I. CONTINUOUS TIME RANDOM WALK

The continuous time random walk (CTRW) was introduced by Montroll and Weiss[1]. Unlike discrete time random walks treated so far, in the CTRW the number of jumps n made by the walker in a time interval $(0, t)$ is a random variable. Considers a random walker which starts on the origin at time $t = 0$. It stays fixed to its position until time t_1, it then makes a jump to $\Delta\mathbf{r}_1$, the particle waits on $\Delta\mathbf{r}_i$ until time $t_2 > t_1$ when its jumps to a new location $\Delta\mathbf{r}_1 + \Delta\mathbf{r}_2$, the process is then renewed. The dots on the time axis $\{t_1, t_2, \cdots\}$ define the times of jumping events. The times $\tau_1 = t_1 - 0$, $\tau_2 = t_2 - t_1$ etc are called waiting times. In the CTRW the waiting times $\{\tau_1, \tau_2 ...\}$ and the displacements $\{\Delta\mathbf{r}_1, \Delta\mathbf{r}_2 ...\}$ are mutually independent identically distributed random variables. The waiting times have a common PDF denoted with $\psi(\tau)$ and the displacements also have a common PDF $f(\Delta\mathbf{r})$. Such a random walk is sometimes called a decoupled CTRW, since the jump lengths are statistically independent of the waiting times. The process is a renewal process and mathematics of previous chapter can be used to analyze the CTRW process.

The total displacement of the particle at time t is

$$\mathbf{r} = \sum_{i=1}^{n} \Delta\mathbf{r}_i \tag{1}$$

and n is the random number of jumps in the interval $(0, t)$. Let $P(t; n)$ be the probability for n jump events in time t. One of our goals is to calculate $P(\mathbf{r}, t)$, the PDF of finding the particle on $\mathbf{r}$ at time t. We obviously have

$$P(\mathbf{r}, t) = \sum_{n=0}^{\infty} P(t; n) P_n(\mathbf{r}), \tag{2}$$

and $P_n(\mathbf{r})$ is the PDF of finding the particle at $\mathbf{r}$ after n jumps. If the random walk is on a lattice then $P(\mathbf{r}, t)$ and $P_n(\mathbf{r})$ are probabilities of finding the particle at lattice point $\mathbf{r}$, not PDFs.

We have obtained already the Laplace $t \to s$ transform of $P(t;n)$ in the context of renewal theory

$$\hat{P}(s;n) = \frac{1-\hat{\psi}(s)}{s}\hat{\psi}^n(s) \tag{3}$$

where

$$\hat{\psi}(s) = \int_0^\infty e^{-st}\psi(t)\,\mathrm{d}t. \tag{4}$$

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

$$\tilde{f}(\mathbf{k}) = \tilde{f}^n(\mathbf{k}). \tag{5}$$

Here we use the d dimensional Fourier transform, with integration over all space

$$\tilde{f}(\mathbf{k}) = \int_V e^{i\mathbf{k}\Delta\mathbf{r}} f(\Delta\mathbf{r})\,\mathrm{d}\Delta\mathbf{r}. \tag{6}$$

For the case of lattice random walks proper replacement of Fourier integrals with Fourier series must be made.

Using Eqs. (2,3,5) we have the Fourier–Laplace transform of $P(\mathbf{r},t)$

$$\hat{\tilde{P}}(\mathbf{k},t) = \sum_{n=0}^{\infty}\frac{1-\hat{\psi}(s)}{s}\hat{\psi}^n(s)\,\tilde{f}^n(\mathbf{k}) \tag{7}$$

thus obtaining

$$\hat{\tilde{P}}(\mathbf{k},s) = \frac{1-\hat{\psi}(s)}{s}\frac{1}{1-\hat{\psi}(s)\,\tilde{f}(\mathbf{k})} \tag{8}$$

where we used the inequality $|\hat{\psi}(s)\,\tilde{f}(\mathbf{k})| \le 1$ to justify the convergence of the series. Eq. (8) is called the Montroll–Weiss equation and is an exact solution in Fourier–Laplace space.

