Chapter 5

Dynamics of particle moving in one dimensional Lorentz lattice gas

5.1 Introduction

Most natural micro-swimmers usually move in complex environment and encounter soft and solid walls, obstacles i.e. a *heterogeneous* environment [Golding & Cox (2006); Moeendarbary et al. (2013); Parry & Jacobs-Wagner (Parry & Jacobs-Wagner)], which can be realised by regular or irregular patterns of obstacles, which control their motion depending on background environment. Their dynamics can vary from confined trajectories, sub-diffusion, diffusion, super diffusion to propagation [Bechinger et al. (2016); Ghosh et al. (2016)]. How does the nature of surroundings affect the dynamics is question addressed in many studies [Golding & Cox (2006); Zeitz & Stark (2017)]. One of the way to model motion of particle in such complex environment is through Lorentz lattice gas [Binder & Young (1986); Cohen & Wang (1995b); Ernst & Binder (1988)]. In the past, there have been a number of ways in which a Lorentz lattice gas (LLG) has been used to model different physical phenomena [Gale (1993);

Langton (1986)]. Most of these studies are for two and higher dimensions [Meng & Cohen (1994); Mishra et al. (2016); Webb & Cohen (2015)]. But study in one-dimension is also interesting which can help us to understand the dynamics of many one dimensional system like: ant moving on a trail [Fonio et al. (2016)], motion of motors on filament [Shelley (2016)], transport of proteins along the channel [Bruce Alberts & Walter (Bruce Alberts & Walter)], etc.. Also one dimensional model have less number of control parameters and hence give more insight to the system.

In a Lorentz [Langton (1986)] lattice gas (LLG) a single particle moves along the bonds of a lattice. When it arrives at a lattice site the particle encounters a scatterer, which scatters the particle according to some fixed rule. In addition to the particle, each scatterer can also have a number of different orientations, or more generally states, that may also change over time as it interact with the particle, etc. Hence a Lorentz lattice gas is defined by (i) underlying lattice (ii) the initial density of scatterer which is called as the LLG's initial configuration. One of the main question we ask here is how does the dynamics of particle changes as we change the density and property of the scatterers.

In our present study we introduce a one dimensional lattice of unit lattice spacing $a = 1$ on which two types of scatterers are present, both are randomly distributed. The one is "reflector" and the another one is "transmitter". Reflector reverse the direction of particle's velocity and transmitter let the particle pass through. The density of scatterers is controlled by a number r which is defined as $r = \frac{C_R}{C_L+C_R}$; where C_R and C_L are the initial concentration of reflector and transmitters respectively. Reflectors (R) and transmitters (T) also flips i.e. $R \leftrightarrow T$ and $T \leftrightarrow R$ with a probability α, once the particle pass through. For $\alpha = 0$ there is always flipping and for $\alpha = 1$ there will be no flipping (i.e. fixed), hence dynamics is deterministic. And for $0 < \alpha < 1$ the flipping is probabilistic.

Now we will briefly discuss our main results. We study the model for range of $\alpha \in [0,1]$ and density $r \in [0,1]$. For $\alpha = 0$ (pure flipping) dynamics is always ballistic, and the direction of the particle velocity depends on the configuration of scatterers in the system. When $r = 0.0$ and $r = 1.0$ (only one kind of scatterers), particle moves in the direction of its initial velocity. For the case when there are both kind of scatterers in the system (i.e. when $r \neq 0.0$ and $r \neq 1.0$) and its first encounter a reflector, followed by a transmitter then the direction of the motion of particle will be opposite to that of its initial velocity. In other case if the particle encounter a transmitter at the start of the motion, on average it will continue to move in the same direction that of it's initial velocity. Also for the pure flipping case speed of the particle decreases with increase in r as $< v >= \frac{1/r}{1/r+2}$. For pure fixed case, when $\alpha = 1$, dynamics of particle is always confined between two nearest reflectors present in the system and span of confinement varies with r. In this case the spread of the confined region i.e. radius of gyration $R_g(= \sqrt{\Delta(t)})$ linearly varies with $1/r$. For the case when $\alpha \neq 0, \neq 1$: the dynamics of the particle is probabilistic. In fig. 5.8 we plot the the full phase diagram for the asymptotic behaviour with respect to (α-r). Dynamics is characterised by mean square displacement (MSD) exponent β, such that at late time MSD, $\Delta(t) \propto t^{\beta}$. For fixed r, decreasing α from 0 to 1., hence going from pure flipping to no flipping, the exponent β decreases from 2 (ballistic) to 0 (confinement). In general, approach to the asymptotic behaviour happens through mainly two states with course of time where the motion continues to progress in the same fashion as the early time behaviour like in the case of ballistic motion, and in other cases the dynamics is initially faster and then slows down to show normal diffusion. But when α is very close to 0 i.e. $0 + \delta$ where $\delta \simeq 0.001$ then the dynamics approaches its asymptotic behaviour mediated my three regimes which is further explained in the results section 5.4. In our model full range of dynamics can be seen by tuning the two parameters α and r. Changing the two parameters system shows a transition from one type of motion to other.

