ABSOLUTE NEGATIVE MOBILITY

A Dissertation Submitted in partial fulfillment

FOR THE DEGREE OF MASTER OF SCIENCE IN PHYSICS

Under Academic Autonomy

NATIONAL INSTITUTE OF TECHNOLOGY, ROURKELA

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CERTIFICATE

This is to certify that the thesis entitled, " **Absolute Negative Mobility** " submitted by Miss. Ashoka Padhi in partial requirements for the award of Master of Science Degree at the National Institute of Technology, Rourkela is an authentic work carried out by her under my supervision and guidance. To the best of my knowledge, the matter embodied in the thesis has not been submitted to any other University / Institute for the award of any Degree or Diploma.

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TO

MY PARENTS

ACKNOWLEDGEMENT

This thesis is the account of one year of devoted work in the field of "Statistical Physics" at National Institute of Technology, Rourkela, India, which would not have been possible without the help of many. A few lines are too short to make a complete account of my deep appreciation for my advisor Prof. Biplab Ganguli. I would like to thank him with immense pleasure for his valuable guidance and constant encouragements which I have received during the last year. I acknowledge my sincere regards to all staff's member, Department of Physics, NIT Rourkela for their enthusiasm in promoting the research in Physics and for their kindness and dedication to students. I am also thankful to my lab mates who worked with me since last one year and to my classmates. Last but not the least, I would like to record deep respect to my parents & friends for selflessly extending their ceaseless support.

Ashoka Padhi

ABSTRACT

An investigation for the motion of mesoscopic particles in equilibrium and non-equilibrium systems is presented . In equilibrium systems Fluctuation Dissipation Theorem (FDT) is valid and hence if a small external field is applied to the system the resulting current is proportional to it and is in the same direction as the applied force. However, for systems away from equilibrium FDT does not hold and thus one can have the current in response to a small external field in the opposite direction to the field. This phenomena is known as Absolute Negative Mobility (ANM). We consider two model systems which display ANM. Then we have applied montecarlo simulation to the model for one dimensional Non-Markovian random walk and found the accuracy.

SYNOPSIS

This thesis entitled " ABSOLUTE NEGATIVE MOBILITY" is submitted by Ashoka Padhi to the Department of Physics,National Institute of Technology, Rourkela in partial fulfillment of the requirement of the M.Sc degree.

In the chapter I We discuss the equilibrium and non-equilibrium state. We have seen that in general most of the system are in non-equilibrium state. So to solve the real life physical system we need an analytical method called simulation.

In chapter II we have studied what is montecarlo simulation , by this which type of problem can be solved and how it is helpful in solving real life problems. We also have studied how montecarlo simulation relates to theoretical and experimental data.

In Chapter III the first part illustrates the stochastic process taking example of Brownian motion of a colloidal particle and second part describes the Random walk. In Random walk section we have got an idea about Binomial distribution and random walk in an one dimensional lattice. Then in third part we discuss about negative mobility with the help of two models in non-equilibrium state.

I

In chapter IV the numerical simulations for ANM is done and in chapter V results are discussed by generalizing the problem for different position of large number of random walkers at different time. As a result we found that for higher value of number of trails the curves become smoother. Also we saw that negative mobility is absent for very high value of N. Here we have calculated negative mobility for random walk in one dimension. It can be extended for two and three dimension where the interaction of particle will play a role.

CONTENTS

1. INTRODUCTION

Statistical Mechanics is the branch of physics which deals with the physical properties of system which consists of a large no of particles. In recent years the field of statistical Physics has expanded dramatically. New results in stochastic theory, transport theory, biophysics have revolutionized. Concepts developed in Statistical Physics underlie all of Physics. Once the forces between microscopic particles are determined, Statistical physics gives us a picture how microscopic particles act in the aggregate to form the macroscopic world. The mesoscopic description of system with large degrees of freedom is based on probabilistic concepts. In general System in nature is either in equilibrium or in non-equilibrium state. If a system is isolated, i.e., does not exchange energy or matter with the outside world then it is expected to be in equilibrium, if left by itself. The macroscopic properties of the system may be described in terms of only a few state variables. These variables do not change with time. When a system is perturbed by an external source it goes out of equilibrium. If the perturbation is small, after it is removed the system is expected to revert to equilibrium after a sufficiently long time. On the other hand, if the system is continuously perturbed it remains in a state of non-equilibrium. Normally equilibrium statistical mechanics is focused and as a consequence Thermodynamics is derived. As a result it is difficult to get the experience of traversing the vast world of Thermodynamics and tough to understand how to apply it to systems which are too complicated for Statistical Mechanics. So it is necessary to have an idea in non-equilibrium statistical mechanics. The use of stochastic theory has many applications in chemical physics, laser physics, population physics and biophysics.

The random walker is a basic paradigm in science that has been applied to a wide range of problems in many different fields. In statistical mechanics and the theory of stochastic processes, it has been studied in great detail and provides a technically simple and conceptually transparent discretized version of the Wiener process. When referring to the erratic motion of thermally agitated particles, the latter is also known as Brownian motion. Motion on the average in a direction against a small external force is impossible. In non-equilibrium, however, there is no fundamental principle that forbids absolute negative mobility. In this paper, we move away from a detailed physical model to show how very simple non Markovian modifications of the basic random walk can result in absolute negative mobility.

In order to describe a real life system when other analyses are mathematically too complicated an analytical method is used known as simulation. Monte-Carlo simulation method is a technique that uses random numbers and probability concept to solve problems.

2.MONTECARLO SIMULATION

Monte Carlo methods are a class of computational algorithm that rely on repeated random sampling to compute their results. These methods are often used for simulating physical systems because of their reliance on repeated computation and random or pseudo-random numbers. As mentioned, Monte Carlo simulation methods are especially useful for modeling phenomena with significant uncertain inputs and in studying systems with a large number of coupled degrees of freedom. Here we attempt to follow the time dependence of a model for which change or growth does not proceed in a predefined way but rather in a stochastic manner. That stochastic process depends upon sequence of random numbers which can be generated during simulation. We require simulation, because computer simulation yields exact information with very very less statistical error. The statistical mechanics of even very simple models such as the 3-dimensional Ising Model cannot be solved exactly and we can know less about the models with realistic potential between atomic degrees of freedom. So computer simulations are designed to check the accuracy of some approximation made in analytical models. But different sequence of random numbers the simulation will not give identical results but will yield values which agree with those obtained from the first Sequence to within some statistical error. The task of equilibrium statistical mechanics is to calculate thermal averages of interacting many particles. Unlike in the application of many analytic techniques, the improvement of the accuracy of Montecarlo result is possible not only in principle but also in particle numbers.

The range of different physical phenomena which can be explored by montecarlo methods is extremely broad. Models which naturally discretized can be considered for montecarlo application. The motion of individual atoms may be examined directly. We can take the DLA growth of colloidal particle for montecarlo simulation. Since their masses are orders of magnitude larger than atomic masses,

The motion of colloidal particle in fluids can be described by random Brownian motion. Hence this system is well suited for montecarlo simulation which uses random number to realize random walk.

Let us consider “micelles formation” in lattice models of micro emulsion, in which each surfactant molecule may be modeled by 2-dimers on the lattice. This model allows the study of the size and shape of the aggregates of surfactant molecules. In reality this is a very slow process. So deterministic molecular dynamics simulation (numerical integration of Newton’s second law) is feasible.

In many cases theoretical treatments are available for models for which there is no perfect physical realization. In this case the only possible test for an approximate theoretical solution is tom compare with data generated from a computer simulation. One more advantage of simulation is that different physical effect which are simultaneously present in real system may be isolated and by separate consideration through simulation e can get better idea about them.

Example: - The phase behavior of Polymers. In which there is subtle interplay between complicated enthalpy contribution and entropic effects. Real system are difficult to understand due to the asymmetries between the constituents of mixtures of system (shape and size , degree of polymerization , exibility). Simulation helps in the case to determine the particular consequence of each contributing factor.

