Homework 4 Solutions

Due Nov. 1, 2016

Problem 1

Starting with the Master equation for a random walker moving via nearest neighbor rates F along the sites of an infinite chain, derive the Einstein formula relating the mean square displacement (msd) of the walker initially localized at one site to the elapsed time. Do this in three ways indicated in class:
(i) by solving the probability propagator in the Fourier domain and differentiating it with respect to q a couple of times;
(ii) solving for the probability propagator in real space and using Bessel function identities;
(iii) directly from the equation WITHOUT solving for the propagator.

From lecture the Master Equation for a random walker:

$$\frac{dP_m(t)}{dt} = F(P_{m+1} + P_{m-1} - 2P_m) \tag{1}$$

(i). To use the discrete Fourier Transform, first multiply both sides of Eq.(1) by e^{iqm}:

$$\sum_m \frac{dP_m e^{iqm}}{dt} = \sum_m e^{iqm} F(P_{m+1} + P_{m-1} - 2P_m)$$

Let

$$P^q(t) = \sum_m P_m e^{iqm}$$

$$\begin{aligned}\frac{dP^q(t)}{dt} &= F(P^q(e^{-iq} + e^{iq} - 2) \\ &= 2FP^q(\cos q - 1)\end{aligned}$$

$$\frac{dP^q(t)}{dt} + 2F(1-\cos q)P^q = \frac{dP^q(t)}{dt} + 4F\sin^2 qP^q = 0$$

$$P^q(t) = P^q(0)e^{(4F\sin^2 q)t}$$

From the initial conditions of the random walker:

$$P^q(0) = \sum_m e^{iqm}P_m(0) = \sum_m e^{iqm}\delta_{m,0} = 1$$

$$P^q(t) = e^{-2FT(1-\cos q)}$$

$$P^q(t) = \sum_m P_m e^{iqm}$$

Note:

$$\frac{d^2P^q}{dt^2} = -\sum_m m^2 P_m e^{iqm} \Longrightarrow -\frac{d^2P^q(t)}{dt^2}\Big|_{q=0} = \langle m^2\rangle$$

$$\frac{dP^q}{dt} = -2Ft(\sin q)e^{-2FT(1-\cos q)}$$
$$\frac{d^2P^q}{dt^2} = -2Ft(\cos q)e^{-2FT(1-\cos q)} + 4F^2t^2(\sin^2 q)e^{-2FT(1-\cos q)}$$

$$\implies \boxed{\langle m^2\rangle = -\frac{d^2P^q(t)}{dt^2}\Big|_{q=0} = 2Ft}$$

(ii).For solving for the probability propagator in real space and using Bessel function identities, we start with

$$P^q(t) = e^{-2FT(1-\cos q)}$$

and the inverse fourier transform

$$P_m(t) = \frac{1}{2\pi}\sum_q e^{iqm}e^{-2FT(1-\cos 1)}$$

where $q = \frac{2\pi}{M}(0, 1, ...)$. In the limit $M \longrightarrow \infty$,

$$P_m(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{iqm}e^{-2FT(1-\cos 1)}dq$$

.
Note that this is the integral representation for I Bessel functions. If $P_m = \delta_{m,0}$

$$P_m(t) = e^{-2Ft}I_m(2Ft)$$
$$\langle m^2\rangle = e^{-2FT}\sum_m m^2 I_m(2Ft)$$

The generation function for these modified Bessel functions:

$$e^{\frac{t}{2}(x+\frac{1}{x})} = \sum_{\infty}^{\infty} I_m(t)x^m$$

$$\frac{d}{dx}e^{\frac{t}{2}(x+\frac{1}{x})} = \frac{1}{2}t\left(1-\frac{1}{x^2}\right)e^{\frac{t}{2}(x+\frac{1}{x})} = \sum_{\infty}^{\infty} mI_m(t)m^{m-1}$$
$$\frac{d^2}{dx^2}e^{\frac{t}{2}(x+\frac{1}{x})} = \frac{1}{4}t^2\left(1-\frac{1}{x^2}\right)^2 e^{\frac{t}{2}(x+\frac{1}{x})} + \frac{te^{\frac{t}{2}(x+\frac{1}{x})}}{x^3} = \sum_{\infty}^{\infty} m^2I_m(t)m^{m-2}$$