Rest of the article is divided in the following manner. In next section 5.2 we first describe our model. Section 5.3 we defined the three types of motion and then in section 5.4 we discuss our results in detail and finally conclude in section 5.5.

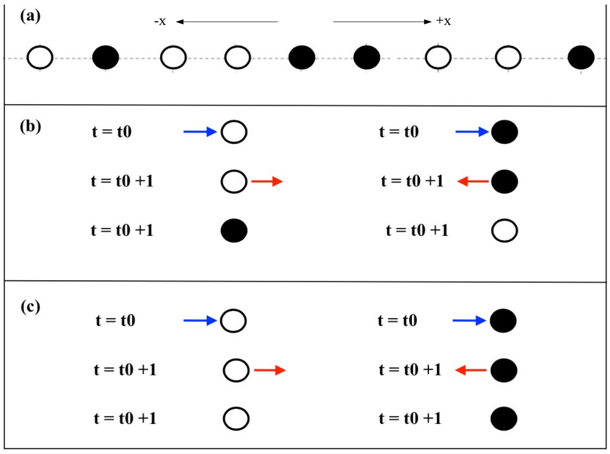

Fig. 5.1 A cartoon of one dimensional Lorentz lattice Gas : filled circles:- reflector, empty circles:- transmitters. Arrow shows the direction of particle's velocity. (a) Part of a typical initial configuration. Interaction of particle with a scatterer and state of scatterer one-step after interaction when (b) $\alpha = 0$ i.e. pure flipping and (c) $\alpha = 1$ i.e. pure fixed.

5.2 Model and numerical details

In our one-dimensional Lorentz lattice gas (LLG) a single particle moves along the bonds of the lattice of unit lattice spacing $a = 1$ in unit time step i.e. $(\Delta t = 1)$. On the lattice the two types of scatterers: "reflectors" and "transmitters" are randomly distributed. Reflectors reverse the direction of the particle's velocity and transmitters let the particle move in the same direction. The reflectors (R) and transmitters (T) also flips (after particle pass through) with probability $\alpha \in [0,1]$. If $\alpha \ = 0$ there will be always flipping and if $\alpha \ = 1$ there will be no flipping, and if $0 < \alpha \ < 1$ then flipping will be probabilistic. We vary the initial density of reflectors R and transmitters T according to a number r, such that if $r = 0$, initially all the scatterers are transmitters and if $r = 1$, all are reflectors, if $r = 0.5$, scatterers are in equal ratio. A cartoon picture of part of the model is shown in fig. 5.1.

We start with a random initial distribution of R and T on the lattice. One of typical initial configuration of R/L is shown in fig. 5.1. A particle start to move along a randomly chosen direction, forward ($+x$ direction) or backward ($-x$ direction), from the center of the lattice and move along the bonds of the lattice. The direction of the particle's velocity changes according to the presence of R or T at each node. For example if particle encounters a R/T then its velocity direction will switch back/remain same (reflected/transmitted). At the same time R/T will change to T/R with probability α. Hence initial configuration of R/T is going to change with the dynamics of the particle. Dynamics of the particle is explored for various choice of initial concentration of R/T i.e. r and flipping probability $1-\alpha$. Although initial condition is generated for fixed lattice size, but particle will never reach the boundary. Hence boundary plays no role. Properties of the system is characterised by calculating (a) Mean square displacement, MSD of particle position defined as $\Delta_{\alpha,r}(t) \ = <[x(t) \ - \ x(0)]^2>$, where $<..>$ denotes the average over many initial realisation of R/T and for a given choice of r and α. (b) Number of different visited sites $N(t)$, (c) density of scatterers on the visited sites $r_{visited}(t)$ and (d) Probability distribution of particle position $P(x,t)$. Also at long time when the motion is diffusion $N(t)$ should satisfies the equation given below,

