Lecture 19: Anomalous diffusion in disordered media

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Abstract

The physical mechanisms of sub-diffusion are overviewed. Long waiting times may occur for extended objects (polymers) diffusing through regular traps or regular objects through complicated traps (beads through a gel). Sinai's problem incorporates random transition rates and Kramer's escape problem incorporates random traps. The thermal phase transition from sub- to normal diffusion is examined for Kramer's escape from exponentially distributed wells. Percolation clusters are introduced and examples are given of random walks on a fractal set. Walk on a comb is formulated and walk on a Sierpinski gasket is shown to be sub-diffusive. Random walk of a tracer particle through arrays of fluid convection rolls is shown to be sub-diffusive. The non-separable continuous random walk is introduced.

1 Physical Mechanisms of sub-diffusion

$< \tau >= \infty$

Here we present several physical mechanisms for sub-diffusion: random walks in 1) disordered media, 2) fractal sets and 3) fluid mechanics.

1.1 Diffusion in disordered media

Long waiting times may occur for extended objects diffusing through regular traps. For example, polymer chains may experience long trapping times in gel electrophoresis (regular traps). Regular objects may also diffuse through complicated traps. An example is a bead in a polymer solution or gel.

Disorder may be introduced into physical problems through traps or transition rates. Sinai's problem incorporates random transition rates; Kramer's escape problem utilizes random traps.

Example 1. Sinai's problem

Consider the motion of a random walker in a random force field in one dimension [1]. We characterize this as a random walk on the integers (Fig. 1), with probability p of stepping to the right. Here p is the random variable, with $< p >= 1/2$. The result is that $< x^2 >\sim (\log t)^4$.

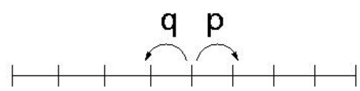
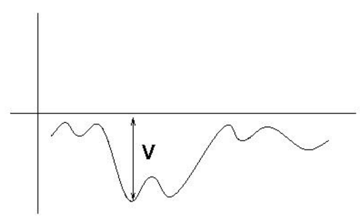


Figure 1: The Sinai problem is an example of a random walk with random transition rates. Here, the walk iis on the integers, with $< p >= 1/2$ and hence $< x^2 >\sim (\log t)^4$.

Example 2: Kramer's escape problem



Consider a random walk over potential wells of depth v shown above. In this example, we assume the probability of moving at each position decreases as the wells increase in depth:

$$p(v) = \frac{1}{v_0} e^{-v/v_0} \tag{1}$$

For the dimension $d \geq 3$, a return to same site is rare, and such a walk is called a "transient walk." At each step we typically sample a new well depth v independently [2]. Kramer studied the rate to escape, r_e. As $r_e \to 0$ and $\tau_e \to \infty$, we have the approximation

$$r_e \sim e^{-\frac{v}{kT}} \tag{2}$$

[1]G. Sinai, Theory Prob. Appl. 27, 256 (1982))

[2]M. Bekele, G. Ananthakrishan and N. Kumar. Mean first passage time approach to the problem of optimal barrier subdivision for Kramers escape rate. Physica A. 270, 149 (1999)

which is valid in the low kT limit. As a result, the mean waiting time to escape τ may be written as

$$\tau \sim \tau_0 e^{\frac{v}{kT} \sim 1/r_e} \tag{3}$$

where τ_0 is a characteristic time scale. Therefore, the PDF for the waiting time τ between steps may be written

$$\psi(\tau) \approx P(v)\frac{dV}{d\tau} \tag{4}$$

where the randomness in ψ is assumed to stem from v rather than τ. Using $v = kT\log(\frac{\tau}{\tau_0})$ we may express ψ as

$$\psi(\tau) \sim \frac{1}{v_0}\left(\frac{\tau}{\tau_0}\right)^{-\frac{kT}{v_0}}\frac{kT}{\tau} \tag{5}$$

$$\sim \frac{kT}{v_0\tau_0^{\frac{kT}{v_0}}}\frac{1}{\tau^{1+\frac{kT}{v_0}}} \tag{6}$$

Recall that sub-diffusion occurs if $0 < \gamma < 1$ and

$$\psi(\tau) \sim \frac{1}{t^{1+\gamma}} \tag{7}$$

$$< x^2 > \sim t^{\gamma} \tag{8}$$

$$< x > \sim 0 \tag{9}$$

Alternatively, normal diffusion occurs if $< \tau >< \infty$ and

$$\psi(\tau) = O(1/\tau^2) \tag{10}$$

In this Kramer's escape problem,

$$\gamma = \frac{kT}{v_0} \tag{11}$$

So, for $T < T_c = v_0/k$, have sub-diffusion with width $\sim e^{\frac{kt}{2v_0}}$. For $T > T_c$ we have normal diffusion with width $\sim \sqrt{\tau}$.

