The standard definition of  $COP P_{ref}$  of a refrigerator is the ratio heat taken from cold reservoir of a refrigerator to the power on the system.

$$P_{ref} = \frac{|\dot{Q}_c|}{|\dot{W}|} = \frac{|\dot{Q}_c|}{|\dot{Q}_h - \dot{Q}_c|} = \frac{E - 2fd}{3fd} \quad (3.17)$$

The upper limit of the load in order for the system to work as a refrigerator is  $f = \frac{E}{2d}$ . To determine analytically the value of the force at which current changes the direction which is the boundary in the parameter space that the model works as heat engine or refrigerator is some what difficult. But we may approximate from the graph. We will see it in the next chapter .

# Chapter 4

## Result and discussion

### 4.1 Dimensionless quantities on which current depends.

The main result in this work is the expression for current ( $J$ ) which we derived in the previous chapter. Current depends on five quantities which characterize our model: the temperature values of the hot and the cold reservoirs ( $T_h$  and  $T_c$ ), the barrier due to the ratchet potential, the trap potential and the load. The expression for current is not that much simple to see their effects, i.e, one can not see the way how current depends on each of these parameters by just looking at the expression for  $J$ . In order to see how current behaves as we vary each of the parameters, we draw various plots of  $J$  as a function of the parameters. For simplicity let us define their corresponding dimensionless quantities, and draw the graph as function of these quantities.

Basically a lattice has its own background temperature. To make sites hot and cold we should supply energy from external sources (for instant shining the sites by electromagnetic radiations). Thus the cold sites are those not shined by radiation and the hot are those shined. So the temperature of the hot sites ( $T_h$ ) will be the sum of the background temperature of the lattice ( $T_c$ ) and the increment ( $\Delta T$ ) due to

shining.  $T_h = T_c + \Delta T$ . We can express the increment by a fraction of the background temperature as  $\Delta T = sT_c$ , where  $s$  is a dimensionless quantity which measures the strength of temperature difference between the reservoirs. Instead of the two variable  $T_h$  and  $T_c$  we can specify the thermal nature of the model by  $s$ .

The other dimensionless parameters characterizing the model,  $u = E/T_c$ ,  $v = \Phi/T_c$  and  $\lambda = fd/T_c$  represent respectively the barrier due to ratchet potential, the trap potential and the load of our model.

Now the scaled current  $j(T_h, T_c, E, \Phi, f)$  will be  $j(s, u, v, \lambda)$ . Thus we can see the behavior of the current as a function of each these four dimensionless quantities. To study the behavior of current as the variation of one of these variables we must fix the remaining three parameters.

#### 4.1.1 Stochastic current and strength of hot locality.

The task of Brownian motor is rectifying thermal noise. Thus thermal noise is one source of current in our model. As we can see from the Figs. 4.1 and 4.2 when  $s = 0$ , i.e,  $T_h = T_c$ , the net current is zero for unbiased system. In our model thermal inhomogeneity is crucial. For nonzero  $s$  there is current and it is monotonically increasing with  $s$ . However the rate of increment of current is fast for small range of  $s$ . For finite but large values of  $s$  the rate will slow down and for ultimately large value of  $s$  current saturates. This is expected result because current directly depends on rate of transition probability and in turn the rate of transition probability depends on temperature of the reservoir. The increment of  $s$  implies increment in  $T_h$  since the background temperature ( $T_c$ ) is constant. The rate of change of transition probability ( $W$ ) with  $s$  is fast in a small range of  $s$  because as  $s$  continue to increase, the particles in hot reservoir get some what enough energy so that the barrier become

relatively easy for the particles to surmount. As  $s$  is increased further  $W$  from hot to cold grows slowly. As  $s$  goes to infinity, increment of  $s$  will not have a significant