$$\frac{d}{dt}N(t) = \frac{c}{N(t)} \tag{5.1}$$

where the value of c depends on the system parameters α and r.

Now we discuss our results for different values of α and r. We find three different kinds of motion on the lattice. First we define the three kinds of motion and then discuss the full phase diagram in the plane of (α,r). The three kinds of motion are characterised by calculating the MSD. In general, with time, MSD varies as $\Delta(t)_{\lim_{t\to\infty}} \simeq t^{\beta}$, where we define, $\beta = \lim_{t\to\infty}\frac{ln\Delta(t)}{ln(t)}$ as the MSD exponent.
All the measurements are done in the asymptotic state when β approaches a constant value at late time. But in general we can define the initial transient state in the system. For all set

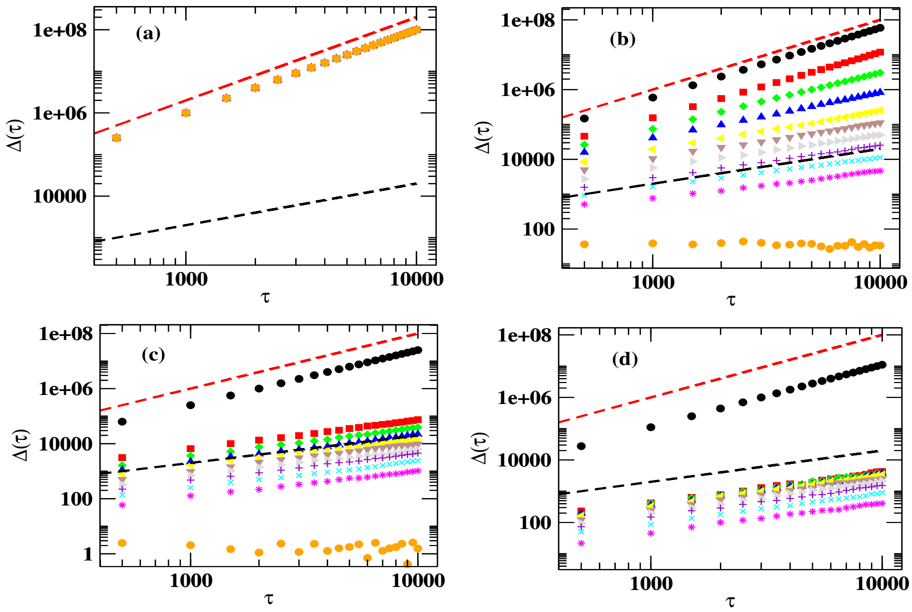

Fig. 5.2 (Color online) MSD $(\Delta(\tau))$ *vs.* time (τ) (upto 10^4 before the asymptotic behaviour observed) Plot: $r = 0.0$ (a), $r = 0.15$ (b), $r = 0.5$ (c) and $r = 1.0$ (d) for $\alpha = 0.0$ (circle), 0.1 (square), 0.2 (diamond), 0.3 (triangle up), 0.4 (triangle left), 0.5 (triangle down), 0.6 (triangle right), 0.7 (plus), 0.8 (x), 0.9 (star), 1.0 (open circle). Black and Red dotted lines have slope = 1 and 2 respectively. Data is averaged over 1000 ensembles.

of parameters (α, r), system shows a transition from early time transient state to late time steady state. Near to the phase boundary transition from early time transient state to late time asymptotic state take very long time and it is almost impossible to achieve in the present available computational facility.