4.1 Consider the CTRW on a one dimensional lattice, where jumps are to nearest neighbors with equal probability, when $\psi(\tau) = \exp(-\Lambda t)$. Show that the probability of finding the particle on lattice site m is

$$P(m,t) = \sum_{n=0}^{\infty}\frac{(\Lambda t)^n e^{-\Lambda t}}{n!}\left(\frac{1}{2}\right)^n \frac{n!}{\left(\frac{n-m}{2}\right)!\left(\frac{n+m}{2}\right)!} \tag{9}$$

when the random walk started on origin $m = 0$. Show that this solution has a Gaussian behavior for long times. Also use Fourier inversion and the integral

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ikm+\Lambda t\cos k\mathrm{d}k} = I_m\left(\lambda t\right) \tag{10}$$

where $I_m\left(x\right)$ is a modified Bessel function, to show that

$$P\left(m,t\right) = e^{-\Lambda t} I_m\left(\Lambda t\right). \tag{11}$$

A. Moments

If the averaged displacement in a single jump is non-zero $\langle\Delta\mathbf{r}\rangle = \int_V \Delta\mathbf{r} f\left(\Delta\mathbf{r}\right)\mathrm{d}\Delta\mathbf{r} \neq 0$ we expect a net drift $\langle\mathbf{r}\rangle \neq 0$. This displacement can be found based on the Montroll–Weiss equation using the small $\mathbf{k}$ expansion

$$\hat{\tilde{P}}\left(\mathbf{k},s\right) \sim 1 + i\mathbf{k}\langle\mathbf{r}(s)\rangle + \cdots \tag{12}$$

hence

$$-i\frac{\partial}{\partial\mathbf{k}} P\left(\mathbf{k},s\right)|_{\mathbf{k}=0} = \langle\mathbf{r}\left(s\right)\rangle. \tag{13}$$

We find using Eq. (8)

$$\langle\mathbf{r}\left(s\right)\rangle = \frac{\hat{\psi}\left(s\right)}{s\left[1-\hat{\psi}\left(s\right)\right]}\langle\Delta\mathbf{r}\rangle, \tag{14}$$

where the identity $-i\partial\tilde{f}(\mathbf{k})/\partial\mathbf{k}|_{\mathbf{k=0}} = \langle\Delta\mathbf{r}\rangle$ was used. We recall from previous chapter that the Laplace transform of the averaged number of jumps is

$$\langle n(s)\rangle = \sum_{n=0}^{\infty} nP(s;n) = \frac{1-\hat{\psi}(s)}{s}\sum_{n=0}^{\infty} n\hat{\psi}^n(s) = \frac{\psi(s)}{s\left[1-\hat{\psi}\left(s\right)\right]}. \tag{15}$$

And hence

$$\langle\mathbf{r}\left(s\right)\rangle = \langle\hat{n}\left(s\right)\rangle\langle\Delta\mathbf{r}\rangle, \tag{16}$$

thus as expected the mean displacement of the random walker is the average number of steps times the average displacement of a single step, namely in the time domain $\langle \mathbf{r}(t) \rangle = \langle n(t) \rangle \langle \Delta \mathbf{r} \rangle$.

