Nonstationary Transport

of

a Brownian Particle in a Model Ratchet Potential

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Abstracts

Considering a sawtooth-shaped symmetric periodic potential, we devise a model ratchet potential by subdividing the potential barrier on one side along the reaction path. For this new model of ratchet potential we examine the inter-well escape rates of a Brownian particle using the known supersymmetric potential approach.We show the existence of an optimal number of barrier subdivision at which a unidirectional motion of the Brownian particle takes maximum speed of nonstationary transport. We find that this speed is substantially larger than the maximum speed that occurs for the classic ratchet potential. This may suggest the best possible way of extracting useful work from random thermal background.

Contents

Chapter 1
Introduction

Macroscopic motion of a particle results in general from the action of macroscopic external forces or potential gradients. From thermodynamics it is known that the long time motion of the particle in an isolated system is diffusive and symmetric. In other words, according to the second law of thermodynamics, no stationary transport of particle occurs under equilibrium fluctuations. To obtain a stationary motion, one has to break somehow detailed balance.

To illustrate some implications of the second law of thermodynamics from the molecular or kinetic point of view, Feynman [1] devised a Brownian motor which has been the basis of many models. Vanes sit in a box with gas at a certain temperature and are subjected to Brownian fluctuations. The vanes are coupled to a ratchet device which, supposedly, should "rectify" these fluctuations to provide motile power. The ratchet sits in a box at some other temperature and can itself perform random walk. Feynman showed that this contraption obeys precisely the formulas for a Carnot cycle, so it is a Brownian analog of a steam engine. He argues convincingly that such a ratchet machine will not provide work or net motion when the vanes and the ratchet are at the same temperature or immersed in a single thermal bath.

A model related to Feynman's ratchet device was devised and used by Magnasco [2] in order to understand biological motors. In this letter Feynman's conclusion concerning the output of the ratchet when the vanes and the ratchet are immersed in a single thermal bath was shown to happen only for an ideal thermal bath, one in which time correlations are negligible. It means a ratchet can extract energy (for free) out of the time correlated pieces of colored (non white) thermal bath remarking that the sufficient ingredients needed to generate motion and forces in the Brownian domain is loss of symmetry and substantially long time correlations. This same author, Magnasco, explored in another letter [3] the relationship between the nonequilibrium fluctuations and the fact that adenosine triphosphate (or ATP) carries energy, and showed that the ratchet described in [2] is a little Brownian machine that eats nonequilibrium fluctuations and walks while a chemical cycle is a little Brownian machine that eats chemical energy and generates nonequilibrium fluctuations.

The effects of a zero-average randomly fluctuating potential barrier or net force on the motion of Brownian particles in asymmetric periodic potentials (ratchets) have been studied extensively by Astumian and Bier [4]. In this study it was shown that a zero-average randomly fluctuating potential barrier or net force can cause a particle on a nonsymmetric periodic potential to move up hill against a constant applied force so long as the period of the oscillation, or, equivalently, the correlation time of the fluctuation, is not much shorter than the relaxation time of the reaction. In other words it means that for a very high frequency of fluctuations, which also have a correlation time approaching zero, net flux does not occur.

In contrast to Magnasco's finding [2], another condition for which broken symmetry dynamics emerges was reported in a work by Hondo and Sawada [5]. In this work, asymmetry of the periodic potential is shown as unnecessary condition if certain chaotic noise works as a driving force. It is argued that the only condition to produce asymmetric motion is an asymmetric distribution of unstable fixed points of the chaotic noise. A large amount of work has been done recently related to rectification of Brownian motion and have been reviewed by Julicher *et al.* [6].

In a more recent work by Brilliantov and Strizhak [7] the motion of the Brownian particles in a ratchet potential under equilibrium white noise was considered. In this study a right-left asymmetry for the mean first passage times (MFPT) of the interwell transitions was found as a result of potential asymmetry. This property of the MFPT gave rise to the nonstationary transport phenomenon.

In the present work, we address the problem of nonstationary transport for a particular kind of ratchet potential. The classic ratchet potential is made up of asymmetric sawtooth-shaped periodic potential barriers. Our particular kind of ratchet potential, on the other hand, is made by converting a symmetric sawtooth-shaped potential barrier to an asymmetric one by subdividing only one side of each potential barrier. Using this model ratchet potential we have studied the motion of a Brownian particle under equilibrium white noise in the high friction limit. We will show that, in the asymmetrically barrier subdivided potential we have devised, the Brownian particle will have a unidirectional nonstationary transport with a velocity that attains a maximum value at an optimal number of barrier subdivision. The magnitude of this velocity is very large when compared with the maximum value of the velocity that could be attained for the motion that occurs for the classic ratchet potential case [7]. This result gives basic information about how useful work can be extracted from random thermal background through the mechanism of asymmetric barrier subdivision. As such it is relevant to problems of tiny heat engines like molecular motors.

The rest of this thesis is organized in the following manner. In chapter 2, we first introduce Kramers' model bistable potential problem [8] and then briefly present two methods of getting the celebrated Kramers' reaction rate. The first method is the classic method which Kramers' and Brinkman [8-11] used while the second method uses supersymmetric (SUSY) technique [12-16] to extract the reaction rate. In chapter 3, the expressions for the escape rates of a Brownian particle over the barriers in a classic ratchet potential is derived using SUSY approach and the result is compared with that found from MFPT method [7]. In chapter 4, we introduce our model potential which is an asymmetrically barrier subdivided model potential that we form from a symmetric sawtooth-shaped potential. Using SUSY technique we derive the expressions for the escape rates of a Brownian particle over the barrier from one well to the adjacent well and vice versa. These expressions are numerically solved, and then the effects of asymmetric barrier subdivision on a unidirectional motion of Brownian particles are discussed in chapter 5. In our concluding remarks we summarize the main results and discuss their implications.

Chapter 2

Kramers' Reaction Rate and Methods of finding it

We discuss Kramers' reaction rate based on his model [8-11]. The model consists of a classical particle of mass m that moves in one-dimensional double well potential field U(x) as shown in fig. (2.1),

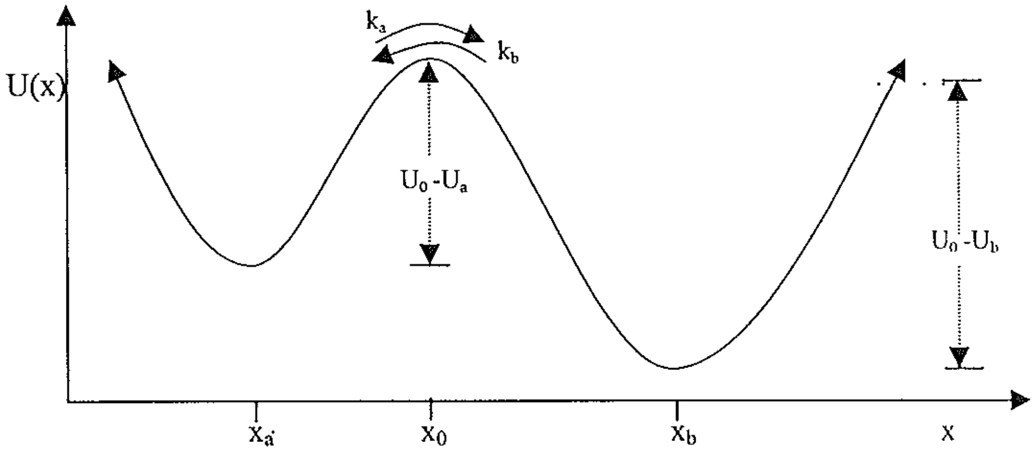


Fig. (2.1). Potential U(x) with two bistable states x_a and x_b. Escape occurs via the forward rate k_a and the backward rate k_b, respectively, and $U_0 - U_a$ and $U_0 - U_b$ are the corresponding activation energies.

where x denotes the particle coordinate that corresponds to the reaction coordinate. The two minima of the potential known as local stable states are at x_a (left of the origin) and x_b (right of the origin). The maximum of U(x) separating these two states known as transition state is at the origin x_0.

The particle is originally caught in either of the potential wells, but it may escape from one well to the other in the course of time by passing over the potential barrier. The transition of the particle from state x_a via the transition state x_0 to the final state x_b or vice versa is represented as a chemical reaction. The energy necessary for the passage through the transition state x_0 is supplied by a heat bath at temperature T which is constituted of the reacting particle and a medium in which the particle is embedded. The total effect of the heat bath on the reacting particle is described by a fluctuating force $\xi(t)$ and by a linear damping force $-m\gamma\dot{x}$, where γ is a damping rate. These forces enter Newton's equation of motion of the particle in the form of the Langevin equation:

$$m\ddot{x} = -U'(x) - m\gamma\dot{x} + \xi(t) \tag{2.1}$$

where prime and dot indicate differentiation with respect to the coordinate x and the time t, respectively. The fluctuating force $\xi(t)$ denotes Gaussian white noise with zero mean,

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

and

$$< \xi(t)\xi(t') >= 2m\gamma k_B T\delta(t - t') \tag{2.3}$$

where k_B is the Boltzmann constant.

In a model representing a chemical reaction the potential barrier is considered high as compared to the thermal energy $k_B T$. In such cases the reaction will relax toward one of the minima of the potential and the system will stay there for an extremely long time until eventually the accumulated action of the random force will drive it over the barrier into a neighboring metastable state. Although rare, such events will surely occur within finite time. The average of this escape time equals the inverse of the escape rate from one local stable state to the other. Therefore, rate processes are phenomena that are characterized by rare events that take place on a long time scale when compared to the dynamic time scales characterizing the states of local stability.

For strong friction γ the particle undergoes a creeping motion, and the Langevin equation, Eq. (2.1), then becomes

$$\dot{x} = \frac{-U'(x)}{m\gamma} + \frac{\xi(t)}{m\gamma}. \tag{2.4}$$

From Eq. (2.4) we obtain via Ito calculus [17] the corresponding Fokker-Planck equation which is usually called the Smoluchowski equation(SE):

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} + \beta U'(x)\right] p(x,t) \tag{2.5}$$

where $p(x,t)$ is the time dependent probability density associated with the particle position, $D = \frac{k_B T}{m\gamma}$ is the diffusion constant, T is the temperature and $\beta = (k_B T)^{-1}$. The SE holds when both $-U'(x)$ and $p(x,t)$ are constant in the thermal length scale $\frac{1}{\gamma}(\frac{k_B T}{m})^{\frac{1}{2}}$.

In the next two sections we will present two ways of solving the SE for a general bistable potential. In the first section we present the original method used by Kramers' while in the second section we present the supersymmetric (SUSY) method that has been recently introduced [12-16].

2.1 Kramers' Method

The steady state solution of Eq. (2.5) is

$$p_0(x) = \frac{e^{-\beta U(x)}}{\int e^{-\beta U(x)}\, dx}.$$

Consider the probability current density in the SE:

$$j(x,t) = -D\left[\frac{\partial}{\partial x} + \beta U'(x)\right] p(x,t). \tag{2.6}$$

Multiplying both sides of eq. (2.6) by $e^{\beta U(x)}$ and integrating from $x = x_a$ to $x = x_b$, one obtains the exact relation

$$\int_{x_a}^{x_b} e^{\beta U(x)} j(x,t)\, dx = -D\left[e^{\beta U(x_b)} p(x_b,t) - e^{\beta U(x_a)} p(x_a,t)\right]. \tag{2.7}$$

Kramers [8] and later Brinckman [11] assumed that the current density j(x,t) near the top of the barrier is spatially constant in space 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 left hand side of eq. (2.7) leading to a factor j(0,t). Introducing as coarse grained variables the particle numbers in the left and right well

$$n_{a(b)}(t) = \int_{-\infty(0)}^{0(\infty)} p(x,t)\, dx \tag{2.8}$$

and using eq. (2.7) with eq. (2.8) leads to the kinetic equations

$$\dot{n}_a(t) = -k_a n_a(t) + k_b n_b(t) \tag{2.9a}$$

$$\dot{n}_b(t) = k_a n_a(t) - k_b n_b(t) \tag{2.9b}$$

where the rate constants follow from eq. (2.7) as

$$k_{a(b)} = D\left[\int_{x_a}^{x_b} e^{\beta U(x)}\, dx \int_{-\infty(0)}^{0(\infty)} e^{-\beta U(x)}\, dx\right]^{-1}. \tag{2.10}$$

The eigenvalues of the rate matrix in eq. (2.9) are $\lambda_0 = 0$ and $\lambda_1 = k_a + k_b$. For a high barrier, assuming parabolic shapes around the extrema of U(x) and using the Taylor expansion, k_a and k_b can be approximately evaluated and we finally get the celebrated Kramers' reaction rate

$$\lambda_1 = \frac{D\beta}{2\pi}\left[(U_a'' U_0'')^{1/2} e^{-\beta(U_0 - U_a)} + (U_b'' U_0'')^{1/2} e^{-\beta(U_0 - U_b)}\right]. \tag{2.11}$$

In this equation, eq. (2.11), U_a'', U_0'' and U_b'' denote the second derivatives of U(x) evaluated at the respective coordinates a, 0 and b, whereas U_a, U_0 and U_b denote the corresponding values of $U(x)$ at these coordinates. Note that $k_{a(b)}$ corresponds to the rate of escape from the left (right) well to the right (left) well.

2.2 The Supersymmetric (SUSY) Method

The SUSY method [12-16] is one of the methods by which we can calculate the escape rate for idealized potentials. It involves converting the SE to a Euclidean Schrödinger equation and finding the eigenvalues of the equation.

