BLOWTORCH EFFECT ON THE ESCAPE AND EQUILIBRATION RATES FOR THE HOPPING MODEL

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Abstract

In bistable systems the transition kinetics between two locally stable states can be altered by heating locally one of the stable states (using blow-torch). As a model for diffusion in a non-homogeneous medium, we consider the hopping model. The kinetic aspect of blow-torch effect is investigated for a model double-well potential with localized heating. That is, we analyze the relaxation behavior of a bistable system when the background temperature profile is non-homogeneous. Using Brinkman's method, we derive the general and analytic expressions for the escape and equilibration rates of the system as a function of the strength, width, and the position of the hot locality, the barrier height and the pit potential of traps for the model that we consider.

Our result shows that the presence of the hot locality enhances the escape rate from the well where it is placed and retards the escape rate from the other well. Our work also shows a remarkable result in relation to the position of the hot locality in that placing the hot locality mid way between the top and bottom of the well has the largest enhancing effect on the escape rate from the hot zone than any other position. This result is similar to the work of Solomon Fekade and Mulugeta Bekele for the case of Landauer's heated pipe model[1]. Moreover, the escape and equilibration rates of the system become decreasing functions of the barrier height and the pit potential of traps.

Contents

1 INTRODUCTION

For a number of decades statistical physics was preoccupied with thermodynamic limit, with equilibrium, or with systems very close to equilibrium[2]. The diffusion of a particle in a high friction homogeneous medium [3, 4] at constant temperature T and in the presence of an external potential $V(x)$, is described by

$$\frac{\partial P(x,t)}{\partial t} = \mu\frac{\partial}{\partial x}\Big(V'(x)P(x,t)\Big) + D\frac{\partial^2}{\partial x^2}P(x,t) \tag{1.1}$$

where P(x,t) is the probability density of the particle at position x at time t, μ is the mobility, D is the diffusion coefficient such that

$$D = k_B T\mu \tag{1.2}$$

where k_B is the Boltzmann constant and $V'(x) = \frac{dV(x)}{dx}$. Then, the equilibrium distribution, $P^e(x)$, of Eq. (1.1) is the Boltzmann's factor

$$P^e(x) = Ce^{[-V(x)/k_B T]} \tag{1.3}$$

which gives us information about the behavior of the particle. It immediately tells us which state is occupied more densely than the other [2]. However, many processes in our daily life take place in an inhomogeneous environment which makes systems not to attain equilibrium state. As a result, these processes are inhomogeneous, non-linear, and operate far from equilibrium and, hence the general arguments of the equilibrium statistical mechanics may not work and one has to study the non-equilibrium nature of systems.

The general diffusion equation for a Brownian particle in non-homogeneous medium proposed by some authors [3, 4] is either

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}[(\mu V'(x)P) + \frac{\partial}{\partial x}(DP)] \tag{1.4}$$

which shows that the difference with Eq. (1.1) consists of an addition drift term, or

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}(\mu V'(x)P) + \frac{\partial}{\partial x}D\frac{\partial P}{\partial x} \tag{1.5}$$

Thus, for the diffusion of a Brownian particle whose diffusion coefficient varies in space, there are two ways [5] in which one can generalize the ordinary diffusion equation. That is, one may write either

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}D(x)P \tag{1.6}$$

or

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}D(x)\frac{\partial P}{\partial x} \tag{1.7}$$

They differ by a term

$$\frac{\partial}{\partial x}[\frac{dD(x)}{dx}P] \tag{1.8}$$

It is true that Eq.(1.7) is more attractive because it can be written as

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial J}{\partial x}. \tag{1.9}$$

where

$$J = -D\frac{\partial P}{\partial x}$$

is the current density. But this is not a decisive argument. To find which one is right one has to start from a precise model and carry out an expansion in some size parameter. Of course, it cannot be concluded that this is always the correct choice. Therefore, for a Brownian particle in non-homogeneous media, one cannot make an a priori choice without examining the underlying diffusion mechanism. Because of this reason, the diffusion equation of a Brownian particle in non-homogeneous medium has been an issue of some debate [4]. The problem is solved after van Kampen, taking three different diffusion equations for three different models which showed the model dependent nature of diffusion equation in non-homogeneous media.

The models are Landauer's heated pipe model, van Kampen's model and the hopping model. As a model for diffusion in a non-constant temperature, Landauer [3, 4] proposed a narrow pipe filled with a Knudsen gas. The wall of the pipe has its own temperature, which varies as a function of the coordinate x along the axis of the pipe. As the molecules (under external potential field, V(x)) of the gas move through the pipe they get thermalized by colliding with the wall of the pipe. Starting from the Kramers' equation for the distribution function of molecules and assuming the radius of the pipe approaching to zero, van Kampen derived a diffusion equation using singular perturbation technique[3, 4].

Van Kampen [1, 4] also derived an equation appropriate for the description of motion of non-interacting Brownian particles in an inhomogeneous medium with a high friction. Starting from one dimensional Kramers' equation and using the generalized method for eliminating fast variables [6, 7], he arrived at the diffusion equation for the model. Van Kampen also proposed hopping model[4] which is the concern of this thesis, the detail of which will be discussed in the next chapter.

In any model, heating the system locally (applying blowtorch effect), will affect the dynamics of the Brownian particle. Most of the investigations related to the blow torch effect study the influence of space dependent temperature on the steady-state relative occupations of the energy minima. There has been no analytical work to study the kinetic aspect of the system, specifically, the calculation of the longest relaxation time in a bistable potential in the presence of a blowtorch long before. In 1990's Mulugeta Bekele, et.al.[8] have started to work on the detailed kinetic aspect of the problem using supersymmetric method. They have calculated the lowest relaxation time in a bistable potential in the presence of a hot locality, for van Kampen's model. Later on, the effect of blowtorch on the escape and equilibration rates on the Landauer's and van Kampen's model is reported by Solomon Fekade and Mulugeta Bekele [1].

The main purpose of this work is to understand the influence of blowtorch effect on the escape and equilibration rates for the hopping model in a bistable potential. We use Brinkman's method [9, 10] to get analytic expressions not only for the equilibration rate but also for the individual escape rates from the two potential wells.

The rest of this thesis is organized as follows. The detail of the hopping model will be discussed in the next chapter. In chapter 3, by considering a bistable potential and space dependent temperature profile, we formulate the general expressions for the escape and equilibration rates. In chapter 4, we consider specific W-potential and a piecewise constant temperature profile to derive analytic expressions for the hopping model. The results of the thesis are discussed in chapter 5. Conclusions of the present work are discussed in the last chapter.

2 THE HOPPING MODEL

For this model we consider the following diffusion mechanism. Both the temperature and the properties of the medium are inhomogeneous. For simplicity, consider one dimension, which will be measured on the macroscopic scale by x. The medium contains randomly located traps with density $\Omega\sigma(x)$. Their random mutual distances are of order Ω^{-1}, which defines the microscopic scale,i.e., Ω is a measure for the number of traps per unit length. An electron hops from one trap to the next, the time spent between traps being negligible. This process constitutes a continuous time random walk, provided that the electron spends enough time in each trap for any memory of its preceding adventures to be erased by the thermal motion of the lattice.

