Lecture 24: Non-Markovian Diffusion Equations

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This lecture concerns separable CTRW, normal diffusion equation for finite mean waiting time and finite step variance, exponential relaxation of Fourier modes, fractional diffusion equations for sub-diffusion, Mittag-Leffler power-law relaxation of Fourier modes, and Riemann-Liouville fractional derivative.

1 Separable CTRW(Continuous Random Walk)

Consider the sum of random variables x_n with random waiting time τ_n, where x_n and τ_n are independent variables:

$$X(t) = \sum_{n=1}^{N(t)} x_n \tag{1}$$

Here, the upper limit of sum $N(t)$ is a random function of continuous time.

We define:

$$\begin{aligned} \psi(t) &= \texttt{PDF for } \tau_n\texttt{(IID)} \\ p(x) &= \texttt{PDF for } x_n\texttt{(IID)} \\ P(x,t) &= \texttt{PDF for } X(t) \end{aligned} \tag{2}$$

Recall that the Montroll-Weiss equation is

$$\tilde{\hat{p}}(k,s) = \left(\frac{1-\tilde{\psi}(s)}{s}\right)\frac{1}{1-\tilde{\psi}(s)\,\hat{p}(k)} \tag{3}$$

As $k \to 0$, $s \to 0$, one can get moments of $X(t)$. We seek what kind of continuum equations for $p(x,t)$ are. Note that in this lecture, $< x >= 0$ by assumption, or in the other word, there is no drift.

2 Normal Diffusion

Now we consider the continuum limit of the continuous time random walk with normal diffusive scaling when CLT (central limit theory) holds. We assume that $< \tau >= \bar{\tau} < \infty$, $\sigma^2 < \infty$, and $\langle \Delta x \rangle = 0$, define $z(t) = \frac{x(t)}{\sigma\sqrt{N(t)}}$, then $\phi(z) = \frac{exp(-z^2/2)}{\sqrt{2\pi}}$, where $\overline{N(t)} = t/\bar{\tau}$.

The walker is assumed to have a finite mean waiting time, so the waiting-time distribution satisfies

$$\psi(t) = o\left(t^{-2}\right),$$

and thus its Laplace transform will have a small s-expansion governed by

$$\tilde{\psi}(s) \sim 1 - \bar{\tau}s, \; s \to 0,$$

and

$$\hat{p}(k) \sim 1 - \frac{\sigma^2 k^2}{2}, \; k \to 0.$$

Substituting into Eq.(3), we have the long-time limit

$$\tilde{\hat{p}}(k,s) \sim \frac{\bar{\tau}}{\bar{\tau}s + \frac{\sigma^2 k^2}{2} + \cdots} \sim \frac{1}{s + Dk^2},$$

where

$$D = \frac{\sigma^2}{2\bar{\tau}}.$$

The definition of Laplace transform is $\tilde{\hat{p}}(k,s) = \int_0^\infty e^{-st}\hat{p}(k,t)dt$. Inverting Laplace Transform leads to

$$\hat{p}(k,t) \sim e^{-Dk^2 t} = e^{-t/\overline{t(k)}}$$

where $\overline{t(k)} = \frac{1}{Dk^2}$, and is the exponential relaxation time for Fourier mode k. Note that large k decays fast. As a result, $p(x,t)$ approaches the solution of the normal diffusion equation,

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

as $t \to \infty$ and $x = O\left(\sqrt{t}\right)$. (This is again the central limit theorem for CTRW.) Since the equation is linear, the same continuum limit holds for any initial condition of the CTRW.

Note

$$z(t) = \frac{X(t)}{\sqrt{2Dt}} = \frac{X}{\sqrt{\sigma^2 t/\bar{\tau}}} = \frac{X(t)}{\overline{N(t)}}$$

To compare $\hat{p}(k,t)$ and $P(x,t)$: 1)$\hat{p}(k,t)$ satisfies ODE

$$\frac{\partial \hat{p}}{\partial t} = -\frac{\hat{p}}{\overline{t(k)}} \; \texttt{with initial condition} \; \hat{p}(k,0) = 1;$$

2)$P(x,t)$ satisfies PDE

$$\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2}, \; P(x,0) = \delta(x).$$

3 Super Diffusion

Assume $\bar{\tau}$ is finite $< \infty$, but $\sigma^2 = \infty$ and symmetric $p(-x) = p(x)$ (This is Levy flight). For example: $\hat{p(k)} = e^{-a|k|^\alpha}$ $(0 < \alpha < 2)$, $p(x) = \ell_{\alpha,a}(x)$.

