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The interpolation between random walk and self-avoiding walk by avoiding marked sites

Trupti R Sharma[1], G Rangarajan[2] and Prashant M Gade[1,*]

[1] PG Department of Physics, Rashtrasant Tukadoji Maharaj Nagpur University, Campus, Nagpur, 440033, India
[2] Department of Mathematics, Indian Institute of Science, Bangalore, 560012, India
E-mail: prashant.m.gade@gmail.com

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Abstract. The self-avoiding walk (SAW) on a regular lattice is one of the most important and classic problems in statistical mechanics with major applications in polymer chemistry. Random walk is an exactly solved problem while SAW is an open problem so far. We interpolate these two limits in 1D and 2D by considering a model in which the walker marks certain sites in time and does not visit them again. We study two variants: (a) the walker marks sites at every k time-steps, in this case, it is possible to enumerate all possible paths of a given length. (b) The walker marks sites with a certain probability p. For $k = 1$ or $p = 1$, the walk reduces to the usual SAW. We compute the average trapping time and distance covered by a walker as a function of the number of steps and radius of gyration in these cases. We observe that 1D deterministic, 1D probabilistic, and 2D deterministic cases are in the same universality class as SAW while 2D probabilistic case shows continuously varying exponents.

Keywords: biopolymer, brownian motion, exclusion processes, loop models and polymers

*Author to whom any correspondence should be addressed.

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Contents

1. Introduction

The study of the random walk has a long history from Lord Rayleigh to the seminal paper by Einstein on Brownian motion and remains a cornerstone of studies in stochastic processes. Several problems in the random walk have not only continued to fascinate mathematicians and physicists but have also found applications ranging from economics to biology. It soon becomes clear that these walks do not represent certain situations such as polymers. Polymers are chains that fold with the condition that no two or more atoms can occupy the same position [1]. These are best modeled by self-avoiding walks (SAW). The SAW is also considered in the context of network theory and in search algorithms [2]. It is common to treat SAWs as dynamic processes. At each time step, walker randomly jumps between adjacent nodes in the network. The walk ends when the walker reaches a dead end and cannot reach the newly unvisited node. Recently, it has been found that the distribution of such dynamically growing SAW path lengths can be calculated analytically in the network [3].

Because many polymer properties can be studied by using self-avoiding random walk (or chain), they have become an important model in polymer chemistry. It is formally the $N \to 0$ limit of $N-$vector model and a fundamental example in the theory of the critical phenomena [4]. Nonetheless, the SAW has not been solved exactly. SAW is a discrete path with no self-intersection. It lives in the entire d-dimensional lattice Z^d consisting of points in R^d whose components are all integers. The elements of Z^d will be referred to as 'site'. Two sites are called nearest neighbors if they are separated by unit Euclidean distance. The SAW at n-step is defined as an ordered set of $n+1$ sites in Z^d for which each

J. Stat. Mech. (2022) 113203

consecutive pair of the sites consists of nearest neighbors and in which no site occurs more than once [5]. By visualizing the walk as a path in the lattice, the self-avoidance constraints imply that the path has no loops. Although a walk is defined as the sequence of sites, it is useful to treat it as a continuum path formed by joining each pair of consecutive sites by the intervening unit line segment. Some researchers prefer the term 'chain' instead of 'walk' [6]. Let c_n denotes the number of n-step SAW which begins at origin. For exact enumeration of c_n is a challenging problem in probability and we do not have an exact formula for c_n. This quantifies the number of possible configurations in the walk. In the case of polymers, the number of possible configurations will be $n+1$ monomers. In the case of a simple random walk that does not have any self-avoidance constraint, the analog of c_n is just $(2d)^n$ as there are $2d$ options for the walk at each step [5]. Let the number of self-avoiding random walks on a d-dimensional hypercubic lattice starting at the origin which never lands on the same lattice point twice in n steps be denoted $c_d(n)$. The first few values are; $c_d(0) = 1,\ c_d(1) = 2d,\ c_d(2) = 2d(2d-1)$. In general, $d^n \leqslant c_d(n) \leqslant 2d(2d-1)^{(n-1)}$. For 2D self avoiding walk on square lattice values of c_n is 4, 12, 36... for $n = 1, 2, 3\ldots$ [7].