1.2 Random walks ($< \tau >< \infty$) on fractal sets

Here we consider random walks on sets with only certain spaces capable of being occupied.

- Percolation clusters

We model percolation as a random coloring of a simple lattice, cubic (Fig. 2) or triangular. We occupy each site in the lattice with probability p (Fig. 2). This process generates clusters of points. Here p may be considered as a concentration of particles so that we expect p fraction of the sites to be occupied.

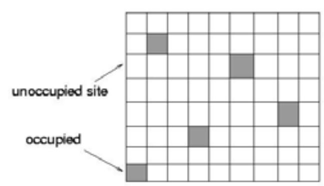


Figure 2: Percolation clusters on a square grid. The probability of occupying a site is p.

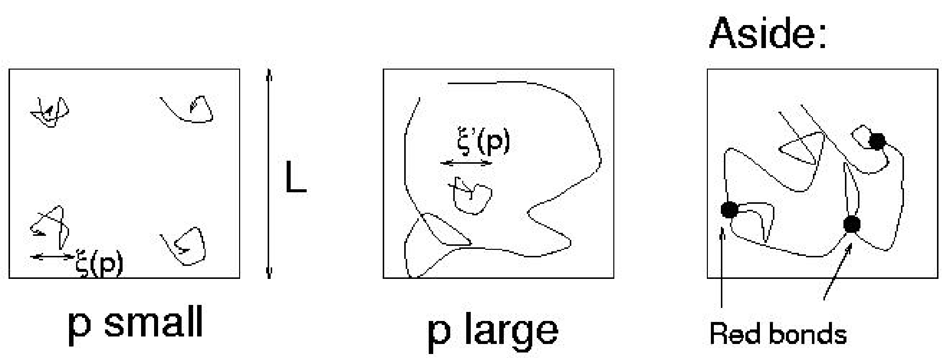


Figure 3: Percolation clusters. The clusters behavior changes from subcritical to supercritical at $p = p_c$. As the length scale of the domain increases, $L \to \infty$, then the second largest length scale $\xi'(p_c)$ also increases.(Aside: Red bonds are those that if cut, one loses spanning.)

The coloring may be described as subcritical or supercritical, as the probability p varies (Fig. 3). The length scale $\xi(p)$ is referred to as the correlation length, the length over which the probability that two points are part of the same cluster is greater than some fixed probability. For the subcritical case (small p), the length scale L of the domain is much larger than the length scale of the largest cluster, ξ: $L \gg \xi(p)$. The transition into the supercritical region occurs at $p = p_c$; the value of p_c varies with the domain under consideration. As $p \to p_c$, the correlation length $\xi \to \infty$. This occurs because two points arbitrarily far apart have a finite probability to be in the same cluster for $p = p_c$.

For the supercritical case, p is large enough that the random walker's trajectory reaches most of the domain. Therefore, the correlation length is meaningless, so we consider instead ξ', the length over which points have a finite probability o be connected but not through the largest cluster that spans the domain. Hence, $\xi'(p)$ is the second largest length scale for the walker's trajectory, and is much smaller than L: $L \gg \xi'(p)$. As the length scale of the domain increases, $L \to \infty$, then the second largest length scale $\xi'(p_c)$ also increases (Fig. 3).

At the critical occupational probability p_c, we have $L << \xi(p)$, and the largest clusters are random fractals (Fig. 4).

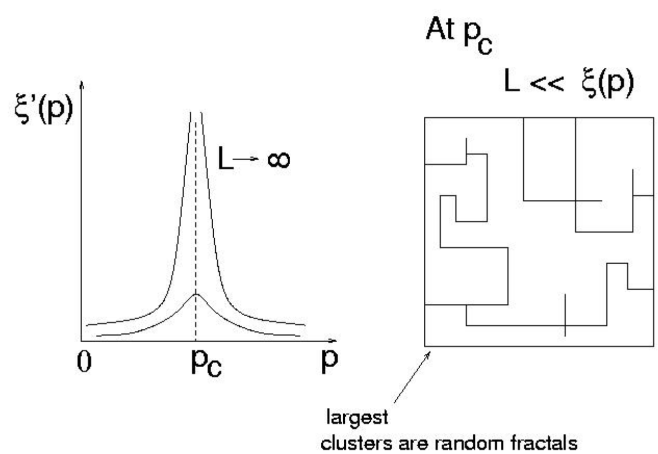


Figure 4: At the critical occupational probability p_c for percolation clusters to form, we have interesting behavior. Here, $L << \xi(p)$, and the largest clusters are random fractals.

