(530190) Methods in Single Molecule Biophysics, Fall 2011

Exercise 3: Wednesday 23.11.2011 at 12:15 in room D116

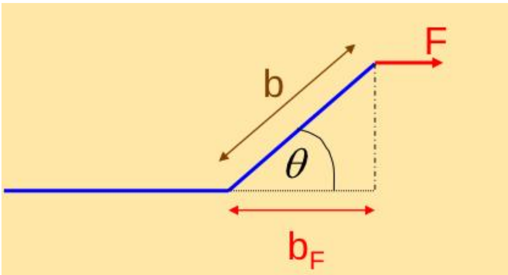
1. Freely Jointed Chain (numerical solution, 1D)

a) Calculate numerically the force-extension curve for a 1D freely joined chain. Choose the number of segments sufficiently high so that you get a nice long chain, but sufficiently low so that the computational time stays reasonable (e.g. N=50). One strategy for numerically calculating the force-extension relationship would be:
- Fix the force f at some value
- Calculate the extension at this force
-- Extension = (1/Z) * Boltzmann probability * extension
- Repeat for next force value

b) Show that the average extension of a 1D FJC is given by: $\frac{\langle z\rangle}{L} = \tanh\left(\frac{FL_{seg}}{k_bT}\right)$

2. Freely Jointed Chain (numerical solution, 2D)

a) Extend the solution of problem 1 to a 2D FJC (see figure) where the angle theta is randomly chosen.
b) Think about extending these ideas into 3D. Does the situation change?



2D FJC

4. Compare the force-extension curves given by FJC and WLC models by plotting them ($L_{seg} = L_p$ = 50 nm, L = 10 µm).

4. (Bonus) Freely Joined Chain model (analytic solution, 2D). This exercise is from Nelson's book (page 389), so you may find help there.

We derived analytically the force-extension relationship for a 1D freely joined chain (Nelson p. 352-353). Try to derive analytically the force-extension relationship for a 3D FJC.

Help and hints: Now the segments not only point in the +z or –z direction, but they are unit tangent vectors $\mathbf{t_i}$ that can point in any direction. Use **r** as the end-to-end vector, and apply the force in the **z** direction. (**r** will point along the **z** direction). The end to end distance will be given by $z = \bar{r}\hat{z}$

We will get a Boltzmann factor that looks similar to the 1D case: $P(t_1 \dots t_n) = Z^{-1} \exp\left[-\frac{-fL\sum_i \bar{t_i}z}{k_BT}\right]$

We already saw the correct solution to this problem in Exercise 1: (from Howard's book, pages 113 and 320):

$\langle X\rangle = nbL\left(\frac{Fb}{k_BT}\right)$, where the Langevin function is $L(x) \equiv \frac{e^x+e^{-x}}{e^x-e^{-x}} - \frac{1}{x}$.