A similar analysis for the mean square displacement using

$$\langle \mathbf{r}^2(s) \rangle = -\frac{\mathrm{d}^2}{\mathrm{d}\mathbf{k}^2} \tilde{\hat{P}}(\mathrm{k}, s) \,|_{\mathbf{k}=0} \tag{17}$$

yields

$$\langle \mathbf{r}^2(s) \rangle = \langle \hat{n}(s) \rangle \langle \Delta \mathbf{r}^2 \rangle + \langle n(n \hat{-} 1)(s) \rangle \langle \Delta \mathbf{r} \rangle^2 \tag{18}$$

where

$$\langle n(n \hat{-} 1)(s) \rangle = \sum_{n=0}^{\infty} n(n-1) P(s;n) = \frac{1-\hat{\psi}(s)}{s} \sum_{n=0}^{\infty} n(n-1) \hat{\psi}^n(s) = \frac{1-\hat{\psi}(s)}{s} \hat{\psi}^2(s) \frac{\mathrm{d}^2}{\mathrm{d}\hat{\psi}(s)^2} \frac{1}{1-\hat{\psi}(s)} = 2 \frac{\hat{\psi}^2(s)}{s \left[1-\hat{\psi}(s)\right]^2}. \tag{19}$$

Eq. (18) tells us that there are two types of contributions to the mean square displacement, the first stemming from fluctuations in the length of the individual microscopical displacements, the other from fluctuations in the number of displacements.

We now assume that

$$\hat{\psi}(s) \sim \begin{cases} 1 - s\langle \tau \rangle & \text{Case1} \\ 1 - s^{\alpha} A & \text{Case2} \end{cases} \tag{20}$$

when $s \to 0$. Here usual $\langle \tau \rangle$ is the average waiting time and for case 2 $\psi(\tau) \propto \tau^{-1-\alpha}$ with $0 < \alpha < 1$ hence the average waiting time is infinite.

The small s behavior of the displacement is

$$\langle \mathbf{r}(s) \rangle \sim \begin{cases} \frac{\langle \Delta \mathbf{r}}{s^2 \langle \tau \rangle} \rangle & \text{Case1} \\ \frac{\langle \Delta \mathbf{r} \rangle}{A s^{1+\alpha}} & \text{Case2} \end{cases} \tag{21}$$

Hence according to the Tauberian theorem

$$\langle \mathbf{r}\,(s)\rangle \sim \begin{cases} \langle \Delta \mathbf{r}\rangle \frac{t}{\langle \tau\rangle} & \text{Case1} \\ \langle \Delta \mathbf{r}\rangle \frac{t^{\alpha}}{A\Gamma(1+\alpha)} & \text{Case2.} \end{cases} \tag{22}$$

The drift is anomalous for the case when the averaged waiting diverges.

We now consider the mean square displacement for unbiased CTRW, when the averaged displacement is zero $\langle \Delta \mathbf{r}\rangle = 0$. Then we have $\langle r^2(s)\rangle = \langle n\,(s)\rangle\langle \Delta \mathbf{r}^2\rangle$ and

$$\langle \mathbf{r}^2\,(t)\rangle \sim \begin{cases} \frac{\langle \Delta \mathbf{r}^2}{\langle \tau\rangle}\rangle t & \text{Case1} \\ \frac{\langle \Delta \mathbf{r}\rangle}{A\Gamma(1+\alpha)} t^{\alpha} & \text{Case2.} \end{cases} \tag{23}$$

We see that when waiting time PDF has a long tailed PDF, the diffusion is anomalous, and slower than the normal diffusion case. Such a diffusion process is called sub-diffusion, which is not rare in Physical systems.

II. PHYSICAL EXAMPLE FOR $\psi\,(\tau)$

The CTRW is a stochastic model for which $\psi\,(\tau)$ and $f\,(\Delta \mathbf{r})$ serve as input functions. To relate the model to physical behavior we have to obtain further insight on these two functions. The main difficulty is to justify the power law tailed waiting time PDF $\psi\,(\tau) \propto \tau^{-1-\alpha}$. There are two types of approaches to gain understanding on the meaning of $\psi\,(\tau)$. The first case is for random walks in disordered materials, a case relevant for example for transport in doped semi-conductors. The second case, considers experiments where the behavior of the random walker mimics very closely the dynamics of the CTRW.

