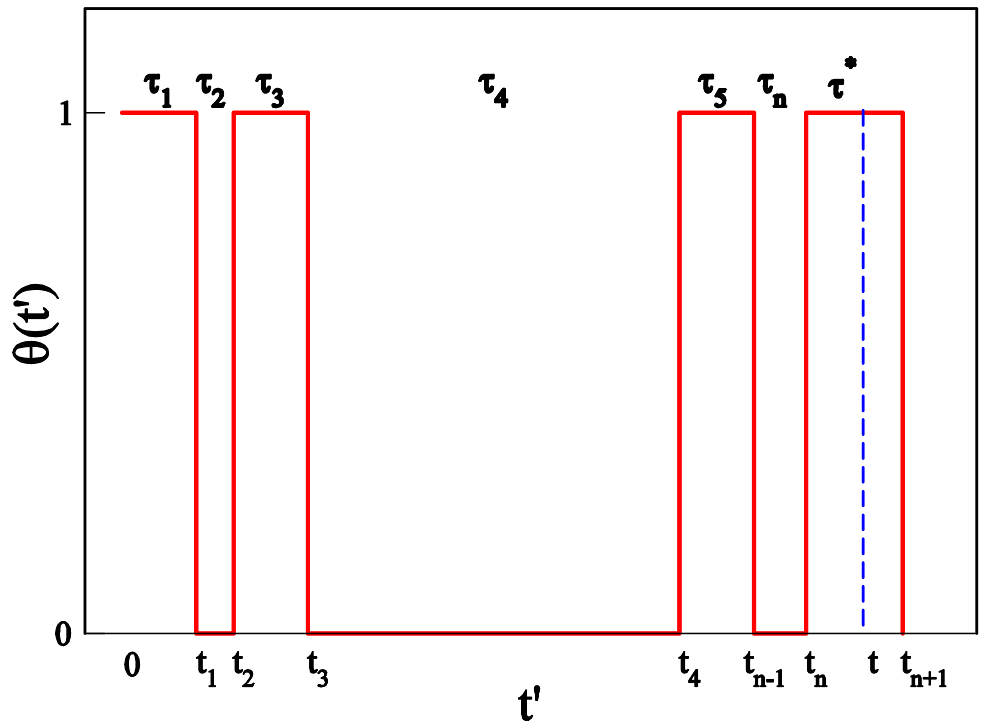

Figure 1: Schematic description of a typical 2-state process.

Occupation time in two-state processes

Many signals exhibit a two-state behavior. Examples include, ion channels switching between "open" state in which current flows through the channel and a "close" state in which no ion can translocate through the channel; and the emission from quantum dots excited by a continuous laser field switches between "on" state, in which many photons are emitted, and an "off" state, in which no photon is emitted. The simplicity of the "state space", namely the fact that there are only two states, makes this kind of processes ideal from pedagogical point of view. We consider a process jumping between an "on" state, $\theta(t) = 1$, and an "off" state, $\theta(t') = 0$. At time $t = 0$ the process starts at $\theta(t = 0) = 1$. Transitions between the states occur at random times, $t_i s$. The sojourn times in the "on" state are labeled with an odd index, $\tau_1, \tau_3, ..$ and the sojourn times in the "off" state are labeled with an even index, $\tau_2, \tau_4, ...$ as shown in the schematic diagram, Figure 1. All the sojourn times are mutually independent, identically distributed random variables characterized by their PDF $\psi(\tau)$. Clearly the above described process is a renewal process. First we analyze the time average of the function θ,

$$\overline{\theta} = \frac{\int\limits_0^t \theta\left(t'\right) dt'}{t}. \tag{1}$$

The time average is a random quantity because it depends on the random realization of the process. However, in the long time limit one may expect that the PDF of $\overline{\theta}$ converges into a delta function centered at $\overline{\theta} = 1/2$, due to the symmetry of the process. Note that the symmetry implies that the ensemble average $\langle\theta\rangle = 1/2$. By ensemble average we mean

$$\langle\theta\rangle = \frac{\sum\limits_{i=1}^{N} \theta_i}{N},$$

where θ_i is the value of θ in a given realization of the process (at any time, long after the process started and many transitions have occurred). The ergodic hypothesis conjectures that in the limit $N \to \infty$ and $t \to \infty$ the two types of average, time and ensemble, coincide. In what follows we will check under which conditions this conjecture holds for the process studied here.