The number of SAW paths of length n is given by

$$c_n \sim \mu^n n^{\gamma-1}. \tag{1}$$

Similarly, mean square displacement $\langle R_n^2 \rangle$ after time n is known as

$$\langle R_n^2 \rangle \sim n^{2\nu} \tag{2}$$

where the exponents γ and ν are exponents which depend only on the dimensionality of the system [8]. There have been a couple of prominent attempts to derive the exponent ν using field-theoretic approaches. Edwards studied probability distribution of configurations of a polymer consisting of freely hinged links of length l and excluded volume v and solved it asymptotically by considering a self-consistent field approach [9]. De Gennes carried out second order expansion and concluded that $2\nu = 1.195$ in 3D using Wilson formulae [10]. In 1D, there are only two possible SAW. The distance will grow linearly in time and we can postulate $\gamma = \mu = \nu = 1$. In 2D, $\gamma = 43/32$ and $\nu = 0.75$. For the particular case of a square lattice $\mu = 2.638$ [11] for SAW while for random walks in 2D $\mu = 4$. Conway and Guttmann enumerated walks of up to length 51 [12] in two dimensions. Jenson extended it and enumerated walks up to the length of 71 [13] on square lattice. Other quantities of interest are the average end-to-end distance of n-step SAW or polymer and radius of gyration. End-to-end distance is defined as the average of squared Euclidean distance between endpoints of the walk. The average is taken over all n-step walk in which each walk is equally weighted.

We do not have an exact formula for the exact enumeration of SAW of certain lengths though various methods are proposed [14]. On the other hand, random walk is a well-understood problem. Hence we interpolate between these two limits which may help understand SAW.

There have been similar attempts in past. The earliest attempt could be the Domb-Joyce model of polymer chains [15, 16]. Here, each self-intersection has a weight $1-w$ where w is between 0 and 1. For any $w > 0$, asymptotic behavior is that of SAW, and for

J. Stat. Mech. (2022) 113203

$w = 0$, random walk behavior is recovered [17]. Later, true self-avoiding walks (TSAW) were introduced. In this case, the walker avoids visiting a frequently visited site again [18]. If there are m neighbors of a given site, the probability of visiting one of the neighbors i is a function of the times v_i the walker has visited the site i in past. For example, if there are two neighbors, $i1$ and $i2$, the probability of visiting site $i1$ is $f(v_{i1})/(f(v_{i1}) + f(v_{i2}))$. Functional forms other than exponential have been studied in [19]. By definition, this walk is never trapped. For TSAW, which uses exponential functional form $f(v) = \exp(-gv)$, distance covered by walk of length N is proportional to N^{μ} with $\mu = 1/2$ for $D \geqslant 2$ and $\mu = 2/3$ in 1D. Thus the asymptotic behavior is not different from a random walk in higher dimensions and we get new behavior only in 1D. For power-law functional form $f(v) = 1/(v+1)^{\alpha}$, the exponent obtained depends on α [19]. Another variant has been proposed known as the z-tolerant random walk. It is a type of random walk in which each site can be visited up to z times. This walk can be trapped. It has been argued that two-tolerant walks are in the same universality class as SAW [20]. Rieger [21] introduced a parameter $\lambda = (z-1)/n$ where n is the length of the walk. In the limit $z \to \infty$, these walks correspond to a case where z/n is kept constant. He argued that this is in the SAW class only for $\lambda = 0$. Initially, z-tolerant walks were studied as a theoretical curiosity. However, it has found application in the domain of liquid-crystal polymer [22]. Another variant of such a walk is useful for foraging animals. Each lattice site contains one food unit and the walker can carry out random walk for S time-steps for food without starving [23]. Chupeau *et al* studied such walk then the depleted site can be renewed after R time-steps and studied the transition from finite to infinite lifetime [24]. This model has been studied in one as well as in higher dimensions and several properties are studied [23–25]. Iba *et al* [26] studied a model in which excluded volume constraints are systematically weakened and argued that such an algorithm correctly reproduces canonical averages at a finite temperature of the HP model of lattice proteins.

2. The model

We use the Monte Carlo simulation to study two variants of SAW in 1D and 2D. The essential difference from SAW is that all sites which are visited previously are not forbidden for the walker. Only marked sites are forbidden. Unlike a true SAW which is also stochastic, the walker gets trapped in the stochastic model studied by us. The walker marks certain sites as he goes along and does not visit the marked sites again. We consider two ways in which sites are marked. **(a) Deterministic model:** we mark sites that are visited after every k timesteps. The deterministic model reduces to SAW for $k = 1$. In this case, exact enumeration is possible. **(b) Stochastic model:** we mark the visited sites with probability p. The stochastic model reduces to RW for $p = 0$ and SAW for $p = 1$. In this case we carried out the simulations to analyze the number of walks and study different properties.

The SAW is considered synonymous with polymer statistics though this assumption has been questioned [27]. Significant departures from Flory exponents have been

J. Stat. Mech. (2022) 113203

obtained in various conditions. They could arise due to weak excluded volume effects due to microchannel confinement [28]. There is a significant departure from Flory exponents for expanding polyion gel [29]. The exponents change for anisotropy in a preferred direction or inclusion of external force [30]. We note that polymer need not be homogeneous. There are periodic copolymers where a periodic sequence of monomers repeats [31] as well as random copolymers where a random sequence of monomers repeats [32]. This work can be considered as a model for a situation where different monomers have a different interactions with the solvent.