5.3 Definitions: Ballistic, Anomalous diffusion and Confined motion

We calculate the MSD i.e $\Delta(t)$ vs. t and extract the exponent β for late time. MSD vs time plot is shown in fig. 5.2 for some choice of values of $r(= 0.0, 0.15, 0.5, 1.0)$ and $\alpha \in [0, 1]$. The dynamics of particle is ballistic if $\beta = 2$, hence particle on average moves in one direction with certain speed $v(t) = \sqrt{\Delta(t)}/t$. Maximum possible speed particle can have is $v(t) = \frac{a}{\Delta t} = 1$, when it always move in one direction. But in general particle can spend some of its time moving forward and backward. But on average moving in one direction. In that situations speed $v(t)$ is less than 1. A ballistic motion of the particle happens when particle do not scatter frequently but moves smoothly i.e. have negligible resistance in the system. Or we can say that the reflectors in the system favours the motion of the particle to be in one direction. We call the dynamics of particle is diffusive type if the exponent of MSD i.e. $\beta \simeq 1$. We call the dynamics of particle is confined if the exponent β approaches zero in long time. Trajectories for such kind of motion is shown in fig. 5.3 for different set of $(\alpha, r) = (1.0, 0.1), (1.0, 0.5), (1.0, 0.9)$.

5.4 Results

Now we discuss our results in detail: First we explain the trivial cases in our model

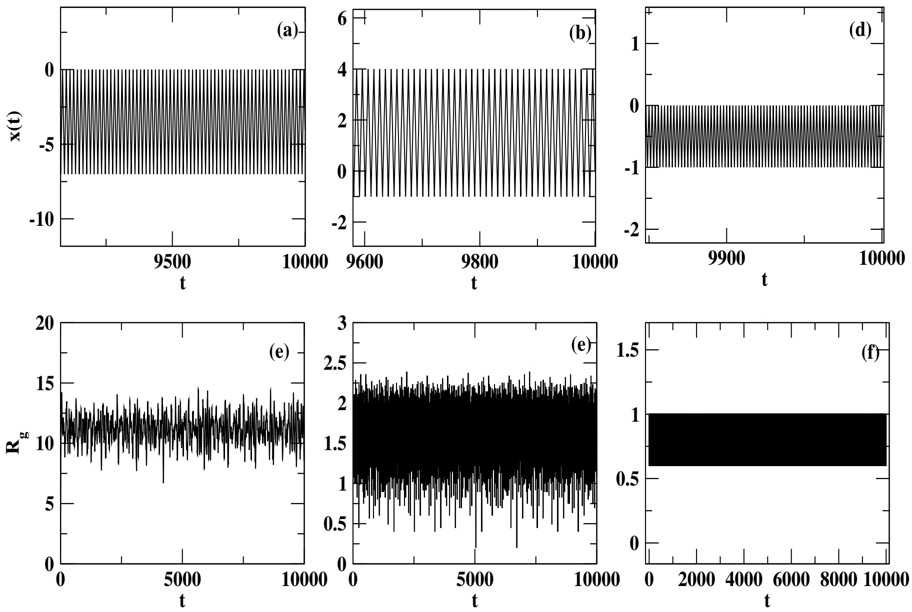

Fig. 5.3 Three different trajectory when particle motion is confined (or periodic): (a), (b) and (c) shows the trajectory for system parameter set (α, r)=(1.0,0.1), (1.0,0.5) and (1.0,0.9) respectively. Figure (d),(e) and (f) shows the RoG of the particle for system parameter set (α, r)=(1.0,0.1), (1.0,0.5) and (1.0,0.9) respectively. Data for $R_g = \sqrt{\Delta(t)}$ is averaged over 100 realisations.

Case I: Pure transmitter $r = 0$:- Initial condition when all obstacles are transmitter type, then whatever is the value of flipping probability $1-\alpha$ particle will always move in a straight line in the direction of its initial velocity with its maximum speed $v_0 = 1$. This is very trivial because in that situation when all of the obstacles are transmitter particle will always pass through and never come back and hence value of α will be irrelevant. Hence $\beta = 2$ and $v(t) = 1.0$.