Now we consider simulated walks on critical percolation clusters, fractals that appear for $p = p_c$. Diffusion in such heterogeneous media containing inhomogeneities of various scales has anomalous properties. We consider walks such that

$$< x^2 >\sim t^{2\nu}, \nu < 1/2 \tag{12}$$

Example: diffusion on a comb.

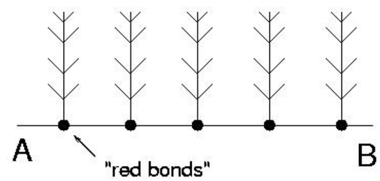


Figure 5: A random walk on a comb, in which $< \tau >= \infty$ on the side branches. The red bond are those that when cut, the walk loses spanning.

Consider a walk on a cluster represented as an infinitely extended backbone and a large number of lateral side branches[3] (Fig. 5). The later branches serve as traps where the particle spends most of its time: on these side branches, $< \tau >= \infty$.

Here, $\psi(t) = f(t) =$ first return time in branch.

Example: Walk on the Sierpinski gasket (a deterministic fractal)

First we define the fractal dimension. The fractal dimension D_f is a non-integer dimension described by the relation:Mass M = no. of sites = L^{D_f}

$$3M \sim 2L^{D_f} \tag{13}$$

$$3 = 2^{D_f} \Rightarrow D_f = \frac{\log 3}{\log 2} < 2 \tag{14}$$

Exact ("real-space") renormalization group analysis

A random walk on the Sierpinski gasket may be examined using this method

[3]a) E.W. Montroll and M.F. Schlesinger, in Studies in Statistical Mechanics, Vol. 11, J. Leibowitz and E.W. Motroll (eds.) North-Holland, Amsterdam (1984) p.1.
b). J.-P. Bouchard and A Georges, Phys. Rep. 195, 127 (1990).
c). M.B. Isichenko, Rev. Mod. Phys. 64, 961 (1992). d). Lubashevskii, I.A. and Zemlyanov, A.A. Continuum description of anomalous diffusion on a comb structure. J. Exp. Theor. Phys. 87 (4), 700 (1998).

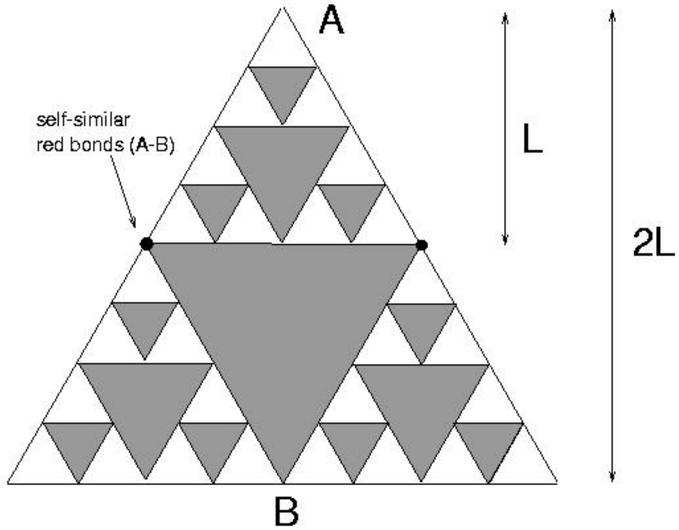


Figure 6: Sierpinski gasket. Random walk on this deterministic fractal may be studied using exact renormalization group analysis.