Starting site is always marked in either model. We compute exact enumeration, average trapping time, distance covered as a function of the number of steps n, end-to-end distance and radius of gyration in both 1D and 2D models. Both deterministic and stochastic variants are not exactly analogous and give slightly different results for some properties. The deterministic model allows exact enumeration of possible paths and this may help analytic studies.

3. Results

3.1. Exact enumeration

We can carry out exact enumeration in the case of the deterministic model. We carried out an exact enumeration of walks of length n for $k = 1 \ldots 6$ in 1D and 2D (tables 1 and 2). In 1D, there are only two SAW. The walker may drift to the right or left. On the other hand, there are 2^n possible walks of length n for a normal random walk. We compute the number of walks of length n and we find that they are of order μ^n where μ interpolates between 1 and 2 in 1D and increases with k. The deterministic walks in 2D yield values of μ between 2.638 and 4 increase with k. Results for $k = 2$ in 1D are trivial. There are only four possible walks at odd n for $n > 1$ and two possible paths for even n. Of course, for $k = 1$ there are only two paths. For $k > 2$, we compute c_n and fit it as μ^n assuming $\gamma = 1$ in 1D. (The behavior for $k = 1$ in 1D can be fitted only with $\mu = \gamma = 1$.) We found values of μ ranging from 1.27 to 1.47 for 1D. In 2D, we compute $c_n/n^{\gamma-1}$ using known value of γ which is 43/32. In 2D, the values of μ range 3 to 3.45 (figures 1(a) and (b)). Different values of μ in 1D and 2D tabulated below (table 3). For $k = 1$ our exact enumeration result matches with standard result [11] in 2D. In all cases, the fit is obtained using values of c_n at multiples of k.

However, it is not possible to explore walks of large lengths using an exact enumeration and hence we employ walks known as kind of walks considered here are kinetic growth SAW [33, 34] in which one randomly chooses the next step among the neighboring unvisited sites and stops growing when none are available. These walks were employed to describe the irreversible growth of linear polymers [35]. We average over 5×10^6 configurations.

J. Stat. Mech. (2022) 113203

Table 1. Exact enumeration for 1D lattice.

n	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
1	2	2	2	2	2	2
2	2	2	2	2	2	2
3	2	4	4	4	4	4
4	2	2	6	6	6	6
5	2	4	6	12	12	12
6	2	2	10	8	20	20
7	2	4	14	16	20	40
8	2	2	12	22	34	30
9	2	4	20	44	48	60
10	2	2	28	24	88	82
11	2	4	24	48	142	164
12	2	2	40	66	130	250
13	2	4	56	132	218	500
14	2	2	48	72	302	318
15	2	4	80	144	550	636

Table 2. Exact enumeration for 2D lattice.

n	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
1	4	4	4	4	4	4
2	12	12	12	12	12	12
3	36	48	48	48	48	48
4	100	124	172	172	172	172
5	284	496	516	688	688	688
6	780	1188	1948	1888	2576	2576
7	2172	4752	6972	7552	7728	10 304
8	5916	11 012	19 904	25 900	29 564	29 036
9	16 268	44 048	75 248	103 600	105 728	116 144
10	44 100	100 508	262 352	272 960	409 760	401 684
11	120 292	402 032	751 080	1091 840	1533 092	1606 736
12	324 932	907 404	2787 224	3666 372	4454 236	5860 732
13	881 500	3629 616	9729 000	14 665 488	1704 6988	23 442 928
14	2374 444	8130 076	27 358 392	37 824 288	59 768 500	64 250 044
15	6416 596	32 520 304	101 736 480	151 297 152	231 834 332	257 000 176

3.2. Average trapping time

In either model, we observe that the walker gets trapped eventually. The walker gets trapped when all neighboring sites are marked. This is not surprising since there is a finite probability that the walker visits the origin again in 1D and 2D. Thus it may get trapped. This is different from first hitting time where the walk gets terminated when the walker visits an already visited (or in our version, marked) site.