Case 2: Pure fixed:- When $\alpha = 1$, or obstacles never change their characteristic then the dynamics of the particle will always be confined between two nearest reflectors. Hence statistically when averaged over large number of initial realisation for a given r, average distance between two nearby reflector is $1/r$. Mean square displacement of the particle trajectory saturates to some finite value after initial transient state. Square root of the of the MSD at late time: i.e. in the stationary state will determined the extend of the particle trajectory or also called as radius of gyration (ROG) $R_g = \sqrt{\Delta(t)}$ for large t, fig. 5.3(d, e and f). This result suggest that in confined motion particle explore different amount of space for different value of r.

Case 3: Pure flipping:-When $\alpha = 0$, i.e when properties of obstacles are pure flipping type, then dynamics of particle is always ballistic in the direction of initially chosen velocity direction. But this case is very different from **case 1**, ($r = 0$), and speed of the particle will depend on the concentration of r on the lattice. It is very trivial exercise to check on a piece of paper that for this case particle will move on average $1/r$ distance in $1/r+2$ time steps. Hence speed of the particle can be estimated to be $v(r) = \frac{1/r}{(1/r)+2}$. As $r \to 0$, speed $v(t)$ approaches 1 (**case 1**) and as $r \to 1.0$, speed $v(t) = 1/3$.

Case 4: Stationary state:- When $r = 0.5$ i.e both types of scatterers are in equal ratio then the motion is always diffusion for all values of α except when $\alpha = 0\ or 1.0$. In this case particle have equal chance to go left and right and this is the case similer to the one dimensional random walk. Also this is the case when the system remains in staionary state irrespective of the time particle have spent in the system. Therefor for other value of r, asymptotically, system approches to its stationary state in which $r_{visited} = 0.5$. To understand this consider the situation that the particle sits on a new site i, visited for the first time. The probability that it will return to this site is either unity or less, say ρ. In the latter case the walker has to move ballistically in either direction, in 1 out of $(1-\rho)^{-1}$ newly visited sites the process renews itself, it never returns to the last site it came from. In the former case the walker will keep returning forever (and the environment of a given site becomes more diffusive and less ballistic with every return). After a number of visits of order $\frac{1}{\alpha}$ the neighbourhood of site i becomes equilibrated, implying $r = \frac{1}{2}$.

When α is close to its boundary values particle takes much longer time to achieve an asymptotic behaviour than that of in the case of other values of α. The asymptotic behaviour shows that particle perform diffusive motion for all values of α except when $\alpha = 0$ and $\alpha = 1.0$, in these cases particle motion is ballistic and confined respectively. When $\alpha \simeq 0.001$ and $r > 0.5$ particle first move ballistically for early simulation time then it shows much slower dynamics for significantly large time (say T) and seems like the motion of particle is sub-diffusion but when we wait further longer then the dynamics again becomes faster comparable to that in the case of normal diffusion where MSD vs. time exponent converges to 1.0 as shown in fig. 5.4(a). Value of T increase as we decrease the value of r i.e particle will take longer time to show asymptotic behaviour for smaller $r < 0.5$ than that of $r > 0.5$. We explain this with the case when initially all the rotators are of reflector type and no transmitter ($r = 1.0$). In this case we know if rotators have pure flipping character $\delta = 0$, then particle will propagate with speed $v(t) = 1/3$. Now if we have finite small δ, rotators have small tendency to retain their character (non-flipping). In general particle is moving on the lattice with speed $1/3$. As soon as it encounter a non-flipping rotator then it get diverted from its propagation direction and will move backward direction with speed $1/3$ to all the previously visited site. Unless it again encounter a non-flipping scatterer and start moving in forward direction it started, with the speed $1/3$. Hence this cycle keeps on and although particle move in propagating mode for some intermediate times but due to small non-flipping character whenever it encounter a non-flipping scatterers, it has to go large distance in backward direction and dynamics is slower but it is never confined. Now if we tune δ to moderate value, then it feels more random kicks from its velocity direction and motion tends to become more random and hence the MSD exponent β increases and approaches to 1 (diffusive type). But during this process the particle also randomize the background lattice such that the value of r on the visited site approaches to 0.5 for $\alpha \neq 0 \neq 1$ i.e $r_{visited} = 0.5$ as shown in fig. 5.6. Also the rate of increase of number of newly visited site $N(t)$ converses to zero therefore at long enough time i.e asymptotically system approaches to its stationary state where $r = 0.5$. This means that at long enough time the motion of the particle will be diffusive i.e the asymptotic behaviour is normal diffusion. We claim this behaviour as asymptotic since the rate of increase of newly visited site converges to zero and the background lattice is being randomize by the particle motion during the total simulation time available and the system reaches to the stationary state. Asymptotic behaviour for $\alpha \simeq 0.999$ and $r < 0.5$ can be understood in the similar way. We have also seen that the number of different site visited $N(t)$ agrees well with equation (5.1) which have the solution $N(t) \propto \sqrt{t}$ which is the case of random walk in one dimension. Plots are given in fig. 5.5 for different sets of parameters (α, r) where $F(t) = \frac{d}{dt}N(t)$ and $G(t) = \frac{1}{N(t)}$. Looking at these plots what we observe that the time derivative of number of different sites visited $\frac{d}{dt}N(t)$ and reciprocal of $N(t)$ converges to zero at long time and also satisfy the equation (5.1) well.