Suppose that each trap consists of a pit in the internal potential of depth Φ. As the particle falls into the trap, at position x' it will be there until it gets a kick, which sends it traveling to the right or to the left. That is having surmounted the energy barrier Φ, the particle will travel to the right or to the left. Then the probability per unit time for this to happen is the escape probability per unit time that can be given by the Arrhenius factor

$$C\ e^{\frac{-\Phi}{k_B T(x\prime)}} \tag{2.1}$$

The temperature is taken at the site of x' of the pit. Let the probability that there is a trap between x and x+dx be $\Omega\sigma(x)dx$ [5,11]. Then, starting at an arbitrary point x' the probability to meet a first trap at a point between x and x+dx , supposing $x > x'$, is

$$dx.\Omega\sigma(x)Exp[-\Omega\int_{x'}^{x}\sigma(x'')dx''] \tag{2.2}$$

In the presence of an externally applied potential $V(x)$, the probability per unit time for a trapped electron to pick up the energy Φ (assumed to be constant for all traps) needed to escape suffices it to roll down the slope of V(x) into the next trap, but not to move up that slope. Suppose let us take the case $\frac{dV(x)}{dx} > 0$. Then the Arrhenius factor of Eq.(2.1) suffices for travel to any $x < x'$, but in order to arrive at some trap uphill, $x > x'$, an additional energy is needed. Then, the probability per unit time for this is

$$CExp[\frac{-(\Phi + V(x) - V(x'))}{k_B T(x')}] \tag{2.3}$$

Therefore, the transition probability per unit time, $W(x|x')$, for a jump from a trap at x' to the next trap at $x < x'$, is

$$C\Omega\sigma(x)Exp[-\Omega \int_x^{x'} \sigma(x'')dx'']Exp[-\Phi/k_B T(x')], for x < x' \tag{2.4}$$

and in order to hop to a trap at $x > x'$ the electron has to surrmount the additional energy $V(x) - V(x')$; So that the transition probability per unit time, $W(x|x')$ is

$$C\Omega\sigma(x)Exp[-\Omega \int_{x'}^{x} \sigma(x'')dx'']Exp[-(\Phi + V(x) - V(x'))/k_B T(x')], for x > x' \tag{2.5}$$

Then, keeping all the above ideas as a background information and using all the expressions given by equations of the transition probabilities for the hopping-model, one can arrive at a gain-loss equation for the probability density $P(x, t)$, which has the general form of a master equation,

$$\frac{\partial P(x,t)}{\partial t} = \int [W(x|x')P(x', t) - W(x'|x)P(x, t)]dx' \tag{2.6}$$

The transition probability $W(x|x')$ per unit time from x' to x involves the information mentioned above. In particular, it involves Ω. The jumps $|x-x'|$ are of order Ω^{-1}. Therefore, for large Ω it is possible to use the standard expansion of the master equation[5, 6, 11], so as to obtain a Fokker-Planck Equation, which is the generalized diffusion equation we are looking for. The result is

$$\frac{\partial P(x,t)}{\partial t} = \frac{C}{\Omega^2}\frac{\partial}{\partial x}[\frac{V'(x)e^{\frac{-\Phi}{k_B T(x)}}}{k_B T(x)\sigma^2(x)}P(x,t) + \frac{1}{\sigma(x)}\frac{\partial}{\partial x}\frac{1}{\sigma(x)}e^{\frac{-\Phi}{k_B T(x)}}P(x,t)] \tag{2.7}$$

In this thesis, we consider the number of available traps for the hopping model to be uniform, and hence $\sigma(x)$ will be independent of position, x. Thus, Eq.(2.7) can have of a form

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}[\frac{C}{\Omega^2\sigma^2}\frac{V'(x)}{k_BT(x)}e^{\frac{-\Phi}{k_BT(x)}}P(x,t) + \frac{\partial}{\partial x}\frac{C}{\Omega^2\sigma^2}e^{\frac{-\Phi}{k_BT(x)}}P(x,t)] \tag{2.8}$$

This is the Fokker-Planck equation for the hopping model for uniform number of traps. Moreover, Eq. (2.8) can be put as

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}[\mu(x)V'(x)P(x,t) + \frac{\partial}{\partial x}(D(x)P(x,t))] \tag{2.9}$$

This is the familiar Smoluchowski equation, where

$$\mu(x) = \frac{C}{\Omega^2\sigma^2 k_BT(x)}e^{\frac{-\Phi}{k_BT(x)}}$$

and

$$D(x) = \frac{C}{\Omega^2\sigma^2}e^{\frac{-\Phi}{k_BT(x)}}$$

and the Einstein's relation

$$D(x) = \mu(x)k_BT(x)$$

is satisfied.

In this thesis, from now onwards, based on the idea that the number of traps are assumed to be uniform, every work or analysis concerning the hopping model relies on Eq. (2.9). The stationary solution of Eq. (2.9) is

$$P_s(x) = C_o e^{\frac{\Phi}{k_BT(x)}} Exp[-\int_{x_o}^{x}\frac{V'(x')}{k_BT(x')}dx'] \tag{2.10}$$

where C_o is a constant which can be determined from initial conditions. From Eq. (2.10), one can see that the first factor is the probability for each trap to be occupied and the second factor is the effect of the external potential.

The effect of the external potential $V(x)$ [2] on the steady state distribution is fully accounted for in the factor

$$e^{[-\int_{x_o}^{x}\frac{V'(x')}{k_B T(x')}dx']} \tag{2.11}$$

In the next chapter we will study in the hopping model the slow dynamics of the Brownian particle in a bistable potential with non-homogeneous temperature background.

3 RATE EQUATIONS IN A BI-STABLE POTENTIAL

Any probability distribution originally peaked near the top of a bistable potential barrier evolves in time and does not remain localized [5]. The evolution occurs in three successive stages. These are

1. The distribution broadens rapidly but fluctuations across the potential barrier are still possible.

2. Fluctuations across the potential barrier die out; the total probability is decomposed into two autonomous parts, left and right of the potential barrier.

3. The peaks reach their local equilibrium shape around the position of these two autonomous parts.

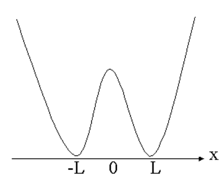

Figure 1: Plot of Bistable potential

In a bistable potential, the two wells can be considered as two separate regions where two kinds of processes take place. These are, the local equilibration process in each well of the potential and the global equilibration process by which the wells exchange the particle.

In general, motion of a Brownian particle in a bistable potential has two time scales in its evolution [1]. One is the time scale which is of the order of the time required for local equilibration in one of the wells (to the left or right of the potential barrier). The other time scale is the time required for the slow process of escaping of the particle from one well to the other. This time scale is of the order of the time required for global equilibration. The time scale for local equilibration is fast as compared to the time scale for global equilibration.