$\overline{\theta} = \frac{T^+}{t}$, where T^+ is the time spent on state "+" (the occupation time of that state). If n, the number of switching events, is odd

$$T^+ = \sum_{k=0}^{\frac{n-1}{2}} \tau_{2k+1},$$

the summation is over the odd sojourn times. Let $f_t\left(T^+\right)$ be the PDF of T^+ and $f_{n,t}\left(T^+\right)$ be the PDF conditioned that n renewals occurred. We consider the case of odd n for which we write,

$$f_{n,t}\left(T^+\right) = \left\langle \delta\left(T^+ - \sum_{k=0}^{\frac{n-1}{2}} \tau_{2k+1}\right) I\left(t_n < t < t_{n+1}\right)\right\rangle; \tag{2}$$

Using s as the Laplace conjugate of t and u as the Laplace conjugate of T^+ we can write the double Laplace transform as,

$$\begin{aligned}\widehat{\widehat{f}}_{n,s}(u) &\equiv \int\limits_0^\infty e^{-st} \int\limits_0^\infty e^{-uT^+} f_{n,t}\left(T^+\right) dT^+ dt \qquad (3)\\ &= \left\langle \int\limits_0^\infty e^{-st} \int\limits_0^\infty e^{-uT^+} \delta\left(T^+ - \sum_{k=0}^{\frac{n-1}{2}} \tau_{2k+1}\right) I\left(t_n < t < t_{n+1}\right) dT^+ dt \right\rangle\end{aligned}$$

$$
\begin{aligned}
&= \left\langle \frac{e^{-st_n}-e^{-st_{n+1}}}{s} e^{-u\sum_{k=0}^{\frac{n-1}{2}}\tau_{2k+1}} \right\rangle \\
&= \left\langle \frac{e^{-s\sum_{i=1}^{n}\tau_i}-e^{-s\sum_{i=1}^{n+1}\tau_i}}{s} e^{-u\sum_{k=0}^{\frac{n-1}{2}}\tau_{2k+1}} \right\rangle \\
&= \left[\widehat{\psi}\left(s+u\right)\right]^{\frac{n+1}{2}}\left[\widehat{\psi}\left(s\right)\right]^{\frac{n-1}{2}}\frac{1-\widehat{\psi}\left(s\right)}{s}
\end{aligned}
$$

In the last line we used the fact that all the $\tau_i s$ are i.i.d.

The calculation for even n is slightly different due to the fact that the statistics of the last sojourn time is different, since it is the backward recurrence time and not a "regular" sojourn time. The details are not provided here but the final result is that for even n,

$$
\widehat{\widehat{f}}_{n,s}\left(u\right) = \left[\widehat{\psi}\left(s+u\right)\right]^{\frac{n}{2}}\left[\widehat{\psi}\left(s\right)\right]^{\frac{n}{2}}\frac{1-\widehat{\psi}\left(s+u\right)}{s+u}. \tag{4}
$$

Using the results above we find

$$
\widehat{\widehat{f}}_{s}\left(u\right) = \sum_{n=0}^{\infty}\widehat{f}_{n,s}\left(u\right) = \left[\frac{1-\widehat{\psi}\left(s+u\right)}{s+u}+\frac{1-\widehat{\psi}\left(s\right)}{s}\widehat{\psi}\left(s+u\right)\right]\frac{1}{1-\widehat{\psi}\left(s+u\right)\widehat{\psi}\left(s\right)}. \tag{5}
$$

For the case of a finite first moment we can obtain the asymptotic behavior by considering the limit of $s\to 0$

$$
\begin{aligned}
\widehat{\widehat{f}}_{s}\left(u\right) &\sim \frac{2}{\left(u+2s\right)} \to \widehat{f}_{s}\left(T_{+}\right) = 2e^{-2sT_{+}} \to f_{t}\left(T_{+}\right) = 2\delta\left(t-2T_{+}\right) = \delta\left(T_{+}-\frac{t}{2}\right) \quad (6) \\
p\left(\frac{T_{+}}{t}\right) &= tf_{t}\left(T_{+}\right) = t\delta\left(T_{+}-\frac{t}{2}\right) = \delta\left(\frac{T_{+}}{t}-\frac{1}{2}\right). \quad (7)
\end{aligned}
$$