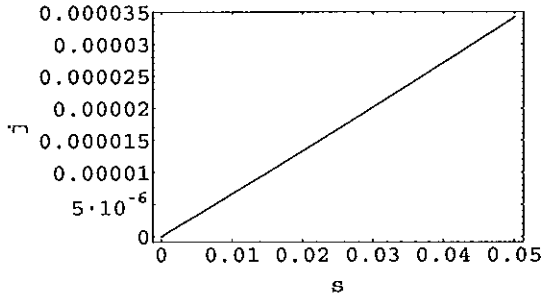


Figure 4.1: The plot of current versus strength of the hot locality taking  $u = 4$ ,  $v = 0$  and  $\lambda = 0$  for  $s$  is between 0 and .05

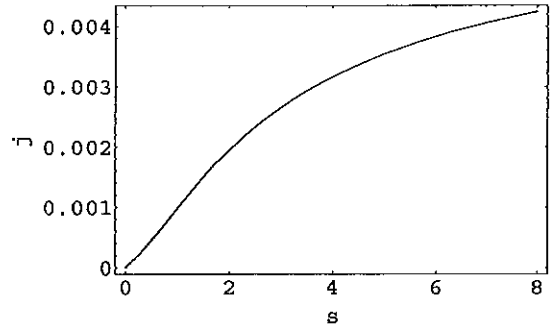


Figure 4.2: The plot of current versus strength of the hot locality taking  $u = 4$ ,  $v = 0$  and  $\lambda = 0$  for  $s$  is between 0 and 8

effect on the transition probability per unit time [19].

This is true for both system with trap and with out trap. We can understand by comparing the graph of Fig.4.2 and Fig.4.4. But the values of  $s$  at which the current gets saturation are different. The values of  $s$  at which the current begins to saturate for system with trap is greater than for system without trap this due to trap increases the barrier. The same is true for biased and unbiased. The presence of both trap and load at the same time does not affect the way how current depends on  $s$  but it affects the value  $s$  at which saturation occurs. Nevertheless it is difficult to determine the exact value of  $s$  at which current becomes saturated for each cases analytically. It may be possible numerically but we have not attempted it here.

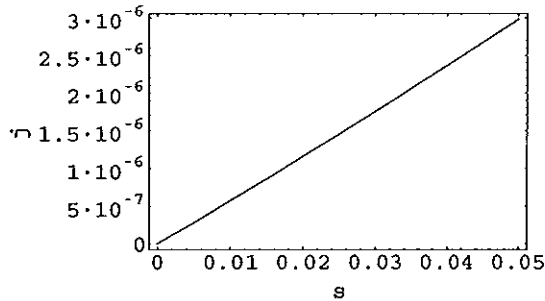


Figure 4.3: The plot of current versus strength of the hot locality taking  $u = 4$ ,  $v = 0$  and  $\lambda = 0$  for  $s$  is between 0 and .05

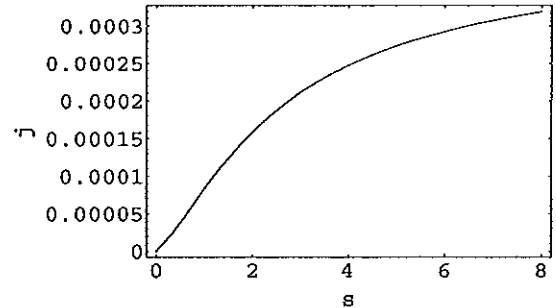


Figure 4.4: The plot of current versus strength of the hot locality taking  $u = 4$ ,  $v = 5$  and  $\lambda = 0$  for  $s$  is between 0 and 8

#### 4.1.2 Stochastic current and barrier potential

The basic parameter that specifies the rectification quality of the model is the barrier due to the ratchet potential. Because it is asymmetric; it highly blocks the backward motion of the particles as compared to the forward motion. Thus the net current is to the right when the load is either zero or very small. This is clearly observed from the graph in Fig.4.5. For  $u = 0$ , current is zero which means that no rectification of the motion takes place when there is no barrier of ratchet. As  $u$  increases the rectification quality will be improved, so that current increases. The improvement of the rectification of the model is only up to certain value of  $u$  at which current gets its optimal value. However further increasing in  $u$  will decrease the quality of rectification. As the barrier height goes high current will tend zero. The increment of  $J$  in  $u$  from zero to a value at which current gets its optimal value is due to  $J^-$  (current to the left) is highly affected by the barrier than  $J^+$  (current to the right). The barrier highly blocks the backward motion as compared to the forward motion of the particles. This is what we mean by rectification of noise. But further increasing of  $u$  will also affect the forward motion of the particles significantly. As  $u$  goes to