Polymer physics Wong et al studied the motion of colloidal tracer particle in an entangled F-actin filament networks (F-actin is a semi-flexible polymer). These networks, embedded in water, have a typical mesh size ξ of order 100 nm - 1 μm. These networks of polymers are important for cellular activity, and as such have attracted considerable research efforts. The radius of the bead is a and importantly it can be controlled by the experimentalist. When $a \ll \xi$ the small bead does not interact with the polymer network and the the bead exhibits a normal Brownian motion. One can imagine this situation as an atom diffusing in a ball of soap (water) and in this soap we have some spaghetti, the atom can easily diffuse around the obstacles (i.e. the spaghetti or the polymers) and hence it motion is still Brownian. When $a > \xi$, the bead cannot penetrate through the network, in this case it is localized in space (with some small thermal fluctuations). The interesting case is $a \simeq \xi$. The authors[6] define waiting time PDFs $\psi(\tau)$ in local cages composed of actin filaments. Using video tracking techniques they show that $\psi(\tau) \sim \tau^{-1-\alpha}$ where the power law behavior is over three orders of magnitude in time and five orders in the PDF. They then show that the mean square displacement of the bead particles behave like $\langle x^2 \rangle \sim t^\alpha$ (the measurement is along one coordinate). Such a behavior is predicted by the unbiased CTRW. Interestingly the authors show (very roughly) that

$$\alpha \simeq \begin{cases} 1 - \frac{a}{\xi} & a/\xi < 1 \\ 0 & a/\xi > 1 \end{cases} \tag{24}$$

Thus when $a/\xi \to 0$ we have normal diffusion and $\alpha = 1$, and as mentioned then the bead interacts only with the water. In the other limit $a/\xi > 0$ we have localization behavior. A detailed microscopic theory which could explain the transition between these two behaviors is still missing.

III. CTRW PROPOGATOR

We now consider the one dimensional CTRW, with displacements Δx (instead of $\mathbf{\Delta} r$) whose PDF is $f(\Delta x)$. We are interested in $P(x,t)$ the probability of finding the particle on

x at time t in the limit of long times. Extension of our results to higher dimensions is in principle straight forward (see[8]). We will assume for simplicity that the variance of $f(\Delta x)$ is finite, and its mean is zero. The variance is denoted with $\sigma^2 = \int_{-\infty}^{\infty} (\Delta x)^2 f(\Delta x) \mathrm{d}\Delta x$.

Before treating the asymptotic in detail let us give some hand waiving ideas on the long time behavior of the problem. As we mentioned already

$$P(x,t) = \sum_{n=0}^{\infty} P_n(t) P(n;x). \tag{25}$$

In the limit of long times we expect that the number of jumps is large hence since only trajectories with large n are important, and position of particle after n steps is $x = \sum_{i=0}^{n} \Delta x_i$, we expect that $P(n;x)$ is Gaussian. Hence we make the replacement

$$P(n;x) \to \frac{1}{\sqrt{2\pi\sigma^2 n}} \exp\left(-\frac{x^2}{2\sigma^2 n} \right) \equiv G(n,x) \tag{26}$$

which is the Gaussian central limit theorem. The number of steps is fluctuating according to our findings in previous chapter on fractal renewal theorem. If the waiting time PDF is moment less, then we found in the limit of long times that the probability of making n jumps is described using the inverse Lévy function

$$P(n;t) \to \frac{1}{\alpha} \frac{t}{n^{1+1/\alpha}} l_{\alpha,1,1} \left(\frac{t}{n^{1/\alpha}} \right) \equiv Il_{\alpha}\left(t;n\right) \tag{27}$$

when $A = 1$ for simplicity. Hence we expect in the limit of long times

$$P(x,t) \sim \int_0^{\infty} \mathrm{d}n Il_{\alpha}(t;n) G(n,x). \tag{28}$$

The equation means that after n jumps the random position is a Gaussian random variable, however the number of jumps is random and described by the inverse Lévy PDF, hence we must average the Gaussian over all possible number of steps (i.e. integrate over n). Eq. (28) is an integral transformation, it maps the Gaussian propogator, to the propogator of the

CTRW with $\alpha < 1$. This transformation is sometimes called inverse Lévy transform which is important for anomalous transport.

