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LETTER TO THE EDITOR

Number of distinct sites visited by a random walker in the presence of a trap

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Abstract. We study the number of distinct sites visited by a random walker in $d=1$ after t steps, $S(t)$, in the presence of a trap. We calculate the distribution $q(S, t)$ of $S(t)$ in the limit of large t. We find an unusual crossover in the probability density at $S \approx S_x \equiv \sqrt{Dt}$. For $S \ll S_x$, $q(S, t) \sim S^{-2}$ and for $S \gg S_x$, $q(S, t) \sim St^{-3/2} \exp(-S^2/4Dt)$. From this crossover it follows that the mean number of distinct sites visited is $\langle S(t) \rangle \sim \ln(t)$.

The number of distinct sites visited by a t-step random walk is one of the most important properties of a discrete-time lattice random walk [1–6]. A large number of physical and chemical processes such as exciton trapping [7] and diffusion limited reactions [4, 8, 9] can be described by first passage time events which are closely related to the number of distinct sites visited.

The mean number of distinct sites visited by a random walker at time t, $\langle S(t) \rangle$, was calculated for any dimension (see e.g. [6]), on fractal systems [4, 10] and for a set of N random walkers [11]. In this letter we present an analytical solution for the number of distinct sites visited by a one-dimensional random walker in the presence of a trap. We find that $\langle S(t) \rangle \sim \ln(t)$, in contrast to the known result $\langle S(t) \rangle \sim \sqrt{t}$ for the unrestricted random walker.

We consider a one-dimensional system with a trap at $x=0$ and a random walker that starts at a given site $x_0 > 0$. Since we are interested in finding $\langle S(t) \rangle$ in the limit of a large number of steps, we shall use the diffusion approximation for the random walk probability density.

Let $\gamma(x, t)$ denote the probability density that a site x will be first visited at time t by the random walker, then the probability of a site x to be visited at least once up to time t is: $\Gamma(x, t) = \int_0^t \gamma(x, \tau)\, d\tau$. The probability density that the right most point visited by the random walker (which corresponds to the number of distinct sites in the discrete case for large t or small x_0) is exactly S up to time t is: $q(S, t) = -[\partial\Gamma/\partial x]_{x=S}$. Using this distribution, the average territory covered by the random walker up to time t can be easily shown to be:

$$\begin{aligned}\langle S(t) \rangle &= \int_{x_0}^{\infty} dS\, Sq(S, t) \\ &= \int_{x_0}^{\infty} dS\, S\left(\frac{-\partial}{\partial S}\int_0^t d\tau\, \gamma(S, \tau)\right).\end{aligned}$$

Using integration by parts and the fact that $\Gamma(x_0, t) = 1$, we get

$$\langle S(t) \rangle = x_0 + \int_0^t d\tau \int_{x_0}^{\infty} dS\, \gamma(S, \tau) \equiv x_0 + \int_0^t d\tau\, I(\tau). \tag{1}$$

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In order to find $\gamma(S, t)$, we introduce another (artificial) trap at $x = S$. We will calculate the probability density $p(x, t|S)$ of a random walker to be at x at time t in the presence of a trap at $x = 0$ and $x = S$. It is easy to see that

$$\gamma(S, t) = -D\left[\frac{\partial p(x, t|S)}{\partial x}\right]_{x=S}.$$

The solution of the diffusion equation, $\partial p/\partial t = D\partial^2 p/\partial x^2$, together with the following boundary conditions:

$$p(x = S, t|S) = 0 \qquad p(x = 0, t|S) = 0 \qquad p(x, t = 0|S) = \delta(x - x_0)$$

is given by:

$$p(x, t|S) = \frac{1}{\sqrt{4\pi D t}} \sum_{n=-\infty}^{\infty} (\mathrm{e}^{-(2nS+x-x_0)^2/4Dt} - \mathrm{e}^{-(2nS+x+x_0)^2/4Dt}). \tag{2}$$

We begin by calculating $\langle S(t)\rangle$ directly in the time domain and later by using the Laplace transformation. The first approach gives a better physical insight into the problem, while the second is mathematically more rigorous. To find $\langle S(t)\rangle$ we begin with calculating $I(t)$, which is defined in (1):

$$\begin{aligned} I(t) &\equiv \int_{x_0}^{\infty} \mathrm{d}S\, \gamma(S, t) \\ &= \frac{-1}{\sqrt{4\pi D t^3}} \sum_{n=-\infty}^{\infty} \int_{x_0}^{\infty} \mathrm{d}S (x_0 + (2n+1)S)\, \mathrm{e}^{-(x_0+(2n+1)S)^2/4Dt} \\ &= \sqrt{\frac{D}{\pi t}} \left(1 - \sum_{m=1}^{\infty} \frac{2}{4m^2-1} \mathrm{e}^{-m^2 x_0^2/Dt}\right). \end{aligned} \tag{3}$$

