International Journal of advancement in electronics and computer engineering (IJAECE)
Volume 3, Issue 3, June 2014, pp.310-312, ***ISSN 2278 -1412***

Monte-Carlo Simulation of Biased Random Walk: A Comparison of One and Three Dimensional Motion

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Abstract *– We have simulated the random walk in one dimensional and three dimensional lattices by applying suitable external biases. A suitable analytical formula for integrating bias with random walk is formulated. Different regime of transport called diffusion and drift regime are identified. By analyzing the mean square difference with time we have identified a time called transition time, where the nature of motion changes from diffusion like to drift like. The biases are scanned in the sale of 0 to 1 and analyzed the variation of transition time with magnitude of bias. It is shown that the effect of bias is more prominent in case of one dimension. This is explained with the help of dependent of random walk properties on the angle between external bias and direction of random walk. This type of study is helpful for the analysis of various systems like semiconductors, plasma, random laser etc.*

I. Introduction

Random walk approach is considered in a variety of field to analyze the collective nature of particles in a large system [1]. Monte-Carlo Simulation is the work horse of such problems, which depends on the generation of pseudo-random number according to a particular probability distribution [2]. In contrast to the pure random walk, electrons in plasma, or in a conductor, tend to move in a direction decided by the externally applied field [3]. Depending upon the magnitude of external field, their motion is expressed as biased random walk. Moreover, the nature of their motion dictates, whether they will undergo one, two or three dimensional motion. This problem of biased random walk, is applicable not only in the material world, but also in the motion of living being like birds, with bias decided by the availability of food or water[4].In this article we have simulated the random walk in one dimensional and three dimensional lattices by applying suitable external biases. By analyzing the mean square difference with time we have identified a time called transition time, where the nature of motion changes from diffusion like to drift like. The biases are scanned in the sale of 0 to 1 and analyzed the variation of transition time with magnitude of bias.

In the past two decades, extensive efforts have been made to investigate biased RW and various models have been presented [5-6]. According to the RW model, the random walker moves along every direction with equal probability. However, in the presence of an external field, the random walker moves to its different directions with different probabilities that show a biased character.

The motion of particles in an eternal bias can be considered as RW in a potential. The walk takes place in a continuous space. At each time step the walker can move in any direction and the length of each step is a unit length. The direction of the external field is chosen as the positive *x*-axis and the angle between the moving direction of the walker and the positive *x*-axis is denoted by θ**.** The Boltzmann distribution is suited to describe the relation between the jump probability and the field strength. So the jump probability can be expressed as $P_\theta = A \exp(B \cos\theta)$ [7]. Here *A* is the normalization constant, which is the jump probability in the absence of any bias. B depends on the magnitude of bias. The relative change in probability because of bias is given by $P_\theta/A = \exp(B \cos\theta)$. It can be noticed that for this kind of bias, along the line of force, the probability increases (nearly 2.75 times) and against the line of force, it goes down to 0.75 of the original value. For perpendicular directions ($\theta = 90^0, 270^0$) the probability is unaffected.

II. Simulation

In our simulations, we have considered more than 10^3 realizations to obtain the accurate mean value. The step length is chosen from Gaussian distribution with a mean specified step length. First, we will investigate the diffusive properties of the particles. Usually, the types of the diffusion processes are determined by the spread of the distance travelled by a random walker. When a particle undergoes random walk in one dimension, the Mean Square Displacement (MSD) is proportional to the time and the proportionality constant is called the diffusion constant and is given by $<R^2> = Dt$.

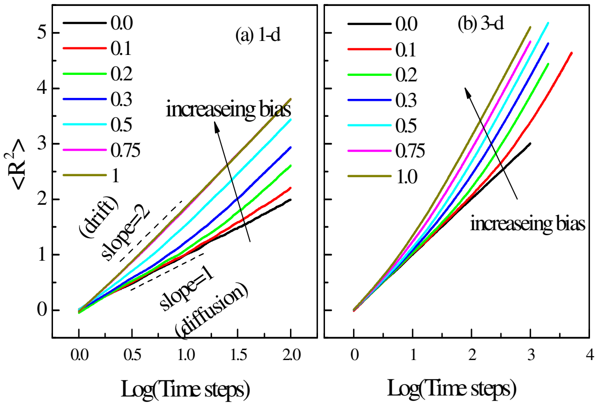

Fig.1. Log-Log plot of mean square displacement ($<R^2>$) as a function of time steps for different applied bias for the case of (a) 1-d motion and(b) 3-d motion