infinity, the barrier will be too high for the particles to surmount; because it will be beyond the thermal kick that builds the capacity of the particle to jump in both directions. This is true for both system, with trap and without trap, and biased and unbiased but the value of  $u$  at which  $J$  gets maximum and the optimal value of the current are different. Again here the numerical determination of the value of the  $u$  at which  $j$  gets its optimal value is open for further study.

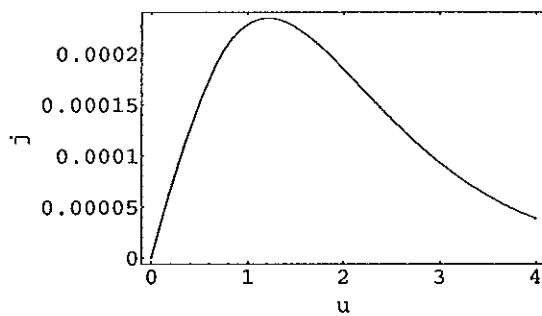


Figure 4.5: The plot of current versus the barrier potential taking  $s = .5$ ,  $v = 5$  and  $\lambda = 0$

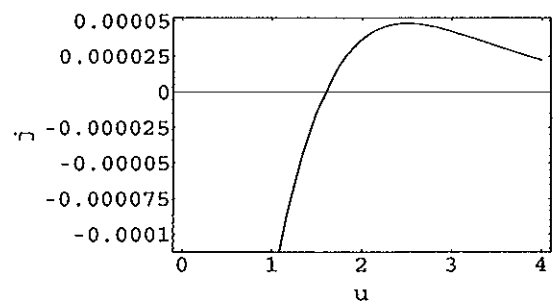


Figure 4.6: The plot of current versus the barrier potential taking  $u = 4$ ,  $v = 0$  and  $\lambda = 0.2$

### 4.1.3 Stochastic current and trap potential

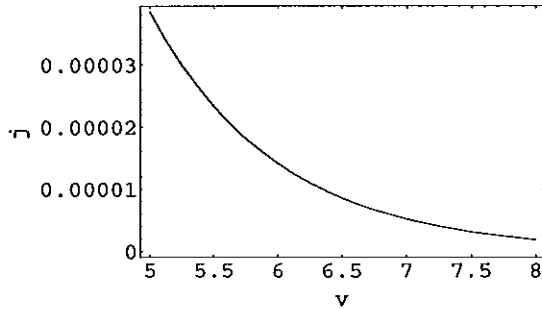


Figure 4.7: The plot of current versus the trap potential taking  $u = 4$ ,  $s = .5$  and  $\lambda = 0$

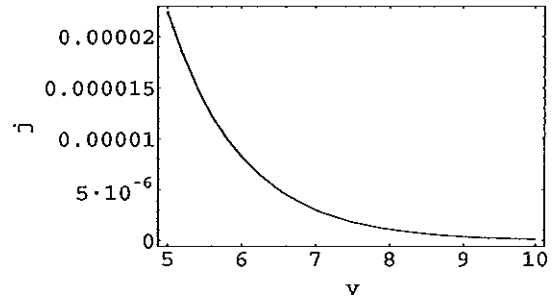


Figure 4.8: The plot of current versus the trap potential taking  $u = 4$ ,  $s = .5$  and  $\lambda = 0.2$

We can see that the current, when there is trap, is smaller than when there is no trap for the same set of other parameters  $s, u$ , and  $\lambda$ .  $j(\text{with trap}) < j(\text{with out trap})$ . For example if we compare the value of  $j$  from the graph in Fig. 4.1 to its value from the graph in Fig.4.3, current of the system with trap is one-tenth that of the current without trap.