To see this let us consider the motion of a Brownian particle in a viscous medium. Then, the dynamics of the particle in the potential wells is described by the Langevin's equation

$$m\frac{d^2x}{dt^2} = -V'(x) - \beta\frac{dx}{dt} + \sqrt{2\beta k_B T}\zeta(t) \tag{3.1}$$

If the mass of the particle, m, is unity, then

$$\frac{d^2x}{dt^2} = -V'(x) - \beta\frac{dx}{dt} + \sqrt{2\beta k_B T}\zeta(t) \tag{3.2}$$

where $-\beta\frac{dx}{dt}$ is the friction force that the Brownian particle experiences from the medium or from the collision as it falls into the traps, ζ is some random fluctuating force. The coefficient β is inversely proportional to the mobility of the particle μ. For high friction limit (large β), the particle will not be free to accelerate. Then,

$$\frac{d^2x}{dt^2} = 0.$$

Hence, $Eq.$(3.2) becomes,

$$\beta\frac{dx}{dt} = -V'(x) + \sqrt{2\beta k_B T}\zeta(t) \tag{3.3}$$

Then, taking the average of both sides, keep track of the displacement of the mean value for $x(t)$, we get,

$$\beta\frac{dx}{dt} = -V'(x) \tag{3.4}$$

Approximating the potential near the minimum points by a parabola of the form

$$\frac{1}{2}\omega(x \pm L)^2 \tag{3.5}$$

where

$$\omega = V''(\pm L).$$

Then Eq. (3.4) becomes

$$\frac{dx}{dt} = -\frac{\omega}{\beta}(x \pm L) \tag{3.6}$$

Solving this differential equation, we get

$$x(t) \pm L = ce^{-\frac{\omega}{\beta}t}, \tag{3.7}$$

where c is a constant which can be determined from initial conditions. Eq. (3.7) can be written as

$$x(t) \pm L = ce^{\frac{-t}{\tau_\ell}}, \tag{3.8}$$

with $\tau_\ell = \frac{\beta}{\omega}$ is the local relaxation time.

To approximate the relaxation time, τ_g, for the global equilibration process, we consider a uniform temperature background for the system ($T(x) = T_o$) and we approximate the potential around the minima by Eq. (3.5) and around the barrier height by

$$V(x) = V(0) - \frac{1}{2}\omega_o x^2 \tag{3.9}$$

where $\omega_o = V''(0)$. Then the relaxation time, τ_g, for global process is

$$\tau_g = \frac{1}{K_A + K_B} \tag{5.10}$$

where escape rates from the potential wells K_A and K_B are given by

$$K_A = K_B = \frac{D(L)e^{\Phi/k_BT(L)}}{\int_{-L}^{L} e^{\int_{-L}^{x}\frac{V'(x')}{k_BT(x')}dx'}dx\int_{-\infty(0)}^{0(\infty)} e^{\Phi/k_BT(x)}e^{-(\int_{-L}^{x}V'(x')/k_BT(x')dx'}dx} \tag{3.11}$$

at uniform temperature.

Note that the detail of the escape rates K_A and K_B is explained in chapter 3 and 4. Now we intend to approximate the values of the integrals in the expressions for the escape rates. Then, using Eq. (3.9), we have

$$\int_{-L}^{L} e^{\int_{-L}^{x} V'(x')/k_B T(x')dx'} dx \;=\; \int_{-L}^{L} e^{(V_o/k_B T_o - \frac{\omega_o x^2}{2k_B T_o})} dx$$

But the potential is significant only near the point $x = 0$ and it drops as we go far away from $x = 0$ in both directions. Hence, the limit of integration can be extended to $-\infty$ and ∞. So that the approximation becomes,

$$\int_{-L}^{L} e^{\int_{-L}^{x} V'(x')/k_B T(x')dx'} dx \;=\; \int_{-\infty}^{\infty} e^{(V_o/k_B T_o - \frac{\omega_o x^2}{2k_B T_o})} dx$$

Then we get,

$$\int_{-L}^{L} e^{\int_{-L}^{x} V'(x')/k_B T(x')dx'} dx \;=\; \sqrt{\frac{2\pi k_B T_o}{\omega_o}} e^{V_o/k_B T_o} \tag{3.12}$$

And the other integrals in K_A and K_B are

$$\int_{-\infty(0)}^{0(\infty)} e^{\Phi/k_B T(x)} e^{(-\int_{-L}^{x} \frac{V'(x')}{k_B T(x')} dx')} dx \;=\; \frac{e^{\Phi/k_B T_o}}{2} \sqrt{\frac{2\pi k_B T_o}{\omega}} \tag{3.13}$$

Then by combining the values of the integrals, we get

$$K_A \;=\; K_B \;=\; \frac{D(L)\sqrt{\omega\omega_o} e^{-V_o/k_B T_o}}{\pi k_B T_o} \tag{3.14}$$

Then, the equilibration time for the global one becomes

$$\tau_g \;=\; \frac{\pi k_B T_o e^{V_o/k_B T_o}}{2\sqrt{\omega_o \omega} D(L)} \tag{3.15}$$

Using the fact that $D(L) = \mu k_B T_o$ and the mobility is inversely proportional to the damping constant, i.e., $\mu = \frac{1}{\beta}$, the time for the global process is

$$\tau_g \;=\; \frac{\pi \beta e^{V_o/k_B T_o}}{2\sqrt{\omega_o \omega}} \tag{3.16}$$

If the parabolas at the minima points and at the maximum point for the potential are assumed to have the same shape, ω and ω_o will have the same value. Hence,

$$\tau_g = \frac{\pi\beta e^{V_o/k_B To}}{2\omega} \tag{3.17}$$

Hence,

$$\tau_g = \frac{c\beta e^{V_o/k_B To}}{\omega} \tag{3.18}$$

where $c = \frac{\pi}{2}$. Thus, comparing with the time for the local one, we get

$$\frac{\tau_g}{\tau_\ell} \sim e^{V_o/k_B T_o} \tag{3.19}$$

This shows that the equilibration time for global equilibration is much greater than the equilibration time for local process. Thus, global equilibration is a slow process compared to local equilibration. Here β is the damping coefficient of the force that the particle experiences from the medium or from collision as it falls into the pits and ω is the measure of the curvature of the potential wells. Comparing these two time scales we see that the global equilibration process is very slow compared to the local one when V_o is larger than $k_B T_o$.

In this chapter, we are interested in the dynamics of the Brownian particle as it approaches to the steady state in a bistable potential.

By considering the two wells as separate regions, we formulate the rate equations governing the dynamics of the Brownian particle for the hopping-model in non-homogeneous medium using Brinkmann's method [9,10].

3.1 Rate Equations In Non-Homogeneous Medium

In this section we study the dynamics of the Brownian particle of the hopping model, where the temperature is non-homogeneous. We consider a double well potential, $V(x)$, whose barrier height is V_o as shown in Fig. (2). Let the peak of the barrier be located at $x = 0$ and the two minima be located at $x_A = -L$ and at $x_B = L$. The non-homogeneous temperature background of the medium is obtained by locally heating a certain portion of the medium in one of the wells.