As $t \to \infty$, the magnitude of the infinite sum can be estimated to be $\sum_{m=1}^{N} 2/(4m^2-1)$ where $N \simeq \sqrt{Dt}/x_0$. The term in parentheses can now be evaluated to be:

$$1 - \sum_{m=1}^{N} \frac{2}{4m^2-1} = \sum_{m=N+1}^{\infty} \frac{2}{4m^2-1} \approx \int_{N}^{\infty} \frac{\mathrm{d}x}{2x^2} = \frac{x_0}{\sqrt{4Dt}}.$$

Thus $I(t) \sim x_0/t$ and

$$\langle S(t)\rangle = x_0 + \int_0^t \mathrm{d}\tau\, I(\tau) \sim x_0 \ln(t). \tag{4}$$

Equation (4) gives only an order of magnitude of the correct result. The source of the difficulties to obtain an exact result is the approximate cut-off used to estimate the infinite sum appearing in (2). The Laplace representation eliminates the infinite sum and both $\langle S(t)\rangle$ and the form of the probability density $q(S, t)$, can be derived rigorously. It can be shown from (2) that:

$$\bar{\gamma}(S, s) \equiv \int_0^{\infty} \mathrm{e}^{-st} \gamma(S, t)\, \mathrm{d}t = \frac{\sinh(\sqrt{s/D}x_0)}{\sinh(\sqrt{s/D}S)}. \tag{5}$$

Using the properties of Laplace transform it can also be shown that $\bar{\Gamma}(S, s) = \bar{\gamma}(S, s)/s$. Thus, the Laplace transform of $q(S, t)$ is:

$$\bar{q}(S, s) = \frac{-1}{s} \frac{\partial \bar{\gamma}(S, s)}{\partial S} = \frac{1}{\sqrt{sD}} \frac{\sinh(\sqrt{s/D}x_0) \cosh(\sqrt{s/D}S)}{\sinh^2(\sqrt{s/D}S)}. \tag{6}$$

The Laplace transform of the mean area $\langle S(t)\rangle$ is:

$$\langle \bar{S}(s)\rangle = \int_{x_0}^{\infty} \mathrm{d}S\, S\bar{q}(S, s)$$
$$= \frac{x_0}{s} - \sqrt{\frac{D}{s^3}} \sinh\left(\sqrt{\frac{s}{D}}\, x_0\right) \ln \tanh\left(\frac{x_0}{2}\sqrt{\frac{s}{D}}\right) \tag{7}$$

and

$$\langle \bar{S}(s\to 0)\rangle = \frac{x_0}{s}\left(1 - \ln\left(\frac{x_0}{2}\sqrt{\frac{s}{D}}\right)\right).$$

Thus, in the large time limit we find:

$$\langle S(t\to\infty)\rangle = x_0\left\{1 + \ln\left(\frac{2\sqrt{D}}{x_0}\right) + \frac{\gamma}{2} + \frac{1}{2}\ln(t)\right\} \sim \frac{x_0}{2}\ln(t) \tag{8}$$

($\gamma = 0.577\,21\ldots$ is Euler's constant) in agreement with the qualitative result, equation (4).

To get a better understanding of the origin of this slow divergence, we study the asymptotic behaviour of the probability density $q(S, t)$ for a fixed and large time t. This can be found using the Laplace representation:

$$\bar{q}(S, s\to 0) = \frac{x_0}{D}\frac{\cosh(\sqrt{s/D}\, S)}{\sinh^2(\sqrt{s/D}\, S)}$$
$$= \begin{cases} \dfrac{x_0}{sS^2} & \text{if } S \ll \sqrt{D/s} \\ \dfrac{2x_0}{D}\mathrm{e}^{\sqrt{s/D}\, S} & \text{if } S \gg \sqrt{D/s}. \end{cases}$$

Thus the form of the probability density of the number of distinct sites for large t is:

$$q(S, t) = \begin{cases} \dfrac{x_0}{S^2} & \text{if } S \ll \sqrt{Dt} \\ \dfrac{x_0 S}{\sqrt{4\pi D^3 t^3}}\mathrm{e}^{-S^2/4Dt} & \text{if } S \gg \sqrt{Dt}. \end{cases} \tag{9}$$

