ME470: Problem sheet 2 - 1D elements

Solutions will be discussed in the exercise session on Thursday, October 10.

(1) Gaussian approximation of binomial distribution Consider a one-dimensional random walk with n steps, each of length b. The probability of being at a distance r after n step follows the binomial distribution as below.

$$P_{1D}(n,r) = \frac{1}{2^n}\binom{n}{\frac{n+r/b}{2}} = \frac{1}{2^n}\frac{n!}{\left(\frac{n+r/b}{2}\right)!\left(\frac{n-r/b}{2}\right)!} \tag{1}$$

Using Stirling's approximation, $n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$, show that the probability above can be approximated by a Gaussian distribution for large n.

$$P_{1d}(n,r) \approx \frac{1}{\sqrt{2\pi\langle r^2\rangle}}\exp\left(-\frac{r^2}{2\langle r^2\rangle}\right) \tag{2}$$

(2) Spring constant of freely jointed chain Given the relation between the extension and applied force for a freely jointed chain,

$$\langle R_z\rangle = nb\left[\coth\left(\frac{bF_z}{k_BT}\right) - \frac{k_BT}{bF_z}\right] \tag{3}$$

show that the spring constant at $F_z \ll 1$ recovers that of an ideal chain.

(3) Entropic filament Imagine you can fabricate steel whiskers with Young's modulus, $E = 200GPa$ of arbitrary length L_c and diameter d (no smaller than atomic dimensions, of course). Approximate the whisker as a filament of circular cross section.

(a) What is called "whiskers" in metallurgy are typically needles with, say, $d = 5\mu m$. Compute (i) the bending rigidity, and (ii) the persistence length ξ_p of such a whisker.

(b) You want to make "floppy" whiskers with persistence length equal to or smaller than the contour length. What minimum contour length must the whisker have if its diameter is (1) $10nm$, or (ii) $0.4nm$ (roughly the minimum d possible)?

(c) You make floppy whiskers with $\xi_p = 1\mu m$ and $L_c = 10\mu m$. What is the root mean square distance $\langle r_{ee}^2\rangle^{1/2}$ for on of these filaments?

(d) We estimate that, because of overlap of many individual whiskers, each whisker takes up a volume of about $V_w \sim \left(\langle r_{ee}^2\rangle^{1/2}\right)^3/10^6$ in a 3D material made from many whiskers as in (c). What is the shear modulus μ of this material as room temperature, if there are no crosslinks between whiskers?

(4) An entropic spring at work A bacteriophage is a virus - an extremely tiny monster (see images) carrying DNA in its polyhedral head (called a *capsid*), which it injects into bacteria to make them produce more bacteriophages. Inside the capsid, the DNA is tightly coiled such that its radius of curvature is given by that of capsid. The capsid can be approximated by a circular cylinder with diameter $44nm$ and height $55nm$. A typical phage DNA is $100,000$ base pairs long ($0.34nm$ per base pair), and the persistence length of DNA is $\xi_p = 53nm$.

(a) Determine the elastic energy stored in the coiled DNA, assuming the DNA coils tightly along the inside of the cylindrical capsid.

(b) Estimate the pressure exerted onto the capsid shell because of this elastic energy (and which is used for DNA injection), assuming that the DNA coil occupies the entire cylinder volume before injection.

(5) Forces on ideal chain Consider biopolymers such as spectrin, actin, and tubulin with persistence lengths of $\xi_p = 15, 15 \times 10^3 nm$, and $2 \times 10^6 nm$, respectively, with a contour length of $100nm$. Assume room temperature conditions for your experiments, $T = 300K$.

(a) Assuming the ideal chain model, calculate the forces required to extend these biopolymers to a length of (i) $50nm$, and (ii) $150nm$.

(b) Why is the extension of $150nm$ unrealistic? Explain the limitations of the ideal chain model.

(6) Ideal chain with numbers Consider a three-dimensional ideal chain of 50 segments, each with length of $10nm$.

(a) Calculate $\langle r_{ee} \rangle$ and $\left\langle \mathbf{r}_{ee}^2 \right\rangle^{1/2}$.

(b) Calculate the effective spring constant (in N/m) at 300K.

(c) If the chain has charges +/-**e** on each end and is placed in a field of $10^6 V/m$, what is the change in the end-to-end distance?

(7) Kuhn segment and persistence length Show that the Kuhn length is equal to twice of the persistence length, $b = 2\xi_p$.