J. Stat. Mech. (2022) 113203

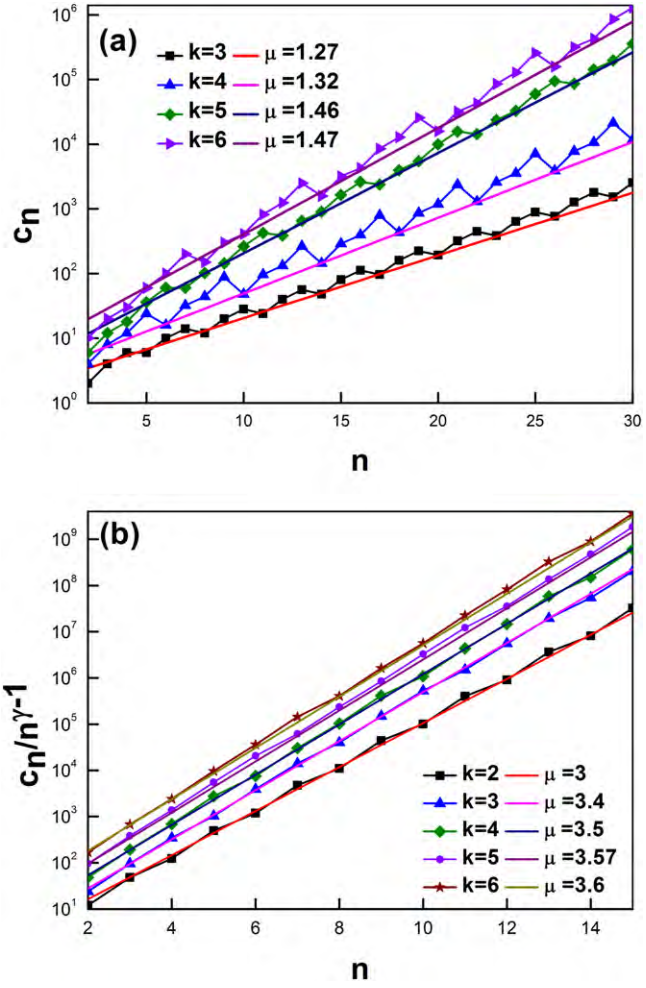

Figure 1. (a) c_n is plotted as a function of n for $k = 3 \ldots 6$ (1D), (b) c_n is plotted as a function of n for $k = 2 \ldots 6$ (2D) (c_n is multiplied by a different constant factor for different k for better visibility.)

Deterministic model:

(i) In 1D, we observe that average trapping time $\langle T(k) \rangle \sim k^{\beta}$. Odd and even values of k have different values of β. We propose $\langle T(k) \rangle = T_0 + k^{\beta}$ for even k and $\langle T(k) \rangle = T_0' + k^{\beta'}$ for odd k. We find $T_0 = 2$ and $\beta = 1.103$ and $T_0' = 8$ and $\beta' = 1.1075$ (figure 2(a)).

(ii) In 2D, we observe that $\langle T(k) \rangle \sim k^{\beta}$ asymptotically with an additive correction. Odd and even values of k have different values of β. We propose $\langle T(k) \rangle = T_0 + k^{\beta}$ for even k and $\langle T(k) \rangle = T_0' + k^{\beta'}$ for odd k. We find $T_0 = 45$ and $\beta = 2.68$ and $T_0' = 160$ and $\beta' = 2.82$ (figure 2(b)).

In both 1D and 2D cases, there is a difference between odd values of k and even values of k. For even values, the average trap time is smaller than odd values. This may be related to the bipartite nature of lattice where walker returns to even sublattice at all even times.

J. Stat. Mech. (2022) 113203

Table 3. Different values of μ for $k = 2 \ldots 6$ in 1D and 2D lattice.

k	μ(1D)	μ(2D)
2	—	3.0 ± 0.02
3	1.27 ± 0.001	3.4 ± 0.02
4	1.32 ± 0.001	3.5 ± 0.005
5	1.46 ± 0.001	3.57 ± 0.003
6	1.47 ± 0.001	3.6 ± 0.0006

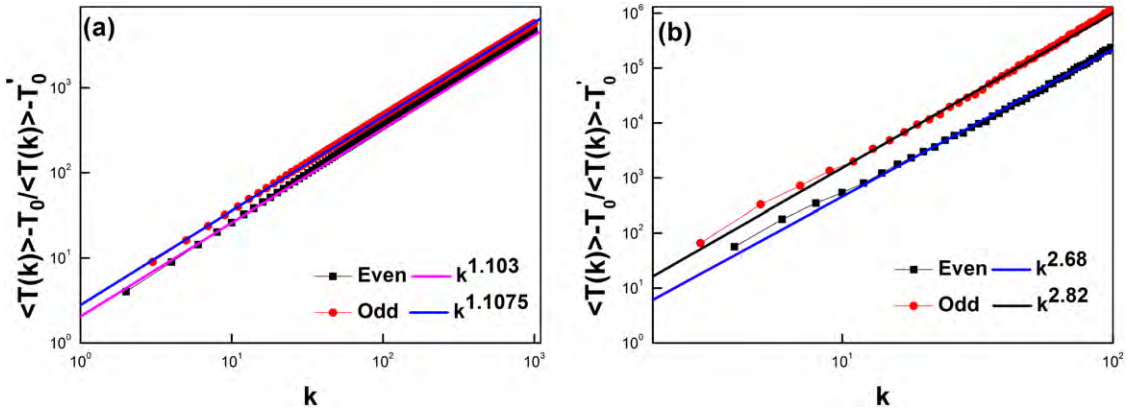

Figure 2. (a) Average time $\langle T(k) \rangle$ for trapping is plotted as a function of k for the deterministic model in 1D on a logarithmic scale. (b) Average time $\langle T(k) \rangle$ for trapping is plotted as a function of k for the deterministic model in 2D on a logarithmic scale. In both cases, odd and even values of k show different behavior.