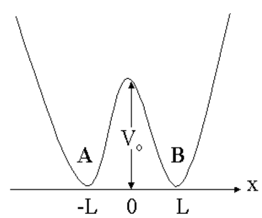

Figure 2: Plot of Bistable potential with barrier height V_o

As we mentioned in the last chapter, the dynamics of the Brownian particle subjected to the non-homogeneous temperature background is governed by the familiar Smoluchowski equation

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}[\mu(x)V'(x)P(x,t) + \frac{\partial}{\partial x}\Big(D(x)P(x,t)\Big)] \tag{3.1.1}$$

where $\mu(x)$ is the mobility of the particle and $D(x)$ is the diffusion coefficient. Eq. (3.1.1) can be written in the form of

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}J(x,t) \tag{3.1.2}$$

where $J(x,t) = -\mu(x)V'(x)P(x,t) - \frac{\partial}{\partial x}\Big(D(x)P(x,t)\Big)$ is the probability current density. In order to solve the problem, we follow Brinkman's approach [9, 10] and define coarse-grained variables $n_A(t)$ and $n_B(t)$ to be the number of particle or population to be found in the left well and the right well at time t, respectively. Then,

$$n_A(t) = \int_{-\infty}^{0} P(x,t)dx \tag{3.1.3}$$

and

$$n_B(t) = \int_{0}^{\infty} P(x,t). \tag{3.1.4}$$

If we differentiate Eq.(3.1.3) with respect to time and substituting Eq.(3.1.2) we get

$$\frac{\partial n_A(t)}{\partial t} = \int_{-\infty}^{0} -\frac{\partial}{\partial x}J(x,t)dx$$

Note that the point $x = -\infty$ is assumed to be a reflecting barrier.Then

$$\frac{dn_A(t)}{dt} = -J(0,t) \tag{3.1.5}$$

Because the probability density has to be normalized, we have

$$\int_{-\infty}^{\infty} P(x,t)dx = 1$$

or

$$n_A(t) + n_B(t) = 1.$$

Hence,

$$\frac{dn_A(t)}{dt} = -\frac{dn_B(t)}{dt}. \tag{3.1.6}$$

Note that the expression for the current density takes the form

$$\frac{\partial}{\partial x}\Big(D(x)P(x,t)\Psi(x)\Big) \;=\; -J(x,t)\Psi(x), \tag{3.1.7}$$

where

$$\Psi(x) \;=\; e^{\int_{-L}^{x}\frac{V'(x')}{k_B T(x')}dx'}$$

and $D(x)$ is the diffusion constant satisfying the Einstein relation

$$D(x) \;=\; \mu(x)k_B T(x). \tag{3.1.8}$$

Now, integrating Eq. (3.1.7) from $-L$ to L , we get

$$P(L,t)D(L)\Psi(L) - P(-L)D(-L) \;=\; -\int_{-L}^{L} J(x,t)\Psi(x)dx. \tag{3.1.9}$$

Clearly $\Psi(-L) \;=\; 1$.

Now the integral on the right hand side of Eq. (3.1.9) can be simplified. For the global equilibration process, the contribution of the current at the peak of the barrier is mainly from the neighboring points of $x \;=\; 0$, that is from the region $(-L, L)$. On the other hand [10] current is very nearly constant in this region. So that the particle density near the top of the barrier will not change very much during the course of time. For this particular condition, Brinkman [9] assumed that the region near the top of the barrier gives the major contribution to the integral and the current density, $J(x,t)$, is spatially constant near the top of the barrier at $x \;=\; 0$ after a transient period and that local equilibrium is established near the two minima. Then $J(x,t)$ is removed from the integrand on the right hand side of Eq. (3.1.9) leading to a factor $J(0,t)$. Hence, Eq. (3.1.9) takes a form

$$-J(0,t) \;=\; \frac{P(L,t)D(L)\Psi(L) - P(-L,t)D(-L)}{\int_{-L}^{L}\Psi(x)dx}. \tag{3.1.10}$$

Again, combining Eqs. (3.1.5) and (3.1.10) gives

$$\frac{dn_A(t)}{dt} = \frac{P(L,t)D(L)\Psi(L) - P(-L,t)D(-L)}{\int_{-L}^{L}\Psi(x)dx}. \tag{3.1.11}$$

In order to determine $P(L,t)$ and $P(-L,t)$, first let us find the non-steady state probability density $P(x,t)$ in terms of the steady state solution of the probability distribution. So, to do this we consider the steady state current density, $J(x,t)$. At steady state the current density is zero,i.e. $J(x,t) = 0$. So that

$$\mu(x)V'(x)P_s(x) + \frac{\partial}{\partial x}\Big(D(x)P_s(x)\Big) = 0 \tag{3.1.12}$$

Hence, the steady state solution of the probability density is

$$P_s(x) = Ce^{\Phi/k_BT(x)}e^{(-\int_{-L}^{x}\frac{V'(x')}{k_BT(x')}dx')}, \tag{3.1.13}$$

where C is the normalization constant which can be determined from initial conditions.

The equilibration process in each well is very fast as compared to the global equilibration process which require escape over the barrier. At large times [9] $P(x,t)$ approaches that of the local thermal equilibrium. Thus, for global equilibration process the probability distribution $P(x,t)$ in each well is not very far away from the steady state distribution and can be approximated by the product of two independent functions. That is,

$$P(x,t) = N(t)P_s(x), \tag{3.1.14}$$

where $N(t)$ is a time dependent non-equilibrium distribution function, which is essentially constant within each well, and changes only in the vicinity of the top of the potential barrier. By combining Eq. (3.1.3) and (3.1.4) with Eq. (3.1.14) $N(t)$ can be found. That is

$$\int_{-\infty}^{0} P(x,t)dx = \int_{-\infty}^{0} N(t)P_s(x)dx = n_A(t)$$

and

$$\int_0^\infty P(x,t)dx \;=\; \int_0^\infty N(t)P_s(x)dx \;=\; n_B(t).$$

Since the non-equilibrium distribution function, $N(t)$, is independent of position, it can be taken out of the integral and we get an expression

$$N_A(t) \;=\; \frac{n_A(t)}{\int_{-\infty}^0 P_s(x)dx}, \tag{3.1.15a}$$

for $x < 0$ and an expression

$$N_B(t) \;=\; \frac{n_B(t)}{\int_0^\infty P_s(x)dx} \tag{3.1.15b}$$

for $x > 0$. Substituting the expression of the steady state solution, $P_s(x)$, from Eq. (3.1.13) into Eq. (3.1.15a) and (3.1.15b) we get the following expression for the non-equilibrium distribution function $N(t)$. That is, for $x < 0$,

$$N_A(t) \;=\; \frac{n_A(t)}{C\int_{-\infty}^0 e^{\Phi/k_BT(x)}e^{-\int_{-L}^x \frac{V'(x')}{k_BT(x')}dx'}dx} \tag{3.1.16a}$$

and for $x > 0$,

$$N_B(t) \;=\; \frac{n_B(t)}{C\int_0^\infty e^{\Phi/k_BT(x)}e^{-\int_{-L}^x \frac{V'(x')}{k_BT(x')}dx'}dx}. \tag{3.1.16b}$$

Inserting Eqs. (3.1.16a) and (3.1.16b) into Eq. (3.1.14), we get the values of $P(-L,t)$ and $P(L,t)$ as

$$P(-L,t) \;=\; \frac{n_A(t)e^{\Phi/k_BT(-L)}}{\int_{-\infty}^0 e^{\Phi/k_BT(x)}e^{-\int_{-L}^x \frac{V'(x')}{k_BT(x')}dx'}dx} \tag{3.1.17a}$$

and

$$P(L,t) \;=\; \frac{n_B(t)e^{\Phi/k_BT(L)}e^{(-\int_{-L}^L \frac{V'(x')}{k_BT(x')}dx')}}{\int_0^\infty e^{\Phi/k_BT(x)}e^{-\int_{-L}^x \frac{V'(x')}{k_BT(x')}dx'}dx}. \tag{3.2.17b}$$

