ME470: Problem sheet 2 - 1D elements - correction

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1 Gaussian approximation of binomial distribution

Using Stirling approximation for large n, we have:

$$
\begin{aligned}
n! &\approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \\
\left(\frac{n+r/b}{2}\right)! &\approx \sqrt{2\pi\frac{n+r/b}{2}}\left(\frac{n+r/b}{2e}\right)^{\frac{n+r/b}{2}} \\
\left(\frac{n-r/b}{2}\right)! &\approx \sqrt{2\pi\frac{n-r/b}{2}}\left(\frac{n-r/b}{2e}\right)^{\frac{n-r/b}{2}}
\end{aligned}
\tag{1}
$$

By substituting these into the expression for $P_{1D}(n,r)$:

$$
P_{1D}(n,r) \approx \frac{1}{2^n}\frac{\sqrt{2\pi n}(\frac{n}{e})^n}{\sqrt{2\pi\frac{n+r/b}{2}}(\frac{n+r/b}{2e})^{\frac{n+r/b}{2}}\sqrt{2\pi\frac{n-r/b}{2}}(\frac{n-r/b}{2e})^{\frac{n-r/b}{2}}}
\tag{2}
$$

That we can simplify as:

$$
P_{1D}(n,r) \approx \frac{\sqrt{n}(\frac{n}{2})^n}{\sqrt{2\pi}\sqrt{\frac{n+r/b}{2}}(\frac{n+r/b}{2})^{\frac{n+r/b}{2}}\sqrt{\frac{n-r/b}{2}}(\frac{n-r/b}{2})^{\frac{n-r/b}{2}}}
\tag{3}
$$

$$
\begin{aligned}
\log(P_{1D}(n,r)) \approx & \frac{1}{2}\log(n) + n\log(n/2) - \frac{1}{2}\log(2\pi) - \frac{1}{2}\log\left(\frac{n+r/b}{2}\right) - \frac{1}{2}\log\left(\frac{n-r/b}{2}\right) \\
& - \left(\frac{n+r/b}{2}\right)\log\left(\frac{n+r/b}{2}\right) - \left(\frac{n-r/b}{2}\right)\log\left(\frac{n-r/b}{2}\right) \\
\approx & \left(n+\frac{1}{2}\right)\log(n) - \frac{1}{2}(n+1)\log\left(\frac{n+r/b}{2}\frac{n-r/b}{2}\right) \\
& + \frac{r}{2b}\log\left(\frac{n-r/b}{n+r/b}\right) - \frac{1}{2}\log(2\pi) - n\log(2)
\end{aligned}
\tag{4}
$$

We expand $1 \pm r/nb$ around 1 which gives an approximate Gaussian form (for large n, r is typically much smaller than n).

$$\log\left(\frac{n - r/b}{n + r/b}\right) \approx -\frac{2r}{bn} \tag{5}$$

$$\log\left(\frac{n + r/b}{2}\frac{n - r/b}{2}\right) \approx \log\left(\frac{n^2(1-(r/bn)^2)}{4}\right) \approx -\log(4) + \log(n^2) + \log(1-(r/bn)^2) \tag{6}$$

Thus,

$$\begin{aligned}\log(P_{1D}(n,r)) \approx &\left(n+\frac{1}{2}\right)\log(n) + (n+1)\log(2) - (n+1)\log(n) + \frac{1}{2}(n+1)\left(\frac{r}{bn}\right)^2 \\ &+ \frac{r}{2b}\left(-\frac{2r}{bn}\right) - \frac{1}{2}\log(2\pi) - n\log(2) \\ \approx &-\frac{1}{2}\log(n) + \log(2) - \frac{1}{2}\frac{r^2}{nb^2} - \frac{1}{2}\log(2\pi) \\ \approx &\log\left(\frac{2}{\sqrt{2\pi n}}\exp\left(-\frac{r^2}{2nb^2}\right)\right)\end{aligned} \tag{7}$$

