Homework 8

Strong stretching behavior of DNA

Consider a DNA double helix with a length $l_0 \approx 10\mu m$ and imagine to apply a force $\vec{F}$ along the $z-$axis on its ends, e.g. with optical tweezers. Recall that DNA is very stiff: its persistence length is about 50 nm, which is quite large with respect its diameter ($\approx 2\ nm$). Hence, a convenient way to model it is to consider a freely jointed chain with $N+1$ monomers and to introduce a *stiffness energy term*:

$$E_s = -\frac{B}{b}\sum_{i=1}^{N-1} \hat{t}_{i+1} \cdot \hat{t}_i \ ,$$

where B is a positive coefficient with dimension Energy×Length, b is the length of a single bond, and $\hat{t}_i$ is the unit vector of the direction of the bond between monomer $i-1$ and monomer i.
The full Hamiltonian is therefore

$$H = -\frac{B}{b}\sum_{i=1}^{N-1} \hat{t}_{i+1} \cdot \hat{t}_i - Fb\sum_{i=0}^{N} t_{iz} \ .$$

Taking correctly the continuous limit gives the worm-like chain Hamiltonian:

$$H = \frac{\xi}{2\beta}\int_0^{l_0}\left(\frac{d\hat{t}(s)}{ds}\right)^2 ds - F\int_0^{l_0} t_z(s)ds \ ,$$

where l_0 is the length of the chain, $\hat{t}(s)$ is the unit tangent vector at position s, and $\xi = B\beta$ is the constant *persistence length*. In the following, we are going to show that the elongation l along the z direction under strong stretching, i.e. $F\xi \gg k_B T$, follows the law

$$\frac{\langle l \rangle}{l_0} \simeq 1 - \frac{1}{2}\frac{1}{(\xi\beta F)^{\frac{1}{2}}} \ .$$

As shown below, this formula fits the experimental results much better than how the freely jointed model does.

1. Firstly, consider that when the chain is strongly stretched then $t_z(s) \sim 1$, while $t_x(s), t_y(s) \ll 1\ \forall s \in [0, l_0]$. Derive an approximate Hamiltonian in terms of the two dimensional tangent vector $\vec{t}_T(s) = (t_x(s), t_y(s))$.

   Hint: Recall that $t_z(s) = \sqrt{1-(t_x^2(s)+t_y^2(s))}$ and develop till order $t_x^2(s)+t_y^2(s) \equiv \left(\vec{t}_T(s)\right)^2$.

2. Imposing the boundary conditions $\vec{t}_T(0) = \vec{t}_T(l_0) = 0$ allows to write $\vec{t}_T(s)$ in terms of its Fourier components, i.e.

   $$\vec{t}_T(s) = \sum_{n=1}^{\infty} \vec{a}_n \sin(k_n s) \ ,$$

   where $k_n = (n\pi)/l_0$. Find the expression for l in terms of the Fourier components $\vec{a}_n$.
   Hint: Recall that the elongation is $l = \int_0^{l_0} t_z(s)ds$.

3. Rewrite the Hamiltonian in the form:

   $$H = \frac{1}{2}\sum_{n=1}^{\infty} J_n \vec{a}_n^2 - Fl_0 \ .$$

   What is the explicit expression for J_n?

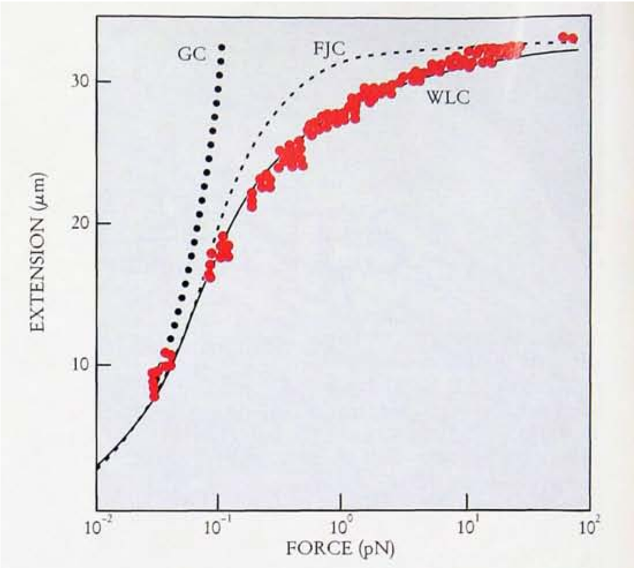

Figure 1: The force-extension curve of a single DNA molecule under traction applied at its ends. The data points from *Smith et al.*, **Science** 1992) vol. **258** pp. 1122 are compared with the theoretical curves for the entropic elasticity of three polymer models: the Gaussian chain, the freely jointed chain and the worm-like chain, which fits the experimental data remarkably well. Taken from *Austin et al.*, **Physics Today** (1997) vol. **50** (2) pp. 32.

4. Exploiting the theorem of equipartition of energy, which gives

$$\frac{1}{2} J_n \langle \vec{a}_n^2 \rangle = 2 \times \frac{1}{2\beta} = k_B T \ ,$$

compute $\langle l \rangle$.
Hint: Evaluate the sum of the expression for l found at point 2 as an integral with

$$\left(\frac{\xi \pi^2}{l_0} \right)^{\frac{1}{2}} \Delta n = \Delta x \simeq dx \ ,$$

where $\Delta n = 1$. This follows from $l_0 \gg \xi$.