3.STOCHASTIC PROCESS

When the outcome of phenomena varies randomly over various possible outcomes the activity is said to be stochastic. Stochastic process or sometimes random process is the counterpart of the deterministic process in probability theory. Instead of dealing with only one possible reality of how the process might evolve under time in a stochastic random process, there is some indeterminacy in its future evolution, i.e. if the initial condition is known then there are many possibilities the process might go to, but some paths are more probable and some are less. Realizations of stochastic process require some knowledge of random numbers and their generation. In simple case a stochastic process amounts to a sequence of random variable known as time series (Markov chain).Another basic type of a stochastic process is a random field, whose domain is a region of space, in other words, a random function whose arguments are drawn from a range of continuously changing values. Although the random values of a stochastic process at different time may be independent random variables, in most commonly considered situation they show complicated statistical correlation. The equation which governs the stochastic dynamics of Markov process is the Master's equation. It is one of the most important equation in Statistical Physics because of its almost universal applicability. It has been applied to solve problems in Chemistry, Laser Physics, Biophysics, Population dynamics. Examples such as Brownian motion and Random walk are included under this process.

a. BROWNIAN MOTION

Brownian motion provides one of the most spectacular evidence on the macroscopic scale of the atomic nature of the matter causing fluctuations which in turn causes observable effect on the Brownian particle._

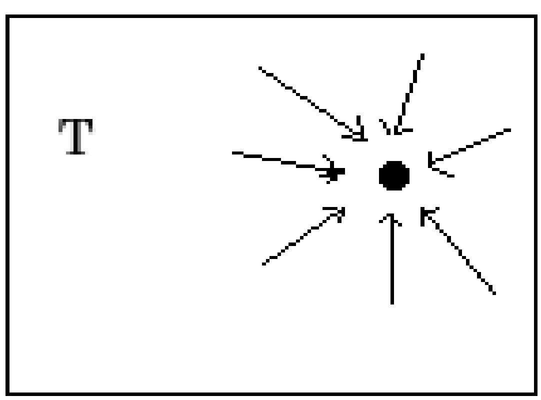

Figure 1: Schematic picture of a Brownian particle inside a fluid at temperature T.

We can define it as random movement of particles suspended in liquid or gases. It can also be called as the random motion of the colloidal particle in a zigzag path. Ex: Stoke market fluctuation. This effect can be clearly observed by the following experiment. Let a mesoscopic particle (e.g., a colloidal particle) be immersed in a fluid of the same density as that of the particle at temperature. When it is viewed under microscope, the particle appears to be in a state of agitation undergoing rapid and random change in velocity. This phenomenon was first observed by Robert Brown. According to his name the motion of the particle in a zigzag path is known as Brownian motion. Now let us consider the motion of a Brownian particle inside the fluid. It is assumed that particle is free to move inside the fluid. The particle experiences two forces, 1. Random kicks by molecules or atoms of the fluid and, 2. Viscous force in the opposite direction to the velocity and proportional to its magnitude. The equation of motion of the particle in the absence of any other applied force may be written the following Langevin equations,

$$\boxed{m\frac{dv(t)}{dt} = -\gamma v_x(t) + \xi_x(t)} \tag{1a}$$

$$\frac{dx(t)}{dt} = v_x(t) \tag{1b}$$

Here,

m = mass of the particle

$v_x(t)$ = velocity of the particle in the x-direction.

x (t) = position of the particle

γ = coefficient of viscosity of the fluid

ξ (t) = Gaussian white noise

Here it is assumed that ξ (t) has zero mean

$$\xi(t)_{\xi} = 0 \qquad (2a)$$

The assumption that the noise is white means the noise is delta correlated.

$$\langle \xi(t_1)\xi(t_2)\rangle_{\xi} = \Gamma\delta(t_2 - t_1)_{\ \xi} \qquad (2b)$$

Where, Γ = strength of the noise.

Similar equations hold for the motion in the y and z directions. Let the initial condition for the motion of the particle be:

$$v = v_0 \quad \text{and} \quad x = x_0 \quad \text{at } t = 0 \qquad (3)$$

Then solving (1) with the above initial conditions, we get,

$$v(t) = v_0 e^{(\frac{\gamma}{m})t} + \frac{1}{m}\int_0^t ds e^{-\frac{\gamma}{m}(t-s)}\xi(s) \qquad (4)$$

Taking average of both sides of equation (4) we see that,

$$\langle v(t)\rangle \approx v_0 e^{-(\frac{\gamma}{m})t}$$

as one would expect from Stoke's law. The two point velocity correlation is,

$$\langle v_x(t_2)v_x(t_1)\rangle_{\xi} = (v_0)^2 - \frac{\Gamma}{2m\gamma}e^{-\frac{\gamma}{m}(t_2+t_1)} + \frac{\Gamma}{2m\gamma}e^{\frac{\gamma}{m}(t_2+t_1)} \qquad (5)$$

For t_1, $t_2 \rightarrow \infty$ with $t_1 - t_2$= fixed, the two point velocity correlation becomes a stationary function:

$$\langle\langle v_x(t_2)v_x(t_1)\rangle\rangle_\xi = \frac{\Gamma}{2m\gamma}e^{-\frac{\gamma}{m}(t_2-t_1)} \qquad (6)$$

Further , if $t_1 = t_2$, mean square velocity at any instant is given by,

$$\langle v_x^2\rangle = \frac{\Gamma}{2m\gamma} \qquad (7)$$

From this we can say that the mean square velocity is independent of the initial velocity. If we demand that the particle should be equilibrating with the fluid as $t \rightarrow \infty$, i.e. it will have Maxwellian distribution, then equipartition theorem holds good and kinetic energy of each degree of freedom is equal to $\frac{1}{2}K_BT$, i.e.

$$\frac{1}{2}m\langle v_x^2\rangle = \frac{1}{2}K_BT \qquad (8)$$

Where, k_B =Boltzmann constant

T=temperature in Kelvin.

From eqns. (7) and (8) we get,

$$\frac{\Gamma}{\gamma} = 2k_BT \qquad (9)$$

This is known as the Fluctuation Dissipation Theorem (FDT).Now, let us consider the position of the Brownian particle, with initial condition (3) after some time t the position of the particle is obtained by integrating eqn (4),

$$x(t) = x_0\,\frac{m}{\gamma}(1-e^{-(\frac{\gamma}{m})t})v_0 + \frac{1}{\gamma}\int_0^t ds(1-e^{-\frac{\gamma}{m}(t-s)})\xi(s) \qquad (10)$$

Mean square displacement is,

$$\langle (x(t) - x_0)^2 \rangle = \frac{m^2}{\gamma^2}(v_0^2 - \frac{\Gamma}{2m\gamma})(1 - e^{-\frac{\gamma}{m}t})^2 \frac{\Gamma}{\gamma^2}[t - \frac{m}{\gamma}(1 - e^{-\frac{\gamma}{m}t})] \qquad (11)$$

For t → ∞, mean square displacement becomes;

$$\langle\langle (x(t) - x_0)^2 \rangle\rangle = 2\frac{K_B T}{\gamma} t \qquad (12)$$

The coefficient of time on R.H.S is known as Diffusion Coefficient D

$$D = \frac{K_B T}{\gamma}$$

We note that the position of the particle does not necessarily attain equilibrium although the velocity has.

b. RAMDOM WALK

Random walk can be stated as a simplified Brownian motion , Or simply it is an application of Binomial distribution.

BINOMIAL DISTRIBUTION

One common application of probability theory is the case of large number N of independent experiments, each have two possible outcomes. The probability distribution for one of the outcome is called Binomial Distribution.

Now let us consider a sequence of N statistically independent trials and assume that each trial can have only one of two outcomes, 0 or +1. Let us denote the probability of outcome, 0, by q and the probability of outcome, +1, by p so that p+q=1. In a given sequence of N trials, the outcome, 0, can occur no times and the outcome, +1 times, is

$$P_N(n_1) = \frac{N!}{n_0!n_1!} q^{n_0} p^{n_1}$$

Since a combination of n_0 outcomes, 0, and n_1, contains ($N!/n_0!n_1!$) permutations. The above equation is called the Binomial distribution.