With the ansatz

$$p(x,t) = \varphi(x) e^{\frac{-1}{2}\beta U(x)} e^{-\lambda t} \tag{2.12}$$

the SE, eq. (2.5), is converted to a time independent Euclidean Schrödinger equation for φ

$$H_+ \varphi_+ = E_+ \varphi_+ \tag{2.13}$$

with $H_+ = A^+ A$ being positive semidefinite, where $E_+ = \frac{\lambda}{D}$,

$$A = \frac{d}{dx} + \frac{1}{2}\beta U'(x) \tag{2.14}$$

and

$$A^+ = -\frac{d}{dx} + \frac{1}{2}\beta U'(x). \tag{2.15}$$

This Hamiltonian H_+ corresponds to the motion of the particle in the potential

$$V_+(x) = [\frac{1}{2}\beta U'(x)]^2 - \frac{1}{2}\beta U''(x). \tag{2.16}$$

For a high potential barrier, the escape rate is determined by the smallest non-zero eigenvalue, $\lambda_1 = DE_+^1$, of the SE where E_+^1 is the eigenvalue of the first excited state of eq. (2.13). On the other hand, this eigenstate is degenerate with the ground state $\varphi_-^0(x)$ of the 'supersymmetric partner potential' $V_-(x)$ given by

$$V_-(x) = [\frac{1}{2}\beta U'(x)]^2 + \frac{1}{2}\beta U''(x) \tag{2.17}$$

which corresponds to the Hamiltonian $H_- = AA^+$ so that

$$H_-\varphi_-^0 = E_-^0\varphi_-^0 \tag{2.18}$$

and

$$E_-^0 = E_+^1. \tag{2.19}$$

The problem is thus simplified to finding the ground state eigenvalue of this 'partner' potential. We will be using this method in the next chapter.

Besides these two methods, there are other methods such as the mean first passage time (MFPT) method [9, 10, 17] that can also be used to determine the escape rates which essentially give the same result. Since SUSY method is more exact and more suited for the kind of potentials we consider than the other methods, for the rest of our work we will use it to determine the escape rates.

In the next chapter we will take the classic ratchet potential and using SUSY method extract the local right and left escape rates. We will then use these escape rates as an input for the coarse grained potential profile to find the velocity of the current that arises for nonstationary transport.

Chapter 3

Classic Ratchet Potential

To realize the effectiveness of our model potential (that will be introduced in the next chapter) in generating a probability current, we have considered the motion of Brownian particles in a classic ratchet potential under the internal white noise discussed in [7]. We derive the expressions for the escape rates of a Brownian particle from one well to the adjacent well and vice versa over the barrier starting from the SE, eq. (2.5), for the ratchet potential given in [7] using SUSY method. In fact, these expressions have already been found in [7] by MFPT method.

We consider a Brownian particle in a periodic ratchet potential as shown in fig. (3.1)

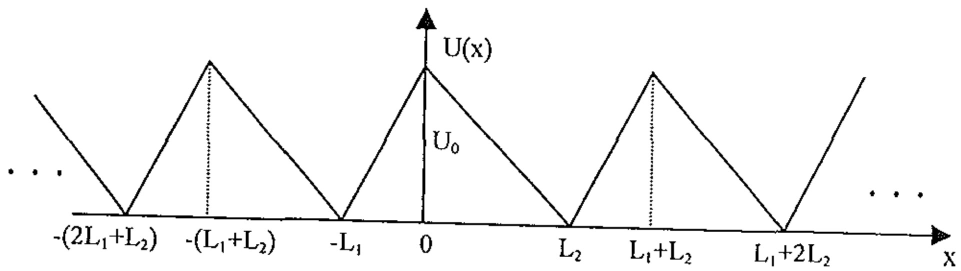


Fig. (3.1).

To determine the escape rates from one well to the neighboring well and vice versa, let us consider the region from $x = -(L_1 + L_2)$ to $x = L_1 + L_2$. When U_0 is large compared to k_BT, this region can be approximated as a bistable W-potential with the outer lines extending to infinity as shown in fig. (3.2). Under this condition, the escape rates can be easily determined.

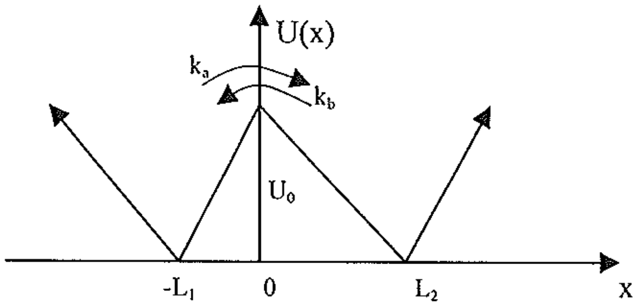


Fig. (3.2).

Let the escape rate to the right and that to the left be denoted by k_a and k_b, respectively. We find the escape rate to the right using the SUSY method by considering fig. (3.3) shown next.

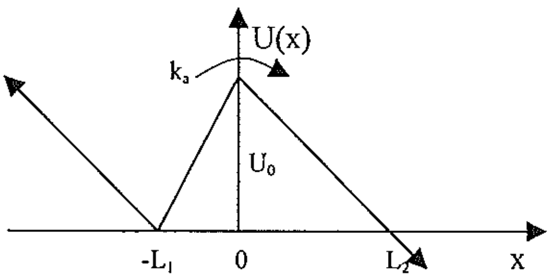


Fig. (3.3).

Using the formula for the supersymmetric 'partner' potential given in eq. (2.17) one can write the corresponding supersymmetric 'partner' potential $V_-(x)$ for the potential shown in fig. (3.3) as

$$V_-(x) = \begin{cases} (\beta\frac{U_0}{2L_1})^2 + 2\beta\frac{U_0}{2L_1}\delta(x+L_1) - \frac{\beta}{2}(\frac{U_0}{L_1} + \frac{U_0}{L_2})\delta(x), & \text{if } x \leq 0; \\ (\beta\frac{U_0}{2L_2})^2, & x > 0. \end{cases}$$

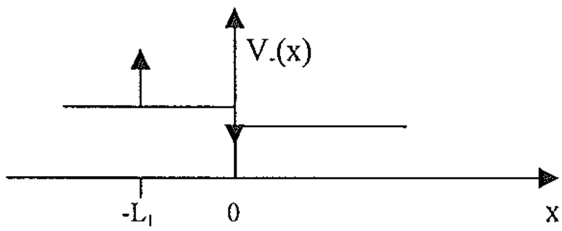


Fig. (3.4).

Note that we have approximated the slope to the left of $x = -L_1$ to be equal to the slope in the region $-L_1 < x < 0$ to simplify the mathematical complication. The effect of this approximation is negligible in the case when the thermal energy k_BT is much less than the barrier height. With $u_0 = \frac{\beta U_0}{2}$ one obtains

$$V_-(x) = \begin{cases} \frac{u_0^2}{L_1^2} + 2\frac{u_0}{L_1}\delta(x + L_1) - (\frac{u_0}{L_1} + \frac{u_0}{L_2})\delta(x), & \text{if } x \leq 0; \\ \frac{u_0^2}{L_2^2}, & x > 0. \end{cases}$$

The corresponding Euclidean Schrödinger equation is

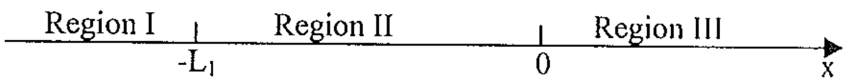
$$H_-\varphi_-^0 = E_-^0\varphi_-^0 \tag{3.1}$$

where H_- is the corresponding Hamiltonian

$$H_-(x) = -\frac{d^2}{dx^2} + V_-(x).$$

As explained earlier in section 2.2, we solve Euclidean Schrödinger equation, eq. (3.1), to find the eigenvalue E_-^0, which in this case is related to the escape rate to the right as $k_a = DE_-^0$, where D is diffusion constant.

We now solve eq. (3.1) considering the following three regions:



Let us consider that $\varphi_0(x)$ be the ground state wave function which is the solution of eq. (3.1) in region I. That is

$$\left(-\frac{d^2}{dx^2}+\frac{u_0^2}{L_1^2}\right)\varphi_0(x)=E_-^0\varphi_0(x).$$

The solution of this equation can be written as

$$\varphi_0(x)=A_0e^{-\kappa(x+L_1)}+B_0e^{\kappa(x+L_1)}$$

where A_0 and B_0 are constants to be determined from the boundary conditions and $\kappa=\sqrt{\frac{u_0^2}{L_1^2}-E_-^0}$.

In region II we consider two solutions as $\varphi_{0'}(x)$ and $\varphi_1(x)$ just at the right of $x=-L_1$ and at the immediate left of $x=0$, respectively. Solving eq. (3.1) one can, therefore, write the solutions as

$$\varphi_{0'}(x)=A_0'e^{-\kappa(x+L_1)}+B_0'e^{\kappa(x+L_1)}$$

and

$$\varphi_1(x)=A_1e^{-\kappa x}+B_1e^{\kappa x}$$

where A_0', B_0', A_1 and B_1 are constants to be determined from the boundary conditions.

In region III we consider only one solution likewise in region I. If this solution is $\varphi_{1'}(x)$, then solving eq. (3.1) one can obtain

$$\varphi_{1'}(x)=A_1'e^{-qx}+B_1'e^{qx}$$

where A_1' and B_1' are constants that we determine from boundary conditions and $q=\sqrt{\frac{u_0^2}{L_2^0}-E_-^0}$.

To determine the constants we use the boundary conditions:

i) $\varphi_0(x)=\varphi_{0'}(x)$ at $x=-L_1$,

ii) $\varphi_1(x) = \varphi_0\prime(x)$ in region ii,

iii) $\varphi_1\prime(x) = \varphi_1(x)$ at $x = 0$,

iv) $\int_{-L_1^-}^{-L_1^+} [-\frac{d^2}{dx^2} + V_-(x)]\, dx = \int_{-L_1^-}^{-L_1^+} E_-^0 \varphi_0\prime\, dx$ or $\frac{d\varphi_0\prime(x)}{dx} - \frac{d\varphi_0(x)}{dx} = 2\frac{u_0}{L_1}\varphi_0(x)$ at $x = -L_1$,

v) $\int_{0^-}^{0^+} [-\frac{d^2}{dx^2} + V_-(x)]\, dx = \int_{0^-}^{0^+} E_-^0 \varphi_0\prime\, dx$

or $\frac{d\varphi_1\prime(x)}{dx} - \frac{d\varphi_1(x)}{dx} = -u_0(\frac{1}{L_1} + \frac{1}{L_2})\varphi_1(x)$ at $x = 0$.

From (i) and (iv) we obtain

$$A_0 + B_0 = A_0' + B_0'$$

and

$$\kappa(A_0 - B_0 - A_0' + B_0') = 2\frac{u_0}{L_1}(A_0 + B_0).$$

These equations can be simplified to

$$A_0' = (1 - \frac{u_0}{L_1\kappa})A_0 - \frac{u_0}{L_1\kappa}B_0$$

and

$$B_0' = \frac{u_0}{L_1\kappa}A_0 + (1 + \frac{u_0}{L_1\kappa})B_0$$

or

$$\begin{pmatrix} A_0' \\ B_0' \end{pmatrix} = \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} \tag{3.2}$$

where $\alpha = \frac{u_0}{L_1\kappa}$

From (ii) we have

$$A_0' e^{-\kappa(x+L_1)} + B_0' e^{\kappa(x+L_1)} = A_1 e^{-\kappa x} + B_1 e^{\kappa x}.$$

This implies that

$$A_1 = A_0' e^{-\kappa L_1}$$

and

$$B_1 = B_0' e^{\kappa L1}$$

or

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} e^{-\kappa L_1} & 0 \\ 0 & e^{\kappa L_1} \end{pmatrix} \begin{pmatrix} A_0' \\ B_0' \end{pmatrix}. \tag{3.3}$$

From (iii) and (v) we obtain

$$A_1 + B_1 = A_1' + B_1'$$

and

$$-A_1'q + B_1'q + A_1\kappa - B_1\kappa = -u_0(\frac{1}{L_1} + \frac{1}{L_2})(A_1 + B_1).$$

Simplifying these equations one can obtain

$$A_1' = \left[\frac{1}{2} + \frac{u_0}{2q}\frac{(L_1 + L_2)}{L_1 L_2} + \frac{\kappa}{2q}\right] A_1 + \left[\frac{1}{2} + \frac{u_0}{2q}\frac{(L_1 + L_2)}{L_1 L_2} - \frac{\kappa}{2q}\right] B_1$$

and

$$B_1' = \left[\frac{1}{2} - \frac{u_0}{2q}\frac{(L_1 + L_2)}{L_1 L_2} - \frac{\kappa}{2q}\right] A_1 + \left[\frac{1}{2} - \frac{u_0}{2q}\frac{(L_1 + L_2)}{L_1 L_2} + \frac{\kappa}{2q}\right] B_1$$

or

$$\begin{pmatrix} A_1' \\ B_1' \end{pmatrix} = \begin{pmatrix} \frac{1}{2} + \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1 L_2} + \frac{\kappa}{2q} & \frac{1}{2} + \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1 L_2} - \frac{\kappa}{2q} \\ \frac{1}{2} - \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1 L_2} - \frac{\kappa}{2q} & \frac{1}{2} - \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1 L_2} + \frac{\kappa}{2q} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}. \tag{3.4}$$

Now we substitute $\binom{A_1}{B_1}$ in eq. (3.4) by its value in eq. (3.3). Then we substitute $\binom{A_0'}{B_0'}$ by its value in eq. (3.2) and obtain

$$\begin{pmatrix} A_1' \\ B_1' \end{pmatrix} = \begin{pmatrix} \frac{1}{2} + \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1 L_2} + \frac{\kappa}{2q} & \frac{1}{2} + \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1 L_2} - \frac{\kappa}{2q} \\ \frac{1}{2} - \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1 L_2} - \frac{\kappa}{2q} & \frac{1}{2} - \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1 L_2} + \frac{\kappa}{2q} \end{pmatrix}$$

$$\begin{pmatrix} e^{-\kappa L_1} & 0 \\ 0 & e^{\kappa L_1} \end{pmatrix} \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}.$$

This equation relates the amplitudes of the ground state wave function at the left of $x = -L_1$ with that of the right of $x = 0$. Such method is known as a matrix transfer method used in [15].