In both biased and unbiased case trap reduces current. This is clearly seen from the graph in Fig.4.7 and 4.8 Current decreases as trap value increases. This is because it elongates the waiting time of the particle at the sites. As trap goes to infinity current becomes zero which means the particle spends a lot of time at the sites. Decrease of current for all ranges of trap shows that trap does not contribute any rectification as a ratchet rather it creates obstacle for the motion of the particles in both direction.

### 4.1.4 Stochastic current and external load

In the case where there is an external load, our sources of current will be both the load and the thermal inhomogeneity controlled by  $s$ . There is competition between these two parameters when  $f > 0$ . If  $s$  is dominant over the strength of the load, the

current will be positive and the model works as heat engine but for the case where load is dominant, current will be negative. So our model works as a refrigerator. From the graph in Fig.4.9, we can see that there is a value of the force which exactly cancels current due to temperature inhomogeneity.

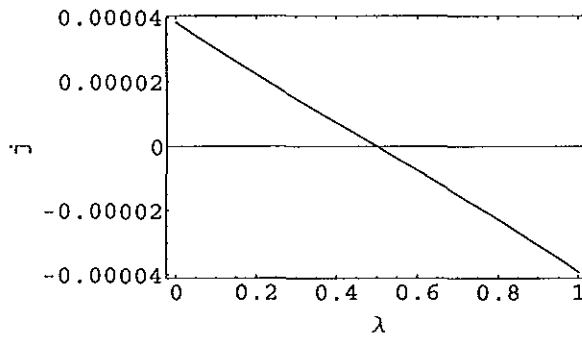


Figure 4.9: The plot of current versus external load taking  $u = 4$ ,  $v = 5$  and  $s = .5$

This force is known as stall force. It is a boundary on the coordinate of force which divide the range of the force where the model works as heat engine or as refrigerator. If the value of the force is in the range between zero and stall force it works as heat engine, but in the range between the stall force and  $E/2d$  it works as refrigerator. For the  $f > E/2d$  it works niter as heat engine nor as refrigerator.

## 4.2 Energetics

As we can see from Eq.3.11 first law of thermodynamics holds true for our system. The amount of energy taken from the hot heat reservoir is equal to the energy given to cold heat reservoir for unbiased system since the work done is zero. Second law of thermodynamics is also true, since as far as  $T_h > T_c$ ,  $\dot{s} > 0$ . Form Eqs. 3.12 and 3.13, we can understand that  $\dot{s}$  is directly dependent on  $J$  which in turn depends on

trap. So trap affects  $\dot{s}$ . As tarp increases,  $\dot{s}$  decreases.

Even if  $\dot{Q}_h$ ,  $\dot{Q}_c$  and  $\dot{W}$  depend on trap through current, efficiency ( $\eta$ ) and  $COP_{ref}$  do not be affected by trap. This is clear from Eqs.3.14 and 3.15

# Chapter 5

## Summary and conclusion

In this thesis we considered two lattice models of Brownian motor. The first is lattice with neglected trap potential. In the second we considered lattice with significant trap potential which is uniformly distributed. When we think about Brownian motor we must give attention for two crucial concepts: noise and rectification. The sources of noise are external fluctuations which might be fluctuation in potential, external load or temperature. The strength of the noise depends on how strong these fluctuations are. Then one has to find a means of rectifying these fluctuations in order to get a useful energy (work or unidirectional current) out of the random noise. In ratchet models the rectification can be easily done by using an asymmetric potential. As such in our model we used an asymmetric periodic potential with non-homogeneous temperature background which is responsible for the strength of the noise. Based on these assumptions we found explicit expressions for current, rate of heat taken from hot reservoir and given to the cold reservoir, power and efficiency as function of dimensionless quantities. From close analysis of these expressions we can understand that:

1. Trap really affects current and quantities which depend on current. As the strength of trap depth increases the current decreases. Trap which opposes

both directions of motion, is obstacle.

2. Strength of hot locality and external load are the sources of current. They are analogous to the potential difference for electric circuit.
3. The ratchet potential which give rises unidirectional motion is our rectifier and it is analogous to the diode for electric circuit.

We proposed a model of tiny engines and predicted the way how it behaves as heat engines and refrigerators. One wonders whether such a model could be realized in the Laboratory.



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