RANDOM WALK IN ONE DIMENSIONAL LATTICE

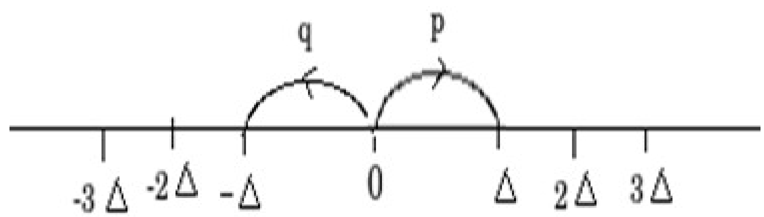

Figure 2: A random walker on a one dimensional lattice. The forward and backward steps occur with probabilities p and q respectively.

This type of random walk is simple so that we can use the concept of Binomial random walk to compute the probability that the walker will reach any other part of the lattice.. Let us consider a particle moving stochastically on a one dimensional lattice (fig.2). It has the probability p of taking a step of length Δ towards right and probability q of a step towards left respectively. Time evolution is discrete and takes place at every τ unit.

Now the position of the particle x(t) may be written as a discrete Langevin equation,

$$x(t+\tau) = x(t) + \varepsilon(t) \tag{13}$$

Here ε(t) is the noise term with prob (ε = +Δ) = p, prob (ε = −Δ) = q.

Continuous limit of eqn (13) is

$$\frac{dx}{dt} = \eta(t) \tag{14}$$

Now the probability of particle at position at x at time t may be written as the following Master's equation, i.e. ,

$$P(x,t) = pP(x-\Delta, t-\tau) + qP(x+\Delta, t-\tau) \tag{15}$$

This equation for evolution of probability defines a Markov process, i.e. the probability at any given time depends only on the probabilities at the previous time. The first term on R.H.S denotes that in the previous time step the particle was at x−Δ and taking a forward step it reaches x. The second term says that at previous time the particle was at x + Δ and by taking a negative step it comes to x at time t.

Now let us consider the continuum limit of eqn(15) i.e. expanding eqn(15) in Taylor series and taking the limit Δ → 0, τ → 0 , $\frac{\Delta^2}{\tau}$ = finite

We get,

$$\frac{dp(x,t)}{dt} = D\frac{\partial^2 p}{\partial^2 x} - v\frac{\partial p}{\partial x} \tag{16}$$

Where $D = (p+q)\frac{\Delta^2}{\tau}$ and $v = (p-q)\frac{\Delta}{\tau}$

This equation is called the drift-diffusion equation and for v = 0 it is known as Fick's law.

Let us now solve eqn(15) for the initial condition P(x, 0) = δ(x) i.e. the particle starts at x = 0, at t = 0.

The characteristics function of P(x,t) is defined as

$$f(k,t) = \int_{-\infty}^{\infty} dx e^{ikx} P(x,t) \tag{17}$$

$$P(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk f(k,t) e^{-ikx} \tag{18}$$

Using P(x, t) in eq.(16) we get,

$$\frac{df(k,t)}{dt} = -Dk^2 f(k,t) + ikvf(k,t) \tag{19}$$

Which has the solution

$$f(k,t) = f(k,0)e^{(-Dk^2+ikv)t} \tag{20}$$

f (k, 0) may be found from the initial condition P(x, 0). i.e.

$$f(k,0) = \int dx e^{ikx} P(x,0) = 1 \tag{21}$$

The probability of finding the particle at position x, at time t is

$$P(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{-ikx} e^{-Dk^2 t + ikvt} = \frac{1}{\sqrt{4\pi Dt}} e^{\frac{-(x-vt)^2}{4Dt}} \qquad (22)$$

The 1st moment, i.e. the mean displacement at time t is given by

$$\langle x(t)\rangle = \int_{-\infty}^{\infty} dx x P(x,t) = vt \qquad (23)$$

The second moment is $\langle x^2 \rangle = \int_{-\infty}^{\infty} dx x^2 P(x,t)$ and the mean square displacement is,

$$\langle x^2 \rangle - \langle x \rangle^2 = 2dt \qquad (24)$$

Hence the mean square displacement is proportional to time t as in the case of Brownian motion (eqn. 12).

In fig (3), it has plotted P(x, t) vs. x at different times,

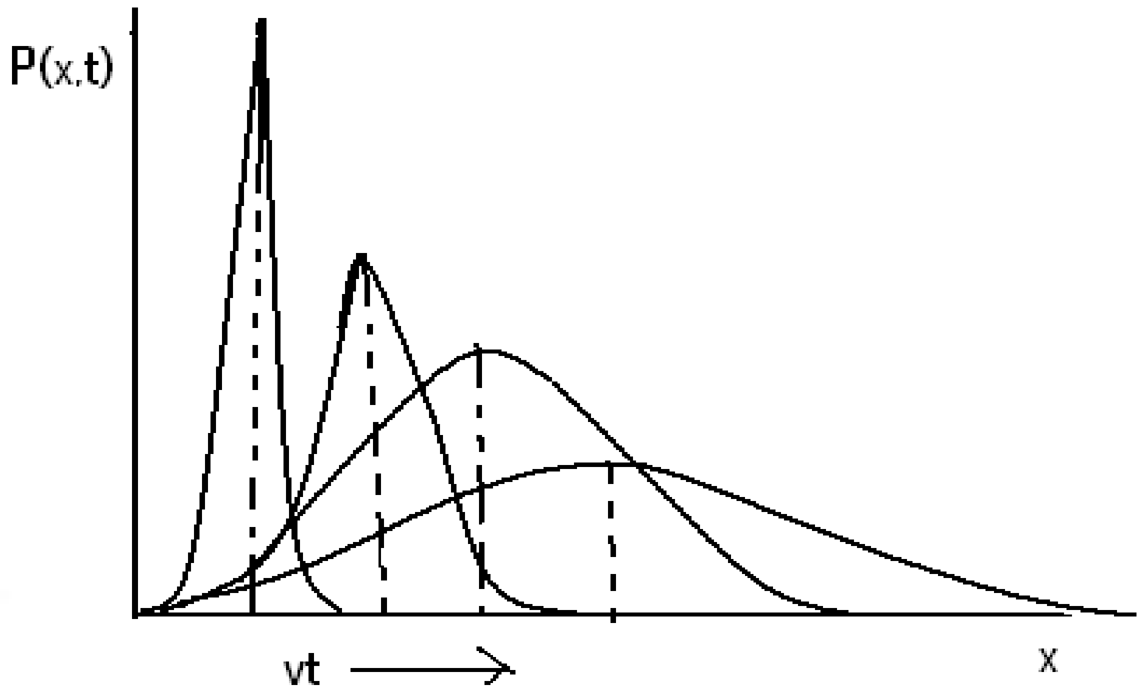

Figure 3: Time evolution of P(x,t). The Gaussian distribution drifts in the positive direction with speed v and spreads as $\sigma(t) \approx \sqrt{2Dt}$

Initially for t = 0, the probability is a delta function. As time goes on the probability distribution P(x, t) spreads and the mean position drifts towards the right with speed v which is proportional to the bias (p − q).

We have made a program in FORTRAN for one-dimensional random walk and executed successfully. Then we plotted a graph taking the outputs. The graph has come as below.

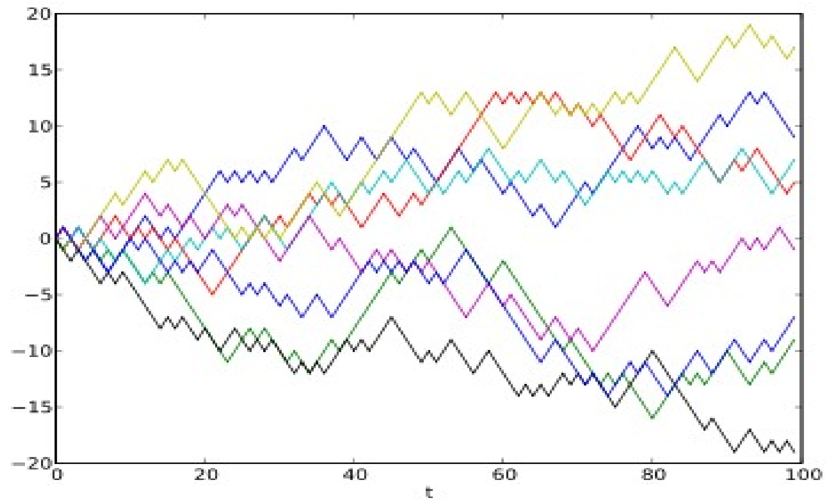

Figure 4: Random walk in one dimension taking different random number generator.