We reduce the constants in this equation to two using the boundary condition at infinity. That is we require $A_0 = B_1' = 0$ so that the solutions $\varphi_0(x)$ and $\varphi_{1'}(x)$ are finite in the regions $x < -L_1$ and $x > 0$, respectively. Hence the above equation will become

$$\begin{pmatrix} A_1' \\ 0 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} 0 \\ B_0 \end{pmatrix}$$

where

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} + \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1L_2} + \frac{\kappa}{2q} & \frac{1}{2} + \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1L_2} - \frac{\kappa}{2q} \\ \frac{1}{2} - \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1L_2} - \frac{\kappa}{2q} & \frac{1}{2} - \frac{u_0}{2q}\frac{(L_1+L_2)}{L_1L_2} + \frac{\kappa}{2q} \end{pmatrix}$$
$$\begin{pmatrix} e^{-\kappa L_1} & 0 \\ 0 & e^{\kappa L_1} \end{pmatrix} \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix}.$$

This implies that

$$M_{22}B_0 = 0$$

and

$$M_{12}B_0 = A_1'.$$

In order that the solution will be nontrivial $M_{22} = 0$ must hold. That is

$$\left[\frac{1}{2} - \frac{\kappa}{2q} - \frac{u_0}{2q}\left(\frac{L_1+L_2}{L_1L_2}\right)\right](-\alpha e^{-\kappa L_1}) + \left[\frac{1}{2} + \frac{\kappa}{2q} - \frac{u_0}{2q}\left(\frac{L_1+L_2}{L_1L_2}\right)\right](1+\alpha)e^{\kappa L_1} \stackrel{\Delta}{=}$$

which implies that

$$\frac{1+\alpha}{\alpha} = \frac{\left[\frac{1}{2} - \frac{\kappa}{2q} - \frac{u_0}{2q}\left(\frac{L_1+L_2}{L_1L_2}\right)\right]}{\left[\frac{1}{2} + \frac{\kappa}{2q} - \frac{u_0}{2q}\left(\frac{L_1+L_2}{L_1L_2}\right)\right]} e^{-2\kappa L_1}. \tag{3.5}$$

E_-^0 is very small when compared with u_0 in the low noise high barrier limit (or $\frac{U_0}{k_BT} \gg 1$). Hence we expand κ and q binomially and take the terms in which there is no higher order of E_-^0. That is

$$\kappa = \sqrt{\frac{u_0^2}{L_1^2} - E_-^0} = \frac{u_0}{L_1}\left(1 - E_-^0\frac{L_1^2}{u_0^2}\right)^{1/2} \approx \frac{u_0}{L_1} - \frac{1}{2}E_-^0\frac{L_1}{u_0},$$

$$q=\sqrt{\frac{u_0^2}{L_2^2}-E_-^0}=\frac{u_0}{L_2}(1-E_-^0\frac{L_2^2}{u_0^2})^{1/2}\approx\frac{u_0}{L_2}-\frac{1}{2}E_-^0\frac{L_2}{u_0}.$$

Therefore the terms in eq. (3.5) can be simplified as

$$\frac{1+\alpha}{\alpha}\approx 2-\frac{1}{2}\frac{L_1^2}{u_0^2}E_-^0,$$

$$\frac{1-\frac{\kappa}{q}-\frac{u_0}{q}\left(\frac{L_1+L_2}{L_1L_2}\right)}{1+\frac{\kappa}{q}-\frac{u_0}{q}\left(\frac{L_1+L_2}{L_1L_2}\right)}\approx\frac{-2u_0L_2+1/2\frac{E_-^0}{u_0}L_1L_2(L_1-L_2)}{-1/2\frac{E_-^0}{u_0}L_1L_2(L_1+L_2)}.$$

Thus, eq. (3.5) will become

$$-\frac{E_-^0}{u_0}L_1L_2(L_1+L_2)+\frac{1}{4}\frac{{E_-^0}^2}{{u_0}^3}L_1^3L_2(L_1+L_2)=e^{-2\kappa L_1}[-2u_0L_2+\frac{1}{2}\frac{E_-^0}{u_0}L_1L_2(L_1-L_2)].$$

We neglect the second term on the left comparing it with the first and then get

$$-\frac{E_-^0}{u_0}L_1L_2[L_1+L_2-(L_1-L_2)e^{-2\kappa L_1}]=-2u_0L_2e^{-2\kappa L_1}.$$

Comparing $(L_1-L_2)e^{-2\kappa L_1}$ with (L_1+L_2) we neglect the former and obtain

$$E_-^0=\frac{2u_0^2e^{-2\kappa L_1}}{L_1(L_1+L_2)}.$$

Consider the exponential part

$$e^{-2\kappa L_1}=e^{-2L_1\sqrt{\frac{u_0^2}{L_1^2}-E_-^0}}=e^{-2u_0(1-\frac{L_1^2E_-^0}{u_0^2})^{1/2}}.$$

We neglect $\frac{L_1^2E_-^0}{u_0^2}$ comparing with 1.

That is $e^{-2\kappa L_1}\approx e^{-2u_0}$.

Therefore, the final expression of the escape rate from the left well to the right well of fig. (3.2) is

$$k_a=DE_-^0\approx\frac{D2{u_0}^2}{(L_1+L_2)L_1}e^{-2u_0}$$

calculated there, is the average time that a random walker, starting from x_0 inside the initial domain of attraction, takes to leave the domain of attraction for the first time. At weak noise this MFPT, $t(x_0)$, becomes essentially independent of the starting point [9], that is, $t(x_0) \approx t_{MFPT}$ for all starting configurations away from the immediate neighborhood of the separatrix. If we note that the probability of crossing the separatrix in either direction equals one half, the total escape time say τ_e equals $2t_{MFPT}$. Thus the rate of escape k itself is given by $k = \frac{1}{2t_{MFPT}}$. Hence we can use the total escape time to the right or left concerning the potential in fig. (3.2) as

$$\tau_{a(b)} = \frac{1}{k_{a(b)}} \tag{3.8}$$

where k_a and k_b are respectively given by eqs. (3.6 and 3.7). This equation shows that $\tau_a \neq \tau_b$ for the potential with asymmetry.

As a consequence of the left-right asymmetry in the escape time, the system develops directed motion in approaching towards stationary probability distribution, $p_{eq} \sim e^{\frac{-U(x)}{k_BT}}$, which is current free, if no density gradients is present in the system. Thus, any initially localized distribution, say $p(x_0, t_0; x, t) = \delta(x - x_0)(t - t_0)$, evolves to the $p_{eq}(x)$, defined on the ratchet, with left and right boundary $-L_\infty, L_\infty \gg L$. In the sequence of the time scales, that characterize the Brownian motion in the over damped case, the shortest time scale corresponds to the intrawell relaxation time say τ. The next time scale is related to the interwell transition times, $\tau_{a(b)}$. Finally, $T_\infty \sim (\frac{L_\infty}{L})\tau_{a(b)}$ defines the global relaxation time. Under condition $e^{\frac{U_0}{k_BT}} \gg 1$, the following hierarchy of time-scales holds, $\tau \ll \tau_{a(b)} \ll T_\infty$, and the nonstationary transport takes place for

$\tau_{a(b)} \ll t \ll T_\infty$. To describe the nonstationary transport we introduce the population of the m-th well of fig. (3.1) as

$$n_m(t) = \int_{L(m)}^{L(m+1)} p(x,t)\, dx$$

and write the kinetic equation:

$$\dot{n}_m(t) = k_b n_{m+1} + k_a n_{m-1} - (k_a + k_b) n_m. \tag{3.9}$$

We transform n_m in the discrete space to $n(x)$ in continuous space coordinate for small L by Taylor expansion of $n(x+L)$ and $n(x-L)$ in powers of L and obtain the coarse grained equation:

$$\frac{\partial n(x,t)}{\partial t} \approx -V \frac{\partial n(x,t)}{\partial x} + \tilde{D} \frac{\partial^2 n(x,t)}{\partial x^2} \tag{3.10}$$

with $V = L(k_a - k_b)$ and $\tilde{D} = \frac{1}{2} L^2 (k_a + k_b)$. Eq. (3.10) shows that the ensemble of Brownian particles moves with a constant velocity V, which depends upon what we define as the net escape rate, $k_+ = k_a - k_b$. The distribution width that depends upon $k_a + k_b$ is described by the renormalized diffusion coefficient $\tilde{D}$.

Using their corresponding values in eq. (3.6) and eq. (3.7) we get an expression for the net escape rate explicitly as

$$k_+ = \left[\left(\frac{U_0}{k_B T} \right)^2 \frac{D e^{\frac{-U_0}{k_B T}}}{2(L_1 + L_2)} \right] \left(\frac{1}{L_1} - \frac{1}{L_2} \right). \tag{3.11}$$

We now look for the particular L_1 and L_2 relation that gives the largest net escape rate. Let L_2 be fixed and L_1 varies. That is

$$k_+(L_1) = C \frac{1}{(L_1 + L_2)} \left(\frac{1}{L_1} - \frac{1}{L_2} \right)$$

where

$$C = \frac{1}{2} \left(\frac{U_0}{k_B T} \right)^2 D e^{\frac{-U_0}{k_B T}}.$$

$$\frac{dk_+(L_1)}{dL_1} = -\frac{C}{(L_1+L_2)^2}\left(\frac{1}{L_1}-\frac{1}{L_2}\right)+\frac{C}{(L_1+L_2)}\left(-1/{L_1}^2\right).$$

We know that $\frac{dk_+(L_1)}{dL_1} = 0$ at the maximum or minimum value of k_+. This implies that

$$L_1 = L_2(1 \pm \sqrt{2}). \tag{3.12}$$

When we compute $\frac{d^2k_+(L_1)}{dL_1^2}$ at $L_1 = L_2(1+\sqrt{2})$, we obtain a value which is greater than 0. This shows that k_+ takes the maximum value to the left when $L_1 = L_2(1+\sqrt{2})$ and takes the maximum value to the right when $L_1 = \frac{L_2}{(1+\sqrt{2})}$.

Now we substitute L_1 in eq. (3.11) by $\frac{L_2}{(1+\sqrt{2})}$ and find the maximum net escape rate to the right:

$$k_+^{max} = \frac{D}{2}\left(\frac{U_0}{k_BT}\right)^2\frac{e^{\frac{-U_0}{k_BT}}}{{L_2}^2}. \tag{3.13}$$

Let us suppose that the ratchet potential we are dealing with is symmetric in such a way that L_1 and L_2 in eq. (3.6) or eq. (3.7) are substituted by $L_0 = \frac{(L_1+L_2)}{2}$. In such a case the expression for the escape rate to the right which is also that to the left will be found as

$$k_0 = \frac{D}{4}\left(\frac{U_0}{k_BT}\right)^2\frac{e^{\frac{-U_0}{k_BT}}}{{L_0}^2}. \tag{3.14}$$

We express L_0 in terms of L_2:

$$L_0 = \frac{1}{2}\left(\frac{L_2}{1+\sqrt{2}}+L_2\right) = \frac{L_2}{2}\left(\frac{2+\sqrt{2}}{1+\sqrt{2}}\right).$$

When we divide k_+^{max} by k_0, we obtain

$$\frac{k_+^{max}}{k_0} = 2\frac{L_0^2}{L_2^2} = \frac{1}{2}\left(\frac{2+\sqrt{2}}{1+\sqrt{2}}\right)^2 = 1. \tag{3.15}$$

From the observed result we see that the maximum net escape rate that can be extracted due to potential asymmetry is as large as k_0. Since the nonstationary transport velocity is directly related to the net escape rate ($V = L(k_a - k_b) = Lk_+$), the largest possible value of V is when $k_+ = k_0$. In other words, the fastest nonstationary transport that can happen for the classic ratchet potential is when $k_+ = k_0$.

In the next chapter, we will introduce our model ratchet potential, find the right- and left- escape rates and then find the corresponding net escape rate. This will then enable us to find the nonstationary transport velocity for our model ratchet potential and compare this with that of the classic ratchet potential.

Chapter 4

Asymmetric Barrier Subdivision in a Periodic Potential

As we tried to explain at the beginning of chapter two, the escape rate of the Brownian particle from a state of local stability to its neighboring minima can happen only via noise-assisted hopping events. We also mentioned that the respective barrier height that separates the adjacent minima is usually much greater than the thermal energy $k_B T$ and the reaction proceeds with a very small rate. But this reaction can turn out to proceed at a substantially higher rate by a mechanism developed by Mulugeta B *et al.* [15]. The mechanism is subdividing the barrier height along the reaction path into a number of discrete steps each requiring a smaller barrier crossing without changing the total height and width of the barrier. The effect of this mechanism for a model W-shaped simplified bistable potential was verified in their study [15]. That is, subdividing the barrier increases the escape rate that attains a maximum value at the optimal number of barrier subdivision. This result is much greater than the escape rate over the potential barrier for the original W-shaped potential of no barrier subdivision.