Consider

$$\tilde{\psi}(s) \sim 1 - \bar{\tau}s, \; s \to 0$$

$$\hat{p}(k) \sim 1 - B|k|^\alpha, \; k \to 0$$

Using Eq.(3), we obtain

$$\widetilde{\hat{p}}(k,s) \sim \frac{\bar{\tau}}{\bar{\tau}s + B|k|^\alpha + \cdots}$$

Invert Laplace Transform

$$\hat{p}(k,t) \sim e^{-\frac{B}{\bar{\tau}}|k|^\alpha t} = e^{-t/\overline{t(k)}}$$

To summarize, we still have exponential relaxation of Fourier modes in time, but now

$$\overline{t(k)} = \frac{\bar{\tau}}{B|k|^\alpha}, \; \alpha < 2.$$

So large k (or small wavelength) features decay more slowly compared to normal diffusion, but small k decay faster. Still

$$\frac{\partial \hat{p}}{\partial t} = -\frac{\hat{p}}{\overline{t(k)}} \; \texttt{ODE}$$

$$\frac{\partial \hat{p}}{\partial t} = -\frac{B}{\bar{\tau}}|k|^\alpha \hat{p}$$

Let $\kappa(t) = k(\frac{Bt}{\tau})^{\frac{1}{\alpha}} \leftrightarrow z = \frac{x}{(\frac{Bt}{\bar{\tau}})^{\frac{1}{\alpha}}}$, $\hat{p} \sim e^{-|\kappa(t)|^\alpha}$, then

$$P(x,t) \sim (\frac{\bar{\tau}}{Bt})^{\frac{1}{\alpha}} \ell_{\alpha,1}\left(\left(\frac{\bar{\tau}}{B}\right)^{\frac{1}{\alpha}} \frac{x}{t^{\frac{1}{\alpha}}}\right)$$

with scales like t^ν, where $\nu = 1/\alpha > \frac{1}{2}$, the supper diffusion.

Note $P(x,t)$ satisfies a fractional diffusion equation

$$\frac{\partial P}{\partial t} = (\frac{B}{\bar{\tau}}|\nabla|^\alpha P)$$

where ∇^α is the Riese fractional derivative which can be defined by:

$$\widehat{|\nabla|^\alpha f(k)} = -|k|^\alpha \hat{f}(k)$$

$$|\nabla|^\alpha f(x) = \int_{-\infty|}^{\infty} e^{ikx}(-|k|^\alpha)\left(\int_{-\infty}^{\infty} e^{-ikx'} f(x')dx'\right)\frac{dk}{2\pi}$$

$$= \int\int f(x')e^{ik(x-x')}|k|^\alpha dx' \frac{dk}{2\pi} = (f * \delta_\alpha)(x)$$

where

$$\delta_\alpha = -\int_{-\infty}^{\infty} e^{ikx}|k|^\alpha \frac{dk}{2\pi}$$

When $\alpha = 0$, this is $\delta(x) = \int e^{ikx}\frac{dk}{2\pi}$ and $\delta(x)$ is localized. This function $\delta_\alpha(x)$ is not localized in x. If α is integer, $|k|^\alpha = k^n$, $\delta_n(x) = \frac{d^n}{dx^n}\delta(x)$, then $|\nabla|^\alpha f \to \frac{d^n f}{dx^n}$.

Hence, boundary conditions for supper diffusion are subtle (fat tails in steps).

4 Subdiffusion

4.1 Mittag-Leffler Power-Law Decay of Fourier Modes

Consider symmetric ($p(x) = p(-x)$), anomalous subdiffusion with an infinite the mean waiting time ($\langle\tau\rangle = \infty$) but finite σ^2 for which the waiting-time distribution satisfies

$$\psi(t) \sim \left(\frac{\tau_0}{\tau}\right)^{1+\gamma},$$

and

$$\overline{N(t)} \sim t^\gamma$$

where $0 < \gamma < 1$ or equivalently $\tilde{\psi}$ has the following small-s expansion of its Laplace transform ,

$$\tilde{\psi}(s) \sim 1 - (\tau_0 s)^\gamma,\ s \to 0.$$

As $k \to 0$,

$$\hat{p}(k) \sim 1 - \frac{\sigma^2 k^2}{2}$$

Thus, we have

$$\widetilde{\hat{p}}(k,s) \sim \left(\frac{(\tau_0 s)^\gamma}{s}\right) \frac{1}{(\tau_0 s)^\gamma + \frac{\sigma^2 k^2}{2} + \cdots}. \tag{4}$$

The factor in front of (4) is not a constant, and in fact is a singularity, as $\gamma - 1 < 0$. This crucial term, which is negligible in the case of normal diffusion, represents walks that have not moved yet.