But random walk can have different property in 3-dimension than in one or two dimension.

C. ABSOLUTE NEGATIVE MOBILITY (ANM)

The velocity or current in an equilibrium system is always in the same direction as that of the applied force. This is the consequence of the Fluctuation Dissipation Theorem. As we found in the previous sections for Brownian motion as well as for the random walk, the velocity is in the same direction as that of the bias (p − q) and proportional to it, i.e.,

$$v \propto (p - q) \tag{25}$$

But if the system is driven away from equilibrium FDT does not remain valid and there is a possibility that one has absolute negative mobility (ANM), i.e. the velocity or current in response to the applied force is in the opposite direction to the force. In this section we consider three such models of non-equilibrium systems where absolute negative mobility is observed. Also we have discussed montecarlo simulation for the 1st model and found its validity.

1. NON-MARKOVIAN RANDOM WALK

Let us consider the random walk model introduced in section (3). Now let us introduce an additional condition which makes the model NonMarkovian. We put the constraint that the maximum number of consecutive steps along the same direction taken by the particle is $N - 1$. Hence whenever the particle hops in the same direction for N successive steps, this excursion is cancelled, i.e., the particle is transferred back to its original position N steps before.

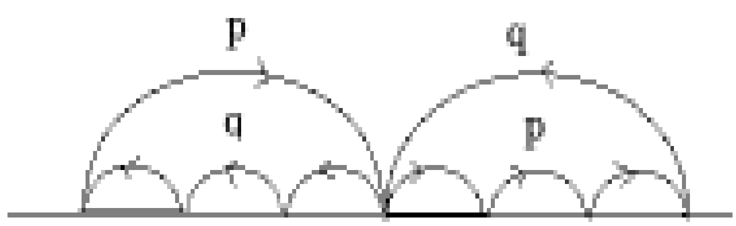

Figure 5: Non-Markovian modification of the random walk in one dimension. The walker is allowed a maximum of $N - 1 = 2$ steps consecutively in either direction.

This can be understood by the following example. A banker offers an investment which, on an average, yields a positive yearly return. The probability for a positive return in a given year is p and the probability of a negative return is q with $p > q$. A nervous investor wants more protection against losses. The banker proposes to cancel the N successive looses. But he argues that in all fairness, he then also has to cancel N successive gains as well. The capital of the investor now undergoes the above described random walk with the paradoxical result that the investment will have on an average a negative return for N =3 and 4.Let us consider a discrete random walk of a particle taking steps of size one to the left or to the right with probabilities *p* and *q* respectively. On average, the particle will acquire a drift velocity equal to 2*p*-1. A well known non-Markovian modification is the so-called random walk with persistence, in which the step directions taken by the walker are correlated with previous ones. In the random walk modification presented here, it is the step sizes that are correlated, rather than their direction. The rule is the following. A particle performs the above described biased random walk. We introduce a new parameter, denoted by *N*-1, which gives the maximal allowed number of consecutive steps in the same direction. Hence, whenever the particle hops in the same direction for *N* successive time steps, this excursion is cancelled, i.e., the particle is transferred back to the original position of *N* steps ago, and its memory is cleared. Our main purpose now is to study how this limitation of large excursions impacts the resulting drift velocity. To do so, we note that the state of the particle is fully described by the knowledge of its position *x*, together with the length *l* of the last sequence of successive steps in the same direction. Let P(x, l, t) denote the probability of the particle being at x at time t with l previous steps in the same direction. Then P(x, l, t) obey the following master equations,

$$P(x, N, t) = pP(x + N - 1, N - 1, t - 1) \quad \textbf{(26a)}$$

$$P(x, j, t) = pP(x - 1, j - 1, t - 1) \quad \textbf{(26b)}$$

$$P(x, 1, t) = pP(x - 1, N, t - 1) + p \sum_{m=-1}^{-N} P(x - 1, m, t - 1) \quad \textbf{(26c)}$$

A similar set of equations can be written for P(x,-l, t) where p is replaced by q. They are,

$$P(x,-N,t) = qP(x-N+1,-N+1,t-1) \quad (27a)$$

$$P(x,-j,t) = qP(x+1,-j+1,t-1) \quad (27b)$$

$$P(x,-1,t) = qP(x-1,-N,t-1) + q\sum_{m=1}^{N} P(x+1,m,t-1) \quad (27c)$$

The particle starts at the origin x = 0at t = 0 and hence the initial conditions for P(x, l, 0) are,

$$P(x,l,0) = (1/2)\delta_{x,0}\delta_{l,\pm N}$$

Now we consider the characteristic function which is the Fourier transform of

$$P(x,t) = \sum_{l=\pm 1}^{\pm N} P(x,l,m),$$

$$F(k,z) = \sum_{x=-\infty}^{\infty} e^{ikx} \sum_{t=0}^{\infty} z^t P(x,t) \quad (28)$$

From eq. (27) and eq.(28) we find that

$$F(k,z) = \frac{1}{f(p,k) + f(1-p,-k) - 1} \quad (29)$$

Where,

$$f(k,z) = (1 - zpe^{ik}) \frac{1-(zp)^N}{(1-zpe^{ik})} \quad (30)$$

From (26) we may obtain various moments of P(x,t) through F (k,z), e.g.,

$$\frac{\partial F}{\partial (ik)}]k = 0 = \sum \langle x(t) \rangle z^t \quad (31)$$

Thus, $\langle x(t) \rangle$ is the coefficient of z^t in the expansion of $\frac{\partial F}{\partial(ik)}]k = 0$, the average speed is,

$$v = \lim_{t\to\infty} \frac{\langle x(t)\rangle}{t} = 2p - 1 + \frac{N(1-p)^N p}{1-(1-p)^N} - \frac{N-(1-p)p^N}{1-p^N} \qquad (32)$$

We have plotted v as a function of p in (fig.8). We see that ANM is observed for N = 3,4 for |p − q| << 1. For large bias (p − q) → 1 positive mobility is observed.

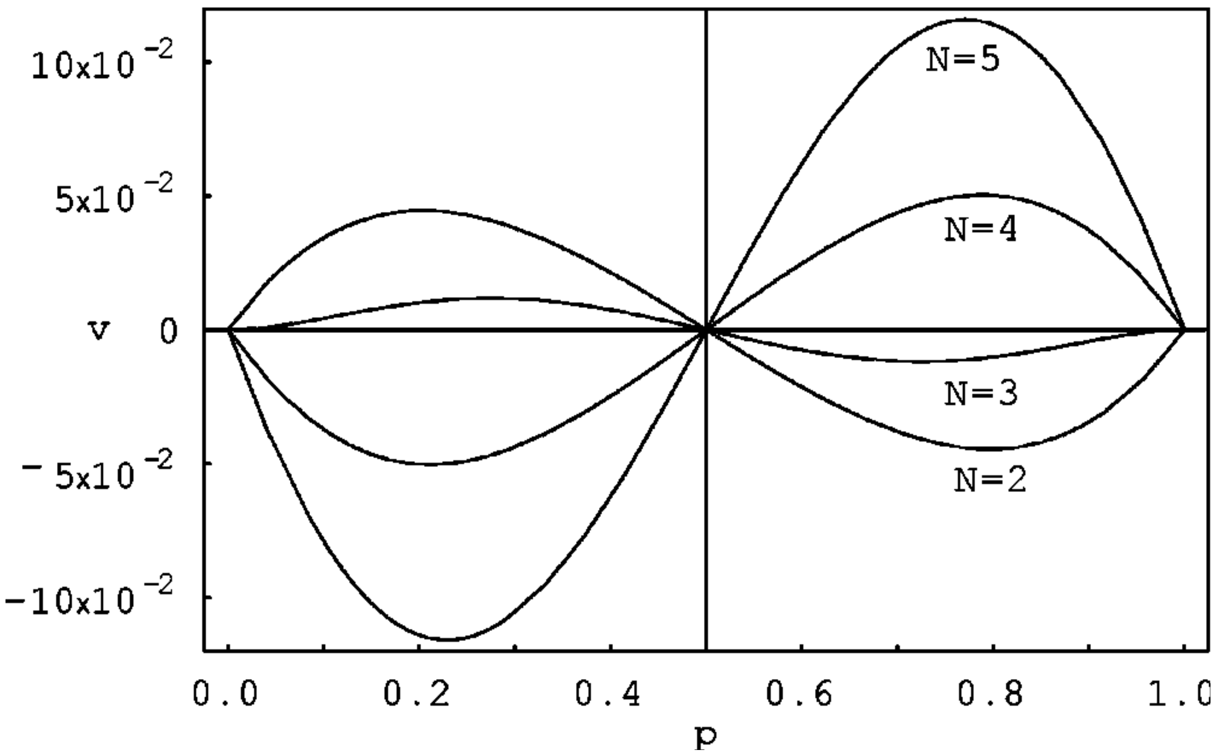

Figure 6: the average speed v of the random walker as a function of p for different values of N