Substituting in the expression above the Laplace transform of the form $\widehat{\psi}\left(s\right)\sim 1-As^{\alpha}$ (where $0<\alpha<1$) and considering the limit of $s\to 0, u\to 0$ and keeping their ratio arbitrary, we obtain

$$
\widehat{\widehat{f}}_{s}\left(u\right) \sim \frac{\left(s+u\right)^{\alpha-1}+s^{\alpha-1}}{\left(s+u\right)^{\alpha}+s^{\alpha}}. \tag{8}
$$

Inverting the double Laplace transform yields

$$
f\left(\overline{\theta}\right) \sim \frac{\sin\left(\pi\alpha\right)}{\pi}\frac{\overline{\theta}^{\alpha-1}\left(1-\overline{\theta}\right)^{\alpha-1}}{\overline{\theta}^{2\alpha}+\left(1-\overline{\theta}\right)^{2\alpha}+2\overline{\theta}^{\alpha}\left(1-\overline{\theta}\right)^{\alpha}\cos\left(\pi\alpha\right)}. \tag{9}
$$

For the case of finite waiting time we find,

$$
f\left(\overline{\theta}\right) \sim \delta\left(\overline{\theta}-1/2\right). \tag{10}
$$

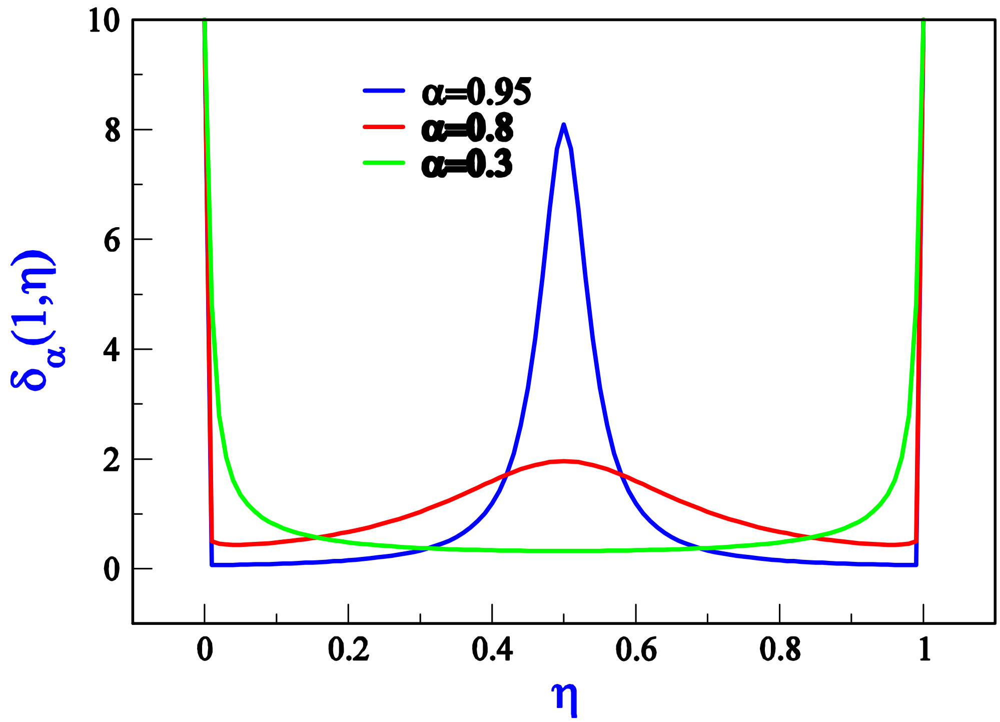

Figure 2: Plots of the PDF of the fraction of occupation time for different values of α. The transition between U shape and a W shape occurs at $\alpha = 0.5946$

The case of $\alpha = 1$ is marginal and is not considered here. For $\alpha = 1/2$ we find

$$f\left(\overline{\theta}\right) \sim \frac{1}{\pi} \frac{1}{\sqrt{\overline{\theta}\left(1-\overline{\theta}\right)}}, \tag{11}$$

whose cumulative distribution is given by the arcsine. Therefore, this distribution is known as the arcsine law.