In chapter 3, we have discussed the nonstationary transport of Brownian particles by internal white noise in the classic ratchet potential addressed earlier in [7]. As was shown there, it is the right-left asymmetry of the inter-well mean first passage times (or equivalently escape rates) for the Brownian particles in a ratchet potential under internal white noise that gives rise to the nonstationary transport. The right-left asymmetry of the MFPT, in this case, occurs as a result of the spatial asymmetry of the ratchet potential. But, now, based on the effect of the mechanism of barrier subdivision shown in [15] we envisage here an alternative scenario where the asymmetry of the interwell MFPT comes from asymmetric barrier subdivision of a symmetric sawtooth-shaped potential. In other words, we take a symmetric sawtooth-shaped potential shown in fig. (4.1),

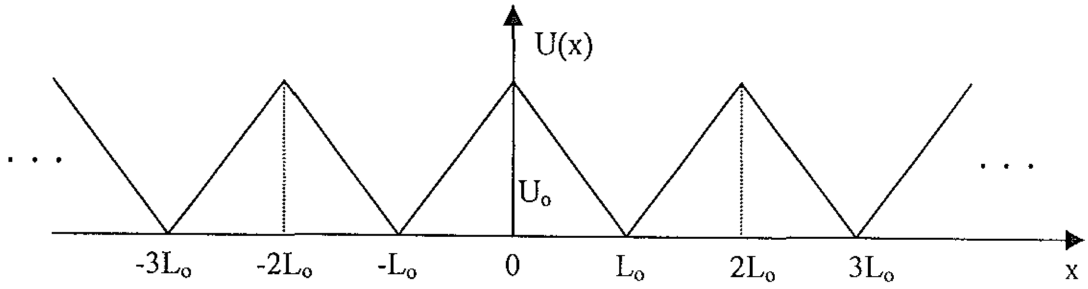


Fig. (4.1).

and then subdivide the potential hills on one side only to get a particular type of ratchet potential shown in fig. (4.2).

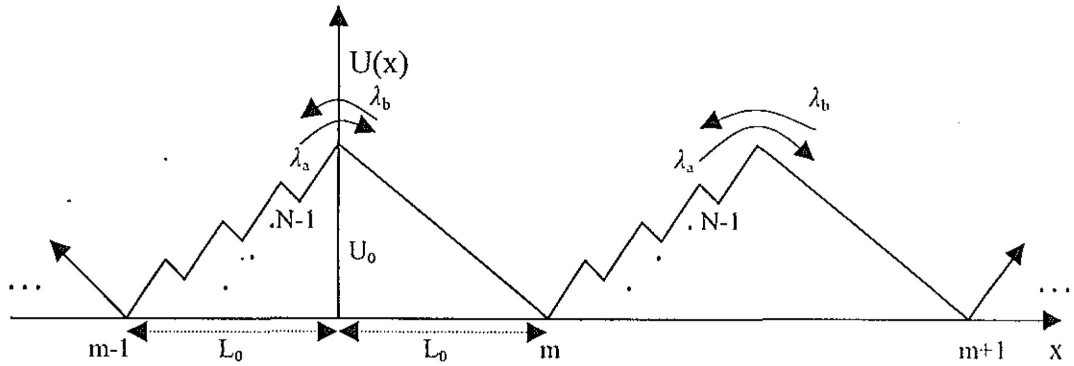


Fig. (4.2).

We expect motion of a Brownian particle over this model potential to have a unidirectional motion with a velocity of greater magnitude than in the classic ratchet potential shown in chapter 3. The main body of our work will dwell on quantitatively finding the strength of such unidirectional motion and comparing it with that of the classic ratchet potential.

4.1 Asymmetric barrier subdivision and their parameterization.

To come to the calculation of the escape rates from one well to the adjacent well and vice versa over the potential barrier of fig. (4.2), we first consider an element of the potential shown in fig. (4.1) which is a symmetric W-shaped potential of barrier height U_0 and width $2L_0$ where L_0 is each distance from the left minimum and the right minimum points to the central maximum points 0 shown in fig. (4.3). We then subdivide the potential barrier of fig. (4.3) on one side only and parameterize the subdivision in a physically reasonable manner so that it becomes the element of the potential in fig. (4.2). The same procedure of approximately taking an element of the periodic potential as a bistable potential was used in the previous chapter on page 11 when finding the escape rates.

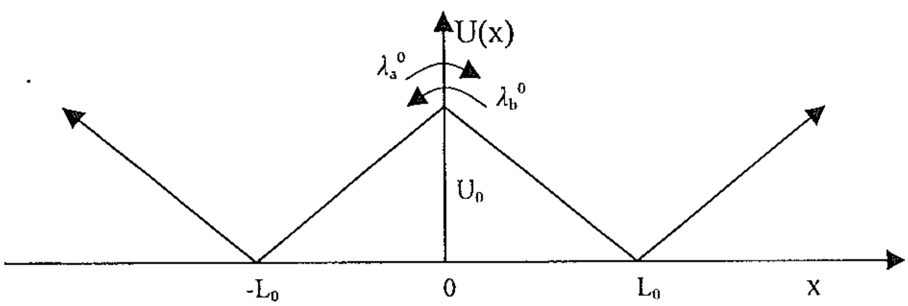


Fig. (4.3).

We now subdivide the barrier between the initial (left minimum) and the transition (central maximum) states into a series of smaller connecting barriers of two equally spaced steps and leave the barrier between the transition state and the final (right minimum) state as it is shown in fig.(4.4).

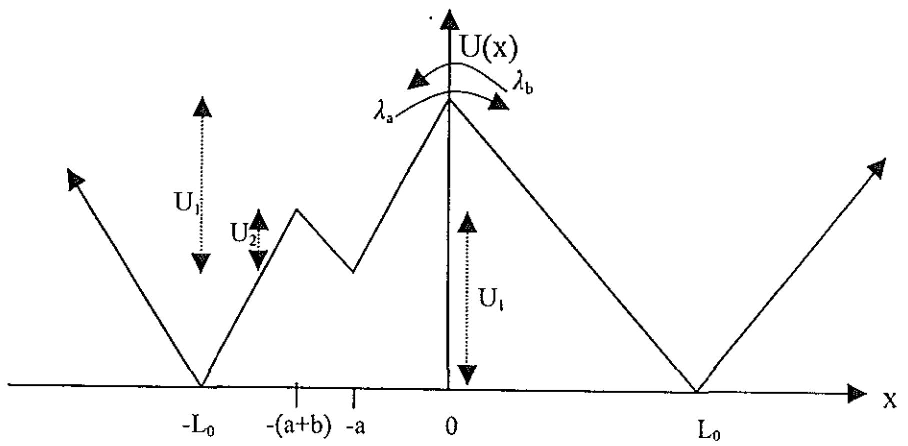


Fig. (4.4).

We then parameterize the subdivision in a physically reasonable manner so that we can examine the effect of asymmetric barrier subdivision on the net escape rate to the right systematically. That is we choose U_1, U_2 and the associated widths a, b (shown in fig. (4.4)) in such a way that $U_1 > U_2$ and $a > b$. We also choose $\frac{U_1}{a} = \frac{U_2}{b}$ to simplify the calculation. With this choice the relations that we can have among the parameters U_1, U_2, a, b, U_0 and L_0 are

$$L_0 = 2a + b$$

$$U_0 = 2U_1 - U_2$$

from which one can also get $\frac{U_2}{2U_1} = \frac{b}{2a}$.

We introduce a parameter ρ defined as

$$\rho \equiv \frac{U_2}{2U_1} = \frac{b}{2a}.$$

What we have done so far concerns only the barrier subdivided into two equally spaced discrete steps. This can be generalized. That is we can accordingly subdivide the barrier into N number of equally spaced discrete steps so that the relations among the parameters for $N \geq 2$ will be

$$L_0 = Na + (N-1)b, \tag{4.1a}$$

$$U_0 = NU_1 - (N-1)U_2, \tag{4.1b}$$

$$\rho \equiv \frac{(N-1)U_2}{NU_1} = \frac{(N-1)b}{Na}. \tag{n4.1c}$$

Such parameterization is physically reasonable as it not only keeps the barrier height and its width fixed, but also keeps the area under the barrier approximately constant as N is varied. The aim is, given U_0 and L_0, to find the net escape rate for different values of barrier subdivision consistent with the high barrier limit. We thus use the SUSY method and find first the escape rate to the right and then to the left.

4.2 The escape rate to the right

The problem of calculating the rate at which a Brownian particle escapes from the left well to the right well surmounting the subdivided potential shown in fig. (4.4) is handled by considering the right minimum as absorbing boundary and the left at infinity as reflecting boundary as shown in fig. (4.5). Such type of consideration is usual in such type of problem.

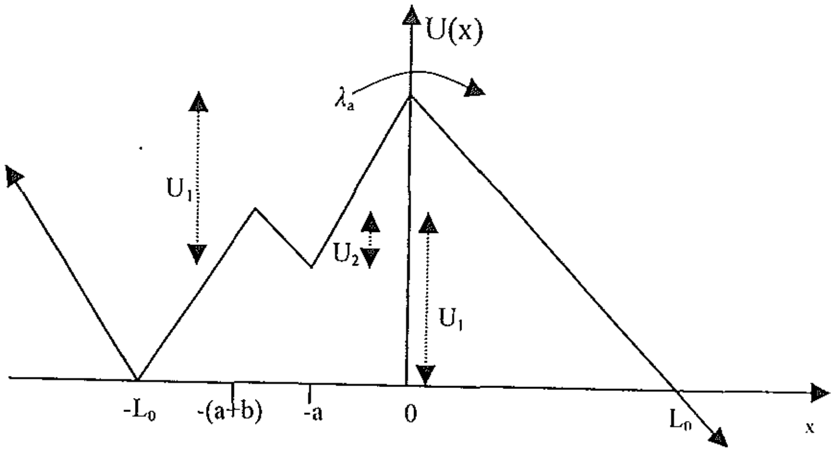


Fig. (4.5).

The supersymmetric 'partner' potential $V_-(x)$ of the potential shown in fig. (4.5) is calculated using the formula in eq. (2.17) and shown in fig. (4.6).

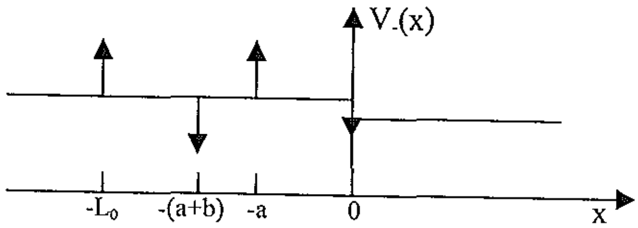


Fig. (4.6).

If we require that $u_{01} = \frac{1}{2}\beta U_1$ and $u_0 = \frac{1}{2}\beta U_0$, then

$$V_-(x) = \begin{cases} (\frac{u_{01}}{a})^2 + \frac{2u_{01}}{a}[\delta(x+2a+b) - \delta(x+a+b) + \delta(x+a)] - (\frac{u_{01}}{a} + \frac{u_0}{L_0})\delta(x), & \text{if } x \le 0; \\ (\frac{u_0}{L_0})^2, & x > 0. \end{cases} \quad (4.2)$$

(Note that we have made the slope to the left of $x = -L_0$ equal to $-\frac{U_1}{a}$, as we have done in chapter 3 to find k_a.)

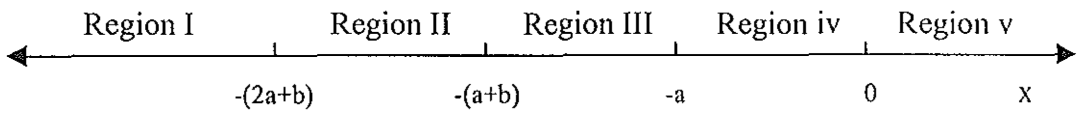
The corresponding Hamiltonian $H_-(x)$ is

$$H_-(x) = -\frac{d^2}{dx^2} + V_-(x)$$

and the corresponding Euclidean Schrödinger equation to be solved is

$$H_- \varphi_-^0 = E_-^0 \varphi_-^0. \tag{4.3}$$

Therefore we find E_-^0 by solving eq. (4.3) in each of the following regions:



Let the solution(s) in:

-region I be denoted by $\varphi_0(x)$,

-region II near $x = -(2a+b)$ be denoted by $\varphi_{0'}(x)$, and $x = -(a+b)$ be denoted by $\varphi_1(x)$,

- region III near $x = -(a+b)$ be denoted by $\varphi_{1'}(x)$ and that near $x = -a$ be denoted by $\varphi_2(x)$,

- region iv near $x = -a$ be denoted by $\varphi_{2'}(x)$ and that near $x = 0$ be denoted by $\varphi_3(x)$,

-region v be denoted by $\varphi(x)$.

