

### Problem Set 5

Due at lecture on Tu Dec 5.

1. **Restoring force of highly stretched polymers.** Consider modeling a polymer in a dilute solution as Rayleigh's isotropic random walk in three dimensions with IID displacements of length,  $a$ . Recall the formula for the PDF of the end-to-end displacement (from PSet 1),

$$P_N(\vec{x}) = \frac{1}{2\pi^2 r} \int_0^\infty u \sin(ur) \left[ \frac{\sin(ua)}{ua} \right]^N du$$

- (a) Use the saddle-point method to derive a globally valid asymptotic approximation for  $P_N(\vec{x})$  for  $N \gg 1$  with  $\xi = |\vec{x}|/Na \leq 1$  fixed, leaving your answer in terms of the inverse  $L^{-1}$  of the Langevin function,

$$L(z) = \coth z - \frac{1}{z}$$

- (b) Use this result to compute and plot the entropic contribution to the free energy,  $F = -TS = -T \log P_N$ , as well as the effective *nonlinear* force  $f(R; T, N, a) = -dF/dR$ , and compare to the approximation in the central region  $R = |\vec{x}| = O(a\sqrt{N})$ .

2. **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,  $\bar{R}_N = \sqrt{\langle R_N^2 \rangle} = a\sqrt{N}$ . 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,  $\theta$ .

- (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,

$$\bar{R}_N \sim a_{eff}(T)\sqrt{N}$$

as  $N \rightarrow \infty$ , with an effective monomer size,  $a_{eff}(T)$ . Sketch  $a_{eff}(T)$ , and discuss its asymptotics for  $T \rightarrow 0, \infty$ .

3. **A persistent Lévy flight.** Consider the Cauchy random walk with IID displacements,  $\Delta x'_n$ ,  $n = 1, \dots, N$ , with PDF,  $p(x) = a/\pi(a^2 + x^2)$ . From this flight, construct another Cauchy random flight with *non-independent* steps,

$$\Delta x_1 = \Delta x'_1, \quad \Delta x_{n+1} = (1 - \rho)\Delta x'_{n+1} + \rho\Delta x'_n, \quad n \geq 2$$

where  $|\rho| < 1$  plays the role of a correlation coefficient between successive steps (although here correlations cannot be defined since the variance is infinite)<sup>1</sup>. Find the exact distribution of the final position,  $X_N = \sum_{n=1}^N \Delta x_n$ . Does the scaling of the half-width depend on  $\rho$ ?

<sup>1</sup>This could model the effect of inertia in the problem of finding the tangential displacement of a particle in a dilute gas bouncing between rough parallel plates, separated by much less than the mean free path. It could also model positive short-time correlations in volatile stock prices.

4. **A continuous-time random walk.** Derive the exact PDF of the position,  $P_N(n, t)$ , of an unbiased CTRW on the integer lattice  $n = 0, \pm 1, \pm 2, \dots$  starting at the origin (with nearest-neighbor hopping) with waiting time PDF,  $\psi(t) = e^{-t}$ .
5. **Self-Avoiding Walk.** (Extra credit) Simulate self-avoiding walks on a cubic lattice in three-dimensions<sup>2</sup>, and try to determine the scaling of the root-mean-square end-to-end length

$$R_n = \langle |\vec{X}_N|^2 \rangle^{1/2} \sim N^\nu$$

by plotting  $\log R_N$  versus  $\log N$  and getting the slope of a (hopefully) straight line. How does your result compare with the Fisher-Flory estimate  $\nu = 3/(d + 2) = 3/5$  and the recent numerical result  $0.5877 \pm 0.0006$ ?

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<sup>2</sup>It is nontrivial to generate large SAW (because most end up “trapped”), so to see the scaling above, you may need to think about more sophisticated sampling algorithms!