2. ANM in an oscillatory non-equilibrium state

Let us take a container having a geometry as in fig(6). The walls of the container are parallel and it has periodically spaced barriers inside it which are of length greater than half the separation between the walls. The inside is filled with a fluid at temperature T and we consider an over damped Brownian particle moving inside. The equations of motion of this Brownian particle may be written as;

$$\gamma \dot{x}(t) = -\partial_x V[x(t), y(t)] + \xi_x(t) \quad (33)$$

$$\gamma \dot{y}(t) = -\partial_y V[x(t), y(t)] + \xi_y(t) + F(t) \quad (34)$$

Where γ is the coefficient of viscosity of the fluid, V(x,y) = hard wall potential and ξ's are the thermal white noise terms. F(t) is the external applied force in the vertical direction.

Now if we apply an oscillating field F(t)=A(t) , in the positive half cycle the particle moves up and eventually gets trapped in one of the left side corners. Similarly the particle gets trapped in one of the right side barriers in the negative half cycle of A(t). Hence the average velocity over a full period of A(t) is zero. Now we apply a constant field F in addition to the oscillating field A0. Hence the total force is given by,

$$F(t) = A(t) + F$$

For the positive half cycle the total field is $F+A_O$ and for negative half cycle the total field is $F - A_0$ (i.e. the particle sees a force $F - A_0$ in the downward direction.

For the positive half cycle, the field is stronger than that in the negative half cycle. For positive half cycle the velocity of the particle is more and hence the flight time to reach successive barriers is small and hence escape probability in the positive cycle is less. But for the negative half cycle the field strength decreases and the velocity of the particle is less and its flight time to reach a barrier is more. Hence the escape probabilities are more in the negative half cycle. The escape probability is sketched in fig 8.

Probability of avoiding the trap in the positive half cycle is,

$$P(F + A_O) = \frac{1}{2} - \frac{1}{2} erf\left(\frac{2b - B}{\sqrt{2k_B T}}\right)\sqrt{F + A_O} \quad \textbf{(35)}$$

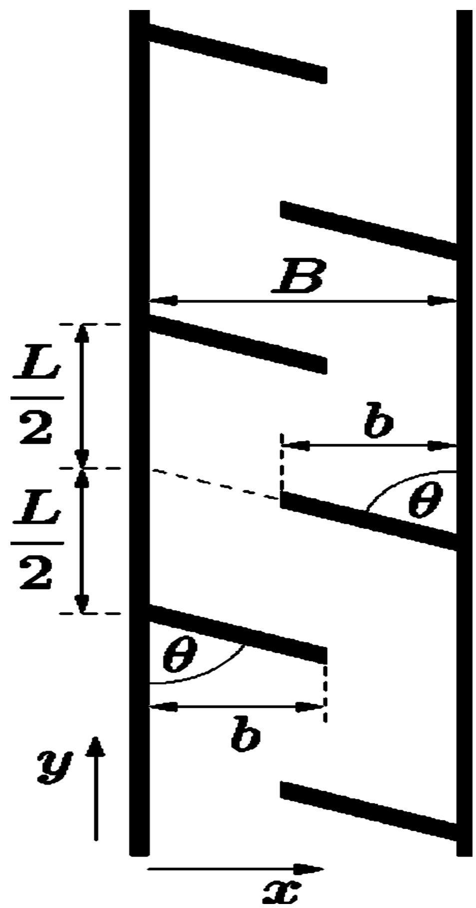

Figure 7: ANM in oscillatory nonequilibrium state

Where,

$$erf(x) = 2\pi^{-\frac{1}{2}} \int_0^x du e^{-u^2} \quad \textbf{(36)}$$

The probability of avoiding the trap for negative half cycle is,

$$P(F - A_0) = \frac{1}{2} - \frac{1}{2} erf(\frac{2b - B}{\sqrt{2k_B T}})\sqrt{F - A_O} \quad \textbf{(37)}$$

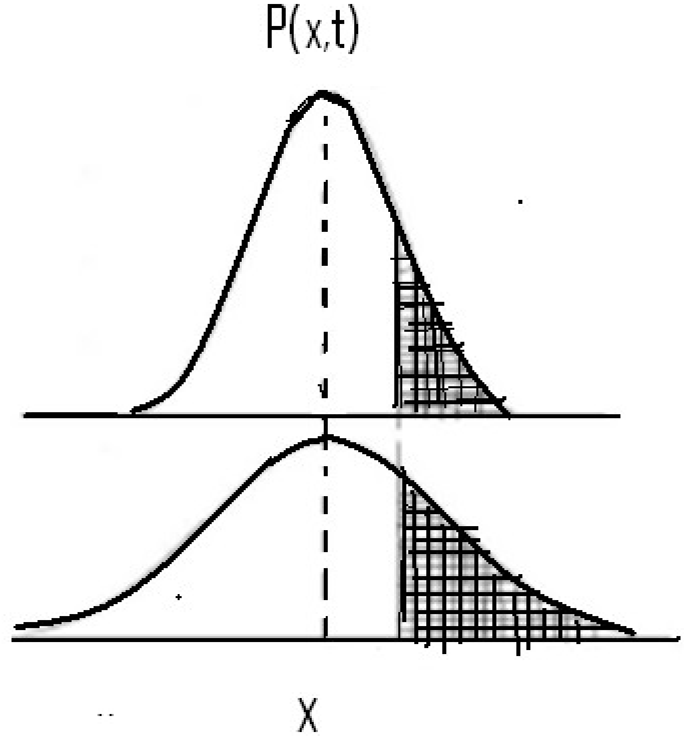

Figure 8: Probability densities when the particle reaches the trapping barrier in the positive half cycle (upper figure) and the negative cycle (lower figure). The shaded regions represent the escape probabilities in either cycle.

The net current is given by,

$$J = \rho[v_+ P(F_+) - v \ P(F_-)]$$

Where

ρ = density of particle

v_+= velocity of the particle in positive half cycle

v_-= velocity of the particle in negative half cycle

$P(F_+)$ = escape probability for positive half cycle

$P(F_-)$ = escape probability for negative half cycle

$$F_+ = F + A_O\,,\ F_- = F - A_O$$

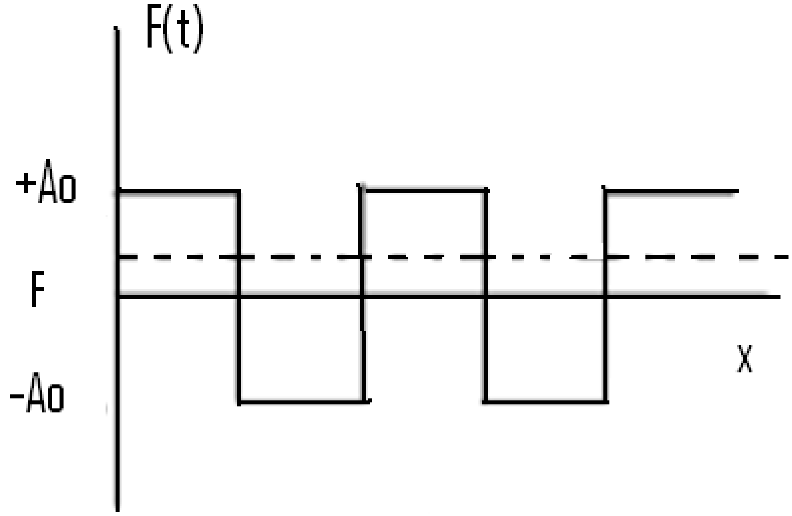

Figure 9: The oscillating field A (t) is a square wave while F is the constant applied field.