A second method is to consider the problem in Fourier Laplace space. Starting with the Montroll–Weiss equation we use a small s small k expansion of the exact solution. We use $f(k) = 1 - \sigma^2 k^2/2 + \cdots$ when $k \to 0$ namely use the assumption that the mean jump length is zero. And also use

$$\psi(s) \sim 1 - s^\alpha \tag{29}$$

when $s \to 0$ and find

$$P(k,s) = \frac{1-\psi(s)}{s} \frac{1}{1 - f(k)\psi(s)} \sim \frac{s^{\alpha-1}}{s^\alpha + \frac{\sigma^2 k^2}{2}}. \tag{30}$$

This long wave length approximation is somewhat ad-hoc at this stage. The claim is that the inverse Fourier–Laplace transform of

$$\frac{s^{\alpha-1}}{s^\alpha + \frac{\sigma^2 k^2}{2}}$$

yields an asymptotic approximation for $P(x,t)$ in the limit of long times. We assume that s^α and $\frac{\sigma^2 k^2}{2}$ are of the same order of magnitude. The main idea behind such small (s,k) expansions is that only a single scale of the jump length PDF, the variance σ^2, controls the long time behavior of $P(x,t)$. On the other hand the rather general small k expansion of $f(k)$ is for a symmetric $f(\Delta x)$ is

$$f(k) = 1 - \frac{k^2\sigma^2}{2} + \frac{m_4 k^4}{4!} - \frac{m_6 k^6}{6!} + \cdots \tag{31}$$

And we assumed that moments m_4 m_6 etc are irrelevant parameters of the problem, namely in the long time limit $P(x,t)$ does not depend on this information. Why this is true is investigated soon. However assuming that all the assumptions we made are correct we have

$$P(k,s) \sim \frac{s^{\alpha-1}}{s^\alpha + \frac{\sigma^2 k^2}{2}} = \int_0^\infty s^{\alpha-1} e^{-ns^\alpha} e^{-\frac{nk^2\sigma^2}{2}} \mathrm{d}n. \tag{32}$$

Now $s^{\alpha-1}e^{-ms^{\alpha}}$ is the Laplace pair of of the inverse Lévy PDF $Il_{\alpha}(t;n)$, and $e^{-\frac{nk^2\sigma^2}{2}}$ is the Fourier pair of the Gaussian $G(n;x)$ hence Eq. (32) has the same meaning as Eq. (28).

A. Why are m_4 m_6 etc irrelevant?

Consider the fourth moment of the displacement of the particle

$$\langle x^4(s)\rangle = \frac{1-\psi(s)}{s}\frac{\mathrm{d}^4}{\mathrm{d}k^4}\frac{1}{1-\psi(s)f(k)}|_{k=0} \tag{33}$$

Using (31) some algebra will convince the reader that

$$\langle x^4(s)\rangle = \frac{1}{s}\left[6\gamma^2(s)\sigma^4 + \gamma(s)m_4\right] \tag{34}$$

where $\gamma(s) = \psi(s)/(1-\psi(s))$. As expected $\langle x^4(s)\rangle$ depends on m_4 and σ^2. In the limit of long times corresponding to small s we have using Eq. (29)

$$\langle x^4(s)\rangle \sim \frac{1}{s}\left[6s^{-2\alpha}\sigma^4 + s^{-\alpha}m_4\right]. \tag{35}$$