Then, by substituting Eqs. (3.1.17a) and (3.1.17b) into Eq. (3.1.11), we get the kinetic equations [9] that describe the transfer of the particle between the two wells or the rate equations for the probabilities of finding the particle in the two wells. That is,

$$\frac{dn_A(t)}{dt} \;=\; -K_An_A(t) + K_Bn_B(t) \tag{3.1.18}$$

and

$$\frac{dn_B(t)}{dt} = K_A n_A(t) - K_B n_B(t) \tag{3.1.19}$$

where

$$K_A = \frac{D(-L)e^{\Phi/k_BT(-L)}}{\int_{-L}^{L} e^{\int_{-L}^{x} \frac{V'(x')}{k_BT(x')}dx'} dx \int_{-\infty}^{0} e^{\Phi/k_BT(x)} e^{(-\int_{-L}^{x} \frac{V'(x')}{k_BT(x')}dx')} dx} \tag{3.1.20}$$

and

$$K_B = \frac{D(L)e^{\Phi/k_BT(L)}}{\int_{-L}^{L} e^{\int_{-L}^{x} \frac{V'(x')}{k_BT(x')}dx'} dx \int_{0}^{\infty} e^{\Phi/k_BT(x)} e^{(-\int_{-L}^{x} \frac{V'(x')}{k_BT(x')}dx')} dx} \tag{3.1.21}$$

are the rates at which the particle jumps from left well to the right well and from right well to the left well, respectively. As Brinkman [10] put, a chemical reaction can be represented by a transition of the particle from one well via the transition state, which is the potential barrier, to the other well or viceversa. Hence, in the process of chemical reaction one can encounter the above kinetic equations. As a result, in chemical reaction process, K_A and K_B are called reaction rates. The escape rates K_A and K_B depend on the form of the potential and the temperature profile. Eqs. (3.1.18) and(3.1.19) can be written as a matrix equation. That is,

$$\frac{d\vec{\rho}}{dt} = G\vec{\rho} \tag{3.1.22}$$

where and Then, the eigen values for the coefficient matrix are $\lambda = 0$ and $\lambda = -\left(K_A + K_B\right)$. Then, the relaxation time or the equilibration time for the global process is

$$\tau_g = \frac{1}{|\lambda|} = \frac{1}{K_A + K_B}. \tag{3.1.26}$$

This is the time needed to see the steady state distribution of the Brownian particle in a double well potential.

In this chapter, we have got the general expressions for the escape rates of the Brownian particle in a bistable potential. In the next chapter, we will consider a simple W-potential and a piece-wise constant temperature profile to get analytic expressions for the escape and the equilibration rates.

4 ANALYTICAL CALCULATION OF THE ESCAPE AND EQUILIBRATION RATES

In the last chapter we have found the general expressions for escape rates. To find these general expressions we considered a general double well potential and a general position dependent temperature profile. But now we consider a specific type of double well potential with a given temperature profile and evaluate the rates at which the Brownian particle escapes from one well to the other. For the bistable potential we consider a symmetric W-potential which is piecewise linear and having the same magnitude in slope through out. It is described by the potential barrier of height V_o and the distance between the two minima located at $x = \pm L$ on either side of the origin is 2L.

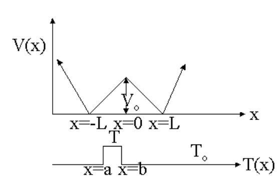

Figure 3: Plot of Symmetric W-potential with hot temperature profile

The W-potential that we consider is described by

$$V(x) = -V_o(\frac{x}{L} + 1) \qquad if \;\; x \leq -L$$

$$\begin{aligned} V(x) &= V_o(\frac{x}{L}+1) \qquad\qquad if \quad -L \leq x \leq 0 \\ V(x) &= V_o(\frac{-x}{L}+1) \qquad\qquad if \;\; 0 \leq x \leq L \\ V(x) &= V_o(\frac{x}{L}-1) \qquad\qquad if \;\; x \geq L \end{aligned} \tag{4.1}$$

The non-homogeneous temperature background is considered to be piecewise constant with the hot locality placed somewhere between the left minimum and the barrier top. To describe the hot locality we used parameters n, v, and s which represent the position of the mid-point of the hot locality from the left minimum, width and the strength of the hot locality, respectively. Hence, we define these parameters as

$$Position \;=\; \ell \;=\; nL \tag{4.2}$$

$$Width \;=\; w \;=\; vL \tag{4.3}$$

$$Strength \;=\; s \;=\; \frac{\Delta T}{T_o} \;=\; \frac{T - T_o}{T_o} \tag{4.4}$$

where ℓ is the position of the midpoint of the hot locality from x = -L, , T is the temperature of the hot region and T_o is the temperature of the rest of the background. Then, the temperature profile, T(x), can be described as

$$\begin{aligned} T(x) &= T \qquad\qquad if \;\; a \leq x \leq b \\ &= T_o \qquad\qquad if \;\; otherwise \end{aligned} \tag{4.5}$$

where

$$\begin{aligned} a &= -L + (n - \frac{v}{2})L \\ b &= -L + (n + \frac{v}{2})L \end{aligned}$$

are the positions of the left and right side of the hot locality from the left minimum (x = -L). For this particular temperature profile, we found the expressions for the escape rates as follows. As we derived in the last chapter, the general expressions for the escape rates of the Brownian particle are

$$K_A = \frac{D(-L)e^{\Phi/k_BT(-L)}}{\int_{-L}^{L} e^{(\int_{-L}^{x} V'(x')/k_BT(x')dx')}dx \int_{-\infty}^{0} e^{\Phi/k_BT(x)}e^{(-\int_{-L}^{x} V'(x')/k_BT(x')dx')}dx}$$

and

$$K_B = \frac{D(L)e^{\Phi/k_BT(L)}}{\int_{-L}^{L} e^{(\int_{-L}^{x} V'(x')/k_BT(x')dx')}dx \int_{0}^{\infty} e^{\Phi/k_BT(x)}e^{(-\int_{-L}^{x} V'(x')/k_BT(x')dx')}dx}$$

Here,we evaluate first the integral found in both expressions of the escape rates K_A and K_B. The expression for this integral by recalling the definition of $\Psi(x)$ from chapter 3, is

$$\int_{-L}^{L} \Psi(x)dx = \int_{-L}^{L} e^{(\int_{-L}^{x} V'(x')/k_BT(x')dx')}dx.$$

Because both the potential and the temperature of the system depend on position, we divide the integral into the corresponding sub intervals. That is

$$\int_{-L}^{L} \Psi(x)dx = \int_{-L}^{a} \Psi(x)dx + \int_{a}^{b} \Psi(x)dx + \int_{b}^{0} \Psi(x)dx + \int_{0}^{L} \Psi(x)dx$$

Then, using the values of a and b, and integrating as usual, the value of these integrals is found to be

$$\int_{-L}^{a} \Psi(x)dx = \left(\frac{k_BT_oL}{V_o}\right)\left(e^{(n-v/2)V_o/k_BT_o} - 1\right)$$
$$\int_{a}^{b} \Psi(x)dx = \left(\frac{k_BTL}{V_o}\right)e^{(n-v/2)V_o/k_BT_o}\left(e^{-vV_o/k_BT} - 1\right)$$
$$\int_{b}^{0} \Psi(x)dx = \left(\frac{k_BT_oL}{V_o}\right)e^{vV_o/k_BT}\left(e^{(1-v)V_o/k_BT_o} - e^{(n-v/2)V_o/k_BT_o}\right)$$
$$\int_{0}^{L} \Psi(x)dx = \left(\frac{k_BT_oL}{V_o}\right)e^{vV_o/k_BT}\left(e^{(1-v)V_o/k_BT_o} - e^{-vV_o/k_BT_o}\right)$$