5.4.1 Anomalous diffusion

We have calculated the probability distribution of particles position for some chosen value of α and r when the particle's dynamics is diffusive i.e. $\beta = 1.0$ (diffusive type). Fig. 5.7 shows the plot of probability distribution of particle position $P(x)$, calculated for 2000 trajectories,

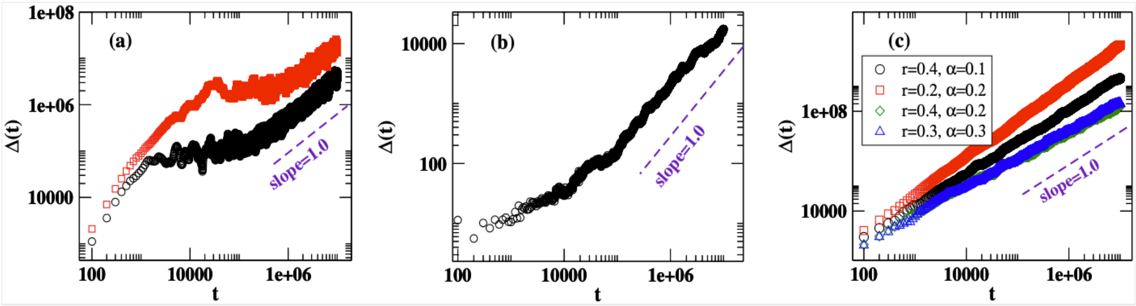

Fig. 5.4 MSD ($\Delta(\tau)$) vs. time (τ) plot when (a) $\alpha = 0.003$ and $r = 0.9$ *and* 0.6, (b) $\alpha = 0.999$ and $r = 0.3$, (c) different set of α *and* r.

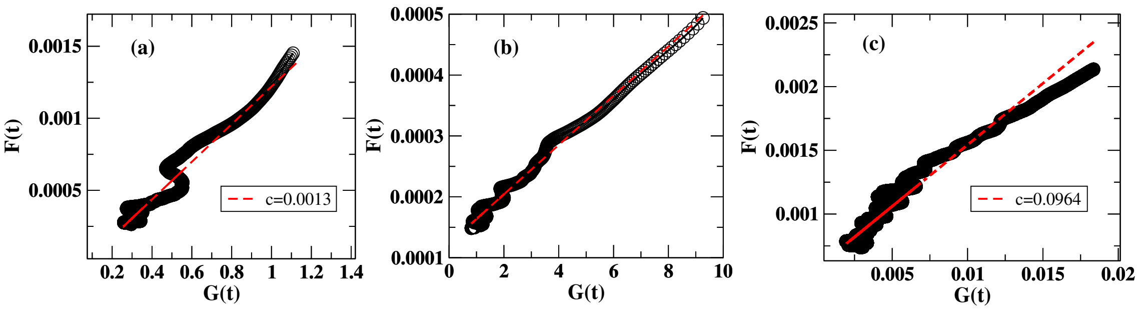

Fig. 5.5 $F(t) = \frac{d}{dt}N(t)$ vs. $G(t) = \frac{1}{N(t)}$ plot when (a)$\alpha = 0.3$ and $r = 0.3$, (b) $\alpha = 0.003$ and $r = 0.6$, (c)$\alpha = 0.003$ and $r = 0.9$. Data (black solid line) is fitted linearly (red dashed line) which give sthe slope c.