Continuous Time Random Walk (CTRW)

The Continuous Time Random Walk (CTRW) was introduced by E. Montroll and G. H. Weiss in 1965. In the CTRW the waiting time between successive jumps is a random variable drawn from a PDF $\psi(\tau)$. Similarly, the displacement on each jump, $\Delta\mathbf{r}$, is drawn from a PDF $f(\Delta\mathbf{r})$. The displacements and the waiting times are mutually independent identically distributed (i.i.d.) random variables. Consider a particle starting in the origin at $t = 0$, waiting there for time τ_1 until at time $t_1 = \tau_1$ it jumps to site $\Delta\mathbf{r}_1$. Then the particle waits there for time τ_2 until it jumps to site $\Delta\mathbf{r}_1 + \Delta\mathbf{r}_2$ at time $t_2 = \tau_1 + \tau_2$ and so on. The first thing to notice about this process is that unlike the case of the discrete time random walk, which we considered so far, the number of jumps taken during a given time period t, is random and not a constant. This renewal process is sometimes called decoupled CTRW due to the decoupling of the displacements and the waiting times. The total displacement of the particle is $\mathbf{r} = \sum_{i=1}^{n} \Delta\mathbf{r}_i$, where n is the number of jumps. In order to characterize the process we would like to find, $p(\mathbf{r}, t)$, the PDF of finding the particle on $\mathbf{r}$ at time t. The following relation exists between the probability (or PDF) of finding the particle in position $\mathbf{r}$ after n steps $P_N(\mathbf{r})$, and $p(\mathbf{r}, t)$

$$p(\mathbf{r}, t) = \sum_{n=0}^{\infty} W(n, t)\, P_n(\mathbf{r}). \tag{12}$$

If the CTRW is on a lattice, then $p(\mathbf{r}, t)$ and $P_n(\mathbf{r})$ are probabilities, while for CTRW in a continuous space they are PDFs. $W(n, t)$ is the probability of making n steps in the time interval $[0, t]$. On our discussion of general renewal processes we found that the Laplace transform, $t \to s$, of $W(n, t)$ is

$$\widehat{W}(n, s) = \left[\widehat{\psi}(s)\right]^n \frac{1 - \widehat{\psi}(s)}{s}. \tag{13}$$

We have also found, in the context of discrete time random walks, that the Fourier transform of $P_n(\mathbf{r})$ is

$$\widetilde{P}_n(\mathbf{k}) = \left[\widetilde{f}(\mathbf{k})\right]^n. \tag{14}$$

Using equations (12), (13) and (14) we find the Fourier-Laplace transform of $p(\mathbf{r}, t)$,

$$\widehat{\widetilde{p}}(\mathbf{k}, s) = \sum_{n=0}^{\infty} \widehat{W}(n, s)\, \widetilde{P}_n(\mathbf{k}) = \frac{1 - \widehat{\psi}(s)}{s} \sum_{n=0}^{\infty} \left[\widehat{\psi}(s)\, \widetilde{f}(\mathbf{k})\right]^n.$$

Summing over n, we find

$$\widehat{\widetilde{p}}(\mathbf{k}, s) = \frac{1 - \widehat{\psi}(s)}{s} \frac{1}{1 - \widehat{\psi}(s)\, \widetilde{f}(\mathbf{k})}. \tag{15}$$

We used the inequality $\left|\widehat{\psi}(s)\, \widetilde{f}(\mathbf{k})\right| \le 1$ to justify the convergence of the sum. Eq. (15) is known as Montroll-Weiss equation and is an exact solution in the Fourier-Laplace space.

To illustrate the use of this equation, let us consider the 1D random walk on a lattice with jumps to the nearest neighbors (with equal probability) for which the sojourn time PDF is given by

$$\psi(\tau) = \Lambda e^{-\Lambda\tau} \to \widehat{\psi}(s) = \frac{\Lambda}{\Lambda + s}. \tag{16}$$

The PDF of the jumps is given by,

$$f(\Delta x) = \frac{1}{2}\left[\delta(\Delta x - 1) + \delta(\Delta x + 1)\right] \rightarrow \widetilde{f}(k) = \frac{1}{2}\left(e^{ik} + e^{-ik}\right) = \cos(k). \tag{17}$$

Therefore,

$$\widehat{\widetilde{p}}(k,s) = \frac{1 - \frac{\Lambda}{\Lambda+s}}{s}\frac{1}{1 - \frac{\Lambda}{\Lambda+s}\cos(k)} = \frac{1}{\Lambda(1-\cos(k)) + s}. \tag{18}$$