It is seen that at $S \approx S_x \equiv \sqrt{Dt}$ there is a crossover from algebraic decay to a Gaussian decay. Thus the origin of the logarithmic dependence is due to:

$$\langle S(t\to\infty)\rangle = \int_{x_0}^{\infty} \mathrm{d}S\, Sq(S, t) \approx \int_{x_0}^{\sqrt{Dt}} \mathrm{d}S\, S\frac{x_0}{S^2} \sim \frac{x_0}{2}\ln(t). \tag{10}$$

It is interesting to compare this result to the average position of the surviving particles at time t. Using the probability density of the random walker in the presence of a single trap (see e.g. [6]):

$$p(x, t) = \frac{1}{\sqrt{4\pi Dt}}\left(\mathrm{e}^{-(x-x_0)^2/4Dt} - \mathrm{e}^{-(x+x_0)^2/4Dt}\right)$$

the survival probability density is:

$$p(t) = \int_0^{\infty} \mathrm{d}x\, p(x, t) = \Phi\left(\frac{x_0}{\sqrt{4Dt}}\right)$$

where $\Phi(x)$ is the probability integral. Thus, the conditional probability for the surviving random walker to be found at x at time t is: $p(x|t)=p(x,t)/p(t)$, and its average position is:

$$\langle x(t)\rangle = \int_0^\infty \mathrm{d}x\, x p(x,t) = \frac{x_0}{p(t)}.$$

For the long time limit of $p(t)$ it follows that

$$\langle x(t)\rangle \sim \sqrt{\pi D t}. \tag{11}$$

Thus we conclude that the average territory covered by the random walker in the presence of a trap is proportional to $x_0 \ln(t)$ in spite of the fact that the surviving random walkers at time t are located around $\sqrt{t}$ (regardless of x_0). This situation is significantly different from the free random walker case. If we define $S(t)$ as the right most point that a random walker, without a trap at $x=0$, visited up to time t, then a similar analysis gives the following trivial results:

$$p(x,t) = \frac{1}{2\sqrt{\pi D t}}\,\mathrm{e}^{-x^2/4Dt}$$

$$\bar{\gamma}(S,s) = \mathrm{e}^{-\sqrt{x^2/DS}}$$

$$q(S,t) = \frac{1}{\sqrt{\pi D t}}\,\mathrm{e}^{-S^2/4Dt}$$

$$\langle S(t)\rangle = \sqrt{\frac{4Dt}{\pi}}$$

$$\langle |x(t)|\rangle = \sqrt{\frac{4Dt}{\pi}}.$$

The reason for the significant difference between the results is that as time evolves, the number of surviving particles decreases due to the trap at the origin. This decrease is so strong that, in spite of the fact that the surviving particles are located around $\sqrt{\pi D t}$, they hardly affect the distribution $q(S,t)$ and the mean territory covered so far—$\langle S(t)\rangle$. When the trap is absent, all the particles survive, so both $\langle S(t)\rangle$ and $\langle |x(t)|\rangle$ have the same meaning and both are proportional to $\sqrt{t}$.

Another physical quantity that exhibits the strong effect of the trap is the average value of the first passage time to reach a location x, $\langle T(x)\rangle$. In general,

$$\langle T(x)\rangle = \frac{\int_0^\infty \mathrm{d}t\, t\gamma(x,t)}{\int_0^\infty \mathrm{d}t\, \gamma(x,t)} = \left[\frac{-\partial\bar{\gamma}(x,s)/\partial s}{\bar{\gamma}(x,s)}\right]_{s=0}. \tag{12}$$

For the free random walk one can easily find that $\langle T(x)\rangle \to \infty$ for any x. However, for a random walk in the presence of a trap one can find that:

$$\langle T(x)\rangle = \lim_{s\to 0} \frac{x\coth(\sqrt{s/D}\,x) - x_0\coth(\sqrt{s/D}\,x_0)}{\sqrt{4Ds}} = \frac{x^2 - x_0^2}{6D} \tag{13}$$

which is a finite quantity. This is due to the fact that for $t \gg x^2/D$ the system is static as can be seen from rewriting (9) in the following form:

$$q(x, t\to\infty) = \begin{cases} \dfrac{x_0}{x^2} & \text{if } t \gg x^2/D \\[2ex] \dfrac{x_0 x}{\sqrt{4\pi D^3 t^3}}\,\mathrm{e}^{-x^2/4Dt} & \text{if } t \ll x^2/D. \end{cases} \tag{14}$$

Thus $\langle T(x)\rangle$ essentially represents the crossover time in (14).

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