which exploits self similarity via recursions [4]. Here it is assumed that the characteristic length scale goes to infinity ($\xi \to \infty$ or $\xi \gg L$). Assume the mean first passage time τ to travel from one point to an adjacent one is known. One enters the triangle at the top vertex and exits at the lower right or lower left vertex. Let τ' be the time it takes to exit the triangle beginning from the entering point shown in Fig. 7. There are two kinds of points that the walker must pass through, labeled A and B. Note that in Fig. 7 there are two points labeled A. We calculate the time to exit τ'; the time a to exit given that we start from point A; and the time b to exit given that we start from point B. This gives us three equations, which we use to solve for the three unknowns, a, b, and τ' in terms of the known time τ. First we calculate a, the time to exit starting from point A (Fig. 8). There are four equally likely paths, $A1$ through $A4$, that a random walker at point A may take. So, $P(A1) = P(A2) = \cdots = 1/4$. The path $A1$ takes time $\tau + \tau'$ because it takes time τ to reach the starting point and time τ' to exit from the starting point. The path $A2$ takes time $\tau + a$ because it takes time τ to reach point A and time a to exit from point A. The path $A3$ takes time

[4]Goldstein, S. Random walks and diffusions on fractals. Percolation theory and ergodic theory of infinite particle systems. IMA Math. Appl., Vol. 8, Kesten, H. (ed.), Springer; Berlin, Heidelberg, New York (1987), 121–129). Also in: Barlow M.T., Perkins A., Brownian motion on the Sierpinski gasket, Probab. Th. Rel. Fields, 79 (1988) 543–623.

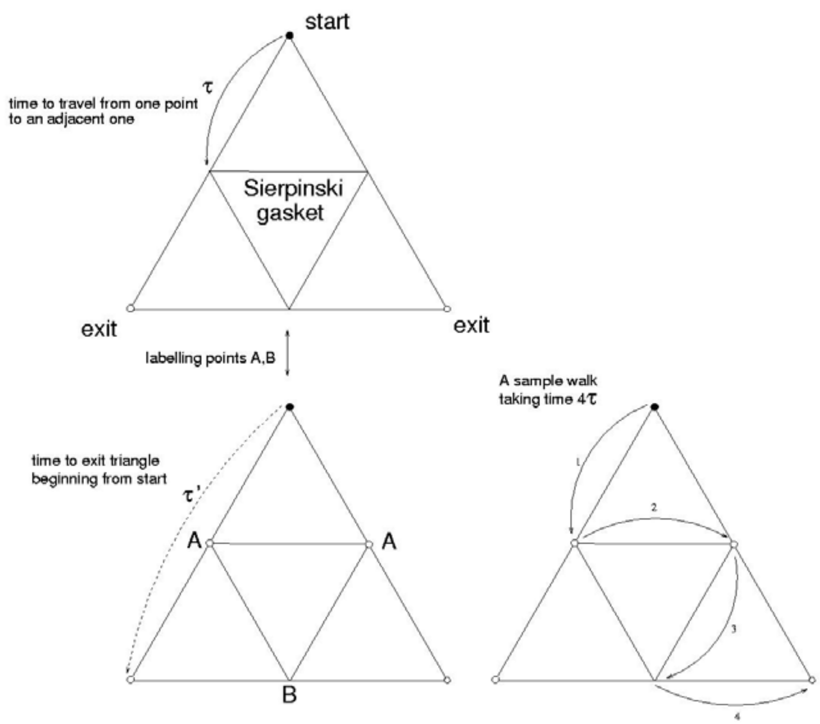


Figure 7: The walk on the Sierpinski gasket. The time to exit may be calculated using renormalization group analysis.

$\tau + b$ because it takes time τ to reach point B and time b to exit from point B. Lastly, the path $A4$ takes time τ because it takes time τ to reach the exit point. Hence, we may write the time a as

$$\begin{aligned} a &= E(\text{time to exit starting from } A) && (15)\\ &= P(A1)A1 + P(A2)A2 + P(A3)A3 + P(A4)A4 && (16)\\ &= \frac{1}{4}(\tau + \tau') + \frac{1}{4}(\tau + a) + \frac{1}{4}(\tau + b) + \frac{1}{4}\tau && (17)\\ &= \tau + \frac{1}{4}(\tau' + a + b) && (18) \end{aligned}$$

Similarly, we may calculate the time to escape b given a start from point B (Fig. 9). At point B, there are two possible kinds of paths, $B1$ and $B2$. So $P(B1) = P(B2) = 1/2$. Path $B1$ takes time τ to exit. Path $B2$ takes time $\tau + a$ to exit. Hence we may write

$$b = \frac{1}{2}\tau + \frac{1}{2}(\tau + a) \tag{19}$$

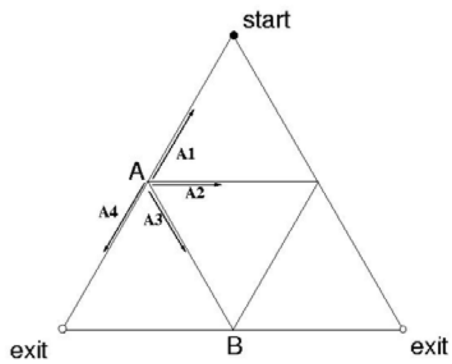


Figure 8: The possible paths that may occur in time a.

