Polymer Properties
Quiz 2
September 5, 2014

1) The following web page has an app that simulates random walks,
http://zeus.plmsc.psu.edu/~manias/MatSE443/Study/7.html.

a) Simulate twenty (or more) random walks, do screen shots of each walk, estimate the end-to-end distance, R, and the step size using a ruler. Calculate $<R^2>$, and $<R>$ (the latter based on independent sums of the x and y coordinates for the walk). Calculate the number of steps, N, using the random walk equation. Explain the expected values for these functions and compare the expected values with your results.

b) From your twenty walks, plot the probability of a walk of length R versus R from –Nl to Nl using the x-axis projection. Comment on the shape of this plot. Some of your walks are very short and some are long, while many have intermediate lengths. Are these outliers an artifact of a flaw in the simulation? Explain.

c) For some of your walks estimate the persistence length using the following equation given by Wikipedia: $\langle \cos\ \theta(s) \rangle = e^{-s/P}$, setting s to P and finding the length where cos(theta) = 1/e. Theta is the angle between the tangent of the chain at an arbitrary point and a point one persistence length away when s = P. Does this value agree with 2* your step length? Explain.

2) When an engine has a loose belt it is often found that the belt squeaks when the engine starts. The squeaking ceases after the engine runs for some time.

a) Use the Gaussian distribution of polymer chain length and the Boltzmann energy function for a thermally activated process to explain this observation. (Consider that the belt is an ideal elastomer.)

b) If the belt were made of leather, which is composed of fiberous native state proteins, would you expect the same behavior? Is it possible that the belt would be tight at startup and slip after the engine runs? Explain your reasoning.

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1) a) $<R^2> = Nl^2$, and $<R> = 0$.

b) P(R) versus R should be a bell shaped curve peaking at 0. It is almost Gaussian. The end to end distance is randomly distributed about 0. It is expected to find long and short walks in a random distribution.

c) The value should agree with 2* the step length.

2) a) This question is asking for you to derive the rubber elasticity equation, F = Kspr * R where the spring constant is $3kT/(nl^2)$. At startup things are cold so the retractive force on the elastomer is small, the belt is loose. When things warm-up the temperature rises and the retractive force increases so the belt gets tight.

b) The normal behavior for non-polymeric materials is that things expand with temperature. So we might expect any other belt material to expand when the belt warms-up. A leather belt is not elastomeric since the fibers are native state proteins and not subject to entropic elasticity.