Choosing two solutions in the same region is advantageous when we use transfer matrix method. Thus solving eq. (4.3) in each of the regions we can write the respective solution as:

$$\varphi_0(x) = A_0 e^{-\kappa(x+2a+b)} + B_0 e^{\kappa(x+2a+b)},$$

$$\varphi_{0'}(x) = A_0' e^{-\kappa(x+2a+b)} + B_0' e^{\kappa(x+2a+b)},$$

$$\varphi_1(x) = A_1 e^{-\kappa(x+a+b)} + B_1 e^{\kappa(x+a+b)},$$

$$\varphi_{1'}(x) = A_1' e^{-\kappa(x+a+b)} + B_1' e^{\kappa(x+a+b)},$$

$$\varphi_2(x) = A_2 e^{-\kappa(x+a)} + B_2 e^{\kappa(x+a)},$$

$$\varphi_{2'}(x) = A'_2 e^{-\kappa(x+a)} + B'_2 e^{\kappa(x+a)},$$

$$\varphi_3(x) = A_3 e^{-\kappa x} + B_3 e^{\kappa x},$$

$$\varphi(x) = Ae^{-qx} + Be^{qx},$$

where $\kappa = \sqrt{\frac{u_{01}{}^2}{a^2} - E_-^0}$, $q = \sqrt{\frac{u_0{}^2}{L_0{}^2} - E_-^0}$, A_0, B_0, A'_0, B'_0, A_1, B_1, A'_1, B'_1, A_2, B_2, A'_2, B'_2, A_3, B_3, A and B are constants to be determined from the boundary conditions.

The wave functions in the adjacent regions of each boundary formed due to delta potentials are continuous at each of the respective boundaries. So we match the ground state wave functions of the adjacent regions at each of the respective boundaries. We also use a relation between the derivative of the functions at the boundary of the adjacent regions that can be obtained from integration of eq. (4.3) across each boundary wherever there is the delta potential. These boundary conditions can be written in equation form as:

a) $\varphi_{0(x)} = \varphi_{0'(x)}$ at $x = -(2a+b)$,

b) $\varphi_{0'(x)} = \varphi_{1(x)}$ in region ii,

c) $\varphi_{1(x)} = \varphi_{1'(x)}$ at $x = -(a+b)$,

d) $\varphi_{1'(x)} = \varphi_{2(x)}$ in region iii,

e) $\varphi_{2(x)} = \varphi_{2'(x)}$ at $x = -a$,

f) $\varphi_{2'(x)} = \varphi_{3(x)}$ in region iv,

g) $\varphi_{3(x)} = \varphi_{(x)}$ at $x = 0$,

h) $\frac{d\varphi_{0'(x)}}{dx} - \frac{d\varphi_{0(x)}}{dx} = 2\frac{u_{01}}{a}\varphi_{0(x)}$ at $x = -(2a+b)$,

i) $\frac{d\varphi_{1'(x)}}{dx} - \frac{d\varphi_{1(x)}}{dx} = -2\frac{u_{01}}{a}\varphi_{1(x)}$ at $x = -(a+b)$,

j) $\frac{d\varphi_{2'(x)}}{dx} - \frac{d\varphi_{2(x)}}{dx} = 2\frac{u_{01}}{a}\varphi_{2(x)}$ at $x = -a$,

k) $\frac{d\varphi_{(x)}}{dx} - \frac{d\varphi_{3(x)}}{dx} = -(\frac{u_0}{L_0} + \frac{u_{01}}{a})\varphi_{3(x)}$ at $x = 0$.

From the boundary conditions expressed in (a) and (h) we obtain

$$A_0' + B_0' = A_0 + B_0$$

and

$$-\kappa A_0' + \kappa B_0' + \kappa A_0 - \kappa B_0 = \frac{2u_{01}}{a}(A_0 + B_0)$$

which can be simplified to

$$A_0' = (1 - \frac{u_{01}}{a\kappa})A_0 - \frac{u_{01}}{a\kappa}B_0$$

and

$$B_0' = \frac{u_{01}}{a\kappa}A_0 + (1 + \frac{u_{01}}{a\kappa})B_0$$

or

$$\begin{pmatrix} A_0' \\ B_0' \end{pmatrix} = \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} \tag{4.4}$$

where $\alpha = \frac{u_{01}}{a\kappa}$.

From b) we have

$$A_0' e^{-\kappa(x+2a+b)} + B_0' e^{\kappa(x+2a+b)} = A_1 e^{-\kappa(x+a+b)} + B_1 e^{\kappa(x+a+b)}$$

which implies that

$$A_1 = A_0' e^{-\kappa a}$$

and

$$B_1 = B_0' e^{\kappa a}$$

or

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} A_0' \\ B_0' \end{pmatrix}. \tag{4.5}$$

From the boundary conditions in c) and i) we have

$$A_1' + B_1' = A_1 + B_1$$

and

$$-\kappa A_1' + \kappa B_1' + \kappa A_1 - \kappa B_1 = -\frac{2u_{01}}{a}(A_1 + B_1).$$

This implies that

$$A_1' = (1 + \frac{u_{01}}{a\kappa})A_1 + \frac{u_{01}}{a\kappa}B_1$$

and

$$B_1' = -\frac{u_{01}}{a\kappa}A_1 + (1 - \frac{u_{01}}{a\kappa})B_1$$

or

$$\begin{pmatrix} A_1' \\ B_1' \end{pmatrix} = \begin{pmatrix} 1+\alpha & \alpha \\ -\alpha & 1-\alpha \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}. \tag{4.6}$$

Now the condition in d) is applied.

That is

$$A_1' e^{-\kappa(x+a+b)} + B_1' e^{\kappa(x+a+b)} = A_2 e^{-\kappa(x+a)} + B_2 e^{\kappa(x+a)}$$

which implies that

$$A_2 = A_1' e^{-\kappa b}$$

and

$$B_2 = B_1' e^{\kappa b}$$

or

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} e^{-\kappa b} & 0 \\ 0 & e^{\kappa b} \end{pmatrix} \begin{pmatrix} A_1' \\ B_1' \end{pmatrix}. \tag{4.7}$$

From the boundary conditions in e) and j) we get

$$A_2' + B_2' = A_2 + B_2$$

and

$$-\kappa A_2' + \kappa B_2' + \kappa A_2 - \kappa B_2 = \frac{2u_{01}}{a}(A_2 + B_2)$$

which can be simplified to

$$\begin{pmatrix} A_2' \\ B_2' \end{pmatrix} = \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}. \tag{4.8}$$

From f) one can finally arrive at

$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} A_2' \\ B_2' \end{pmatrix}. \tag{4.9}$$

Finally we consider the boundary conditions expressed in g) and k) that lead to

$$A + B = A_3 + B_3$$

and

$$-qA + qB + A_3\kappa - B_3\kappa = -(\frac{u_{01}}{a} + \frac{u_0}{L_0})(A_3 + B_3)$$

or

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} A_3 \\ B_3 \end{pmatrix} \tag{4.10}$$

where

$$Q = \begin{pmatrix} \frac{1}{2} + \frac{\kappa}{2q} + \frac{u_{01}}{2aq} + \frac{u_0}{2L_0 q} & \frac{1}{2} - \frac{\kappa}{2q} + \frac{u_{01}}{2aq} + \frac{u_0}{2L_0 q} \\ \frac{1}{2} - \frac{\kappa}{2q} - \frac{u_{01}}{2aq} - \frac{u_0}{2L_0 q} & \frac{1}{2} + \frac{\kappa}{2q} - \frac{u_{01}}{2aq} - \frac{u_0}{2L_0 q} \end{pmatrix} \tag{4.11}$$

and $q = \sqrt{\frac{{u_0}^2}{{L_0}^2} - E_-^0}$.

Now we have got eqs. (4.4 - 4.10). We combine them using transfer matrix method. That is we start with eq. (4.10) and substitute $\binom{A_3}{B_3}$ in it by its value in eq. (4.9) and obtain

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} A_2' \\ B_2' \end{pmatrix}.$$

Now we substitute $\binom{A_2'}{B_2'}$ by its value in eq. (4.8) and obtain

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}.$$

One can keep on doing the same thing and finally get an equation:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} e^{-\kappa b} & 0 \\ 0 & e^{\kappa b} \end{pmatrix}$$
$$\begin{pmatrix} 1+\alpha & \alpha \\ -\alpha & 1-\alpha \end{pmatrix} \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}.$$

This equation relates the amplitudes of the ground state wave function in the left region of $x = -L_0$:

$$\varphi_0(x) = A_0 e^{-\kappa(x+2a+b)} + B_0 e^{\kappa(x+2a+b)}$$

with the amplitudes of the wave function in the right region of $x = 0$:

$$\varphi(x) = Ae^{-qx} + Be^{qx}.$$

Here we require $A_0 = B = 0$ so that we can have a well behaved function as $|x| \to \infty$. So the equation that we will be dealing with is

$$\begin{pmatrix} A \\ 0 \end{pmatrix} = LT \begin{pmatrix} 0 \\ B_0 \end{pmatrix} \tag{4.12}$$

where

$$L = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix}. \tag{4.13}$$

and

$$T = \begin{pmatrix} e^{-\kappa b} & 0 \\ 0 & e^{\kappa b} \end{pmatrix} \begin{pmatrix} 1+\alpha & \alpha \\ -\alpha & 1-\alpha \end{pmatrix}$$
$$\begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix}. \tag{4.14}$$

We started with the barrier subdivided into two steps and obtained the relation between $\binom{A}{0}$ and $\binom{0}{B_0}$ as shown in eq. (4.12). One can do similarly for the barrier subdivided into $N > 2$ number of steps and get a general relation for $N \geq 2$ as

$$\begin{pmatrix} A \\ 0 \end{pmatrix} = LT^{N-1}\begin{pmatrix} 0 \\ B_0 \end{pmatrix}$$

or

$$\begin{pmatrix} A \\ 0 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} 0 \\ B_0 \end{pmatrix} \tag{4.15}$$

where

$$LT^{N-1} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}. \tag{4.16}$$

From eq. (4.15) we have $M_{12}B_0 = A$ and $M_{22}B_0 = 0$.
This implies that

$$M_{22} = 0 \tag{4.17}$$

for the fact that $B_0 = 0$ gives a trivial solution.

From eqs. (4.13, 4.14 and 4.16) we obtain

$$M_{22} = L_{21}{T_{12}}^{N-1} + L_{22}{T_{22}}^{N-1} \tag{4.18}$$

and

$$L = \begin{pmatrix} (1-\alpha)Q_{11}e^{-\kappa a} + Q_{12}\alpha e^{\kappa a} & Q_{11}(-\alpha)e^{-\kappa a} + Q_{12}(1+\alpha)e^{\kappa a} \\ (1-\alpha)Q_{21}e^{-\kappa a} + Q_{22}\alpha e^{\kappa a} & Q_{21}(-\alpha)e^{-\kappa a} + Q_{22}(1+\alpha)e^{\kappa a} \end{pmatrix}, \tag{4.19}$$

$$T = \begin{pmatrix} (1-\alpha^2)e^{-\kappa(a+b)} + \alpha^2 e^{\kappa(a-b)} & -\alpha(1+\alpha)e^{-\kappa(a+b)} + \alpha(1+\alpha)e^{\kappa(a-b)} \\ -\alpha(1-\alpha)e^{-\kappa(a-b)} + \alpha(1-\alpha)e^{\kappa(a+b)} & (1-\alpha^2)e^{\kappa(a+b)} + \alpha^2 e^{-\kappa(a-b)} \end{pmatrix}. \tag{4.20}$$

We find the elements of matrix T^{N-1} by decomposing matrix T as a product of three matrices as used in [15].

That is, $T = R\Lambda r$,
where $\Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$ provided that λ_1 and λ_2 are the eigenvalues of T that are given by

$$\lambda_1 = [T_{11} + T_{22} + \sqrt{(T_{11} - T_{22})^2 + 4T_{12}T_{21}}]/2, \tag{4.21a}$$

$$\lambda_2 = [T_{11} + T_{22} - \sqrt{(T_{11} - T_{22})^2 + 4T_{12}T_{21}}]/2 \qquad (4.21b)$$

and R is the right eigenvector of T that are expressed as

$$R = \begin{pmatrix} 1 & \frac{T_{12}}{\lambda_2 - T_{11}} \\ \frac{\lambda_1 - T_{11}}{T_{12}} & 1 \end{pmatrix} \qquad (4.22)$$

and r is the inverse of R which is the left eigenvector of T:

$$r = (\frac{\lambda_2 - T_{11}}{\lambda_2 - \lambda_1}) \begin{pmatrix} 1 & \frac{-T_{12}}{\lambda_2 - T_{11}} \\ \frac{T_{11} - \lambda_1}{T_{12}} & 1 \end{pmatrix}. \qquad (4.23)$$

With the decomposition $T = R\Lambda r$, T^{N-1} will, therefore,become

$$T^{N-1} = R\Lambda^{N-1}r$$

where

$$T^{N-1} = \begin{pmatrix} R_{11}r_{11}\lambda_1^{(N-1)} + R_{12}r_{21}\lambda_2^{(N-1)} & R_{11}r_{12}\lambda_1^{(N-1)} + R_{12}r_{22}\lambda_2^{(N-1)} \\ R_{21}r_{11}\lambda_1^{(N-1)} + R_{22}r_{21}\lambda_2^{(N-1)} & R_{21}r_{12}\lambda_1^{(N-1)} + R_{22}r_{22}\lambda_2^{(N-1)} \end{pmatrix}. \qquad (4.24)$$

We, therefore, substitute L_{21}, L_{22}, $T_{12}^{(N-1)}$ and $T_{22}^{(N-1)}$ in eq. (4.18) by their corresponding values from eqs. (4.19 and 4.24) and then equate it to 0. That is

$$(1-\alpha)R_{11}r_{12}Q_{21}\lambda_1^{(N-1)}e^{-\kappa a} + (1-\alpha)R_{12}r_{22}Q_{21}\lambda_2^{(N-1)}e^{-\kappa a} + \alpha R_{11}r_{12}Q_{22}\lambda_1^{(N-1)}e^{\kappa a} +$$

$$\alpha R_{12}r_{22}Q_{22}\lambda_2^{(N-1)}e^{\kappa a} - \alpha R_{21}r_{12}Q_{21}\lambda_1^{(N-1)}e^{-\kappa a} - \alpha R_{22}r_{22}Q_{21}\lambda_2^{(N-1)}e^{-\kappa a} +$$

$$(1+\alpha)R_{21}r_{12}Q_{22}\lambda_1^{(N-1)}e^{\kappa a} + (1+\alpha)R_{22}r_{22}Q_{22}\lambda_2^{(N-1)}e^{\kappa a} = 0.$$

Substituting r and R by their respective values from eqs. (4.22 and 4.23) will yield

$$T_{12}({\lambda_2}^{N-1} - {\lambda_1}^{N-1})[(1-\alpha)Q_{21}e^{-\kappa a} + \alpha Q_{22}e^{\kappa a}] +$$

$$[(\lambda_2 - T_{11}){\lambda_2}^{N-1} - (\lambda_1 - T_{11}){\lambda_1}^{N-1}][Q_{22}(1+\alpha)e^{\kappa a} - \alpha Q_{21}e^{-\kappa a}] = 0 \quad (4.25)$$

This is the equation that we will be using to evaluate E_-^0 numerically, for a given u_0, L_0, ρ and N. The escape rate to the right, λ_a, is then given by $\lambda_a = DE_-^0$

4.3 The escape rate to the left

The problem to be solved in this section is more or less similar to that we have gone through in section 4.2 except that this time escaping is from the right well to the left well of the potential shown in fig. (4.4). The boundary condition that we have to consider is thus the vice versa of the previous one. That is, the left minimum at $x = -L_0$ is taken as absorbing boundary whereas the reflecting boundary is considered at infinity from the right side as shown in fig. (4.7).