The $m_4 s^{1-\alpha}$ term is a small term and hence can be neglected, we have

$$\langle x^4(s)\rangle \sim \frac{1}{s}6s^{-2\alpha}\sigma^4, \tag{36}$$

which is independent of m_4. We see that m_4 is not relevant for the calculation of $\langle x^4(t)\rangle$ in the limit of long times. Note that $\langle x^4(t)\rangle \propto t^{2\alpha}$ and hence the first non zero moments exhibit simple scaling $\langle x^2(t)\rangle^2 \propto \langle x^4(t)\rangle \propto t^{2\alpha}$ or in other words x scales with $t^{\alpha/2}$. Using a similar method one can show that the sixth moment $\langle x^6(s)\rangle$ does not depend on m_4 and m_6 (it is a trivial fact that the $\langle x^6(s)\rangle$ does not depend on m_8 etc). Hence m_{2n} with $n > 2$ are not important, as we assumed in previous sub-section.

More precise statement is that the expression in (32) yields the moments of the random walk $\langle x^2(s)\rangle$, $\langle x^4(s)\rangle$ etc when s is small. To see this notice the expansion

$$\frac{s^{\alpha-1}}{s^{\alpha}+\frac{\sigma^2k^2}{2}} = \frac{1}{s}\left[1 - \frac{\sigma^2k^2}{2s^{\alpha}} + \frac{\sigma^4k^4}{4s^{2\alpha}}\cdots\right]$$

which gives the correct small s behavior of the moments $\langle x^2(s)\rangle$, $\langle x^4(s)\rangle$ etc.

B. The Green Function

We now find the long time behavior of $P(x,t)$ using first the inverse Fourier transform

$$P(x,s) \sim \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{s^{\alpha-1}}{s^{\alpha}+\frac{\sigma^2 k^2}{2}}\mathrm{d}k. \tag{37}$$

Using Cauchy integral formula

$$P(x,s) = \frac{1}{\sigma}\frac{s^{\alpha/2-1}}{\sqrt{2}}e^{-\sqrt{2s^{\alpha}}\frac{|x|}{\sigma}}. \tag{38}$$

This can be rewritten

$$P(x,s) = \frac{1}{|x|\alpha} - \frac{\mathrm{d}}{\mathrm{d}s}e^{-\sqrt{2}s^{\alpha/2}\frac{|x|}{\sigma}}. \tag{39}$$

Noting that $e^{-\sqrt{2}s^{\alpha/2}\frac{|x|}{\sigma}}$ is the Laplace pair of the one sided Lévy PDF and that a derivative with respect to s yields a multiplication in t space we have

$$P(x,t) = \frac{t}{|x|\alpha}l_{\alpha/2,\frac{\sqrt{2}|x|}{\sigma},1}(t) = \frac{1}{\alpha}\left(\frac{\sigma}{\sqrt{2}}\right)^{2/\alpha}\frac{t}{|x|^{1+2/\alpha}}l_{\alpha/2,1,1}\left[\frac{t\sigma^{2/\alpha}}{\left(\sqrt{2}|x|\right)^{2/\alpha}}\right]. \tag{40}$$

Or rewriting we may use the inverse Lévy function

$$P(x,t) \sim \frac{\sqrt{2}}{\sigma}Il_{\alpha/2}\left(t;\frac{\sqrt{2}|x|}{\sigma}\right). \tag{41}$$

We see that in the limit of long time $P(x,t)$ is expressed in terms of a scaling function

$$P(x,t) \to \frac{1}{t^{\alpha/2}}f\left(\frac{x^{2/\alpha}}{t}\right).$$

In particular the behavior on the origin is slower than normal diffusion case, since $P(x=0,t) \propto t^{-\alpha/2}$. When $\alpha = 1$ we recover from Eq. (41) the Gaussian PDF, for $\alpha < 1$ we see that Lévy central limit theorem gives the correct description of the anomalous diffusion process.

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[1] Montroll and Weiss

[2] Weiss book

[3] Scher Montroll

[4] Tunaley

[5] Shlesinger

[6] Wong Weitz PRL

[7] Margolin on case when $\langle \tau^2 \rangle$ is infinite.

[8]