Stochastic model:

(i) In 1D, we observe that trapping time is non-monotonic and U-shaped (figure 3(a)). For $p = 1$, every visited site is marked and the walker has to drift to right or left. Thus it will never get trapped. Similarly, for $p = 0$, no site is marked and the walker will continue to carry out random walk without getting trapped ever. For any finite p, we expect the walker to be trapped. This leads to non-monotonic behavior.

(ii) In 2D, the empirical fit goes as $\langle T(p) \rangle \sim T_0 + (1/p)^{\delta}$ (figure 3(b)) in 2D with $T_0 = 60$ and $\delta = 2.2$. The behavior in the deterministic case is like k^{β}. This the similarity in qualitative behaviors suggests that $k \sim 1/p$ though exponents are different.

3.3. Distance covered as function of number of steps *n*, end-to-end distance and radius of gyration

We have clubbed all these quantities together because end-to-end distance as well as distance covered after n steps scale like square-root of the radius of gyration for a walk of n steps. As mentioned above, we carry out 5×10^6 walks for both deterministic as well as the stochastic case. However, for longer times, the fraction of walks that contribute

J. Stat. Mech. (2022) 113203

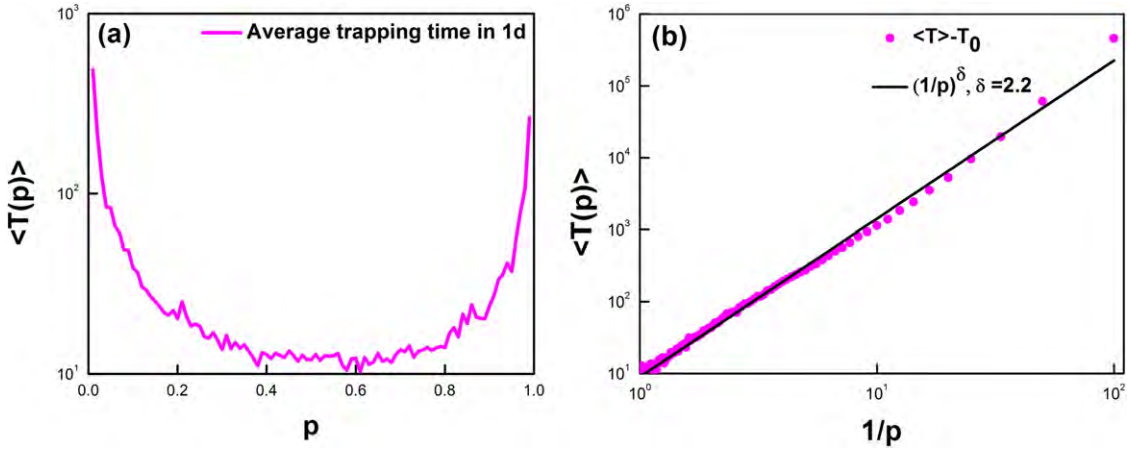

Figure 3. Average trapping time $\langle T(p)\rangle$ is plotted as a function of (a) p in 1D for the stochastic model. (b) $1/p$ in 2D for the stochastic model. It can be fitted as $\langle T\rangle = T_0 + (1/p)^{\delta}$ with $T_0 = 60$ and $\delta = 2.2$.

decays exponentially. For example, for $k = 6$, the fraction of walks that contribute at $n = 10, 100, 1000$ is 0.99, 0.76 and 0.0013. This leads to large fluctuations for large values of n and this data has not been plotted. However, it has been included in logarithmic binning.

3.3.1. Radius of gyration. It is the average squared distance of any point in the walk from its center of mass. This is an important quantity since it can be found experimentally for polymers. For a walk of n sites, it is defined as $R_n^2 = \frac{1}{n}\sum_{i=1}^{n} S_i^2$ where S_i is the distance of the walker from the center of mass of the walk. The average over several configurations is denoted by $\langle R_n^2\rangle$ and it is known that $\langle R_n^2\rangle \sim n^{2\nu}$ and thus $\sqrt{\langle R_n^2\rangle} \sim n^{\nu}$. We have computed the radius of gyration of the walk in both 1D and 2D.

3.3.2. Distance covered in ***n*** *steps.* We also compute distance $d(n)$ covered in n steps. It is larger than $\sqrt{\langle R_n^2\rangle}$ but expected to behave in same manner, i.e. $d(n) \sim n^{\nu}$. This expectation is indeed fulfilled. **In 1D**

(i) Deterministic case: in 1D, the radius of gyration $\sqrt{\langle R_n^2\rangle}$ grows as n for $k = 2, 3, 4, 5, 6$ (figure 4(a)). Distance $d(n)$ at step n also grows linearly (figure 4(b)).

(ii) Stochastic case: the behavior in the probabilistic case is no different. Both quantities $\sqrt{\langle R_n^2\rangle}$ and $d(n)$ grow linearly (figures 4(c) and (d)).