$$V_{\pm} = \frac{1}{\gamma} F_{\pm}$$

Where $1/\gamma = \mu$ = mobility

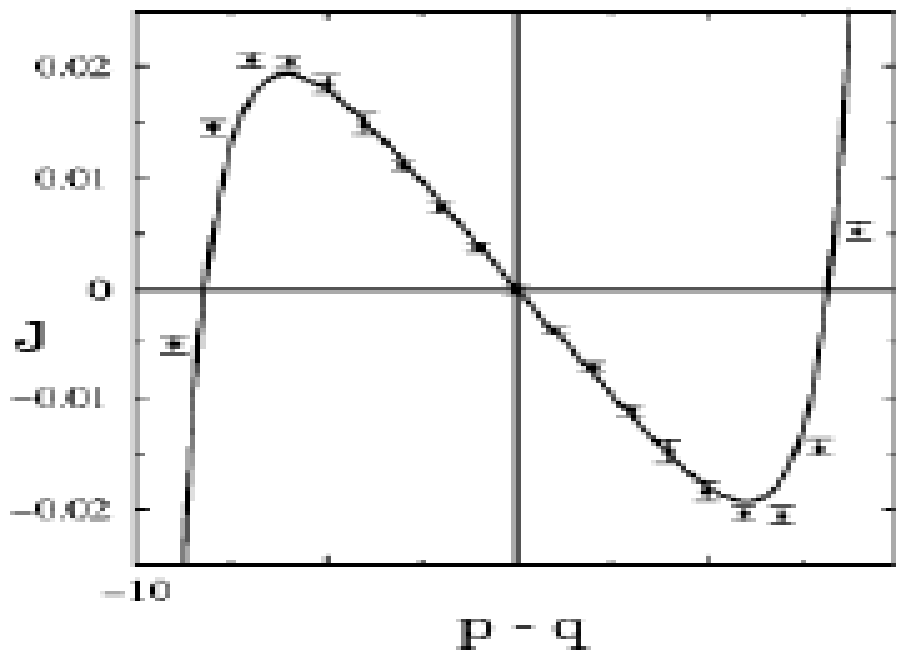

Figure 10: The time average current J eq.(41) as a function of the average force F. For small F we obtain ANM

In fig.10, we plot J vs F. We observe ANM of small values of F ($|F| << A_0$) For large value of $F >> A_0$ there is no negative half cycle and hence current is in the same direction as F.

4. RESULT & DISCUSSION

First of all we have plotted a graph for simple random walk in one-dimension. Then plotting a graph between the average of position of different walker with different time interval we will have a graph like fig:11. Here we have taken we have taken the average random walk of 100, 1000, 10000 walkers at different time as input choosing iseed (random number generator) as 12345.Then extending that for the average of the position square with respect to different time.

We found graphs like fig: 12. From those graph we can conclude that as the no of trails increases the rate of fluctuation decreases and the curves become smoother.

Here
avgrw u 1:2 curve is for dimension=100
avgrw1 u 1:2 curve is for dimension=1000
avgrw 2 u 1:2 curve is for dimension=10000

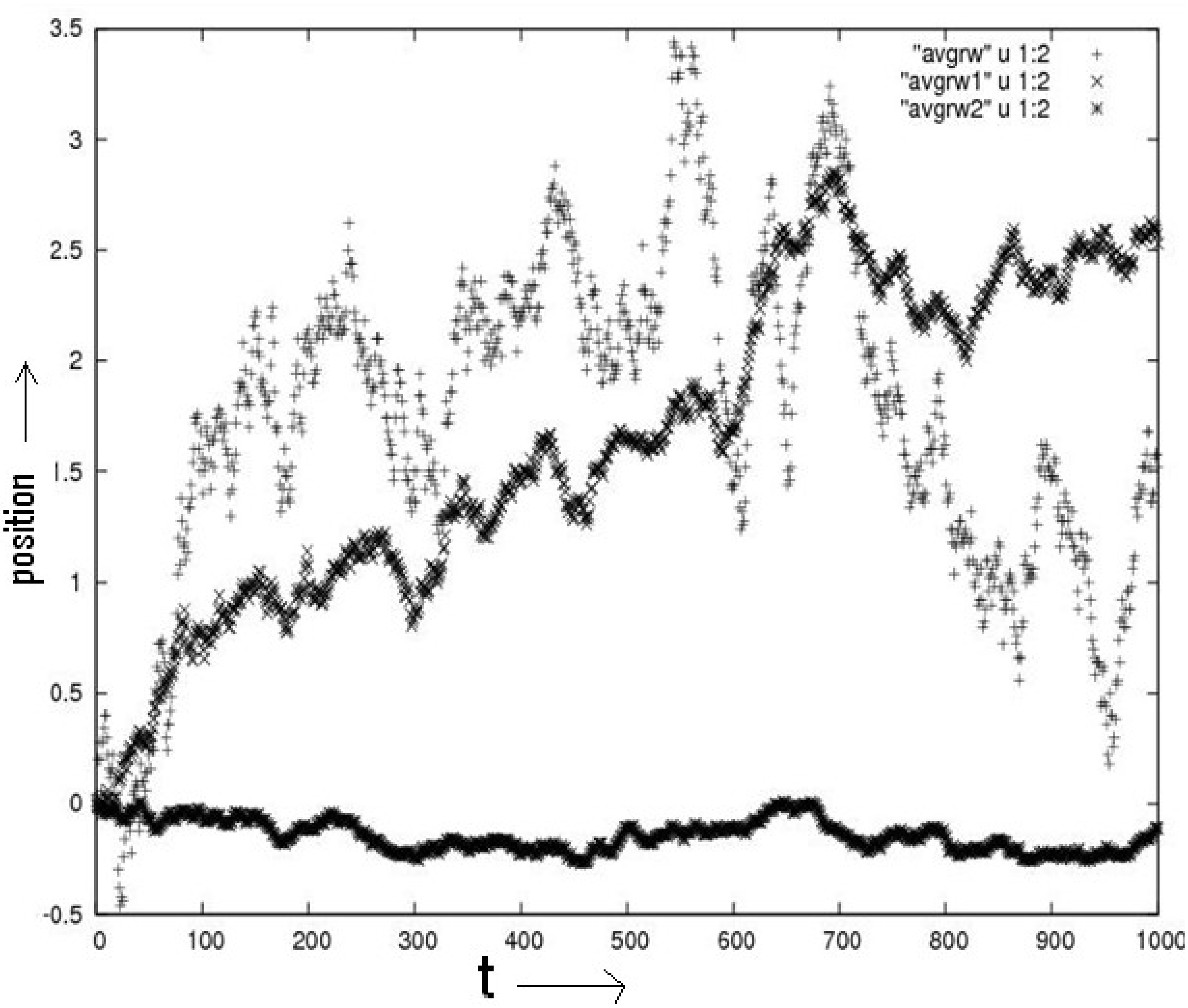

Figure 11: average of random walk of different walkers at different time.