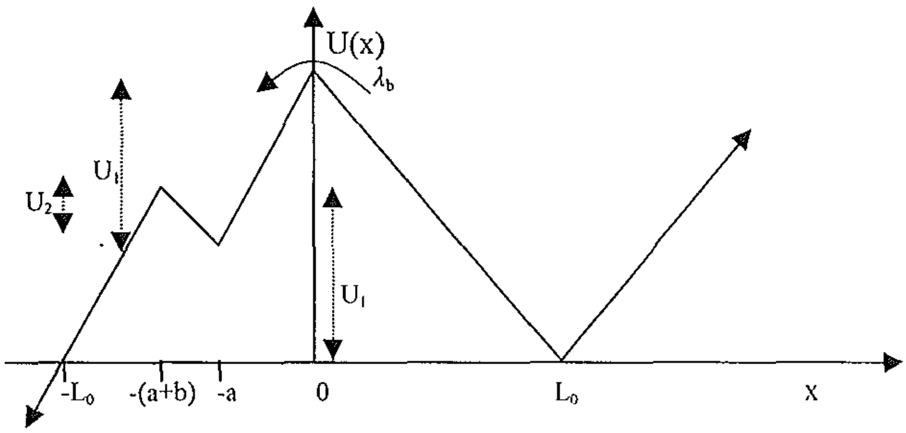


Fig. (4.7).

The supersymmetric 'partner' potential $V_-(x)$ of the potential shown in fig. (4.8)

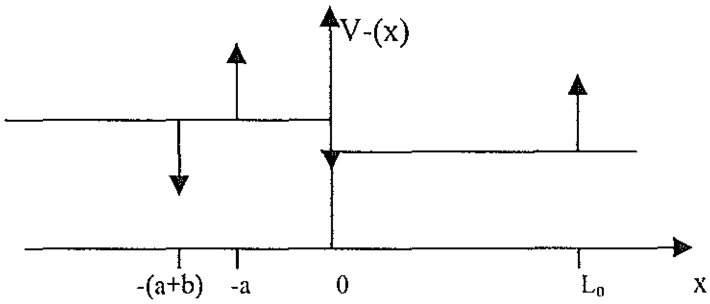


Fig. (4.8).

is found from the formula in eq. (2.17). If we require that $u_{01} = \frac{1}{2}\beta U_1$ and $u_0 = \frac{1}{2}\beta U_0$, then

$$V_-(x) = \begin{cases} (\frac{u_{01}}{a})^2 + \frac{2u_{01}}{a}[-\delta(x+a+b) + \delta(x+a)] - (\frac{u_{01}}{a} + \frac{u_0}{L_0})\delta(x), & \text{if } x \leq 0; \\ (\frac{u_0}{L_0})^2 + \frac{2u_0}{L_0}\delta(x - L_0), & x > 0. \end{cases} \quad (4.26)$$

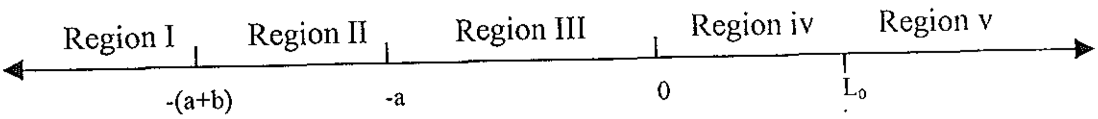
The corresponding Hamiltonian $H_-(x)$ is

$$H_-(x) = -\frac{d^2}{dx^2} + V_-(x)$$

and the corresponding Euclidean Schrödinger equation is

$$H_-\varphi_-^0 = E_-^{0\prime}\varphi_-^0. \quad (4.27)$$

We find $E_-^{0\prime}$ by solving eq. (4.27) using transfer matrix method in the regions shown next



Let us denote the solution as $\varphi_1(x)$ in the left region of $x = -(a+b)$ and $\varphi_4'(x)$ in the right region of $x = L_0$. In each of the rest three regions we choose a pair of solutions at different positions with different amplitudes. Let the solution(s) in:

-region II near $x = -(a+b)$ be denoted by $\varphi_{1'}(x)$ and that near $x = -a$ be denoted by $\varphi_2(x)$,

-region III near $x = -a$ be denoted by $\varphi_{2'}(x)$ and near $x = 0$ be denoted by $\varphi_3(x)$,

-region iv near $x = 0$ be denoted by $\varphi_{3'}(x)$ and near $x = L_0$ be denoted by $\varphi_4(x)$.

So we solve eq. (4.27) in each region and write the corresponding solution using the above notation as:

$$\varphi_1(x) = A_1 e^{-\kappa(x+a+b)} + B_1 e^{\kappa(x+a+b)},$$

$$\varphi_{1'}(x) = A_1' e^{-\kappa(x+a+b)} + B_1' e^{\kappa(x+a+b)},$$

$$\varphi_2(x) = A_2 e^{-\kappa(x+a)} + B_2 e^{\kappa(x+a)},$$

$$\varphi_{2'}(x) = A_2' e^{-\kappa(x+a)} + B_2' e^{\kappa(x+a)},$$

$$\varphi_3(x) = A_3 e^{-\kappa x} + B_3 e^{\kappa x},$$

$$\varphi_{3'}(x) = A_3' e^{-qx} + B_3' e^{qx},$$

$$\varphi_4(x) = A_4 e^{-q(x-L_0)} + B_4 e^{q(x-L_0)},$$

$$\varphi_{4'}(x) = A_4' e^{-q(x-L_0)} + B_4' e^{q(x-L_0)},$$

where $\kappa = \sqrt{\frac{u_{01}{}^2}{a^2} - E_-^{0\prime}}$, $q = \sqrt{\frac{u_0{}^2}{L_0{}^2} - E_-^{0\prime}}$, A_1, B_1, A_1', B_1', A_2, B_2, A_2', B_2', A_3, B_3, A_3', B_3', A_4, B_4, A_4' and B_4' are constants to be determined from the boundary conditions.

The wave functions in the adjacent regions of each boundary formed due to delta potentials are continuous at each of the respective boundaries. So we match the ground state wave functions of the adjacent regions at each of the respective boundaries. We also use a relation between the derivative of the functions at the boundary of the adjacent regions that can be obtained from integration of eq. (4.27) across each boundary wherever there is the delta potential. These boundary conditions can be written in equation form as:

a) $\varphi_{1(x)} = \varphi_{1'(x)}$ at $x = -(a+b)$,

b) $\varphi_{1'(x)} = \varphi_{2(x)}$ in region ii,

c) $\varphi_{2(x)} = \varphi_{2'(x)}$ at $x = -a$,

d) $\varphi_{2'(x)} = \varphi_{3(x)}$ in region iii,

e) $\varphi_{3(x)} = \varphi_{3'(x)}$ at $x = 0$,

f) $\varphi_{3'(x)} = \varphi_{4(x)}$ in region iv,

g) $\varphi_{4'}(x) = \varphi_4(x)$ at $x = L_0$,

h) $\frac{d\varphi_{1'(x)}}{dx} - \frac{d\varphi_{1(x)}}{dx} = -2\frac{u_{01}}{a}\varphi_{1(x)}$ at $x = -(a+b)$,

i) $\frac{d\varphi_{2'(x)}}{dx} - \frac{d\varphi_{2(x)}}{dx} = 2\frac{u_{01}}{a}\varphi_{2(x)}$ at $x = -a$,

j) $\frac{d\varphi_{3'(x)}}{dx} - \frac{d\varphi_{3(x)}}{dx} = -(\frac{u_0}{L_0} + \frac{u_{01}}{a})\varphi_{3(x)}$ at $x = 0$,

k) $\frac{d\varphi_{4'}(x)}{dx} - \frac{d\varphi_{4(x)}}{dx} = 2\frac{u_0}{L_0}\varphi_4(x)$ at $x = L_0$.

When we use the boundary conditions a) and h) we obtain

$$A_1' + B_1' = A_1 + B_1$$

and

$$-\kappa A_1' + \kappa B_1' + \kappa A_1 - \kappa B_1 = -\frac{2u_{01}}{a}(A_1 + B_1).$$

This is equivalent to

$$A_1' = (1 + \frac{u_{01}}{a\kappa})A_1 + \frac{u_{01}}{a\kappa}B_1$$

and

$$B_1' = -\frac{u_{01}}{a\kappa}A_1 + (1 - \frac{u_{01}}{a\kappa})B_1$$

or

$$\begin{pmatrix} A_1' \\ B_1' \end{pmatrix} = \begin{pmatrix} 1+\alpha & \alpha \\ -\alpha & 1-\alpha \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \tag{4.28}$$

where $\alpha = \frac{u_{01}}{a\kappa}$.

From b) we obtain

$$A_2 = A_1' e^{-\kappa b}$$

and

$$B_2 = B_1' e^{\kappa b}$$

or

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} e^{-\kappa b} & 0 \\ 0 & e^{\kappa b} \end{pmatrix} \begin{pmatrix} A_1' \\ B_1' \end{pmatrix}. \tag{4.29}$$

From the boundary conditions expressed in c) and i) we obtain

$$A'_2 + B'_2 = A_2 + B_2$$

and

$$-\kappa A'_2 + \kappa B'_2 + \kappa A_2 - \kappa B_2 = 2\frac{u_{01}}{a}(A_2 + B_2)$$

which is equivalent to

$$\begin{pmatrix} A'_2 \\ B'_2 \end{pmatrix} = \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}. \tag{4.30}$$

From d) we obtain

$$A_3 = A'_2 e^{-\kappa a}$$

and

$$B_3 = B'_2 e^{\kappa a}$$

or

$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} A'_2 \\ B'_2 \end{pmatrix}. \tag{4.31}$$

From e) and j) we get

$$A'_3 + B'_3 = A_3 + B_3$$

and

$$-qA'_3 + qB'_3 + \kappa A_3 - \kappa B_3 = -(\frac{u_{01}}{a} + \frac{u_0}{L_0})(A_3 + B_3)$$

which is equivalent to

$$\begin{pmatrix} A'_3 \\ B'_3 \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} A_3 \\ B_3 \end{pmatrix} \tag{4.32}$$

where

$$Q = \begin{pmatrix} \frac{1}{2} + \frac{\kappa}{2q} + \frac{u_{01}}{2aq} + \frac{u_0}{2L_0 q} & \frac{1}{2} - \frac{\kappa}{2q} + \frac{u_{01}}{2aq} + \frac{u_0}{2L_0 q} \\ \frac{1}{2} - \frac{\kappa}{2q} - \frac{u_{01}}{2aq} - \frac{u_0}{2L_0 q} & \frac{1}{2} + \frac{\kappa}{2q} - \frac{u_{01}}{2aq} - \frac{u_0}{2L_0 q} \end{pmatrix}. \tag{4.33}$$

From the boundary conditions expressed in c) and i) we obtain

$$A_2' + B_2' = A_2 + B_2$$

and

$$-\kappa A_2' + \kappa B_2' + \kappa A_2 - \kappa B_2 = 2\frac{u_{01}}{a}(A_2 + B_2)$$

which is equivalent to

$$\begin{pmatrix} A_2' \\ B_2' \end{pmatrix} = \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}. \tag{4.30}$$

From d) we obtain

$$A_3 = A_2' e^{-\kappa a}$$

and

$$B_3 = B_2' e^{\kappa a}$$

or

$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} A_2' \\ B_2' \end{pmatrix}. \tag{4.31}$$

From e) and j) we get

$$A_3' + B_3' = A_3 + B_3$$

and

$$-qA_3' + qB_3' + \kappa A_3 - \kappa B_3 = -(\frac{u_{01}}{a} + \frac{u_0}{L_0})(A_3 + B_3)$$

which is equivalent to

$$\begin{pmatrix} A_3' \\ B_3' \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} A_3 \\ B_3 \end{pmatrix} \tag{4.32}$$

where

$$Q = \begin{pmatrix} \frac{1}{2} + \frac{\kappa}{2q} + \frac{u_{01}}{2aq} + \frac{u_0}{2L_0 q} & \frac{1}{2} - \frac{\kappa}{2q} + \frac{u_{01}}{2aq} + \frac{u_0}{2L_0 q} \\ \frac{1}{2} - \frac{\kappa}{2q} - \frac{u_{01}}{2aq} - \frac{u_0}{2L_0 q} & \frac{1}{2} + \frac{\kappa}{2q} - \frac{u_{01}}{2aq} - \frac{u_0}{2L_0 q} \end{pmatrix}. \tag{4.33}$$

From f) we obtain

$$A_4 = A'_3 e^{-qL_0}$$

and

$$B_4 = B'_3 e^{qL_0}$$

or

$$\begin{pmatrix} A_4 \\ B_4 \end{pmatrix} = \begin{pmatrix} e^{-qL_0} & 0 \\ 0 & e^{qL_0} \end{pmatrix} \begin{pmatrix} A'_3 \\ B'_3 \end{pmatrix}. \tag{4.34}$$

From g) and k) we get

$$A'_4 + B'_4 = A_4 + B_4$$

and

$$-qA'_4 + qB'_4 + qA_4 - qB_4 = 2\frac{u_0}{L_0}(A_4 + B_4)$$

which is simplified to

$$\begin{pmatrix} A'_4 \\ B'_4 \end{pmatrix} = \begin{pmatrix} 1-\delta & -\delta \\ \delta & 1+\delta \end{pmatrix} \begin{pmatrix} A_4 \\ B_4 \end{pmatrix} \tag{4.35}$$

where $\delta = \frac{u_0}{L_0 q}$.