For a one-dimensional random walk with n steps, each of length b the mean square displacement is:

$$\langle r^2 \rangle = nb^2 \tag{8}$$

So,

$$P_{1D}(n,r) = K\frac{2}{\sqrt{2\pi n}}\exp\left(-\frac{r^2}{2nb^2}\right) \tag{9}$$

where K is a normalization constant.
Moreover,

$$\int_{-\infty}^{+\infty} P_{1D}(n,r)dr = 1 \tag{10}$$

So,

$$K = \frac{1}{2b} \tag{11}$$

Finally,

$$P_{1D}(n,r) = \frac{1}{\sqrt{2\pi\langle r^2\rangle}}\exp\left(-\frac{r^2}{2\langle r^2\rangle}\right) \tag{12}$$

2 Spring constant of freely jointed chain

For $F_z \ll 1$,

$$\coth\frac{bF_z}{k_bT} \simeq \frac{k_bT}{bF_z} + \frac{bF_z}{3k_bT}.$$

Then,

$$\langle R_Z \rangle \simeq nb \left[\frac{k_b T}{bF_z} + \frac{bF_z}{3k_b T} - \frac{k_b T}{bF_z} \right]$$

and

$$F_Z = \frac{3k_b T}{nb^2} \langle R_Z \rangle .$$

3 Entropic filament

a)
i)

$$\kappa_b = EI = E\frac{\pi d^4}{64} = 6.136 \cdot 10^{-12}\text{Jm}$$

ii) Assuming room temperature $T = 300\text{K}$,

$$\xi_p = \frac{\kappa_b}{k_b T} = 1.482 \cdot 10^9\text{m}$$

b) Floppy if $L_c \geq \xi_p$.

i) For $d = 10\text{nm}$, $\xi_p = 23.7\text{mm}$ and $L_c \geq 23.7\text{mm}$.
ii) For $d = 0.4\text{nm}$, $\xi_p = 60.7\text{nm}$ and $L_c \geq 60.7\text{nm}$.
The atomic radius of Fe is around 0.1 nm, so $d > 0.1\text{nm}$

c) $\xi_p = 1\mu\text{m}$, $L_c = 10\mu\text{m}$

$$\left\langle \vec{r_{ee}^2} \right\rangle = nb^2 = 2\xi_p L_c - 2\xi_p^2(1 - e^{-L_c/\xi_p}) = 1.8 \cdot 10^{-11} m^2$$

Then $\sqrt{\left\langle \vec{r_{ee}^2} \right\rangle} = 4.24\mu\text{m}$.

By comparison, for the ideal chain $\left\langle \vec{r_{ee}^2} \right\rangle = 2\xi_p L_c = 2 \cdot 10^{-11} m^2$ and $\sqrt{\left\langle \vec{r_{ee}^2} \right\rangle} = 4.47\mu\text{m}$.

d) Consider pure shear and assume affine deformation

$$\vec{R} = (x, y, z) \to \vec{r} = (r_x, r_y, r_z)$$
$$\left\langle r_x^2 \right\rangle = \lambda_x^2 \left\langle x^2 \right\rangle$$
$$\left\langle r_y^2 \right\rangle = \lambda_y^2 \left\langle y^2 \right\rangle$$
$$\left\langle r_z^2 \right\rangle = \left\langle z^2 \right\rangle$$

$$\langle \Delta F(r) \rangle = \frac{3k_B T}{2nb^2} \left\langle r^2 - R^2 \right\rangle = \frac{3k_B T}{2nb^2} \left(\lambda_x^2 \left\langle x^2 \right\rangle + \lambda_y^2 \left\langle y^2 \right\rangle - \left\langle x^2 \right\rangle - \left\langle y^2 \right\rangle \right).$$

Here, $\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{1}{3} nb^2$. Then,

$$\langle \Delta F(r) \rangle = \frac{1}{2} k_B T \left(\lambda_x^2 + \lambda_y^2 - 2 \right).$$

For volume conservation, $\lambda_x = \lambda, \quad \lambda_y = \frac{1}{\lambda}$. Then

$$\langle \Delta F(r) \rangle = \frac{1}{2} k_B T \left(\lambda^2 + \frac{1}{\lambda^2} - 2 \right).$$

Given a strain ε, $\lambda = 1 + \varepsilon$, with $\varepsilon \ll 1$. Then,

$$\begin{aligned} \langle \Delta F(r) \rangle &= \frac{1}{2} k_B T \left[(1+\varepsilon)^2 + \frac{1}{(1+\varepsilon)^2} - 2 \right] \\ &\simeq \frac{1}{2} k_B T \left[1 + 2\varepsilon + \varepsilon^2 + 1 - 2\varepsilon + \varepsilon^2 - 2 \right] = 2\varepsilon^2 k_B T. \end{aligned}$$