In 2D (i) deterministic case: in the 2D deterministic case, the radius of gyration $\sqrt{\langle R_n^2\rangle}$ grows as n^{ν} with $\nu = 0.75$ for $k = 2, 3, 4, 5, 6$ (figure 5(a)). The value of ν is independent of k and identical to that for SAW. We also plot $\sqrt{\langle R_n^2\rangle}/d(n)$ as a function of n which saturates asymptotically. Thus asymptotic behavior of $d(n)$ is the same as that of $\sqrt{\langle R_n^2\rangle}$ as expected (figure 5(b)). There are strong fluctuations for large values of n and to overcome those we find exponent using logarithmic binning. Let $G(i) = \sqrt{\langle R_i^2\rangle}$. Let, $S(n) = \sum_{i=r^n}^{r^{n+1}} G(i)$ where $r = 10^{1/10}$. We plot $S(n)/\ln(r)$ as a function of n. The exponent b obtained thus is related to true exponent ν as $b = \nu + 1$ and we expect

J. Stat. Mech. (2022) 113203

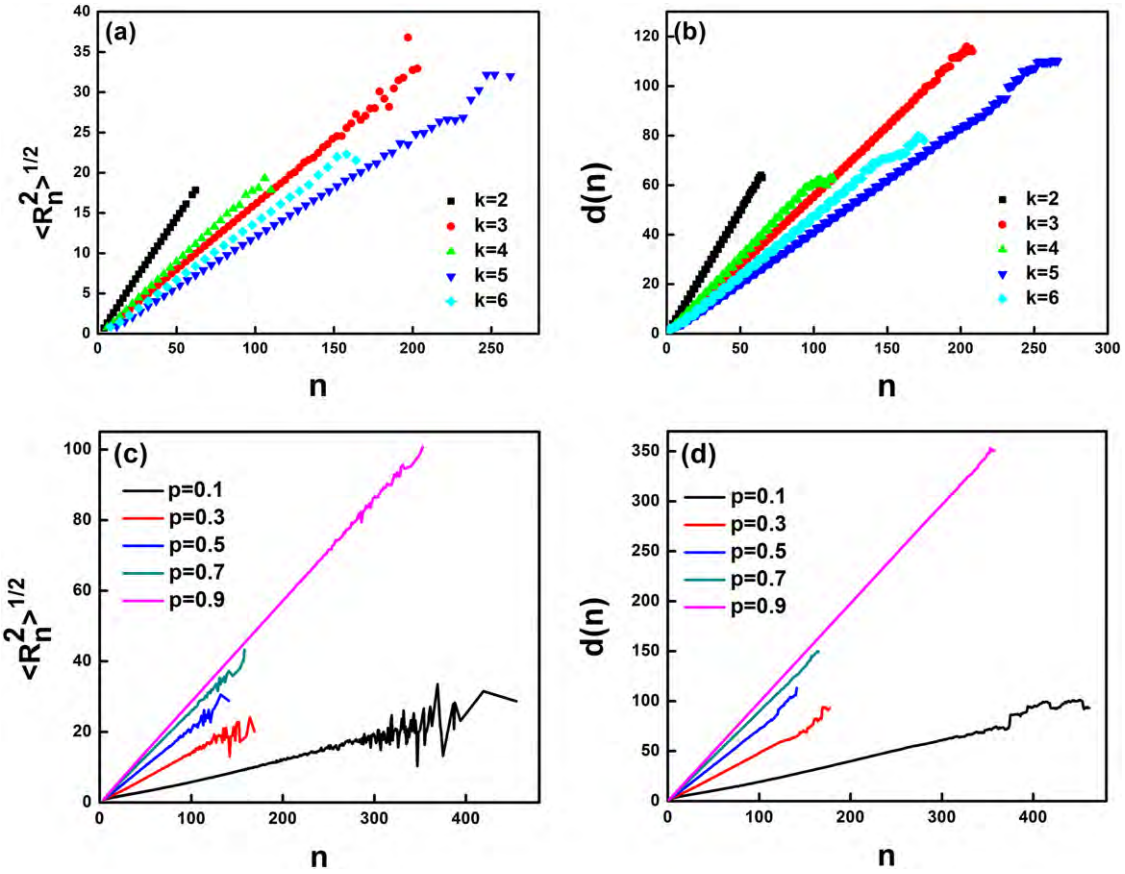

Figure 4. (a) We plot $\sqrt{\langle R_n^2 \rangle}$ as a function of n for 1D deterministic case. (b) $d(n)$ is plotted as a function of n for 1D deterministic case. (c) We plot $\sqrt{\langle R_n^2 \rangle}$ as a function of n of 1D stochastic case. (d) $d(n)$ is plotted as a function of n for 1D stochastic case. All above quantities grow linearly with n.

$S(n) \sim n^b$ with $b = 1.75$ and the deterministic case is in the same universality class as SAW (figure 5(c)).