When $x - 1$

$$\sum_{\infty}^{\infty} m^2I_m(t)m^{m-2} = te^t$$

Set $t = 2Ft$,

$$\implies \langle m^2\rangle = e^{-2FT}\sum_m m^2I_m(2Ft) = e^{-2FT}e^{2FT}(2Ft) = \boxed{2Ft}$$

(iii). To solve Eq. (1) directly, multiply both sides by m^2:

$$\frac{1}{F}\frac{d}{dt}\sum_m m^2P_m = \sum_m m^2P_{m+1} + \sum_m m^2P_{m-1} - \sum_m 2m^2P_m$$

where:

$$(m+1)^2 = m^2 + 2(m+1) - 1 \implies m^2 = (m+1)^2 - 2(m+1) + 1)$$

$$(m-1)^2 = m^2 - 2(m-1) - 1 \Longrightarrow m^2 = (m-1)^2 + 2(m+1) + 1)$$

This gives

$$\sum_m m^2 P_{m+1} = \sum_m (m+1)^2 P_{m+1} - 2\sum_m (m+1)P_{m+1} + \sum_m P_{m+1}$$
$$\sum_m m^2 P_{m-1} = \sum_m (m-1)^2 P_{m-1} - 2\sum_m (m-1)P_{m-1} + \sum_m P_{m-1}$$

Note:

$$\sum_m (m+1)^2 P_{m+1} = \langle m^2\rangle; \quad \sum_m (m+1)P_{m+1} = \langle m\rangle; \quad \sum_m P_{m+1} = 1$$
$$\sum_m (m-1)^2 P_{m-1} = \langle m^2\rangle; \quad \sum_m (m-1)P_{m-1} = \langle m\rangle; \quad \sum_m P_{m-1} = 1$$

Thus,

$$\frac{1}{F}\frac{d\langle m^2\rangle}{dt} = \left[\cancel{\langle m^2\rangle} - 2\cancel{\langle m\rangle} + 1\right] + \left[\cancel{\langle m^2\rangle} + 2\cancel{\langle m\rangle} - 1\right] - 2\cancel{\langle m^2\rangle}$$
$$\frac{1}{F}\frac{d\langle m^2\rangle}{dt} = 2 \quad \Rightarrow \boxed{\langle m^2\rangle = 2Ft}$$

Problem 2

Show explicitly by evaluating the propagator in terms of special functions in real space that motion in the horizontal and vertical directions in a 2-dimensional counterpart of the nearest-neighbor chain (without oblique i.e. diagonal hops) are independent of each other.

The gain-loss Master equation in 2-dimensions, where the walker can only go one lattice site in up-down, and left-right steps is

$$\frac{dP_{m_x,m_y}}{dt} = F(P_{m_x+1,m_y} + P_{m_x-1,m_y} - 2P_{m_x,m_y}) + F(P_{m_x,m_y+1} + P_{m_x,m_y-1} - 2P_{m_x,m_y}) \tag{2}$$

Solving for the time derivative of P_{m_x,m_y} yields

$$\begin{aligned}\frac{dP_{m_x,m_y}}{dt} &= \frac{P_{m_x}}{dt}P_{m_y} + P_{m_x}\frac{dP_{m_y}}{dt}\\ &= F(P_{m_x+1} + P_{m_x-1} - 2P_{m_x})P_{m_y} + F(P_{m_y+1} + P_{m_y-1} - 2P_{m_y})P_{m_x}\\ &= F(P_{m_x+1,m_y} + P_{m_x-1,m_y} - 2P_{m_x,m_y}) + F(P_{m_x,m_y+1} + P_{m_x,m_y-1} - 2P_{m_x,m_y})\end{aligned}$$

Thus, we can see that the two random walks are independent of each other. Recall for 1-dimension, if $P_m(0) = \delta_{m,0}$

$$P_{m_x}(t) = e^{-2Ft}I_{m_x}(2Ft)$$

Combining the solutions for each dimension gives

$$\boxed{P_{m_x,m_y} = e^{-4Ft}I_{m_x}(2Ft)I_{m_y}(2Ft)}$$