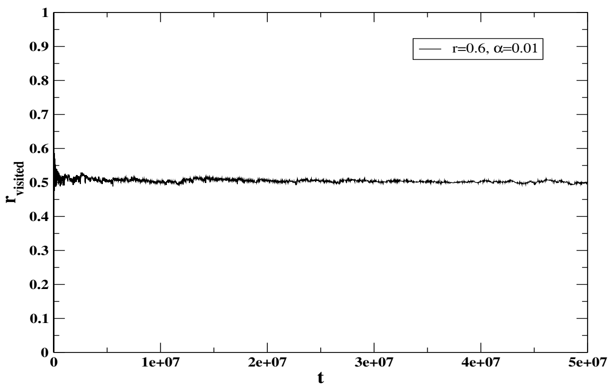

Fig. 5.6 Plot of $r_{visited}$ vs time for $\alpha = 0.01$ and $r = 0.6$.

Table 5.1 List of the values of D_{eff} and D_{est} for different values of r when $\alpha = 0.5$.

r	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
D_{eff}	12.142	3.434	1.592	0.770	0.467	0.335	0.268	0.212	0.172	0.123
D_{est}	12.500	3.125	1.389	0.781	0.500	0.347	0.255	0.195	0.154	0.125
β	01.003	1.067	1.087	1.003	1.022	1.029	1.060	0.960	0.984	1.004

for certain value of parameters $(r,\alpha) = (0.5,0.5),(0.5,0.9),(0.9,0.5),(0.9,0.9)$, when the exponent $\beta = 1$. Bars are the data from the simulation and lines are fit to the Gaussian. Data fits well with the Gaussian. $P(x)$ is calculated by collecting particle's position at few random times for each 2000 trajectories.

We also calculate the effective diffusion coefficient D_{eff} using,

$$D_{eff} = \lim_{t\to\infty} \frac{\Delta(t)}{2t}$$

in the numerical simulation and also estimate it as follows: consider the case when $\alpha = 0$ (pure flipping **case 3**) typical path length of straight motion is $1/r$, hence $1/r$ is like mean free path for pure flipping case. Now when we deviate α from 0 ($\alpha > 0.0$), the average mean free path will decrease and typical speed of the particle when it moves in straight is $V \simeq (\frac{1-\alpha}{r})\frac{1}{\tau}$ where the rate τ at which particle changes its trajectory is $\frac{1}{1-\alpha}$. Hence estimated diffusion coefficient can be given by $D_{est} \simeq \frac{V^2}{\tau} = \frac{(1-\alpha)^2}{r^2}\alpha$. In table 5.1 we list the value of effective diffusivity D_{eff} from simulation and estimated D_{est} for $\alpha = 0.5$. Numerical data matches very well with estimated D_{est}. The same argument do not hold as we go away from $\alpha = 0.5$ values because randomness decreases. For $r = 0.5$, D_{eff} approaches 0.5, which is the value for one dimensional random walk. Now as we tune r, it can be tuned to larger values (for small r) and diverges for $r \to 0$ and to smaller values (for large r) and approaches 0 for $r = 1$.

Phase Diagram:- We have calculated the phase diagram for the asymptotic behaviour from numerical simulation as well as analytical estimation in the plane of $\alpha - r$. Phase