We can rewrite (4) as

$$\widetilde{\hat{p}}(k,s) \sim \frac{1}{s}\left(\frac{1}{1 + (\bar{t}(k)s)^\gamma}\right), \tag{5}$$

where

$$\bar{t}(k)^{-\gamma} = \tau_0^{-\gamma} \frac{\sigma^2 k^2}{2}.$$

Or,

$$\bar{t}(k) = \frac{\tau_0}{k^{2/\gamma}} \left(\frac{2}{\sigma^2}\right)^{\frac{1}{\gamma}} \propto \frac{1}{k^{2/\gamma}}$$

Inverting Laplace transform gives

$$\hat{p}(k,t) = E_\gamma\left(-(t/E(k))^\gamma\right)$$

where $E_\gamma(z)$ is Mittg-Leffler function, and $E_\gamma(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1+\gamma n)}$.

Note

$$E_1(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1+n)} = \sum_{n=0}^{\infty} \frac{z^n}{n!} = e^z,$$

So we recover $\hat{p}(k,t) = e^{-t/\bar{t}(k)}$ for $\gamma = 1$.

$$E_{1/2}(z) = e^{z^2} erfc(-z),$$

where erfc (x) is the complementary error function $(erf(z) = \frac{2}{\pi}\int_0^z e^{-x^2}dx,\ erfc(z) = 1 - erf(z))$. In this case,

$$\hat{p}(k,t) = e^{t/\bar{t}(k)} erfc(\sqrt{t/\bar{t}(k)})$$

Asymptotics:

$$\hat{p}(k,t) = E_\gamma(-t/\bar{t}(k)^\gamma)$$

For the non-exponential cases $0 < \gamma < 1$, the asymptotic expansions of the Mittag-Leffler functions are

$$E_\gamma\left(-\left(t/\bar{t}(k)\right)^\gamma\right) \sim \begin{cases} \exp\left(-\frac{(t/\bar{t}(k))^\gamma}{\Gamma(1+\gamma)}\right), & t \to 0 \\ \frac{1}{\Gamma(1-\gamma)}\left(\frac{\bar{t}(k)}{t}\right)^\gamma, & t \to \infty \end{cases},$$

so we have stretched-exponential decay at short times and power-law decay at long times.

Now what is the continuum relaxation equation?

$$\widetilde{\frac{df}{dt}}(s) = s\tilde{f}(s) - f(0) = \int_0^\infty e^{-st}\frac{df}{dt}(t)dt$$

$$\frac{\partial\tilde{\hat{p}}}{\partial t}(k,s) = s\tilde{\hat{p}}(k,s) - \hat{p}(k,0)$$

At the long time limit in the central region

$$\begin{aligned} \frac{\partial\tilde{\hat{p}}}{\partial t}(k,s) &\sim \frac{1}{1+(\tau(k)s)^{-\gamma}} - 1 \\ &= -\frac{(\bar{t}s)^{-\gamma}}{1+(\bar{t}s)^{-\gamma}} \\ &= -\bar{t}(k)^{-\gamma}s^{1-\gamma}\tilde{\hat{p}}(k,s) \end{aligned} \tag{6}$$

Here, $\bar{t}(k)^{-\gamma} = \frac{\sigma^2}{2\tau_0^\gamma}k^2 = D_\gamma k^2 = -D_\gamma k^2\, {}_0\mathcal{D}_t^{1-\gamma}P(k,s)$.

For $\hat{p}$, it satisfies equation

$$\frac{\partial\hat{p}}{\partial t} = -D_\gamma k^2\, {}_0\mathcal{D}_t^{1-\gamma}\hat{p}$$

where ${}_0\mathcal{D}_t^\beta$ is the Riemann-Lionvill fractional derivative. So $p(x,t)$ satisfies

$$\frac{\partial p}{\partial t} = D_\gamma\left({}_0\mathcal{D}_t^{1-\gamma}\right)\nabla^2 p. \tag{7}$$

This is a fractional diffusion equation. For subdiffusion, boundary conditions are easy, but initial condition is subtle. Besides,${}_0\mathcal{D}_t^{1-\gamma}$ is nonlocal in time, depending on the history.