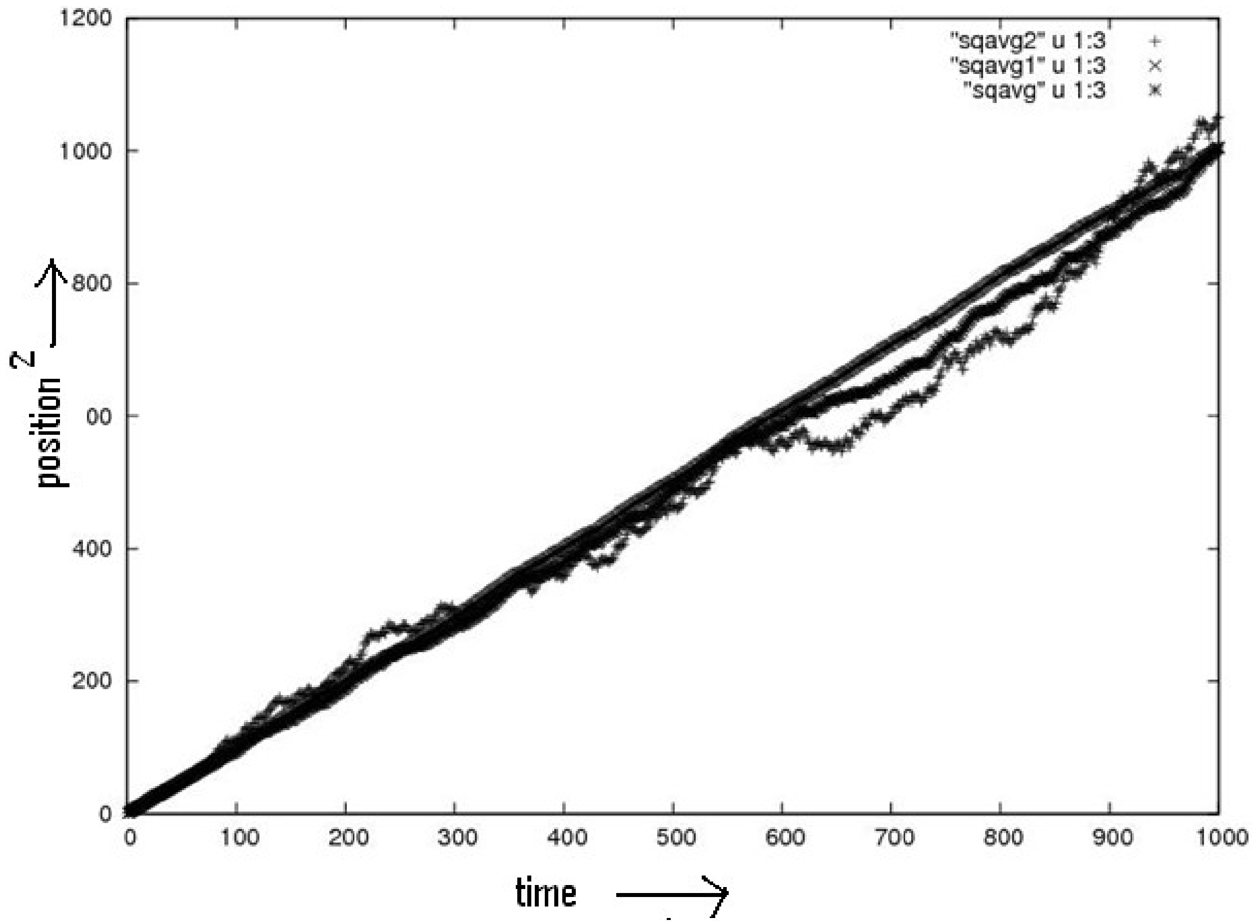

Figure 12: Average of square of position of different random walker with respect to different time

Here

sqavg2 u 1:3 curve is for N=100

Sqavg u 1:3 curve is for N=1000

Sqavg1 u 1:3 curve is for N=10000

2. For biased random walk i.e. When some constraints are given to the random walker, we have plotted a graph between the position of 100, 1000 and 10000 random walkers (i.e. N=100, 1000, 10000) with respect to different time. We have applied the condition that probability of taking positive step is greater than probability of taking negative step. i.e. $(p > q)$. $p = 0.6$, $q = 0.4$. Here we have used iseed=1234 and have the plot like fig: 13.

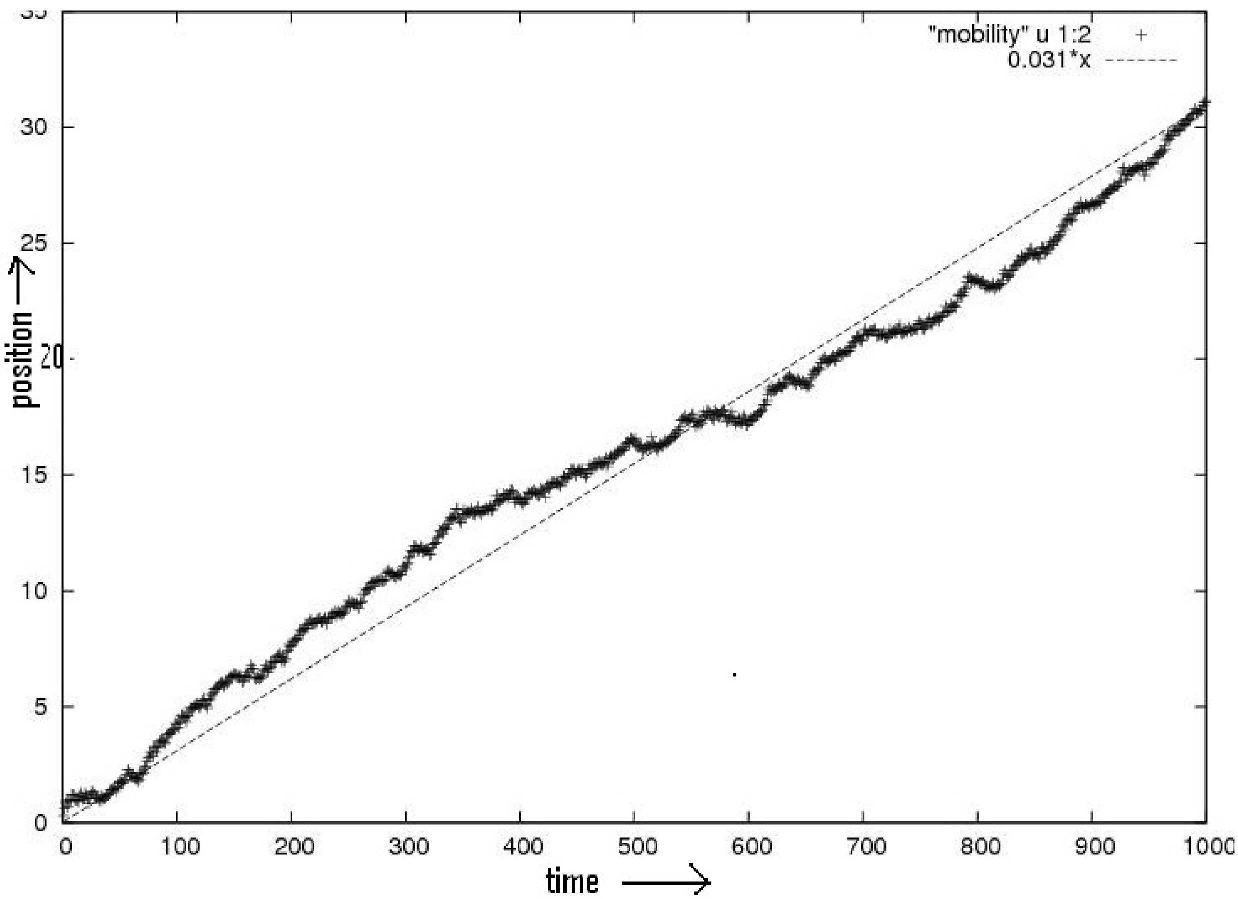

Figure 13: Average random walk for biased case

3. In Non-Markovian Random walk we have taken p=0.6 and q=1-p=0.4. Then added a new parameter N-1 to make the system non-equilibrium. Iseed used= 1234. Value of N=3 for fig: 14, and value of N= 6 for fig: 15. Plotting graph of position of 1000 random walker with respect to different time we got a figure like below. We have got negative mobility for N=2, 3, 4. But for very large value of N we have positive mobility.