As we did in section 4.2, we combine here also eqs. (4.28-4.35) into one equation that relates $\binom{A'_4}{B'_4}$ with $\binom{A_1}{B_1}$. So substituting eq. (4.34) into eq. (4.35), we obtain a relation between $\binom{A_4}{B_4}$ and $\binom{A'_3}{B'_3}$. We keep on substituting until we arrive at the equation:

$$\begin{pmatrix} A'_4 \\ B'_4 \end{pmatrix} = \begin{pmatrix} 1-\delta & -\delta \\ \delta & 1+\delta \end{pmatrix} \begin{pmatrix} e^{-qL_0} & 0 \\ 0 & e^{qL_0} \end{pmatrix} \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix}$$
$$\begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} e^{-\kappa b} & 0 \\ 0 & e^{\kappa b} \end{pmatrix} \begin{pmatrix} 1+\alpha & \alpha \\ -\alpha & 1-\alpha \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}. \tag{4.36}$$

Here we demand $A_1 = B'_4 = 0$ in order that we can have a well behaved function as $|x| \to \infty$. Thus eq. (4.36) becomes

$$\begin{pmatrix} A'_4 \\ 0 \end{pmatrix} = SW \begin{pmatrix} 0 \\ B_1 \end{pmatrix} \tag{4.37}$$

where

$$S = \begin{pmatrix} 1-\delta & -\delta \\ \delta & 1+\delta \end{pmatrix} \begin{pmatrix} e^{-qL_0} & 0 \\ 0 & e^{qL_0} \end{pmatrix} \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \tag{4.38}$$

and

$$W = \begin{pmatrix} e^{-\kappa a} & 0 \\ 0 & e^{\kappa a} \end{pmatrix} \begin{pmatrix} 1-\alpha & -\alpha \\ \alpha & 1+\alpha \end{pmatrix} \begin{pmatrix} e^{-\kappa b} & 0 \\ 0 & e^{\kappa b} \end{pmatrix} \begin{pmatrix} 1+\alpha & \alpha \\ -\alpha & 1-\alpha \end{pmatrix}. \tag{4.39}$$

From eq. (4.37) we can conclude the general expression that relates the amplitudes of the groundstate wave functions at the left of $x = -(a+b)$, $\binom{A'}{0}$, with that at the right of $x = L_0$, $\binom{0}{B}$, for the barrier subdivided into $N \geq 2$ as

$$\begin{pmatrix} A' \\ 0 \end{pmatrix} = SW^{N-1} \begin{pmatrix} 0 \\ B \end{pmatrix}.$$

That is,

$$\begin{pmatrix} A' \\ 0 \end{pmatrix} = \begin{pmatrix} M'_{11} & M'_{12} \\ M'_{21} & M'_{22} \end{pmatrix} \begin{pmatrix} 0 \\ B \end{pmatrix} \tag{4.40}$$

where

$$SW^{N-1} = \begin{pmatrix} M'_{11} & M'_{12} \\ M'_{21} & M'_{22} \end{pmatrix}. \tag{4.41}$$

From eq. (4.40) one can obtain

$M_{12}{}'B = A'$ and $M'_{22}B = 0$. $B = 0$ results in trivial solution. Thus we require $M'_{22} = 0$. That is,

$$M'_{22} = S_{21}W_{12}{}^{N-1} + S_{22}W_{22}{}^{N-1} = 0 \tag{4.42}$$

where

$$S = \begin{pmatrix} Q_{11}(1-\delta)e^{-qL_0} - Q_{21}\delta e^{qL_0} & Q_{12}(1-\delta)e^{-qL_0} - Q_{22}\delta e^{qL_0} \\ Q_{11}\delta e^{-qL_0} + Q_{21}(1+\delta)e^{qL_0} & Q_{12}\delta e^{-qL_0} + Q_{22}(1+\delta)e^{qL_0} \end{pmatrix} \tag{4.43}$$

and

$$W = \begin{pmatrix} (1-\alpha^2)e^{-\kappa(a+b)} + \alpha^2 e^{-\kappa(a-b)} & \alpha(1-\alpha)e^{-\kappa(a+b)} - \alpha(1-\alpha)e^{-\kappa(a-b)} \\ \alpha(1+\alpha)e^{\kappa(a-b)} - \alpha(1+\alpha)e^{\kappa(a+b)} & (1-\alpha^2)e^{\kappa(a+b)} + \alpha^2 e^{\kappa(a-b)} \end{pmatrix}. \tag{4.44}$$

Following the same method that was used to find the elements of T^{N-1}, eq. (4.24), in section (4.2) we obtain

$$W^{N-1} = \begin{pmatrix} D_{11}d_{11}{\lambda_1}'^{(N-1)} + D_{12}d_{21}{\lambda_2}'^{(N-1)} & D_{11}d_{12}{\lambda_1}'^{(N-1)} + D_{12}d_{22}{\lambda_2}'^{(N-1)} \\ D_{21}d_{11}{\lambda_1}'^{(N-1)} + D_{22}d_{21}{\lambda_2}'^{(N-1)} & D_{21}d_{12}{\lambda_1}'^{(N-1)} + D_{22}d_{22}{\lambda_2}'^{(N-1)} \end{pmatrix} \quad (4.45)$$

where λ_1' and λ_2' are the eigenvalues of W which are expressed as

$$\lambda_1' = [W_{11} + W_{22} + \sqrt{(W_{11} - W_{22})^2 + 4W_{12}W_{21}}]/2, \qquad (4.46a)$$

$$\lambda_1' = [W_{11} + W_{22} - \sqrt{(W_{11} - W_{22})^2 + 4W_{12}W_{21}}]/2 \qquad (4.46b)$$

and D is the right eigenvector of W and d is the inverse of D:

$$D = \begin{pmatrix} 1 & \frac{W_{12}}{\lambda_2' - W_{11}} \\ \frac{\lambda_1' - W_{11}}{W_{12}} & 1 \end{pmatrix} \qquad (4.47a)$$

and

$$d = \left(\frac{\lambda_2' - W_{11}}{\lambda_2' - \lambda_1'}\right) \begin{pmatrix} 1 & -\frac{W_{12}}{\lambda_2' - W_{11}} \\ -(\frac{\lambda_1' - W_{11}}{W_{12}}) & 1 \end{pmatrix}. \qquad (4.47b)$$

Hence putting for S_{21}, ${W_{12}}^{N-1}$, S_{22} and ${W_{22}}^{N-1}$ their corresponding values in eq. (4.42) one can obtain an equation:

$$W_{12}\left(\lambda_2'^{(N-1)} - \lambda_1'^{(N-1)}\right)\left[e^{-qL_0}\delta Q_{11} + e^{qL_0}(1+\delta)Q_{21}\right]$$
$$+ \left[(\lambda_2' - W_{11})\lambda_2'^{(N-1)} - (\lambda_1' - W_{11})\lambda_1'^{(N-1)}\right]\left[\delta Q_{12}e^{-qL_0} + (1+\delta)Q_{22}e^{qL_0}\right] = 0. \qquad (4.48)$$

For a given u_0, L_0, ρ and N, root of this equation will give us the value of $E_-^{0\prime}$. The escape rate to the left, λ_b, is then given by $\lambda_b = DE_-^{0\prime}$

In the following chapter, the inter-well escape rates will be evaluated numerically for various kinds of potential profile, that is, for different values of u_0, ρ and N. These local escape rate values will then be used as an input to determine the unidirectional motion that arises for non-stationary transport. This result of unidirectional motion will then be compared with the unidirectional motion one finds for the classic ratchet potential.

Chapter 5

Results and Discussion

5.1 Effect of asymmetric barrier subdivision on the net escape rate

Now we consider eqs. (4.25 and 4.48) which contain variables E_{-}^{0} and $E_{-}^{0\prime}$, respectively. In these equations the total barrier height u_0, the slope of the local barrier height ρ, and the width under the potential from the maximum to either the right or the left minimum point L_0 are assumed to be known. The parameters u_{01}, a and b are expressed from eqs. (4.1a and 4.1b or 4.1c) in terms of u_0, $L_0 = 1$, ρ and N as

$u_{01} = \frac{u_0}{N(1-\rho)}$; $a = \frac{L_0}{N(1+\rho)}$; $b = \frac{\rho L_0}{(N-1)(1+\rho)}$.

We have solved these equations, eq. (4.25) and eq. (4.48), numerically for E_{-}^{0} and $E_{-}^{0\prime}$, respectively, using a FORTRAN program on a computer for specified values of u_0, L_0, and N. The corresponding escape rates are, therefore, expressed from the relation $\lambda_0 = DE_{-}^{0}$, discussed in section 2.2. That is the escape rate to the right denoted by λ_a is

$$\lambda_a = DE_{-}^{0}, \tag{5.1}$$

and the escape rate to the left denoted by λ_b is

$$\lambda_b = DE_{-}^{0\prime}, \tag{5.2}$$

where D is the diffusion coefficient.

We denote the amount by which escape rate to the right exceeds escape rate to the left by λ_+ given by

$$\lambda_+ = D(E_-^0 - E_-^{0\prime}). \tag{5.3}$$

We call λ_+ as net escape rate. This net escape rate, λ_+, is now compared with the escape rate, λ_a^0, from one well to the adjacent well for the potential of no barrier subdivision as a function of ρ, u_0 and N. Fig. (5.1) is a plot of the ratio $\frac{\lambda_+}{\lambda_a^0}$ versus N for fixed ρ and various values of u_0

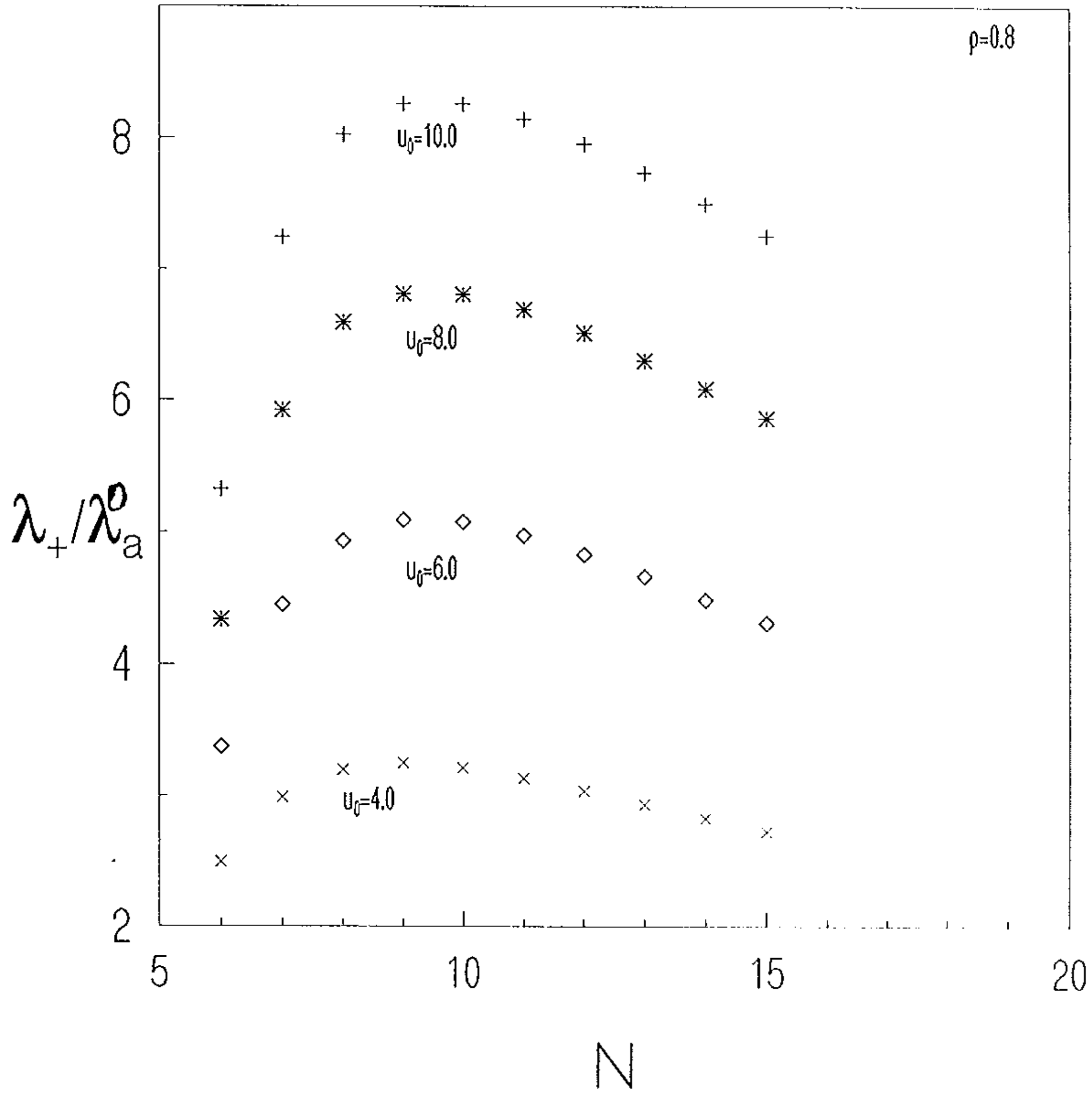


Fig. (5.1).

while fig. (5.2) is plot of the same variables for fixed u_0 and various values of ρ.