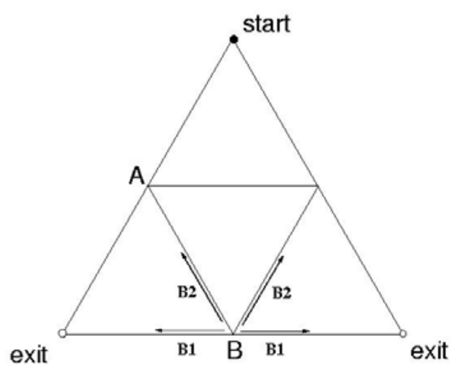


Figure 9: The possible paths that may occur in time b

Finally, we write τ', the time to exit beginning from the starting point. At the starting point, we may only travel to point A. Therefore,

$$\tau' = \tau + a \tag{20}$$

Using three equations (18),(19) and (20) to solve for three unknowns, we find

$$\tau' = 5\tau, \quad a = 4\tau, \quad b = 3\tau \tag{21}$$

We assume that the time τ is a function of the length of the triangle, L: $\tau(L) = L^{1/\nu}$. The time τ' is the time to exit the triangle of length $2L$. Together, $(2L)^{1/\nu} = \tau' = 5\tau = 5L^{1/\nu}$. Multiplying by ν gives

$$2L = 5^{\nu} L \tag{22}$$

where the coefficient ν satisfies $2 = 5^{\nu}$ and thus

$$\nu = \frac{\log 2}{\log 5} = \frac{1}{2.32} < 1/2 \qquad (23)$$

Hence, this a random walk through the Sierpinski gasket is a sub-diffusive process.

1.3 Experiment: advection-diffusion in a linear array of convection rolls

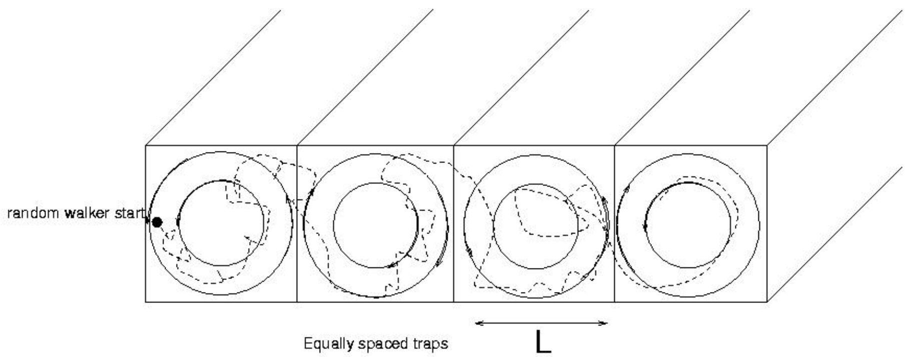


Figure 10: A tracer particle moving in a one-dimensional array of convection rolls undergoes convection and molecular diffusion (Bouchard and Georges, 1990). Different visits to a given roll lead to different diffusion histories; hence the total travel time t will be the sum of independent variables.

Consider the motion of a tracer particle in a one-dimensional array of convection rolls[5] (Fig. 12). The particle both convects along flow lines and undergoes molecular diffusion (D_0), which allows jumps between flow lines. The observation is that the rolls act as equally spaced traps with a release time distribution decaying as $\psi(\tau) = \tau^{-1+\mu}$ for $\tau \leq L2/D_0$ where L is the diameter of the roll. The return from finite interval may lead to sub-diffusion at smaller times

$$x^2 \sim t^{\gamma} \rightarrow t, \quad t \gg L^2/D \qquad (24)$$

Note in fluids, we often find superdiffusion with $\nu > 1/2$ How? The problem cannot be a Levy flight because $< \sigma^2 >= \infty$

[5] Bouchard, J.-P. Georges, A. Anomalous diffusion in disordered media: statistical mechanics, models and physical applications. Phys. Rep. 195:4 and 5, 127-293 (1990)