Therefore, adding the value of each of these separate integrals gives

$$\int_{-L}^{L} \Psi(x)dx = \left(\frac{k_BT_oL}{V_o}\right)e^{V_o/k_BT_o}M \tag{4.6}$$

where

$$M = 2e^{(\frac{-sv}{1+s})V_o/k_BT_o} + se^{(n-v/2)V_o/k_BT_o}\left(e^{(\frac{v}{1+s}-1)V_o/k_BT_o} - e^{-V_o/k_BT_o}\right)$$
$$-e^{-V_o/k_BT_o} - e^{-(1+\frac{sv}{1+s})V_o/k_BT_o}$$

But the last two terms are negligible as compared to the other terms ($V_o >> k_BT_o$). Then, M can be written as

$$M = 2e^{(\frac{-sv}{1+s})u} + se^{(n-v/2)u}\left(e^{(\frac{v}{1+s}-1)u} - e^{-u}\right) \tag{4.7}$$

with $u = \frac{V_o}{k_BT_o}$.

Again, we calculate the other two integrals that are found in the expressions of the escape rates. These are,

$$\int_{-\infty}^{0} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx$$

and

$$\int_{0}^{\infty} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx.$$

With the same reason as above, each of these integrals has to be expressed as the sum of the corresponding sub intervals. That is,

$$\int_{-\infty}^{0} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx = \int_{-\infty}^{-L} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx + \int_{-L}^{a} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx + \int_{a}^{b} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx + \int_{b}^{0} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx$$

Then, the values of each of these integrals is

$$\int_{-\infty}^{-L} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx = \left(\frac{k_BT_oL}{V_o}\right)e^{\Phi/k_BT_o}.$$
$$\int_{-L}^{a} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx = \left(\frac{k_BT_oL}{V_o}\right)e^{\Phi/k_BT_o}\left(1 - e^{-(n-v/2)V_o/k_BT_o}\right)$$
$$\int_{a}^{b} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx = \left(\frac{k_BTL}{V_o}\right)e^{\Phi/k_BT}e^{-(n-v/2)V_o/k_BT_o}\left(1 - e^{-vV_o/k_BT}\right)$$
$$\int_{b}^{0} \frac{e^{\Phi/k_BT(x)}}{\Psi(x)}dx = \left(\frac{k_BT_oL}{V_o}\right)e^{\Phi/k_BT_o}e^{-vV_o/k_BT}\left(e^{-(n-v/2)V_o/k_BT_o} - e^{-(1-v)V_o/k_BT_o}\right)$$

Then,

$$\int_{-\infty}^{0} \frac{e^{\Phi/k_B T(x)}}{\Psi(x)} dx \;=\; \left(\frac{k_B T_o L}{V_o}\right) e^{\Phi/k_B T_o} F \tag{4.8}$$

where

$$F \;=\; 2 + e^{-(n-v/2)V_o/k_B T_o}\left[(1+s)e^{(-s/1+s)\Phi/k_B T_o}(1 - e^{-(v/1+s)V_o/k_B T_o}) - 1 + e^{-(v/1+s)V_o/k_B T_o}\right]$$

$$-e^{-(1-\frac{sv}{1+s})V_o/k_B T_o}$$

Then,

$$F \;=\; 2 + e^{-(n-v/2)u}[(1+s)e^{(-s/1+s)h}(1 - e^{-(v/1+s)u}) - 1 + e^{-(v/1+s)u}] - e^{-(1-\frac{sv}{1+s})u}. \tag{4.9}$$

with $\frac{\Phi}{k_B T_o} \;=\; h.$

Similarly,

$$\int_{0}^{\infty} \frac{e^{\Phi/k_B T(x)}}{\Psi(x)} dx \;=\; \int_{0}^{L} \frac{e^{\Phi/k_B T(x)}}{\Psi(x)} dx + \int_{L}^{\infty} \frac{e^{\Phi/k_B T(x)}}{\Psi(x)} dx$$

Then,the value of each of these separate integrals is

$$\int_{0}^{L} \frac{e^{\Phi/k_B T(x)}}{\Psi(x)} dx \;=\; \left(\frac{k_B T_o L}{V_o}\right) e^{\Phi/k_B T_o} e^{(sv/1+s)V_o/k_B T_o}\left(1 - e^{-V_o/k_B T_o}\right)$$

$$\int_{L}^{\infty} \frac{e^{\Phi/k_B T(x)}}{\Psi(x)} dx \;=\; \left(\frac{k_B T_o L}{V_o}\right) e^{\Phi/k_B T_o} e^{(sv/1+s)V_o/k_B T_o}$$

Hence, we have

$$\int_{0}^{\infty} \frac{e^{\Phi/k_B T(x)}}{\Psi(x)} dx \;=\; \left(\frac{k_B T_o L}{V_o}\right) e^{\Phi/k_B T_o} Q \tag{4.10}$$

where

$$Q \;=\; 2e^{(sv/1+s)V_o/k_B T_o}\left(1 - e^{-V_o/k_B T_o}\right).$$

For $V_o \;>>\; k_B T_o$, the contribution of the exponential inside the bracket to the expression is negligible. Hence, Q can be written as

$$Q \;=\; 2e^{(sv/1+s)u}. \tag{4.11}$$

Since the temperature of the background at the two minima points is the same in our model potential then,

$$T(-L) \;=\; T(L) \;=\; T_o$$

and

$$D(-L) \;=\; D(L) = \frac{C}{\Omega^2\sigma^2}e^{\Phi/k_BT_o}.$$

Therefore, the rate at which the Brownian particle escape from the left well to the right well of the W-potential that associates with a locally heated temperature background is

$$K_A \;=\; \frac{C_o\left(\frac{u}{L}\right)^2 e^{-(u+h)}}{MF} \tag{4.12}$$

while the escape rate at which the particle escapes from right well to the left well is

$$K_B \;=\; \frac{C_o\left(\frac{u}{L}\right)^2 e^{-(u+h)}}{MQ}. \tag{4.13}$$

Where M, P, and Q are given by Eqs. (4.7), (4.9)and (4.11), respectively. So that the equilibration rate of the global(slow) process of the system is

$$K \;=\; K_A + K_B \;=\; \frac{C_o\left(\frac{u}{L}\right)^2 e^{-(u+h)}}{M}\left(\frac{1}{F}+\frac{1}{Q}\right) \tag{4.14}$$

Since the W-potential we considered is symmetric, the escape rate to the right and to the left of the barrier height are equal when there is no distinction of temperature profile; that is, when there is no hot locality(s = 0). Hence, the escape rates for isothermal background become

$$K_A^o \;=\; K_B^o \;=\; C_o\left(\frac{u}{2L}\right)^2 e^{-(u+h)}. \tag{4.15}$$

In this chapter, we obtained analytic expressions for the escape and equilibration rates of the Brownian particle by choosing a simple W-potential for non-isothermal background by heating locally somewhere in the region between -L and 0 to have piecewise constant temperature profile. The escape rates that we found are functions of the parameters n, v, s, u, and h. In the next chapter we will discuss the behavior of the escape and equilibration rates as the values of these parameters vary.