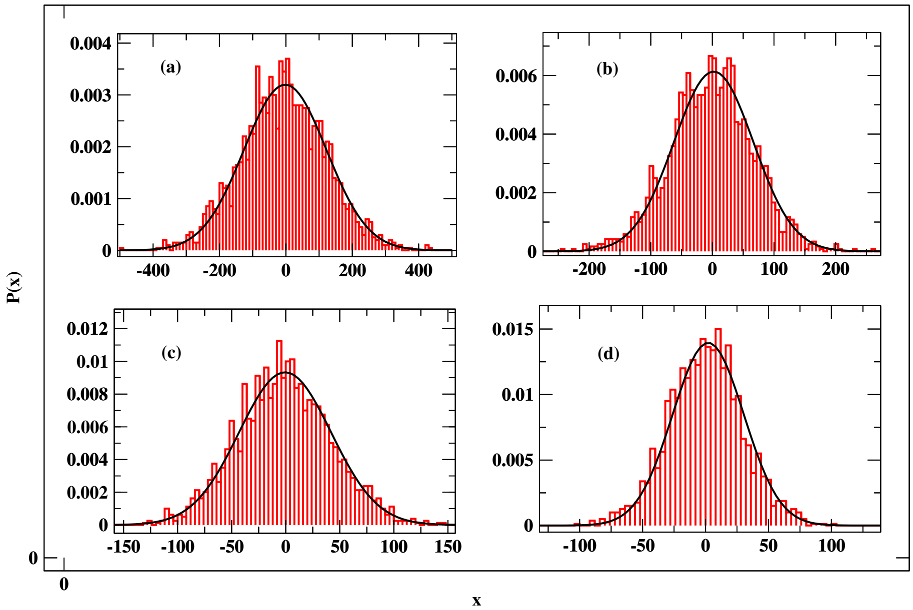

Fig. 5.7 Probability distribution of particles position (bars) and fitted with Gaussian distribution (solid line) when (a) $r = 0.5$ and $\alpha = 0.5$, (b) $r = 0.5$ and $\alpha = 0.9$, (c) $r = 0.9$ and $\alpha = 0.5$, (d) $r = 0.9$ and $\alpha = 0.9$.

boundaries between ballistic motion and diffusion have been drawn in the phase diagram shown in fig. 5.8.

5.5 Discussion

We have studied the dynamics of a single particle moving on a one-dimensional lattice-gas with randomly distributed reflectors and transmitters. Particle moves along the bonds of the lattice of unit spacing. Reflectors reflect the direction of particle velocity and transmitters leave it unchanged. Scatterers also change their character after interaction with particle with probability $1-\alpha$. Hence for $\alpha = 1$, nature of scatterers remain unchanged and for $\alpha = 0$, they always flip. Otherwise for $\alpha \neq 0 \neq 1$, flipping is probabilistic. Hence initial density of right/left scatterers and probability (r, α) are the two control parameters in our model.

For $\alpha = 0$ and 1, dynamics of particle is pure deterministic: and it is completely confined

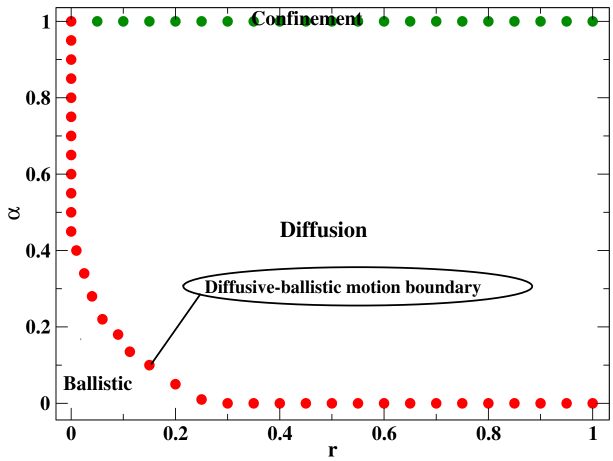

Fig. 5.8 Phase diagram in the plane of (r, α). Data points shows the asymptotic phases of the system, based on the values of MSD exponent (β) for different set of (r, α), when the system reaches the steady state.

or periodic for $\alpha = 1$ and ballistic for $\alpha = 0$ for all r. Region of confinement and speed of propagation depends on initial r. For $\alpha \in (0, 1)$, dynamics of particle shows a crossover from initial transient feature to late time steady state behaviour and asymptotically shows diffusive motion. Approach to the steady state behaviour in general is quick and happens through a short transient state. But when the parameters α and r are close to 0 or 1.0, particle take a much longer time to reach its steady state and show asymptotic behaviour.