(ii) Stochastic case: this case is very different from all three previous cases studied and we observe continuous dependence of exponent ν on the probability p with which sites are marked. We have plotted the radius of gyration as a function of n for $p = 0.1, 0.3, 0.5, 0.7$ and 0.9 (figure 6(a)). The exponent ν varies continuously and tends to 0.75 as $p \to 1$. We also plot $\sqrt{\langle R_n^2 \rangle}/d(n)$ and find that the ratio tends to a constant asymptotically showing that they have similar behavior as expected (figure 6(b)). We have carried out logarithmic binning as in deterministic case to average out strong fluctuations. We plot $S(n)/\ln(r)$ as a function of n and obtained exponent b which shows continuous variation as p.

In both cases, we observe strong fluctuations at a long time because the number of walks that contribute to the statistics is much lower. Though the number of walks grows exponentially, they grow slower than $(2d)^n$ and thus the observed number of walks found by kinetic growth decrease exponentially with n.

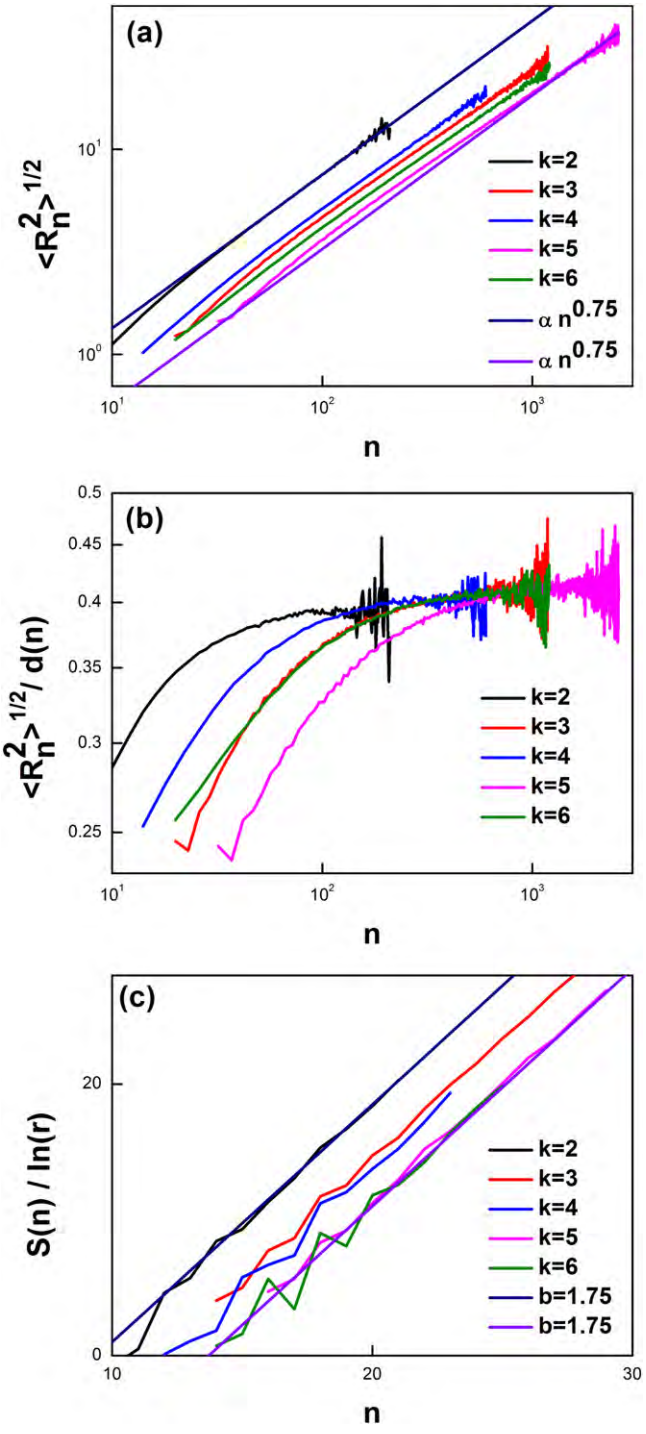

Figure 5. (a) $\sqrt{\langle R_n^2 \rangle}$ is plotted as a function of n in a deterministic 2D model, (b) $\sqrt{\langle R_n^2 \rangle}/d(n)$ is plotted as a function of n in the deterministic 2D model. The observations show that both $\sqrt{\langle R_n^2 \rangle}$ and $d(n)$ behave as n^{ν} with $\nu = 0.75$. (c) The quantity $S(n)/\ln(r)$ is plotted as a function of n in above model. It goes as $n^{1+\nu}$.