5 RESULT AND DISCUSSION

In the last chapter we obtained analytical expressions for the escape and equilibration rates. These expressions are functions of the parameters v, n and s which have been used to describe the hot locality. Moreover, these escape and the equilibration rates are functions of the potential barrier, u, and the pit depth, h, of the traps. We quantitatively study the effect of the hot locality on the escape and the equilibration rates using these parameters.

In order to study the change of escape and equilibration rates due to the presence of the hot locality, we define a dimensionless factor by which the rates mentioned above are improved. We call this factor as improvement or enhancement factor, which is defined as

$$R_{A(B)} = \frac{K_{A(B)}}{K^o_{A(B)}} \tag{5.1}$$

where $K_{A(B)}$ is the escape rate in the presence of the hot locality while $K^o_{A(B)}$ is the escape rate in the absence of the hot locality.

Then, substituting the corresponding values for the escape rates that are obtained in the presence and absence of the hot locality, the expressions for the improvement factors, R_A and R_B, are found to be

$$R_A = \frac{4}{MF}, \tag{5.4}$$

and

$$R_B = \frac{4}{MQ}. \tag{5.5}$$

Moreover, the improvement factor for the equilibration rate is given as

$$R = \frac{K_A + K_B}{K^o_A + K^o_B} . \tag{5.6}$$

Then, substituting the corresponding values for the quantities in the numerator and denominator of Eq. (5.6) one gets

$$R = \frac{2}{M}(\frac{1}{F} + \frac{1}{Q}) \tag{5.7}$$

and from Eqs. (4.12), (4.13) and (5.14), for the expressions of escape and equilibration rates we have

$$K_A = \frac{C_o \left(\frac{u}{L}\right)^2 e^{-(u+h)}}{MF} , \tag{5.8}$$

,

$$K_B = \frac{C_o \left(\frac{u}{L}\right)^2 e^{-(u+h)}}{MQ} , \tag{5.9}$$

and

$$K = K_A + K_B = \frac{C_o \left(\frac{u}{L}\right)^2 e^{-(u+h)}}{M} \left(\frac{1}{F} + \frac{1}{Q}\right) \tag{5.10}$$

where M, F, and Q are the usual expressions encountered in the last chapter.

Fixing the values of n, v, u and h, the behavior of R_A as a function of the strength, s, of the hot locality is shown in Fig. (4).

From the plot that the improvement factor of the escape rate to the right well increases as s increases. The presence of the hot locality in the left well causes a strong thermal kick on the particle that enables it to jump better over the potential barrier. This shows that the escape rate to the right well increases as the strength of the hot locality increases.

Again, for fixed values of n, s, u and h we plot the improvement factor, R_A, versus the width, v, of the hot locality as shown in Fig. (5).

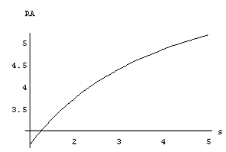

Figure 4: Plot of R_A versus s, for v=0.2, n=0.5, u=10, h=0.1.

The improvement factor for the escape rate to the right well increases by a large amount as the width of the hot locality increases. When the width of the hot locality increases, the part of left well gets thermalized gradually so that the pumping effect of the hot locality on the particle in the left well increases. This shows that the escape rate to the right well increases quite significantly as v increases.

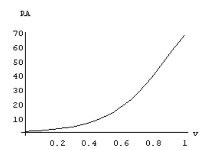

Figure 5: Plot of R_A versus v, for s=1, n=0.5, u=10, h=0.1.

The variation of the position of the hot locality has an effect on the escape rate to the right well as shown in Fig. (6). For fixed values of v, s, u and h, it is possible to observe how the escape rate to the right well depends on the position of the hot locality, n.

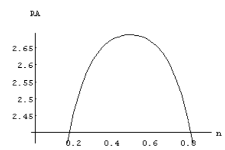

Figure 6: Plot of R_A versus n, for s=1, v=0.2, u=10, h=0.1.

The improvement factor for the escape rate to the right well, R_A, increases when the position of the hot locality increases upto some intermediate values, and R_A decreases with further increase in the position of the hot locality. Hence, R_A is highly dependent on the position of the hot locality and there is an intermediate value of n which is the optimal position of the hot locality at which R_A gets maximum value. This implies that the escape rate to the right well increases upto some intermediate values of n and then decreases when the hot locality is very far away from the left minimum or very close to the potential barrier.

Fixing the values of s, v, n, h and other constants ($C_o = L = 1$), the behavior of the escape rate to the right well, K_A, as a function of the barrier height, u, is shown in Fig. (7). The escape rate to the right of the potential barrier decreases as the barrier height increases.This is because when the value of the potential barrier increases the particle will face difficulty to jump over the potential barrier. Hence, when u increases it will not be easy for the particle to escape to the right of the potential barrier. This implies that when the

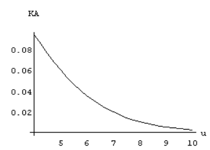

Figure 7: Plot of K_A versus u, for s=1, v=0.2, n=0.5, h=0.1.

barrier height increases the escape rate to the right well decreases.

By fixing the values of s, v, n, u and other constants ($C_o = L = 1$) the behavior of escape rate to the right well, K_A,

As it is depicted on the plot, the escape rate to the right decreases when h increases. This is because in addition to the external barrier height the Brownian particle experiences difficulty to over come the pit depth, h, of traps. Therefore, when the pit depth, h, of traps increases it will be more difficult for the particle to escape. As a result escape rate to the right of the potential well decreases as h increases.

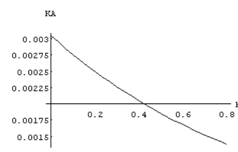

Figure 8: Plot of K_A versus h, for s=1, v=0.2, n=0.5, u=10.

The escape rate to the left well depends on the parameters s, n, v, u, and h. For fixed values of n, v, u, and h, the the improvement factor for the escape rate to the left of the potential barrier, R_B, as a function of the strength of the hot locality, s, is shown in Fig. (9). The improvement factor for the escape rate to the left of the potential barrier, R_B, decreases as the strength of the hot locality increases. That is, whenever there is a jump of the Brownian particle from the right well to the left well there is a thermal kick upon the particle that causes the particle to bounce back to the right well. Therefore, due to the bouncing effect of the hot locality, the Brownian particle would like to spend more time in the right well. So that the escape rate to the left well decreases as the strength of the hot locality increases. However, the amount of the decrease of the escape rate is very insignificant.

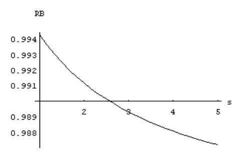

Figure 9: Plot of R_B versus s, for v=0.2, n=0.5, u=10, h=0.1.

If we look at the effect of the width of the hot locality on R_B for fixed values of n, s, u and h, the behavior of R_B is affected as v varies as shown in Fig. (10).

The plot shows that the improvement factor for the escape rate to the left well, R_B, decreases as the width of the hot locality increases. Because when the width of the hot locality increases, the bouncing effect of the hot locality on the particle from the right well increases. Thus, the Brownian particle likes to stay in the right well. Therefore, R_B decreases when the width of the hot locality increases. This shows that the escape rate to the left well decreases as v increases.

