Polymer Diffusion in a Gel

A polymer is a long chain molecule which takes on new, emergent behavior at very large size. Often times, it is convenient to model a polymer as a continuous chain of length L. Its position in space is then given by a vector field $\mathbf{x}(s,t)$, with t denoting time. A very simple of model of polymer motion in some liquid is given by a diffusive equation

$$\frac{\partial \mathbf{x}}{\partial t} - D\frac{\partial^2 \mathbf{x}}{\partial s^2} = \text{noise}$$

For simplicity, you can set the noise terms to 0 in this problem. The boundary conditions for this diffusion equation are

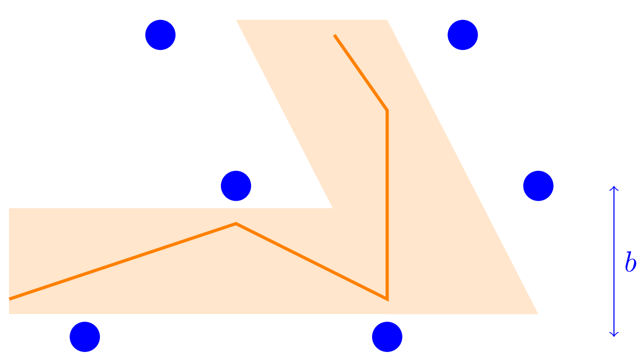
$$\mathbf{0} = \left.\frac{\partial \mathbf{x}}{\partial s}\right|_{s=0,L}.$$

You also do not need to worry about configurations such as $\mathbf{x} = \mathbf{x}_0$, which is unphysical because the polymer cannot scrunch up to a point – the noise terms often "take care of those" for us without altering what we're after.

Ultimately, what we want to ask is: how long does it take for this polymer to "lose track" of its starting position? This is a qualitative question and therefore deserves a qualitative answer – you may ignore all O(1) constants in this problem.

(a) In the simple diffusive model above, what is the time scale over which the polymer moves to a completely new configuration?

Now, let us consider a polymer diffusing in a gel. Let us approximate a gel as a liquid, but with hard rods which the polymer cannot pass through. The typical distance between two such rods is b. As shown in the figure below, the polymer is restricted by the gel-like rods to diffuse only in thin tubes of size b. These tubes themselves can be thought of as random walking through the gel – ultimately, this is what will allow the polymer to enter new configurations.



The diffusive pictures above describe the dynamics of a polymer given an initial configuration. On very large length scales, the typical "shape" of the polymer should be "similar" to what it is without the gel – what the gel does is make it much harder to get between configurations! What sorts of initial configurations are common to a polymer? If we think of the polymer growing as a random walker, we can find useful information about the initial conditions.

(b) Using the random walk picture for initial conditions, we would expect to find

$$\left\langle (\mathbf{x}(s,0) - \mathbf{x}(0,0))^2 \right\rangle = as^\nu$$

What is ν? For the rest of the problem you'll need to include the constant a from this part.

(c) Compare what the two random walk models predict for $\langle(\mathbf{x}(L,0) - \mathbf{x}(0,0))^2\rangle$. About how many disjointed steps does the gel break the random walk of the polymer into?

(d) Use the result of part (c) to determine what the effective diffusion constant is. What the time scale for the polymer to move to a new configuration? Compare to the case of part (a) and comment.

Despite our incredibly simple model, it turns out the results of part (d) are seen quantitatively in quite a few numerical simulations of the problem.