"Many particle systems out of equilibrium" Problems, Series 7, 2006-07.

Problem 16. Continuous time random walks and single file diffusion

In a continuous time random walk a moving particle makes jumps between integer sites na and $(n \pm 1)a$ at random times, with average jump frequency ν. The probability $p(n,t)$ of finding the particle on site na at time t satisfies the *master equation*

$$\frac{\partial p(n,t)}{\partial t} = \frac{\nu}{2}\left[p(n-1,t) + p(n+1,t) - 2p(n,t)\right]. \tag{1}$$

The *generating function* $G(x,t)$ is defined as

$$G(x,t) = \sum_{n=-\infty}^{\infty} x^n p(n,t) \tag{2}$$

a) Show that this function is of the form

$$G(x,t) = \exp\left[\frac{\nu(x-1)^2}{2x}t\right] G(x,0). \tag{3}$$

(Hint: first derive a differential equation for it.) What is $G(x,0)$ if the moving particle starts out at the origin at $t = 0$? Find expressions for $p(n,t)$ under this initial condition (see the mathematical relationships at the end).

Single file diffusion is a process in which diffusing particles on a line cannot pass each other. A specific realization is a process on a one-dimensional lattice, with a dilute set of vacancies, each making a continuous random walk of the type described above. At each jump of a vacancy it exchanges positions with the particle (or occasionally another vacancy) at the site towards which it jumps. Realizations of this process may be characterized by set of time instants $tr_m^{(i)}$ and $tl_n^{(i)}$ at which vacancy i jumps to the right, respectively to the left. The velocity of this vacancy as function of time may then be defined as.

$$v^{(i)}(t) = a\left[\sum_m \delta(t - tr_m^{(i)}) - \sum_n \delta(t - tl_n^{(i)})\right]. \tag{4}$$

Similarly the velocity of particle p may be defined as

$$v^{(p)}(t) = a\sum_i \left[-\sum_m \delta(t - tr_m^{(i)})\delta_{n_{ip}(tr_m^{(i)}-),-1} + \sum_n \delta(t - tl_n^{(i)})\delta_{n_{ip}(tl_n^{(i)}-),1}\right]. \tag{5}$$

Here $an_{ip}(t) = a(n_i(t) - n_p(t))$ is the difference in position between i and p at time t and $\delta_{i,j}$ denotes a Kronecker delta. In words: the velocity of particle p is

$a\delta(t-t_{jump})$ at instants it exchanges with a vacancy on the right and $-a\delta(t-t_{jump})$ at instants it exchanges with a vacancy on the left.

For a calculation of the velocity autocorrelation function of a tagged particle at low vacancy concentration it suffices to consider correlations between position exchanges with *the same* vacancy. Why is this so?

b) Show that in this approximation the tagged particle velocity autocorrelation function assumes the form

$$C(t) = \rho_{vac} \frac{\nu a^2}{2} \left[\delta(t-0^+) - \nu\{p(0,t) - p(1,t)\} \right], \tag{6}$$

with ρ_{vac} the average density of vacancies. Hint: for the first term consider the mean square displacement at very short times and use $C(t) = \frac{1}{2}\partial^2\langle(x(t)-x(0))^2\rangle/\partial t^2$. The delta-function $\delta(t-0^+)$ is defined such that $\int_0^\epsilon dt\, \delta(t-0^+) = 1$. Another possibility is approximating the velocity by a function having a large constant value $a/(\Delta t)$ during a very short time intervals of length Δt, constructing the autocorrelation function of this at very short times and taking the limit $\Delta t \to 0$.

c) Using the explicit form of $p(n,t)$ found before, determine the diffusion coefficient of the tagged particle and find the asymptotic behavior of the velocity autocorrelation function and the mean square displacement for long times. Check the positivity of the real part of the z-dependent diffusion coefficient for $Re(z) \geq 0$ and $z \neq 0$.

Some useful mathematical relationships:

$$\begin{aligned}
\exp \frac{1}{2}\left(x + \frac{1}{x}\right) t &= \sum_{k=-\infty}^{\infty} x^k I_k(t) \\
\int_0^\infty dt\, \exp(-zt) I_n(ct) &= \frac{c^n}{\sqrt{z^2-c^2}(z+\sqrt{z^2-c^2})^n} = \frac{(z-\sqrt{z^2-c^2})^n}{c^n\sqrt{z^2-c^2}} \\
\exp(-t) I_n(t) &\approx \frac{1}{\sqrt{2\pi t}}\left(1 - \frac{(n+\frac{1}{2})(n-\frac{1}{2})}{2t}\right) \quad \text{for } t \to \infty
\end{aligned}$$

Here $I_n(t)$ is a Bessel function of imaginary argument.