18.366 Random Walks and Diffusion, Spring 2005, M. Z. Bazant.

Problem Set 4

Due at lecture on Th May 5.

1. **Linear Polymer Structure.** Consider a chain of N monomers, each of length a, in $d = 3$ dimensions. Let R_N be the end-to-end distance, with PDF, $P(R, N)$. In the absence of correlations, we have the usual scaling, $\overline{R}_N = \sqrt{\langle R_N^2 \rangle} = a\sqrt{N}$. Now suppose that monomers also tend to be aligned linearly at each link, with an energy, $\varepsilon(\theta) = -\alpha \vec{\Delta x}_n \cdot \vec{\Delta x}_{n+1} = -\alpha a^2 \cos\theta$, for $1 \leq n \leq N-1$, which yields a PDF, $p(\theta) \propto e^{-\varepsilon(\theta)/kT}$, for each angle, θ.
   (a) Normalize $p(\theta)$ and calculate the mean total energy, $\langle E_N \rangle = (N-1)\alpha a^2 \rho$, where $\rho(T) = \langle \vec{\Delta x}_n \cdot \vec{\Delta x}_{n+1} \rangle / a^2$, is the correlation coefficient between 'steps' (monomer vectors).
   (b) Show that the same scaling holds,
   $$\overline{R}_N \sim a_{eff}(T)\sqrt{N}$$
   as $N \to \infty$, with an effective monomer size, $a_{eff}(T)$. Sketch $a_{eff}(T)$, and discuss its asymptotics for $T \to 0, \infty$.

2. **Polymer Surface Adsorption.** Consider a long polymer chain in solution attached ('adsorbed") onto a flat surface at a discrete set of points, $\vec{r}_n = (x_n, y_n, z = 0)$. Model the polymer as a continuous stochastic process in the half-space, $(x, y, z > 0)$, with zero drift and "diffusivity", $D = a^2/2$, where a is the monomer length and "time" is measured in monomers. Take discreteness into account by starting the stochastic process at $\vec{r}_n + a\hat{z} = (x_n, y_n, a)$ before it returns for the next adsorption at $\vec{r}_{n+1}$.
   (a) Calculate the PDF for the displacement between successive adsorption sites, proportional to the eventual hitting probability density on the surface. [Hint: use the electrostatic analogy with an "image charge".]
   (b) Calculate the PDF of the position $\vec{r}_{N_s}$ of the N_sth adsorption site (a Lévy flight).
   (c) *(Extra credit)* For a polymer of length N, show that the expected number of adsorption sites $\langle N_s(N) \rangle$ scales like $\sqrt{N}$, which is also the scaling of the surface displacement, $\vec{r}_{N_s(N)}$, and the bulk radius of the polymer.

3. **Solution to the Telegrapher's Equation.** Let $c(x, t)$ be the solution to[1]
   $$c_{tt} + rc_t = v^2 c_{xx}$$
   for $-\infty < x < \infty$, $t > 0$ subject to the initial conditions, $c(x, 0) = \delta(x)$ and $c_t(x, 0) = 0$.
   (a) Show that the Fourier[2]-Laplace[3] transform of the solution is
   $$\hat{\tilde{c}}(k, s) = \frac{s + r}{s(s + r) + v^2 k^2}$$

[1] As explained in class, this continuum problem describes the long-time PDF of the position , $p_n(m) = \sigma c(m\sigma, n\tau)$, of a persistent random walk on a lattice of spacing σ with correlation coefficient, ρ, between successive steps of time interval τ, in the limit $\rho \to 1$ where $v = \sigma/\tau$, $r = 1/\tau_c$, $\tau_c = \tau n_c$, $n_c = -2/\log\rho$.

[2] $\hat{f}(k) = \int_{-\infty}^{\infty} e^{-ikx} f(x) dx$

[3] $\tilde{g}(s) = \int_0^{\infty} e^{-st} g(t) dt$.

