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Diffusive behaviour of self-attractive walks

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Abstract. We study an attractive random walk called the SATW in one dimension and show that the walk is diffusive. We show rigorously that asymptotically $S_N^2 \geqslant CN$, where S_N^2 is the average of the square of the number of distinct points visited by the walk in N steps. Since $\langle X_N^2 \rangle$, the average square of the distance to the origin, is of the same order as S_N^2 we get the result that $\langle X_N^2 \rangle \propto N$ asymptotototically.

The self-avoiding walk (SAW), and its variants such as the true self-avoiding walk (TSAW), the kinetic self-avoiding walk etc, have been extensively studied as models of polymers [1–9]. In a recent paper Sapozhinikov [10] proposed a kind of attractive random walk (SATW) in which the probability for making a transition to a neighbouring site is proportional to $\exp(-nu)$, where u is a negative parameter and $n = 1$ or 0 depending on whether the site to which the transition is made has been visited earlier or not. Using plausible approximations, he showed that the walk was diffusive in one dimension. However, in a recent paper, Fabio and Aarão Reis [11], obtained results at variance with this. Using a series analysis of exact enumeration studies up to 30 steps, they came to the conclusion that the walk shows sub-diffusive behaviour if $\langle x_N^2 \rangle \propto N^\nu$, ν is less than one. Here, x_N is the distance travelled in N steps. According to them the exact value of ν depends on the dimensionality and the strength of the biasing parameter u. In this paper, we rigorously prove the following:

$$S_N^2 \geqslant C_2 N. \tag{1}$$

Here, S_N^2 is the average of the square of the number of distinct points visited by an SATW in N steps in one dimension and C_2 is a constant of O(1). Since the walk is attractive, $\langle x_N^2 \rangle$, the mean square distance after N steps, is less than or equal to N. We also show that asymptotically $\langle X_N^2 \rangle \propto S_N^2$. Combining the two, we get the desired result, namely $\langle X_N^2 \rangle \propto N$.

Let Ω_N be the set of all N step one-dimensional SATWs $\omega = (0, x_1, x_2, \ldots, x_N)$ starting from zero. Let $p(\omega)$ be the probability of the walk ω. We then have

$$x_{i+1}(\omega) = x_i(\omega) + \xi_i(\omega). \tag{2}$$

Here, $\xi_i(\omega)$ takes on values $+1$ or -1:

$$x_{i+1}^2(\omega) = x_i^2(\omega) + 1 + 2x_i(\omega)\xi_i(\omega) \tag{3}$$

$$\langle x_{i+1}^2 \rangle = \langle x_i^2 \rangle + 1 + 2\langle x_i \xi_i \rangle. \tag{4}$$

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Here $\langle\ \rangle$ denotes averaging over the set Ω:

$$\langle x_N^2\rangle = N + 2\sum_{i=0}^{N-1}\langle x_i\xi_i\rangle. \tag{5}$$

Then, we have

$$\langle x_N^2\rangle = N + \sum_{\omega\in\Omega} p(\omega)\sum_{i=1}^{N} x_i(\omega)\xi_i(\omega). \tag{6}$$

We note that the average over the second term cancels out for an unbiased ordinary random walk. The only difference between an SATW and an ordinary random walk occurs when x_i happens to be an extremity that is

$$\begin{aligned} &\text{either } x_i \geqslant x_k \qquad \text{for } k = 0, 1, 2, \ldots, i-1 \\ &\text{or } x_i \leqslant x_k \qquad \text{for } k = 0, 1, 2, \ldots, i-1. \end{aligned} \tag{7}$$

Using this as well as the fact that when x_i is at an extremity there is a bias for an inward step, we get the inequality $\langle x_N^2\rangle < N$. Further since $-|x_i(\omega)| \leqslant x_i(\omega)\xi_i(\omega)$

$$\langle x_N^2\rangle \geqslant N - \sum_{\omega\in\Omega} p(\omega)\sum_{i=1}^{N}|x_i(\omega)|\mathrm{ind}(i,\omega). \tag{8}$$

Here $\mathrm{ind}(i,\omega)$ is a function which takes on values 1 or 0 depending on whether the SATW is at an extremity at i or not. We rewrite the equation as

$$\langle x_N^2\rangle \geqslant N - \sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty}\sum_{\omega\in\Omega_N^{l_1,l_2}} p(\omega)\sum_{i=1}^{N}|x_i(\omega)|\mathrm{ind}(i,\omega). \tag{9}$$

Here, $\Omega_N^{l_1,l_2}$ is the set of all N step SATWs which extend from $-l_1$ to l_2. Clearly, for all such walks, $|x_i| \leqslant (l_1 + l_2)$,

$$\langle x_N^2\rangle \geqslant N - \sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty}(l_1+l_2)\sum_{\omega\in\Omega_N^{l_1,l_2}} p(\omega)\sum_{1}^{N}\mathrm{ind}(i,\omega). \tag{10}$$

We note that $\sum_1^N \mathrm{ind}(i,\omega)(=K)$ is nothing but the total number of times the particular walk took an inward step from an extremity. We now prove that $q(K;l_1,l_2)$, the probability that an N step SATW extending from $-l_1$ to l_2 makes exactly K inward steps at extremities, satisfies the inequality

$$q(K;l_1,l_2) \leqslant \exp[l(1+\log[(K+l)/l])] + K\log(\alpha) + l\log(\beta)] \tag{11}$$

where $\alpha = \exp(-u)/(1-\exp(-u))$ and $\beta = 1/(1+\exp(-u))$. Basically, the proof is based on the fact that if a walk extending from $-l_1$ to l_2 takes a total of K inward steps at the extremities, these K steps as well as l outward steps are fixed. It has at most two options in the remaining $N-K-l$ steps. So, the total number of such walks is less than $2^{(N-K-l)}P_N(K)$. Here, $P_N(K)$ is the number of ways of distributing the K inward steps among the l lattice sites from $-l_1$ to l_2.

