Homework 8

Strong stretching behavior of DNA

1. Using the Taylor expansion

$$\sqrt{1-\epsilon} \overset{\epsilon\to 0}{\simeq} 1 + \frac{1}{2}\frac{-1}{\sqrt{1-\epsilon}}\bigg|_{\epsilon=0} \epsilon = 1 - \frac{\epsilon}{2} ,$$

we have

$$t_z(s) = \sqrt{1-\left(t_x^2(s)+t_y^2(s)\right)} \simeq 1 - \frac{1}{2}\left(t_x^2(s)+t_y^2(s)\right) \equiv 1 - \frac{1}{2}\left(\vec{t}_T(s)\right)^2 .$$

Therefore, the elongation is

$$l = \int_0^{l_0} t_z(s)ds \simeq l_0 - \frac{1}{2}\int_0^{l_0} \left(\vec{t}_T(s)\right)^2 ds . \tag{1}$$

In handling the first term of the Hamiltonian, we note that

$$\left(\frac{d\hat{t}(s)}{ds}\right)^2 = \left(\frac{dt_x(s)}{ds}\right)^2 + \left(\frac{dt_y(s)}{ds}\right)^2 + \left(\frac{dt_z(s)}{ds}\right)^2 , \tag{2}$$

and that

$$\frac{dt_z}{ds} = \frac{d}{ds}\sqrt{1-\left(t_x^2(s)+t_y^2(s)\right)} \simeq -t_x\frac{dt_x}{ds} - t_y\frac{dt_y}{ds} ,$$

By comparing the third term in eqn (2) with the other two, we notice that their ratio is $O(t_x^2, t_y^2)$, so that it is negligible with respect to the other two terms. Summarizing, the Hamiltonian can be written as

$$H = \frac{\xi}{2\beta}\int_0^{l_0}\left(\frac{d\vec{t}_T(s)}{ds}\right)^2 ds + \frac{F}{2}\int_0^{l_0}\left(\vec{t}_T(s)\right)^2 ds - Fl_0 .$$

2. Introducing the Fourier series in (1) gives

$$\begin{aligned}
l &= l_0 - \frac{1}{2}\int_0^{l_0}\left(\hat{t}_T(s)\right)^2 ds \\
&= l_0 - \frac{1}{2}\int_0^{l_0}\left(\sum_{n=1}^{\infty}\vec{a}_n\sin(k_n s)\right)^2 ds \\
&= l_0 - \frac{1}{2}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\int_0^{l_0}\vec{a}_n\sin(k_n s)\vec{a}_m\sin(k_m s)ds \\
&= l_0 - \frac{1}{2}\sum_{n=1}^{\infty}(\vec{a}_n)^2\int_0^{l_0}\sin^2(k_n s)ds \\
&= l_0 - \frac{1}{2}\sum_{n=1}^{\infty}(\vec{a}_n)^2\frac{1}{2}l_0 .
\end{aligned}$$

Recall: If $n \neq m$

$$\int_0^{l_0} \sin(k_n s)\sin(k_m s) ds = \frac{l_0}{\pi}\int_0^{\pi} \sin(nx)\sin(mx) dx = 0 \ ,$$

because

$$\int \sin(mx)\sin(nx)dx = \sin(mx)\left(-\frac{\cos(nx)}{n}\right) - \int \cos(mx) m \left(-\frac{\cos(nx)}{n}\right) dx$$

$$\int \cos(mx)\cos(nx)dx = \cos(mx)\left(\frac{\sin(nx)}{n}\right) - \int \left(-\sin(mx)m\right)\frac{\sin(nx)}{n} dx \ ,$$

so

$$\int_0^{\pi} \sin(mx)\sin(nx)dx = \frac{1}{1-\frac{m}{n}}\left[\cos(mx)\frac{\sin(mx)}{n} - \sin(mx)\frac{\cos(nx)}{n}\right]_0^{\pi} = 0 \ .$$

3. The Fourier expansion of $\frac{d\hat{t}_T(s)}{ds}$ is simply

$$\frac{d\hat{t}_T(s)}{ds} = \sum_{n=1}^{\infty} \vec{a}_n k_n \cos(k_n s) \quad k_n = \frac{n\pi}{l_0} \ ,$$

therefore

$$H = \frac{1}{2}\left[\frac{\xi}{\beta}\sum_{n=1}^{\infty}(\vec{a}_n)^2 k_n^2 \frac{1}{2} l_0 + F\sum_{n=1}^{\infty}(\vec{a}_n)^2\frac{1}{2}l_0\right] - Fl_0 = \frac{1}{2}\sum_{n=1}^{\infty}\frac{l_0}{2}\left[\frac{\xi}{\beta}k_n^2 + F\right](\vec{a}_n)^2 - Fl_0 \ ,$$

and

$$J_n = \frac{l_0}{2}\left[\frac{\xi}{\beta}k_n^2 + F\right] \ .$$

4. Finally,

$$\begin{aligned}
\frac{\langle l\rangle}{l_0} &= \left[1 - \frac{1}{2}\sum_{n=1}^{\infty}\frac{1}{2}\langle\vec{a}_n^2\rangle\right] = \left[1 - \frac{1}{2}\sum_{n=1}^{\infty}\frac{1}{\beta J_n}\right] = \left[1 - \frac{1}{2}\sum_{n=1}^{\infty}\frac{1}{\frac{\beta l_0}{2}\left[\frac{\xi}{\beta}k_n^2 + F\right]}\right] \\
&= \left[1 - \sum_{n=1}^{\infty}\frac{1}{\xi\frac{\pi^2 n^2}{l_0^2}l_0 + Fl_0\beta}\right] = \left[1 - \sum_{n=1}^{\infty}\Delta n\left(\frac{\xi\pi^2}{l_0}\right)^{\frac{1}{2}}\left(\frac{l_0}{\xi\pi^2}\right)^{\frac{1}{2}}\frac{1}{n^2\frac{\pi^2\xi}{l_0} + Fl_0\beta}\right] \\
&= \left[1 - \sum_{n=1}^{\infty}\Delta x\left(\frac{l_0}{\xi\pi^2}\right)^{\frac{1}{2}}\frac{1}{x^2 + Fl_0\beta}\right] \\
&\simeq \left[1 - \left(\frac{l_0}{\xi\pi^2}\right)^{\frac{1}{2}}\int_0^{\infty}\frac{1}{x^2 + Fl_0\beta}dx\right] = \left[1 - \left(\frac{l_0}{\xi\pi^2}\right)^{\frac{1}{2}}\frac{1}{(Fl_0\beta)^{\frac{1}{2}}}\int_0^{\infty}\frac{1}{y^2+1}dy\right] \\
&\simeq \left[1 - \frac{1}{(\xi\beta F)^{\frac{1}{2}}\pi}\left[\arctan y\right|_0^{\infty}\right] = \left[1 - \frac{1}{(\xi\beta F)^{\frac{1}{2}}\pi}\frac{\pi}{2}\right] \\
&= \left[1 - \frac{1}{2(\xi\beta F)^{\frac{1}{2}}}\right] \ .
\end{aligned}$$