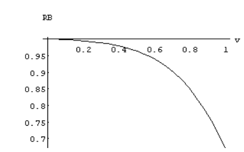

Figure 10: Plot of R_B versus v, for s=1, n=0.5, u=10, h=0.1.

To discuss the dependence of R_B on the position of the hot locality, we fix the values of s, v, u, h and plot R_B as a function of n as shown in Fig. (11).

From Fig. (11) it is noticed that the improvement factor of the escape rate to the right well, R_B, decreases as the position of the hot locality from the left minimum increases. This is because when the hot locality approaches the potential barrier its bouncing effect on the particle that tries to jump to the left well increases. So that the escape rate to the left well decreases as the position of the hot locality increases from the left minimum. Note that the hot locality practically no effect as long as it is positioned in the lower half of the well.

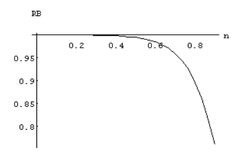

Figure 11: Plot of R_B versus n, for s=1, v=0.2, u=10, h=0.1.

To see the dependence of the escape rate to the left well on the potential barrier, we fix the values of s, v, n, h and other constants ($C_o = L = 1$) and the plot of K_B as a function of u is shown in Fig. (12).

The plot shows that when the barrier height increases, the escape rate to the left well decreases. The reason is similar with what we have seen for the case of escape rate to the right. That is, if the value of the barrier height increases, it will be difficult for the particle to escape to the left well.

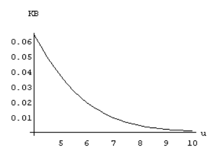

Figure 12: Plot of K_B versus u, for s=1, v=0.2, n=0.5, h=0.1.

Fixing the values of s, v, n, u and other constants ($C_o = L = 1$), the behavior of the escape rate to the left well, K_B, as a function of the pit depth, h, of traps is shown in Fig. (13). P We have seen that in addition to the barrier height the Brownian particle experiences difficulty from the potential of the pit depth, h. Hence, when h increases K_B decreases.

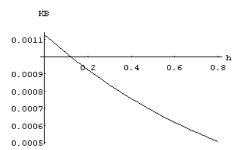

Figure 13: Plot of K_B versus h, for s=1, v=0.2, n=0.5, u=10.

Again, we have studied the dependence of the equilibration rate on the parameters. Fixing the values of v, n, u and h, the behavior of the improvement factor associated with the equilibration rate , R, as a function of the strength of the hot locality, s, is shown in Fig. (14). The improvement factor, R, associated with equilibration rate increases as the strength of the hot locality increases. That means, if the strength of the hot locality increases the process of global equilibration will be so fast. Then, the time needed to see this equilibration process will be small.

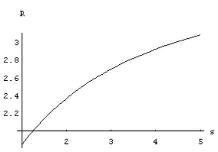

Figure 14: Plot of R versus s, v=0.2, n=0.5, u=10, h=0.1.

The behavior of the equilibration rate, R, with respect to the width of the hot locality, v, for fixed values of s, n, u, and h is plotted as shown in Fig. (15). The improvement factor associated with the equilibration rate increases as the width of the hot locality increases. This means that when the width of the hot locality increases the time needed for global equilibration decreases.

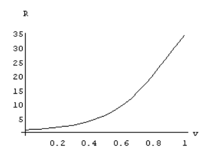

Figure 15: Plot of R versus v, for s=1, n=0.5, u=10, h=0.1.

Moreover, by fixing the values of s, v, u and h, the behavior of R is shown as a function of the position of the hot locality in Fig. (16).

When the value of n increases, the equilibration rate increases upto some intermediate values of n and then decreases when the value of n increases further. So that, the equilibration rate of the system is also highly dependent on the position of the hot locality. It is easy to see from the plot that there is an optimal value of n at which the improvement factor, R, becomes maximum. This shows that the equilibration rate gets maximum value for some intermediate values of n and decreases otherwise.

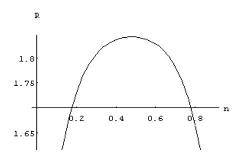

Figure 16: Plot of R versus n, for s=1, v=0.2, u=10, h=0.1.

The variation of the barrier height affects the equilibration rate. By fixing the values of s, v, n, h and other constants ($C_o = L = 1$) we plot the equilibration rate, K, as a function of the barrier height, u, as shown in Fig. (17). From the plot, one can see that when the potential barrier height increases, the equilibration rate decreases. That means, if the value of the barrier height gets larger and larger, the difficulty of escaping of the particle from both wells increases. Hence, it takes long time to have equilibration between the two wells when the barrier height increases.

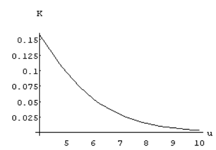

Figure 17: Plot of K versus u, for s=1, v=0.2, n=0.5, h=0.1.

Next we have studied the behavior of K as a function of the pit depth, h, by fixing the values of s, v, n, u, h and other constants ($C_o = L = 1$) as shown in Fig. (18). From the plot it is possible to say that when h increases the equilibration rate, K, decreases. This happens because of the fact that in addition to the barrier height, the increment of h makes the escape of the particle difficult from both wells and hence the equilibration rate decreases as h increases. This shows that when h increases the time needed to see equilibration between the two wells will be long.

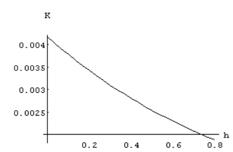

Figure 18: Plot of K versus h, for s=1, v=0.2, n=0.5, u=10

6 CONCLUSION

In this work, we considered a model known as the hopping model for the study of diffusion of a Brownian particle in non-homogeneous medium. Based on this, we studied the dynamics of a Brownian particle in a bistable potential with non-uniform temperature background so as to formulate the general expressions for the escape and equilibration rates. In particular, we considered a simple W-potential having a piecewise constant temperature profile, where we put the hot locality somewhere within the left well. For this specific choice of potential and temperature profile we found analytical expressions for the escape and equilibration rates using Brinkman's method.

The escape and equilibration rates are functions of the strength, width and position of the hot locality, the height of the potential barrier and the pit potential of traps. The presence of the hot locality causes a strong pumping effect of particle to the right well and a retarding effect on the escape rate of the particle to the left well. To sum up, the hot locality enhances both the equilibration rate of the system and the escape rate to the right well significantly as compared to the well without the hot locality.

A remarkable result that we found in this work is that the escape rate of the particle to the right well and the equilibration rate of the system have optimal positions at which these attain their maximum values, which is similar to the work of Solomon Fekade and Mulugeta Bekele for Landauer's heated pipe model.

From the dependance of escape and equilibration rates on the height of the potential barrier and the pit potential of traps, our result reveals that even though there is a thermal kick (fluctuation) from the hot locality that enhances the escape of the particle, a particle in one well, separated by a large potential barrier (in addition to the pit potential) from the other, will have no chance of a transition in times that are of interest. Clearly, the particle will spend more time in cold region where it moves slowly.

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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 acknowledged.

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Signature: ____________________

This thesis has been submitted for examination with my approval as University advisor.

Name: Mulugeta Bekele, PhD

Signature: __________________

Place and date of submission:

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June 2003