(b) Use part (a) to determine the variance of the position,

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

Show that this agrees with the scaling function for the persistent walk obtained in class (for the ballistic to diffusive transition in the limit $\rho \to 1$).

(c) By comparing (a) with the Fourier-Laplace transform of the Diffusion Equation, $c_t = Dc_{xx}$, show that the Telegrapher's Equation reduces to the Diffusion Equation after long times, $t \gg \tau_c$ (or $s \ll r$), where $D = v^2/r$. (This essentially proves the Central Limit Theorem for the persistent random walk.)

(d) *(Extra credit)* Invert the transforms in (a) to obtain the exact solution [4],

$$c(x,t) = \frac{e^{-rt/2}}{2}\left\{\delta(x-vt)+\delta(x+vt)+\frac{r}{4v}\left[I_0(z)+\frac{I_1(z)}{2z}\right]H(vt-|x|)\right\}$$

where

$$z = \frac{r\sqrt{v^2t^2-x^2}}{2v}$$

which smoothly interpolates between the Green functions for the Wave Equation, $c_{tt} = v^2 c_{xx}$, and the diffusion equation, $c_t = Dc_{xx}$, respectively[5]

4. **Inelastic Diffusion**. Consider a ball bouncing on a rough surface. Each time the ball hits the surface it is scattered in a random direction. For any real surface, the collision is *inelastic*, i.e. the ball only retains a fraction $0 < r < 1$ of its kinetic energy ($r =$ "the coefficient of restitution"). Therefore, the ball's expected height and horizontal displacement are reduced by factors of r and $\sqrt{r}$, respectively, with each successive bounce.

A reasonable model for this situation might be an 'inelastic random walk', with exponentially decreasing step lengths[6]. Let ΔX_n be IID random variables with zero mean and cumulants $c_l < \infty$ ($l \geq 2$), which represent the typical displacement after an elastic bounce. The inelastic nature of the collisions is reflected in a rescaling of this distribution with each step. Specifically, our model is the random walk

$$X_N = \sum_{n=1}^{N} a^n \Delta X_n$$

with non-identical steps, where $0 < a < 1$ is a constant ($a = \sqrt{r}$). Do the analysis below for the case of one dimension (which would model transverse diffusion on a surface with random parallel grooves), but keep in mind that your results are easily generalized to higher dimensions.

(a) Express the PDF, $P_N(x)$, of X_N in terms of the PDF, $p(x)$, of ΔX_n.

(b) Find the cumulants $C_{N,l}$ of X_N (in terms of c_l).

(c) Let $C_l = \lim_{N\to\infty} C_{N,l}$ and $a = 1-\epsilon$ ($\epsilon > 0$). Show that $C_{2m}/C_2^m = O(\epsilon^{m-1})$ as $\epsilon \to 0$.

(d) Let $\phi(\zeta,\epsilon) = C_2^{1/2} P_\infty(\zeta C_2^{1/2})$, and show that "the Central Limit Theorem holds" as $a \to 1$. In other words, show that

$$\phi(\zeta,\epsilon) \to \phi_o(\zeta) = e^{-\zeta^2/2}/\sqrt{2\pi}$$

as $\epsilon \to 0$ with ζ fixed[7] This, of course, agrees with the limit of a simple random walk ($a = 1$).

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[4] You may wish to use the following identities for modified Bessel functions: $I_0(z) = \int_0^\pi \cosh(z\cos\theta)d\theta$, $I_1(z) = I_0'(z)$.

[5] The former is obvious (delta function terms), and you may expand the solution in the limit $rt \gg 1$ and $x = O(\sqrt{t})$ to obtain the latter (from the Bessel function terms), although it is also implied by (c).

[6] See Lecture 14, 18.366 notes (2003).

[7] Note, however, that the CLT does not applyfor any fixed $\epsilon < 0$ as $N \to \infty$. For a dramatic example of the violation of the CLT, where ΔX_n is a Bernoulli random variable, see Lecture 15, 18.366 notes (2003).