Quiz 4 Polymer Physics
February 7, 2020

The persistence length is half the Kuhn step length. The persistence length is easily calculated from computer simulations of chain structure. For example, BS Hanson, D Head and L Dougan from the University of Leeds (*The hierarchical emergence of worm-like chain behaviour from globular domain polymer chains* Soft Matter **15**, 8778-89 (2019)) studied the persistence length of polymers formed by globular proteins. An example of this is G-actin which acts as a monomer for F-actin (shown below). F-actin acts like a polymer (*it has randomness caused by kT*) but the monomers are complex folded native state proteins. Actin is an active component of muscle in humans, along with titin and myosin, but also exists in almost the same form in all life down to single cell algae. Hanson modeled actin using spheres and springs (*they are physicists obviously*). This model partly derives from studies of titin which is the largest protein, about 2 microns in length, composed of natively folded proteins (beads) and unfolded protein (Gaussian springs). When stressed, the folded native state is unfolded, and when stress is released, titin refolds reversibly. The model considered by Hanson et al. is a simpler bead spring model.

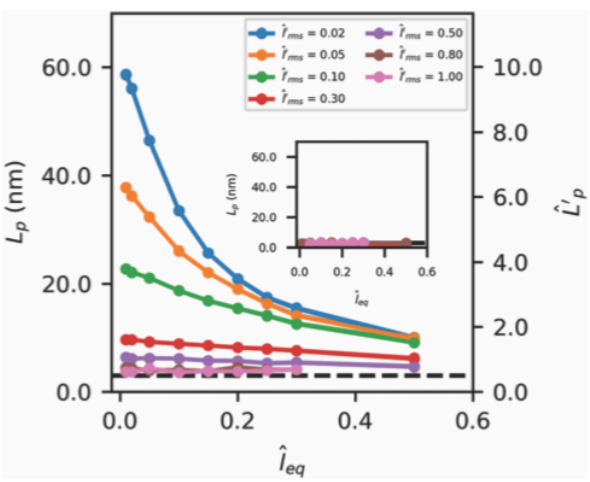
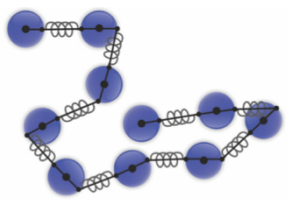
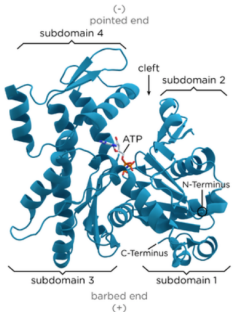
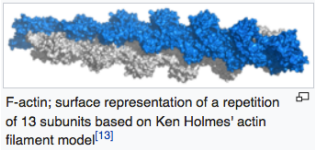


Fig. 5 The effect of the linker equilibrium length on the persistence length of a globular domain polymer, for a variety of relative fluctuation magnitude values, $\hat{l}_{rms}'$, and in the presence and absence of the steric interaction, as represented by the globular domain stiffness k_{st}. Main k_{st} = 192.31 pN nm and inset k_{st} = 0 pN nm.





G-actin

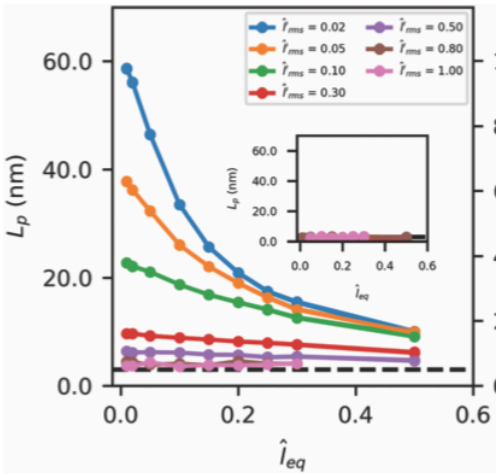

F-actin; surface representation of a repetition of 13 subunits based on Ken Holmes' actin filament model[13]