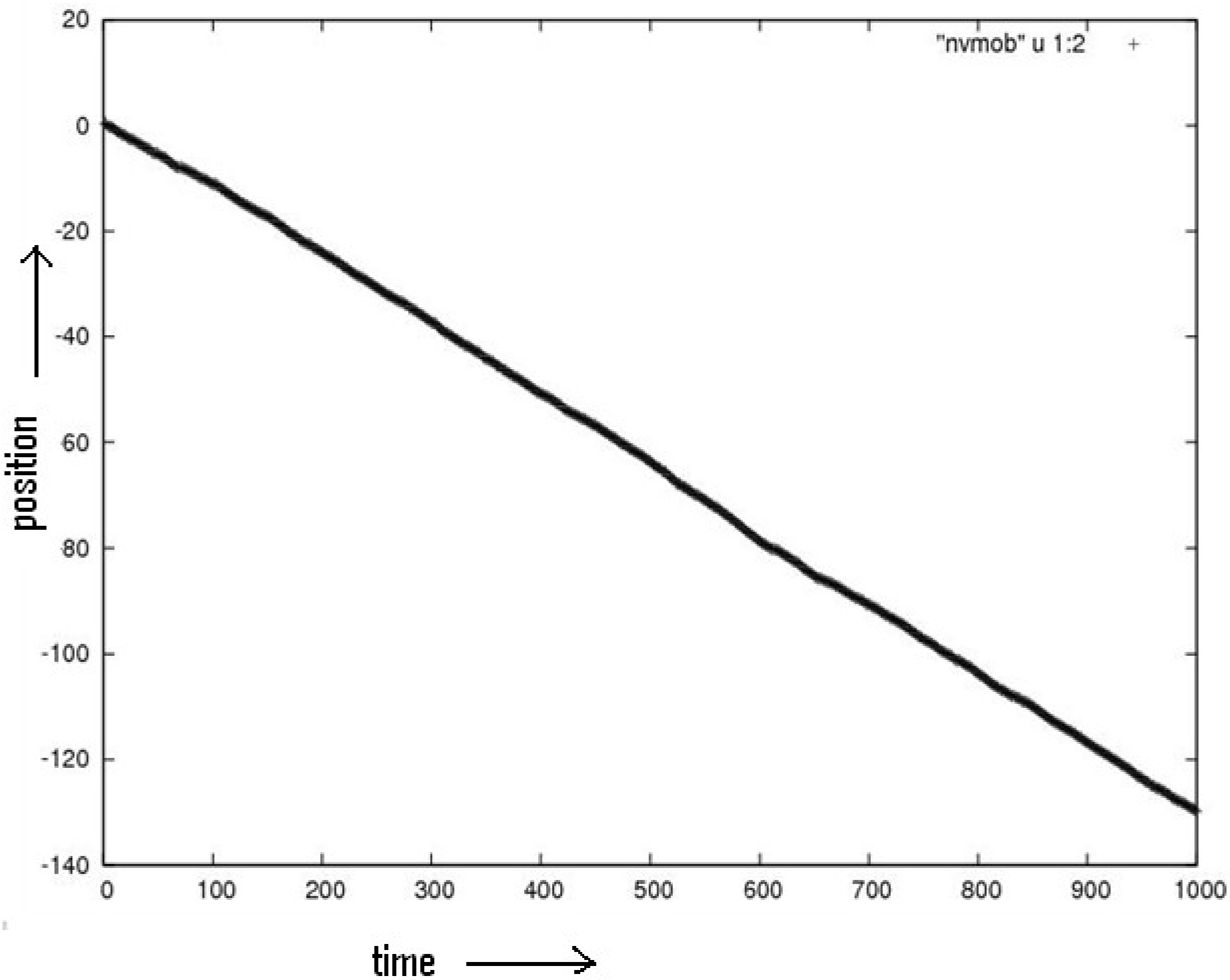

Figure 14: Negative mobility for N=3

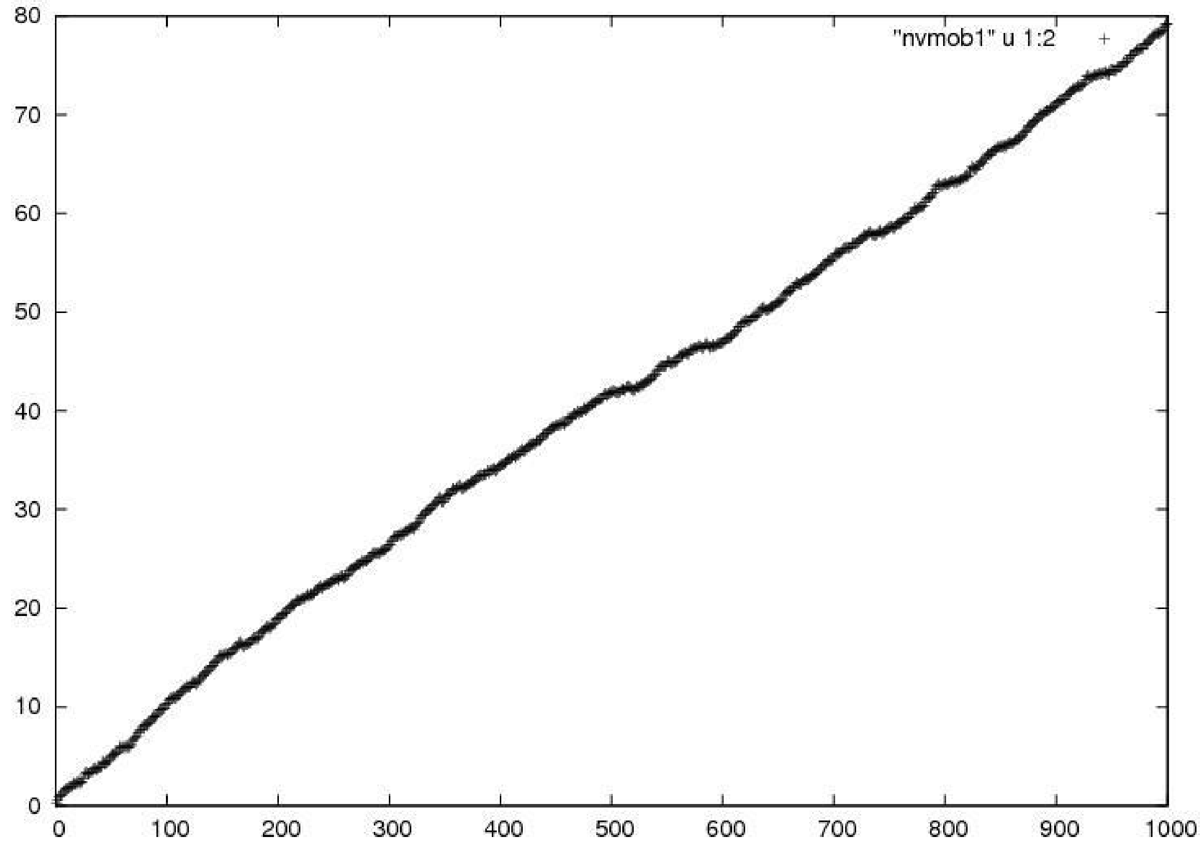

Figure 15: for large value of N we'll get positive mobility. Here N=6

5. CONCLUSION

We close with a discussion of the distinctive features of walks with negative mobility and a broad overview of related results. First, such walkers are reservoirs of energy that become available *upon request*. Rather than dissipating energy supplied by an external force, the walker, which moves in a direction opposite to the force, actually performs work. Second, whereas usual walkers get trapped in the minima of an external potential, the ones with negative mobility move towards the maxima. The roles of stability and instability are thus interchanged.

In this paper, also we have discussed that a single, classical Brownian particle in a periodic, symmetric, two-dimensional potential landscape can exhibit the paradoxical phenomenon of absolute negative mobility under suitable far from non-equilibrium conditions.

Fluctuation Dissipation Theorem (FDT) holds good in equilibrium states. FDT implies that response to small external field is in the same direction as the field. For system driven away from equilibrium FDT does not remain valid and the response to an external field may be in the opposite direction to the field. This is known as absolute negative mobility (ANM). We studied three examples of non-equilibrium systems which display ANM. The first one is a random walker with Non-Markovian dynamics, the second one is a Brownian particle moving in an oscillating non-equilibrium state.. In all these system ANM is observed for small applied fields and for large fields normal positive mobility results.

We have studied all these effects by taking consideration of single Brownian particle or a number of noninteracting particles. It would be interesting to study collective effects in these systems when interactions between particles cannot be ignored.

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