# Multiscale Modeling and Methods

## Problem Set 2 by Jacob Woods

(Out Mon 09/30/2024, Due Mon 10/7/2024)

### Problem 1

For each of the following examples of wait time and jump length PDF Fourier or Laplace space asymptotic behavior, derive the mean squared displacement

$$\langle x^2(t) \rangle = \int_{-\infty}^{\infty} x^2 p(x,t) dx$$
 (1)

or show it diverges for long times. Use the Montroll–Weiss formula:

$$\hat{p}(k,u) = \frac{1 - \bar{w}(u)}{u} \frac{1}{1 - \bar{w}(u)\hat{\lambda}(k)}$$
(2)

where  $\bar{w}(u)$  is the Laplace transform of the wait time PDF and  $\hat{\lambda}(k)$  is the Fourier transform of the jump length PDF.(HINT: look at the formula for  $\hat{p}(k, u)$  in terms of  $\hat{p}(x, u)$ )

(a)

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

$$\bar{w}(u) \sim 1 - \tau u .$$
(3)

(b) let  $0 < \alpha < 1$  (subdiffusion)

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

$$\bar{w}(u) \sim 1 - (\tau u)^{\alpha} .$$
(4)

(c) let  $1 < \beta < 2$  (Levy flights)

$$\hat{\lambda}(k) \sim 1 - (\sigma k)^{\beta}$$
  

$$\bar{w}(u) \sim 1 - \tau u .$$
(5)

#### Problem 2

Simulate random walks for  $t \in [0, 1000]$  to confirm the mean squared displacement scaling as a function of time for subdiffusion. For the step length and wait time PDF use:

$$w(x) = \begin{cases} 0, & \text{if } x < 1\\ \frac{\alpha - 1}{x^{\alpha}}, & \text{if } x \ge 1 \end{cases}$$

$$\tag{6}$$

$$\lambda(t) = \frac{1}{2\pi} e^{\frac{-x^2}{2}} .$$
 (7)

(a) For  $\alpha = 3$  conduct a convergence experiment or give an argument to decide how many random walks are sufficient to recover the expected slope for the mean squared displacement as a function of time when plotted in log-log scale.(slope=1)

(b) Produce a plot for a sufficiently large number of random walks for  $\alpha = 1.25, 1.5, 1.75, 2, 3$  to demonstrate the relationship between mean squared displacement and time in question 1. Explain why in the case of  $\alpha = 2$  vs  $\alpha = 3$  this relationship looks similar.

#### Instructions

Email your solutions (i.e., a scan or typed version of your pen-and-paper part; and programming codes in a way that they can be run by someone else) to tuf98099@temple.edu with the email subject Math 8200. Homework 2 and all the submitted filenames starting with your family name.