Inverting the Laplace transform we find

$$\widetilde{p}(k,t) = e^{-\Lambda(1-\cos(k))t}. \tag{19}$$

Inverting the Fourier transform we find

$$\begin{aligned}
p(m,t) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ikm} e^{-\Lambda(1-\cos(k))t} dk \\
&= \frac{e^{-\Lambda t}}{2\pi}\int_{-\pi}^{\pi} e^{ikm} e^{\Lambda t\cos(k)} dk \\
&= \frac{e^{-\Lambda t}}{2\pi}\sum_{n=0}^{\infty}\frac{(\Lambda t)^n}{n!}\int_{-\pi}^{\pi} e^{ikm}\left(\cos(k)\right)^n dk \\
&= \frac{e^{-\Lambda t}}{2\pi}\sum_{n=0}^{\infty}\frac{(\Lambda t)^n}{n!}\sum_{l=0}^{n}\frac{n!}{l!\,(n-l)!}\left(\frac{1}{2}\right)^n\int_{-\pi}^{\pi} e^{-ik(n-2l-m)} dk \\
&= e^{-\Lambda t}\sum_{n=0}^{\infty}\frac{(\Lambda t)^n}{n!}\sum_{l=0}^{n}\frac{n!}{l!\,(n-l)!}\left(\frac{1}{2}\right)^n \delta_{l,\frac{n-m}{2}} \\
&= e^{-\Lambda t}\sum_{n=0}^{\infty}\frac{(\Lambda t)^n}{\left(\frac{n-m}{2}\right)!\left(\frac{n+m}{2}\right)!}\left(\frac{1}{2}\right)^n
\end{aligned}$$

Changing the summation variable according to $k = (n-m)/2$ and accounting for the parity condition

$$\begin{aligned}
&= e^{-\Lambda t}\sum_{k=0}^{\infty}\frac{(\Lambda t/2)^{m+2k}}{k!(m+k)!}; \\
p(m,t) &= e^{-\Lambda t} I_m(\Lambda t),
\end{aligned} \tag{20}$$

where $I_m(\Lambda t)$ is the modified Bessel function.