1.4 Experiment: n traps in a ring

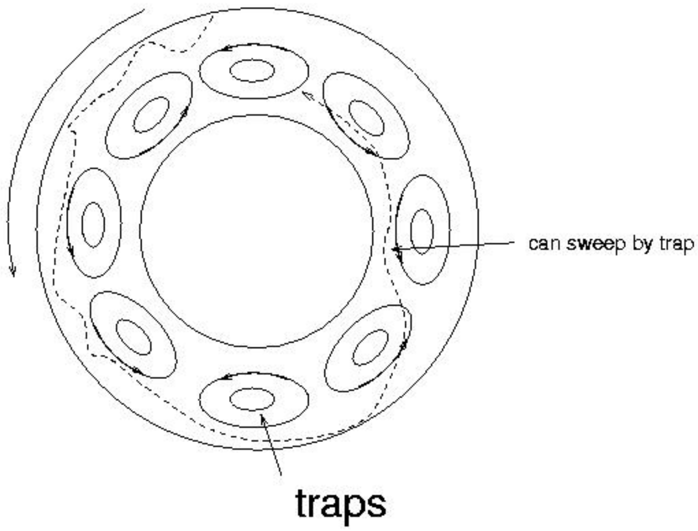


Figure 11: Solomon, Weeks, Swinney examined the chaotic transport of tracer particles laminar fluid flow through a circular chain of n vortices in a rotating annulus.

Solomon, Weeks, Swinney 1993[6] examined the chaotic transport of tracer particles laminar fluid flow through a circular chain of n vortices in a rotating annulus. Although the velocity field is laminar, passive tracers in the flow have chaotic trajectories, intermittently sticking near the vortices as in Bouchard Georges. They found that the variance of the displacement grows with time as t^γ with $\gamma = 1.65$. The flight times have power law distributions:

$$p(\text{passing n traps}) \sim \frac{1}{n^{1+\alpha}} \sim \frac{1}{t^{1+\alpha}} \tag{25}$$

where $\alpha \sim 1.3 < 2$, which indicates that the trajectories can be described quantitatively as Levy flights. Levy motion and anomalous diffusion has been analyzed theoretically[2] for model system and these analyses yield an exponent $\gamma = 3 - \alpha$, that is 1.65 should equal 1.33. Swinney et al state that the measured values of α and γ are in good accord with this relation when considering uncertainty in the exponent values.

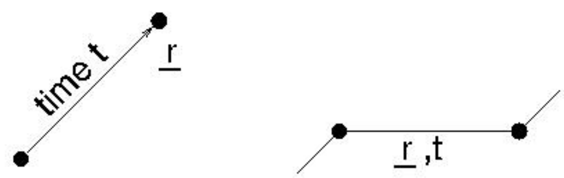
[6] T. H. Solomon, Eric R. Weeks, and Harry L. Swinney."Observation of anomalous diffusion and Levy flights in a two-dimensional rotating flow", "Observation of anomalous diffusion and Levy flights in a two-dimensional rotating flow", Phys. Rev. Lett. 71 3975-3978 (1993).

2 Non-separable CTRW

Now we introduce the non-separable continuous random walk (Lec 20) in which we will examine leapers and creepers. A step with size $\vec{r}$ and duration t has the joint PDF ϕ

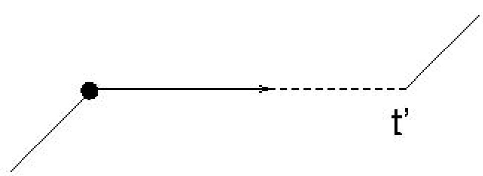
$$\phi(\vec{r}, t) \neq p(\vec{r})\psi(t) \tag{26}$$

That is the distributions for the waiting time ψ and step length p can no longer be separated. Each $\vec{r}$ and time t are random but not independent:



$$\phi = p(\vec{r}|t)\psi(t) \tag{27}$$

Let $\Psi(\vec{r}, t)$ be the PDF of a displacement $\vec{r}$ at time t since the last turning point and having taken no "steps".



Then

$$\Psi(\vec{r}, t) = p(\vec{r}|t) \int_t^{\infty} \psi(t')dt' \tag{28}$$

if the turning point has not been reached yet. Hence we only need $\psi(t), p(\vec{r}|t)$ to obtain ϕ and Ψ.