More formally, let $\Omega_N^{\bar{k},l_1,l_2}$ be the set of all N step SATWs $\omega = (0, x_1, x_2, \ldots, x_N)$ with the following constraints

$$l_2 = \sup_{1\leqslant i\leqslant N} x_i \qquad -l_1 = \inf_{1\leqslant i\leqslant N} x_i \tag{12}$$

$$\bar{k} = (k_{-l_1}, k{-}l_1+1, \ldots, k_{-1}, k_1, \ldots, k_{l_2}) \tag{13}$$

where k_l is the number of steps l to $l-1$ (respectively $l+1$) taken by the walk before the first step l to $l+1$ (respectively $l-1$) when l is positive (respectively negative). We consider all such walks with the additional restriction that

$$\sum_{l=-l_1}^{l_2} k_l = K. \tag{14}$$

All such walks can be mapped to strings $\bar{\psi}$ of length $N_1 (= N - K - l)$ as follows. Define

$$\bar{\psi} = (\psi_1, \psi_2, \ldots, \psi_{N_1}) \tag{15}$$

where the ψ_i take on values $+1$ or -1 only. A string $\bar{\xi} = (\xi_1, \xi_2, \ldots, \xi_N)$ can easily be generated with $\xi_i = x_i - x_{i-1}$. From this string of length N, we delete the entries ξ_i for which x_{i-1} is an extremity of the walk ω to generate a string $\bar{\psi}$ of length N_1.

Clearly, one can get $\bar{\psi}$ given ω. Further, the mapping is unique, that is given $\bar{\psi}$ and $\bar{k}$, one can obtain ω. Therefore, the total number of walks with a given $\bar{k}$ is less than or equal to the total number of strings of length N_1. The number of strings of length N_1 is 2^{N_1}. Further, the number of different $\bar{k}$'s which give the same K is merely the number of ways of distributing K identical objects in l distinguishable boxes:

$$P_N(K) = \frac{(K+l-1)!}{K!(l-1)!}. \tag{16}$$

Therefore, $q(K; l_1, l_2)$, the probability to get exactly K in a SATW extending from $-l_1$ to l_2, is given by

$$q(K; l_1, l_2) \leqslant 2^{N_1} P_N(K) (0.5)^{N_1} \alpha^K \beta^l. \tag{17}$$

Using Sterling's approximation, we have

$$q(K; l_1, l_2) \leqslant \exp[l(1 + \log[(K+l)/l]) + K \log(\alpha) + l \log(\beta)]. \tag{18}$$

For $K \gg l$, this term tends to zero exponentially. We may, therefore, in the limit write the inequality (10) as

$$\langle x_N^2 \rangle \geqslant N - \sum_{l_1=0}^{\infty} \sum_{l_2=0}^{\infty} u(l_1, l_2) c (l_1 + l_2)^2 \tag{19}$$

where $u(l_1, l_2)$ is probability that the walk extends from $-l_1$ to l_2:

$$\langle x_N^2 \rangle \geqslant N - C \langle (l_1 + l_2)^2 \rangle. \tag{20}$$

Since $\langle x_N^2 \rangle \leqslant \langle (l_1 + l_2)^2 \rangle$,

$$S_N^2 = \langle (l_1 + l_2)^2 \rangle > N / C_2. \tag{21}$$

It is fairly obvious that the average number of distinct points with a SATW will be less than the number for an ordinary random walk since there is an inward bias at the extremities (it can also be rigorously proved quite easily). The average of the square of the number of distinct points traversed by an ordinary random walk is $O(N)$. Combining this fact wth equation (21), we get the result that $\langle S_N^2 \rangle \propto N$. It is also fairly easy to show that $\langle X_N^2 \rangle \propto \langle S_N^2 \rangle$. One way of proving this is as follows.

Consider a realization with the extremities at $-l_1$ and l_2 with $l = l_1 + l_2 = O(N^{0.5})$. Let $l_2 \geqslant l_1$, so that $l_2 = O(N^{0.5})$. Let N_1 be the last time the SATW hits l_2 and let $N' = N - N_1$. After time N_1, the SATW behaves exactly like an ordinary random walk when it is at $x_i, 0 < x_i < l_2$. When the random walk is at $x_i, -l_1 \leqslant x_i \leqslant 0$, there is a possible bias towards the right in some of the steps. Therefore, the conditional probability $p_c(x, N; l_1, l_2)$ for the SATW is greater than or equal to the conditional probability $q_c(x, N; l_1, l_2)$ for the ordinary random walk of finding the particle at x, $0 < x < l_2$ at time N. It is known that $\sum_{x=0}^{l_2} q_c(x, N; l_1, l_2)x^2 \propto l_2^2$. This combined with the fact that $S_N^2 \propto N$ yields the result $X_N^2 \propto N$ asymptotically.

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