The moments of CTRW

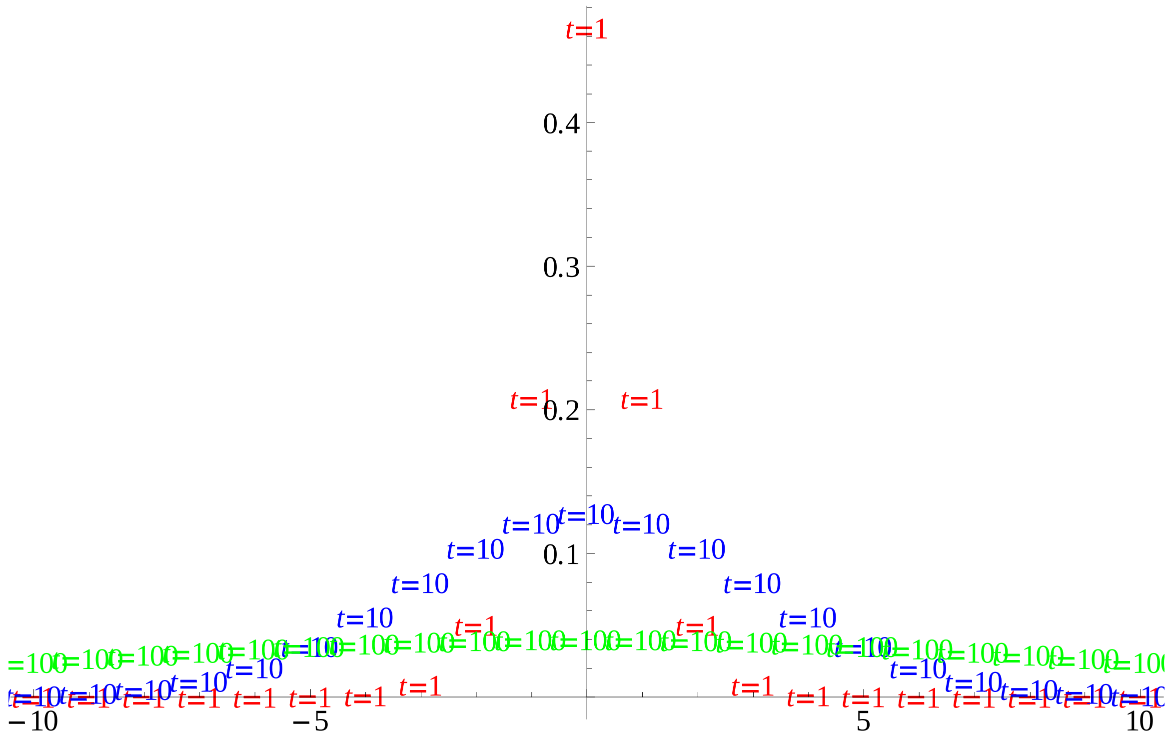

Figure 3: $p(m,t)$ with $\Lambda = 1$ for different times, $t = 1, t = 10, t = 100$ as indicated in the figure.

Getting back to the more general case, we turn to calculate the moments of the CTRW. If the average displacement in a single jump is non zero, $\int_{dV} f(\Delta\mathbf{r})\,\Delta\mathbf{r}\,d\Delta\mathbf{r} = \langle\Delta\mathbf{r}\rangle$, we expect an overall drift, $\langle\mathbf{r}\rangle \neq 0$. Using eq. (15) we find

$$\begin{aligned}
\langle\widehat{\mathbf{r}}(s)\rangle &= \frac{1}{i}\frac{d}{d\mathbf{k}}\widehat{\widetilde{p}}(\mathbf{k},s)\,|_{\mathbf{k}=0} \\
&= \frac{1}{i}\frac{1-\widehat{\psi}(s)}{s}\frac{\widehat{\psi}(s)}{\left[1-\widehat{\psi}(s)\widetilde{f}(\mathbf{k}=\mathbf{0})\right]^2}\frac{d}{d\mathbf{k}}\widetilde{f}(\mathbf{k})\,|_{\mathbf{k}=0} \\
&= \frac{\widehat{\psi}(s)\langle\Delta\mathbf{r}\rangle}{s\left[1-\widehat{\psi}(s)\right]}.
\end{aligned} \tag{21}$$

On our discussion of renewal processes, we found that the Laplace transform of the average number of jumps is:

$$\langle\widehat{n}(s)\rangle = \frac{\widehat{\psi}(s)}{s\left[1-\widehat{\psi}(s)\right]}.$$

Hence,

$$\langle\widehat{\mathbf{r}}(s)\rangle = \langle\widehat{n}(s)\rangle\langle\Delta\mathbf{r}\rangle.$$

In the time domain we may express it as:

$$\langle\mathbf{r}(t)\rangle = \langle n(t)\rangle\langle\Delta\mathbf{r}\rangle.$$

As expected (for decoupled CTRW), the mean displacement is equal to the average number of jumps times the average displacement in a single jump. A similar analysis for the mean square displacement yields,

$$\begin{aligned}
\left\langle\widehat{\mathbf{r}}^2(s)\right\rangle &= -\frac{d^2}{d\mathbf{k}^2}\widehat{\widetilde{p}}(\mathbf{k},s)\,|_{\mathbf{k}=0} \\
&= -\frac{d}{d\mathbf{k}}\left[\frac{1-\widehat{\psi}(s)}{s}\frac{\widehat{\psi}(s)}{\left[1-\widehat{\psi}(s)\widetilde{f}(\mathbf{k})\right]^2}\frac{d}{d\mathbf{k}}\widetilde{f}(\mathbf{k})\right] \\
&= -\frac{1-\widehat{\psi}(s)}{s}\frac{\widehat{\psi}(s)}{\left[1-\widehat{\psi}(s)\widetilde{f}(\mathbf{k})\right]^2}\frac{d^2}{d\mathbf{k}^2}\widetilde{f}(\mathbf{k})\,|_{\mathbf{k}=\mathbf{0}} \\
&\quad -\frac{1-\widehat{\psi}(s)}{s}\frac{2\left[\widehat{\psi}(s)\right]^2}{\left[1-\widehat{\psi}(s)\widetilde{f}(\mathbf{k})\right]^3}\left(\frac{d}{d\mathbf{k}}\widetilde{f}(\mathbf{k})\right)^2|_{\mathbf{k}=\mathbf{0}} \\
&= \frac{\widehat{\psi}(s)\left\langle\Delta\mathbf{r}^2\right\rangle}{s\left[1-\widehat{\psi}(s)\right]} + \frac{2\left[\widehat{\psi}(s)\right]^2\langle\Delta\mathbf{r}\rangle^2}{s\left[1-\widehat{\psi}(s)\right]^2}
\end{aligned}$$