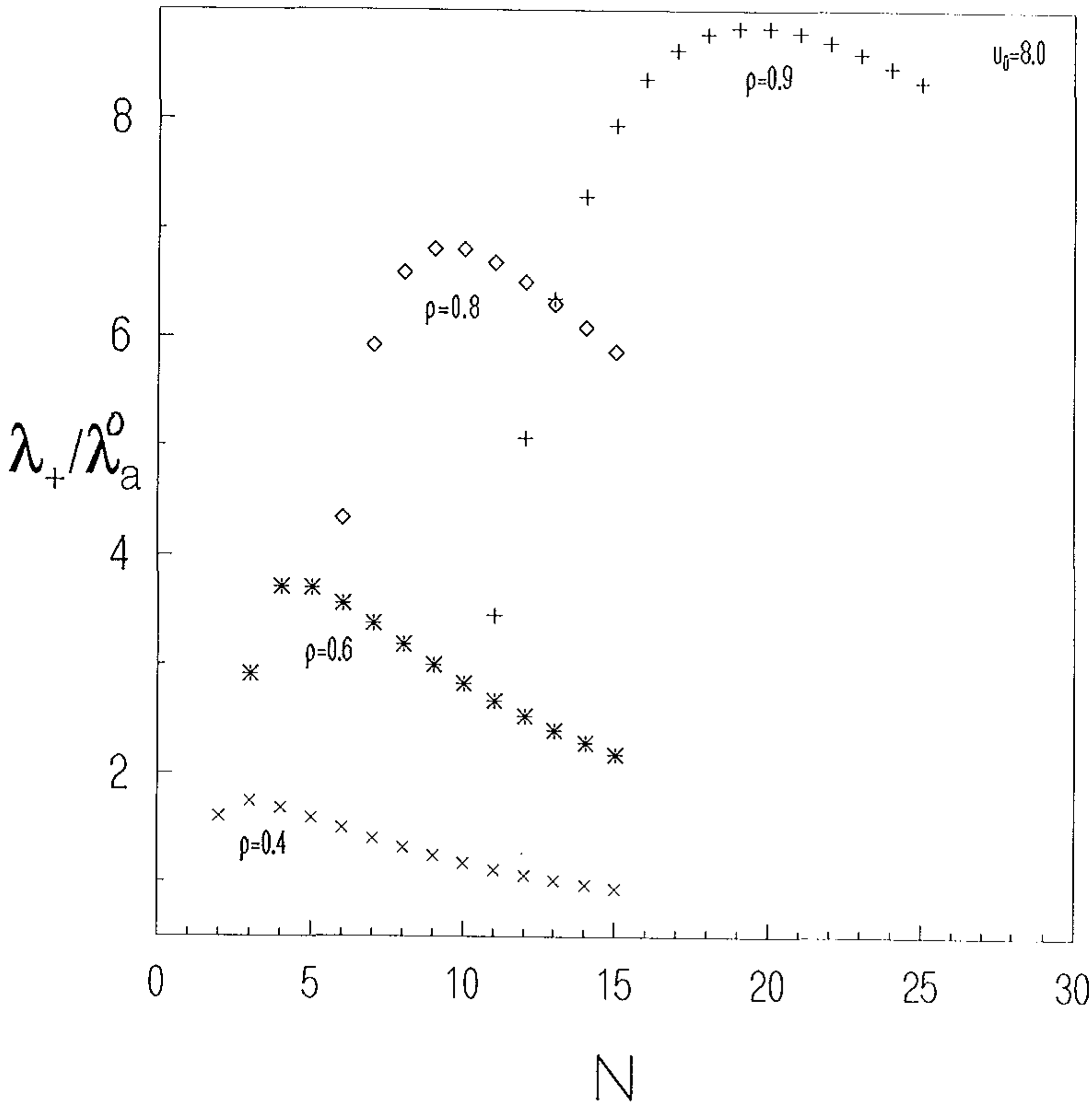


Fig. (5.2).

From the plots in both figures we see that λ_+ arises as a result of barrier subdivision. For the specified values of ρ and u_0 the magnitude of λ_+ varies with the number of barrier subdivision and reaches maximum value at an optimal number of barrier subdivision, N_{op}. At the optimal number of barrier subdivision, as shown in fig. (5.1), λ_+ is as large as: $3.3\lambda_a^0$ for $u_0(=4)$, $5.1\lambda_a^0$ for $u_0(=6)$, $6.8\lambda_a^0$ for $u_0(=8)$ and $8.3\lambda_a^0$ for

$u_0(= 10)$. That is λ_+ increases as u_0 increases and reaches a value as high as 8.3 times λ_a^0 for $u_0(= 10)$ while N_{op} remains constant (here 9) suggesting that the steepness of the local barrier height determines N_{op}. But for specified value of barrier height (in our case $u_0 = 8$), as shown in fig. (5.2), both optimal number of barrier subdivision N_{op} and the net escape rate λ_+ increases as ρ increases.
(Note that in both figures we have chosen $a > b$ and $U_1 > U_2$. This choice restricted N to have values greater than or equal to 2, 3, 6 and 11 respectively for ρ equal to 0.4, 0.6, 0.8 and 0.9.)

It is now appropriate to compare net escape rate for classic ratchet potential with the net escape rate for our model ratchet potential. The net escape rate for the classic ratchet potential is at most equal to λ_a^0 and independent of u_0. On the other hand, the net escape rate for our model ratchet potential depends on N, ρ and u_0 and can attain substantially large values.

The results verified in fig. (5.1) and fig. (5.2) are general. Thus, there is an optimal value of barrier subdivision, N_{op}, at which the net escape rate to the right reaches the maximum value. This effect, the effect of asymmetric barrier subdivision on the net escape rate of the Brownian particle, has a consequence of a net unidirectional motion of the Brownian particle. We describe this motion for a potential of period $2L_0$ shown in fig. (4.2) in the high barrier low noise limit. Each distance from the central maximum point to the adjacent right or left minimum point is equal to L_0, and the barrier height is U_0. Therefore the rate at which the particle escapes from any well to the neighboring right or left well over the respective barrier height is respectively denoted by λ_a or λ_b which is the same as the corresponding escape rates to the right and to the left found for the asymmetric barrier subdivided W-shaped potential. As was verified for W-shaped asymmetric barrier subdivided model potential $\lambda_+ = \lambda_a - \lambda_b$ has a non-zero positive value that reaches a maximum value at an optimal number of barrier subdivision. The occurrence of λ_+ with non-zero value, as already discussed for ratchet potential in chapter 3, results in directed motion for the time scale which is much more greater than the MFPT. So the motion of the Brownian particle in the asymmetric barrier subdivided model potential is likewise that in a ratchet potential of fig. (3.1). Hence the same coarse grained equation, eq. (3.10), can govern this motion. In this equation the constant velocity V with which the ensemble of Brownian particles move was described as

$$V = L(k_a - k_b) = Lk_+. \tag{5.4}$$

The corresponding velocity denoted by v for the motion in the potential of fig. (4.2) is, therefore, described as

$$v = 2L_0(\lambda_a - \lambda_b) = 2L_0\lambda_+. \tag{5.5}$$

If we suppose $L_1 + L_2 = 2L_0$, then the escape rate to the right for the potential of no barrier subdivision shown in fig. (4.3), λ_a^0, is exactly equal to k_0. Where k_0 is the escape rate to the right or left described in eq. (3.13). Thus the maximum net escape rate over the barrier of the ratchet potential of fig. (3.1) shown in eq. (3.15) is exactly equal to λ_a^0 and the maximum possible velocity that can be attained due to potential asymmetry is

$$V_{max} = 2L_0\lambda_a^0, \tag{5.6}$$

while the maximum velocity that can be attained for the motion in asymmetric barrier subdivided model potential which is reached at an optimal number of barrier subdivision is

$$v_{max} = 2L_0\lambda_+^{max} \tag{5.7}$$

where λ_+^{max} is; for instance, $8.3\lambda_a^0$ when $\rho = 0.8$ and $u_0 = 10$, $8.8\lambda_a^0$ when $\rho = 0.9$ and $u_0 = 8$. The value of λ_+^{max} can increase than this when u_0 increases. This shows that v_{max} can be much larger than V_{max}. Therefore a Brownian particle can move with a substantially large velocity in our modified ratchet potential.

5.2 The effect of asymmetric barrier subdivision on the current

In the previous section we discussed the net escape rate, λ_+, that could occur as a result of asymmetric barrier subdivision. Now we discuss its effect on the probability current. Let us, therefore, consider fig. (5.3). Because of the net escape rate to the right, particles that are supplied to say $(m-1)$-well with energy a few k_BT below the barrier height U_0 leave the well over the barrier to m-well after thermalization. In m-well also they are first thermalized and then removed to $(m+1)$-well. In a similar way they move to the next well and so on until they are eventually removed by the sink at the right end. (Note that this process as we mentioned in chapter 3 takes place in a finite time which is much greater than the time needed for the escaping from one well to the adjacent well which in turn is much greater than the relaxation time in each well.) If particles are continuously fed into the well at the extreme left by a source, then due to the net escape rate to the right they will move to the right and also removed continuously if a sink exists at the extreme right. This results in a steady-state current j. So we deal with a motion in which the net escape rate over the barrier is constant by considering a stationary situation in which a steady-state probability current from one well to the adjacent right well is maintained by a source and a sink. The total probability flux (which usually is normalized to one particle) over the barrier is given [9] by the product of the net escape rate from say m-well to $(m+1)$-well, λ_+, and the population of the m-well, n_m. This can be written as

$$j = \lambda_+ n_m. \tag{5.8}$$

From this equation we see that as a result of asymmetry j, which is zero over the original W-shaped potential of no barrier subdivision, could increase until the maximum value is attained at an optimal number of barrier subdivision.

rier heights and for local barrier heights of steeper slope. However, the optimal number of barrier subdivision is determined only by the slope of the local barrier height.

The net escape rate that occurs as a result of asymmetric barrier subdivision gives rise to the nonstationary transport of Brownian particles with a certain velocity. The possible maximum value of velocity was found to be much larger when compared with the corresponding velocity for the motion that takes place for the classic ratchet potential.

Finally, we remark that we have devised a model ratchet potential through the mechanism of asymmetric barrier subdivision in which a random thermal noise could be used to produce a unidirectional motion or in other words to do a useful work. This result gives basic information about how best useful work can be extracted from random thermal background.

References

[1] R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics* (Addison-Wesley, Reading, MA, 1963); Vol. I, chap. 46.

[2] M. O. Magnasco, Phys. Rev. Lett. 71, 1477(1993).

[3] M. O. Magnasco, Phys. Rev. Lett. 72, 2656(1994).

[4] R. D. Astumian and M. Bier, Phys. Rev. Lett. 72, 1766(1994).

[5] T. Hondo and Y. Sawada, Phys. Rev. Lett. 75, 3269(1995).

[6] F. Julicher, A. Ajdari and J. Prost, Rev. Mod. Phys. 69, 1269(1997).

[7] N. Brilliantov and P. Strizhak, Cond-mat/9609246, Nonstationary Transport by Internal White Noise and "Localization" in Ratchets.

[8] H. A. Kramers, Physica 7, 284(1940).

[9] P. Hanggi, P. Talkner and M. Borkovec, Rev. Mod. Phys. 62, 251(1990).

[10] N. G. van Kampen, *Stochastic processes in physics and chemistry* (North-Holland, 1992).

[11] H. C. Brinkman, Physica, 22, 149(1956).

[12] M. Bernstein and L. S. Brown, Phys. Rev. Lett. 52, 1933(1984).

[13] W. Y. Keung, E. Kovacs, and U. P. Sukhatme, Phys. Rev. Lett. 60, 41(1988).

[14] K. Schonhammer, Z. Phys. B78, 63(1990).

[15] Mulugeta Bekele, Ananthakrishna and N. Kumar, Pramana - J. Phys. 46, 403(1996).

[16] Richard W. Robnett, *Quantum Mechanics* (New york, Oxford University Press, 1997)

[17] C. W. Gardiner, *Handbook of Stochastic Methods* (springer-verlag, 1983).