However, if we consider biased random walk, there will be some component of directional motion along the field along with the pure random motion. The directional motion is called drift and is characterized by drift velocity **(*v*)** where as the random motion is called diffusion and is characterized by diffusion constant **(D).** This can be written mathematically as $<R^2> = Dt + v^2t^2$. Therefore, $\boldsymbol{<R^2>}$ can be taken to be dependent on *t* as

$$\left\langle R^2 \right\rangle \alpha t^a \quad (1<a<2) \qquad (1)$$

The mean square displacement $\boldsymbol{<R^2>}$ has been simulated by the Monte Carlo method and plotted against time steps as the log–log plot in figure 1. Different values of biases (B) are considered ranging from 0 to 1.

As we are considering motion along 1-d only, $cos(\theta) = \pm 1$. Therefore, bias can be given by ±B. For small bias, the motion of the particle is governed by the random motion and therefore diffusion dominates over drift (figure 1). In contrast, for relatively higher bias, the directional motion governs the motion of the particle and therefore drift dominates over diffusion. These two situations are explained quite well by figure 1. In the case of intermediate field strengths, the motion of carriers is governed by a combination of random motion (diffusion) and directional motion (drift). As can be noticed from equation 1, for small ***t***, the first term ***Dt*** dominates the motion; and for large ***t***, the second term $\boldsymbol{v^2t^2}$ plays a major part. Therefore, there is smooth transition from the diffusion like motion (*a = 1*) to drift like motion (*a* = 2) as time increases. This is also observed in figure 2. ***a*** is calculated from figure 1. as

$$a = \frac{d\left(\log\left\langle R^2 \right\rangle\right)}{d\left(\log(t)\right)} \qquad (2)$$

There is smooth transition from the diffusion like motion to drift like motion as time increases. The transition time (from diffusion dominated to drift) depends on the applied bias. However, in the long-time regime, ***a* = 2**, irrespective of the applied bias causing the particles to move in well directed manner.

The transition time ($\boldsymbol{\tau_c}$) can be calculated from figure 2 as explained in the inset of figure 3. Since $\boldsymbol{\tau_c}$ is the point of inflation, therefore it is calculated as the maximum of the slope of ***a*** plotted against time step. Similar calculations are also done for 3-d random walks and presented in figure 1 and 2 It should be noted that by the application of bias, the transition time shifts towards lower time scales (figure 3). This is explainable in the sense that when bias increases, particles tend to attain drift like motion very early in their motion. For small bias, it takes long time to average out the random motion.

Therefore, transition time increases. It should be noted that the effect of bias is less in 3-d as compared to 1-d motion. It is because in 1-d, we have bias in the moving direction and there is no motion in the perpendicular directions. However, in 3-d motion, in addition to motion along the bias, there are motions in two directions perpendicular to bias. In these directions, the probability of motion is unchanged because of bias. Therefore, effective influence of bias decreases.

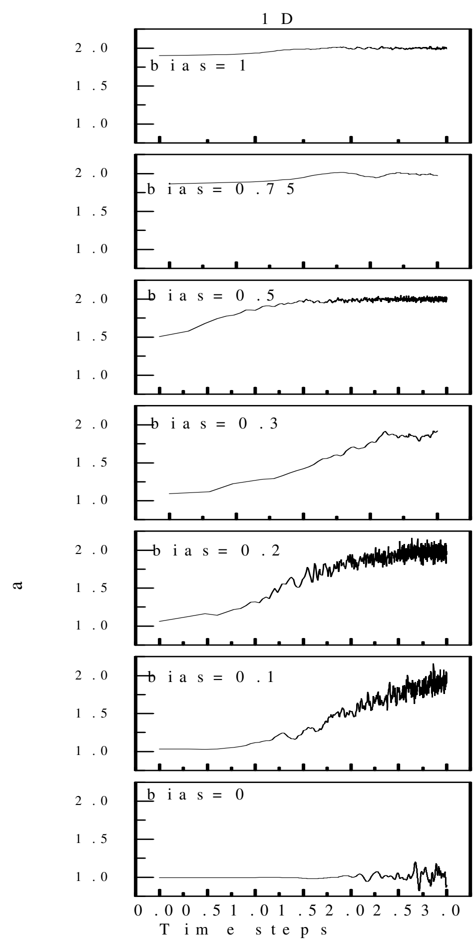

Fig. 2 (a) Plotted against log(time steps) for different bias for the case of 1-dmotion