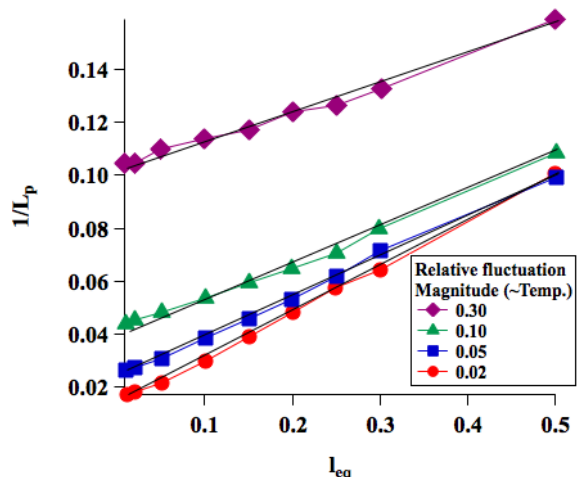
F-actin

a) Hanson et al. found the behavior shown in Fig. 5 above for his bead and spring simulations. As the linker (spring) becomes longer, l_{eq} in the x-axis, the persistence length becomes smaller, L_p in the y-axis. Explain why this might be the case.

b) The different curves in Fig. 5 are for different value of the "*mean fluctuation magnitude*", which can be thought of as the temperature. The top curve is at a low "temperature" the bottom at a high "temperature". Why might persistence length decrease with "temperature" or fluctuation magnitude? Does your explanation also explain why the dependence on the linker spring length diminishes with higher temperature?

c) The plot below shows the top four curves of Fig 5 replotted as $1/L_p$ versus l_{eq}.





What does $1/L_p$ reflect? Why would $1/L_p$ be linear in the length of the linker spring, l_{eq}? Why would $1/L_p$ increase with increasing temperature (relative fluctuation magnitude)? (*Hanson didn't notice this dependence.*)

d) Write an equation with two constants that reflects the linear plot and explain what the two constants measure. Does the temperature and linker length dependencies of the two constants that you observe in this plot agree with your description of the parameters?

e) Hanson et al. uses an equation (equation 14) to predict the mechanical behavior of a bead and spring protein,

$$F = \frac{k_B T}{L_p}\left(\frac{1}{4}\left(\left(1-\frac{\Delta x}{L_c}\right)^{-2}-1\right)+\frac{\Delta x}{L_c}\right)$$

This equation has two parts, the second part is,

$$F \sim (kT/L_p)\,(\Delta x/L_c)$$

Where F is the force applied to the ends of the chain, L_c is the contour length of the chain. What is the origin of this part of the equation? Does this give relevance to the parameter $1/L_p$? The first part of the equation has the term $(1 - \Delta x/L_c)$. What happens to the molecule when this term is 0? What happens to the force?

Answers: Quiz 4 Polymer Physics February 7, 2020

a) Hanson et al. found the behavior shown in Fig. 5 above for his bead and spring simulations. As the linker (spring) becomes longer, l_{eq} in the x-axis, the persistence length becomes smaller, L_p in the y-axis. Explain why this might be the case.

Polymer chains have a modulus that follows kT/MW. Longer linker chains have a larger MW so the modulus is lower. Lower modulus makes a more flexible spacer and a lower L_p.

b) The different curves in Fig. 5 are for different value of the "*mean fluctuation magnitude*", which can be thought of as the temperature. The top curve, large L_p, is at a low "temperature" the bottom at a high "temperature". Why might persistence length increase with "temperature" or fluctuation magnitude? Does this explanation also explain why the dependence on the linker spring length diminishes with higher temperature?

The chain beads are moving with kT. As they move faster their mean position fluctuates more. This apparently leads to a smaller persistence length.

c) Write an equation with two constants that reflects the linear plot and explain what the two constants measure. Does the temperature and linker length dependencies of the two constants that you observe in this plot agree with your description of the parameters?

$1/L_p = K_1 + K_2 l_{eq}$

K_1 is $1/L_p$ for no spring, with just beads. This increases with temperature due to the relative motion of the beads. K_2 reflects how changes in the spring length impact the base bead persistence length. One might expect $K_2 \sim 1/kT$ following rubber elasticity. So the slope of the linear plots should decrease with temperature, as is observed.

d) Hanson et al. uses an equation (equation 14) to predict the mechanical behavior of a bead and spring protein,

$$F = \frac{k_B T}{L_p}\left(\frac{1}{4}\left(\left(1-\frac{\Delta x}{L_c}\right)^{-2}-1\right)+\frac{\Delta x}{L_c}\right)$$

This equation has two parts, the second part is,

$F \sim (kT/L_p)\,(\Delta x/L_c)$

Where F is the force applied to the ends of the chain, L_c is the contour length of the chain. What is the origin of this part of the equation? Does this give relevance to the parameter $1/L_p$? The first part of the equation has the term $(1 - \Delta x/L_c)$. What happens to the molecule when this term is 0? What happens to the force?

The second part is from rubber elasticity as derived in class, $F \sim 3kT/nl^2$. The first part pertains to the finite extensibility of the chain. When the chain is fully extended the force becomes infinite.