J. Stat. Mech. (2022) 113203

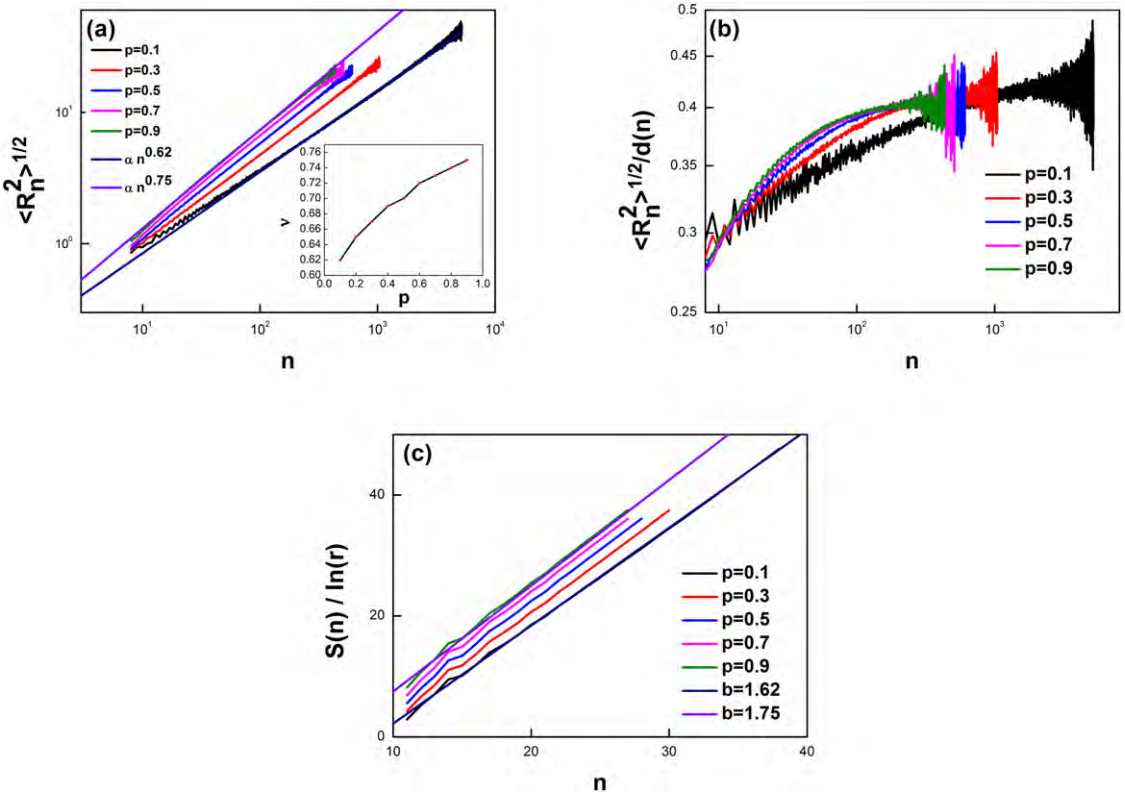

Figure 6. (a) $\sqrt{\langle R_n^2 \rangle}$ is plotted as a function of n in the stochastic 2D model, (b) $\sqrt{\langle R_n^2 \rangle}/d(n)$ is plotted as a function of n in the deterministic 2D model. It is clear that the exponent ν varies continuously with p. (c) The quantity $S(n)/\ln(r)$ is plotted as a function of n in the above model. The variation in the exponent as a function of p is confirmed. The quantity on the y axis is multiplied by arbitrary constant for better visibility.

4. Discussion

We have introduced a variant of the random walk which interpolates between SAW and RW. We mark sites and these sites are forbidden for the walker. We study two cases (a) deterministic: the sites are marked after every $k-$time-steps and (b) stochastic: the sites are marked with probability p. We can carry out exact enumeration for the deterministic case and these results are presented. In Monte-Carlo simulations, the walk continues till the walker is trapped, i.e. all the neighboring sites are marked. In both cases, we have studied an average trapping time, distance covered, and radius of gyration as a function of the number of steps n. We note that instead of continuing the walk till it is trapped, the walk can be continued till it visits the previously marked site. This is the first hitting time studied in the context of random network [36–38] and on directed lattice [39]. Instead of trapping, we could also study the first hitting time where the walk terminates as soon as it hits the marked site. We could also consider a non-backtracking version. The number of marked sites in both deterministic and stochastic

J. Stat. Mech. (2022) 113203

case is proportional to n. For the deterministic case, the number of marked sites is $\mathrm{Int}[n/k] + 1$ and for the probabilistic case, the expected number of marked sites is $pn + 1$. However, the trapping happens due to local density fluctuations. The role of local density fluctuations in trapping could also be of interest. These studies are considered for future work.

We find that the 1D and 2D deterministic cases and the 1D stochastic case are in the same universality class as SAW in 1D and 2D. However, for the 2D stochastic case, we observe exponents that interpolate between random walk and SAW limits as we vary p. We have carried out preliminary studies in 3D. For deterministic case, the exponent ν is close to 0.58 [6] which is the expected value for SAW. However, for the stochastic case, it varies continuously from 0.5 to 0.58. Thus our main conclusions do not change in 3D.

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J. Stat. Mech. (2022) 113203

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J. Stat. Mech. (2022) 113203