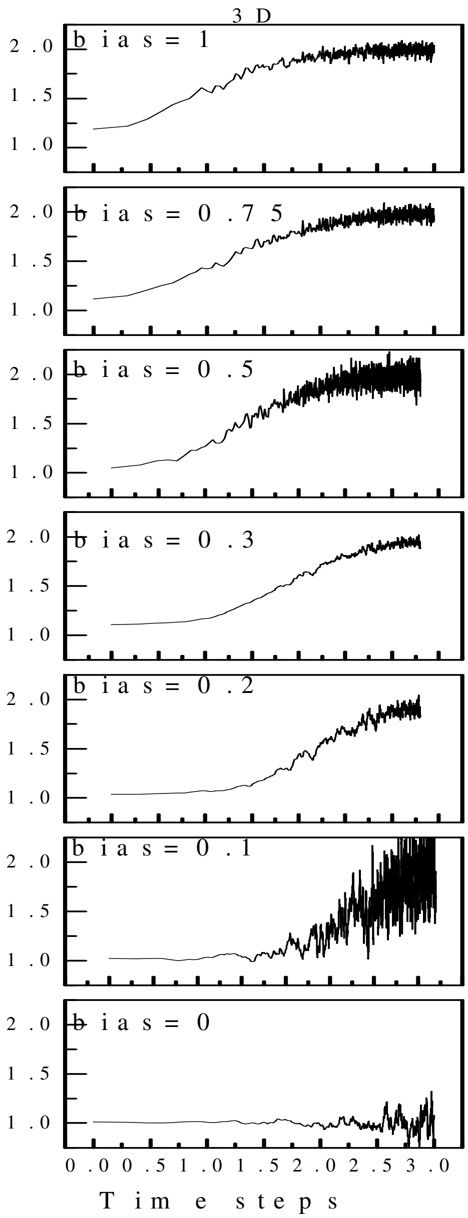

Fig. 2 (b) Plotted against log(time steps) for different bias for the case of 3-d motion

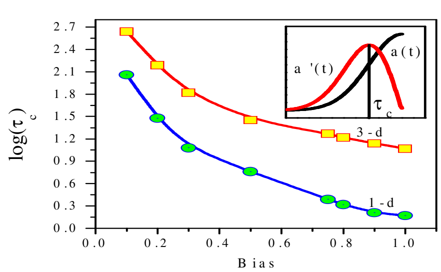

Fig. 3. (a) The transition time as a function of bias for 1-d and 3-d motion. Note that bias is more effective for the case of 1-d incomparison to 3-d. Inset shows the method of calculation of τ_c from the plot of a~t.

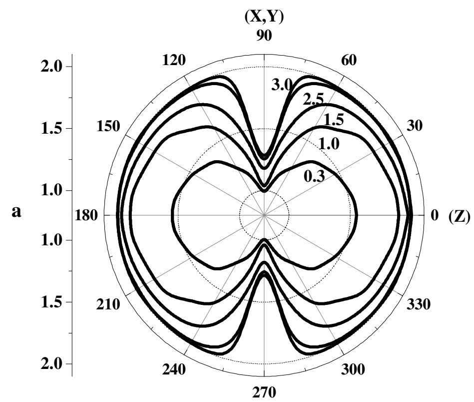

Fig. 3. (b) Angular dependent value of the exponent *a*. Note that at higher bias the angle dependency become lower and for all most all angle, the value of *a* approaches 2

This can be even better understood, if we consider the motion of the particle in a particular direction for a particular bias. This is done by fixing a bias and than allowing the particle to undergo random walk in 1-d along a particular angle to the direction of bias. The above figure is plotted for a bias of 0.2 and for different times ranging from log(t) = 0.3 to 3.0. It can be seen that for the direction of bias (θ = 0 or 180) the value of $\boldsymbol{a}$ is higher than any other direction. This can be compared with figure 4. As time passes, the value of $\boldsymbol{a}$ approaches two for every direction. However, the progress is slow for $\theta = 90^o$ or 270^o, indicating lesser effect of applied bias. Though it is a two dimensional plot, it can be easily extended to three-dimensional plot as the effect of bias on X and Y-axes are the same. In this case, its shape will be donut type. Since the effect of bias is lower for both the perpendicular directions, $\boldsymbol{\tau_c}$ is larger for 3-d case than 1-d case.

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