$$\left\langle \mathbf{r}^2(s) \right\rangle = \langle \widehat{n}(s) \rangle \left\langle \Delta\mathbf{r}^2 \right\rangle + \langle \widehat{n}(s)(\widehat{n}(s)-1) \rangle \langle \Delta\mathbf{r} \rangle^2, \tag{22}$$

where we used

$$\begin{aligned}
\langle \widehat{n}(s)(\widehat{n}(s)-1) \rangle &= \sum_{n=0}^{\infty} n(n-1)\widehat{W}(n,s) \\
&= \frac{1-\widehat{\psi}(s)}{s} \sum_{n=0}^{\infty} n(n-1)\left[\widehat{\psi}(s)\right]^n \\
&= \frac{1-\widehat{\psi}(s)}{s} \left[\widehat{\psi}(s)\right]^2 \frac{d^2}{d\widehat{\psi}(s)^2} \sum_{n=0}^{\infty} \left[\widehat{\psi}(s)\right]^n \\
&= \frac{1-\widehat{\psi}(s)}{s} \left[\widehat{\psi}(s)\right]^2 \frac{d^2}{d\widehat{\psi}(s)^2} \frac{1}{1-\widehat{\psi}(s)} \\
&= \frac{1-\widehat{\psi}(s)}{s} \left[\widehat{\psi}(s)\right]^2 \frac{d}{d\widehat{\psi}(s)} \frac{1}{\left[1-\widehat{\psi}(s)\right]^2} \\
&= \frac{2\left[\widehat{\psi}(s)\right]^2}{s\left[1-\widehat{\psi}(s)\right]^2}.
\end{aligned}$$

Eq. (22) tells us that there are two contributions to the MSD. The first comes from the fluctuations in the single step length and the second one stems from the fluctuations in the number of steps. Now we will consider again two cases

$$\widehat{\psi}(s) \sim_{s\to 0} \begin{cases} 1-\langle\tau\rangle s & \text{case1} \\ 1-As^{\alpha} \quad 0<\alpha<1 & \text{case2} \end{cases}.$$

The mean displacement is

$$\langle \widehat{\mathbf{r}}(s) \rangle \sim_{s\to 0} \begin{cases} \frac{\langle \Delta\mathbf{r} \rangle}{\langle\tau\rangle s^2} & \text{case1} \\ \frac{\langle \Delta\mathbf{r} \rangle}{As^{\alpha+1}} & \text{case2} \end{cases}.$$

Hence, according to the Tauberian theorem

$$\langle \mathbf{r}(t) \rangle \sim_{t\to\infty} \begin{cases} \frac{\langle \Delta\mathbf{r} \rangle t}{\langle\tau\rangle} & \text{case1} \\ \frac{\langle \Delta\mathbf{r} \rangle t^{\alpha}}{A\Gamma(1+\alpha)} & \text{case2} \end{cases}.$$

When the mean waiting time diverge, the drift is anomalous. For the unbiased CTRW, , we find that the MSD is

$$\left\langle \widehat{\mathbf{r}}^2(s) \right\rangle \sim_{s\to 0} \begin{cases} \frac{\left\langle \Delta\mathbf{r}^2 \right\rangle}{\langle\tau\rangle s^2} & \text{case1} \\ \frac{\left\langle \Delta\mathbf{r}^2 \right\rangle}{As^{1+\alpha}} & \text{case2} \end{cases}.$$

In the time domain it has the following limiting behavior

$$\left\langle \mathbf{r}^2(t) \right\rangle \sim_{t\to\infty} \begin{cases} \frac{\left\langle \Delta\mathbf{r}^2 \right\rangle}{\langle\tau\rangle} t & \text{case1} \\ \frac{\left\langle \Delta\mathbf{r}^2 \right\rangle t^{\alpha}}{A\Gamma(1+\alpha)} & \text{case2} \end{cases}.$$

When the mean waiting time diverges the diffusion is anomalous and is slower than the normal diffusion. When the diffusion exponent is smaller than 1 the process is called sub-diffusion. Examples of diverging mean waiting time include bid diffusion in F-Actin, diffusion of mRNA inside the cell and the dynamics of lipid granules inside living cells.