This is the energy difference per whisker. For bulk energy per volume

$$\Delta f_{bulk} = \rho \langle \Delta F(r) \rangle = 2\varepsilon^2 \rho k_B T,$$

with ρ the number of whiskers per volume. Here each whisker takes up a volume of $V_w \sim \left(\langle r_{ee}^2 \rangle^{1/2} \right)^3 / 10^6$. Then

$$\rho \sim \frac{N_c}{V} = \frac{V/V_w}{V} = 1/V_w.$$

For a pure shear with $\lambda = 1 + \varepsilon$

$$\begin{cases} \varepsilon_{xx} = \varepsilon \\ \varepsilon_{yy} = \frac{1}{1-\varepsilon} - 1 \simeq 1 - \varepsilon - 1 = -\varepsilon \\ \varepsilon_{zz} = 0 \end{cases}$$

For an isotropic material

$$u = \mu \left(\varepsilon_{ik} - \frac{1}{3} \delta_{jk} \varepsilon_{ll} \right)^2 + \frac{K}{2} \varepsilon_{ll}^2 = \mu \varepsilon_{ik}^2 = 2\mu\varepsilon^2,$$

Where we have used the fact that $\varepsilon_{ll} = 0$. Then,

$$2\mu\varepsilon^2 = 2\varepsilon^2 \rho k_B T, \quad \mu = \rho k_B T.$$

At room temperature $T = 300\text{K}$, $k_B = 1.38 \cdot 10^{-23} J K^{-1}$,

$$\mu = \frac{4.14 \cdot 10^{-15}}{\langle r_{ee}^2 \rangle^{3/2}}$$

4 An entropic spring at work

$\xi_p = 53\text{nm}$, $d = 44\text{nm}$, $h = 55\text{nm}$.

a) The curvature is $K = 1/(d/2) = 2/d$. Then the bending energy is

$$U_b = \frac{1}{2} \kappa_b L_c \frac{1}{R^2} = \frac{1}{2} \kappa_b L_c K^2.$$

For DNA, $L_c = nb = 34\mu\text{m}$ and $\kappa_b = \xi_p k_B T$. Then,

$$U_b = \frac{1}{2}\xi_p k_B T L_c \frac{4}{d^2} = 1862 k_B T = 7.71 \times 10^{-18} J$$

b)

$$H = U_b + U_{iuso} = \frac{1}{2}\xi_p k_b T L_c \frac{4}{d^2} + p\frac{\pi d^2}{4}h,$$

where $U_{iuso} = pV$. Imposing $\mathrm{d}H = 0$,

$$\frac{\partial H}{\partial d} = \frac{4\xi_p k_B T L_c}{d^3} + p\frac{2\pi d}{4}h = 0.$$

$$p = \frac{4}{\pi d h}\frac{2\xi_p k_B T L_c}{d^3} \simeq 89\text{kPa}.$$

5 Forces on ideal chain

Remember $F = \frac{3k_B T}{nb^2}x = \frac{3k_B T}{2\xi_b L_c}x$.
a) i)

$$F_{spectrin} = \frac{3 \cdot 300 \cdot 1.38 \cdot 10^{-23}}{2 \cdot 15 \cdot 10^{-9} \cdot 100 \cdot 10^{-9}} = 2.65 \cdot 10^{-13}\text{N}.$$

$$F_{actin} = 2.05 \cdot 10^{-16}\text{N}.$$

$$F_{tubulin} = 1.55 \cdot 10^{-14}\text{N}.$$

ii) is just 3 times i).
b) 150 nm > L_c

6 Ideal chain with numbers

a)

$$\langle r_{ee}\rangle = 0 \quad \text{and} \quad \sqrt{\langle r_{ee}^2\rangle} = b\sqrt{n} = 70.7nm \tag{13}$$

b)

$$K_{sp} = \frac{3k_b T}{2\xi_p L_c} = \frac{3k_b T}{nb^2} = 2.4810^{-6} N/m \tag{14}$$

c)

$$F = qE = 1.610^{-19} * 10^6 = 1.610^{-13} N \Delta x = \frac{F}{K_{sp}} = 64.5nm \tag{15}$$

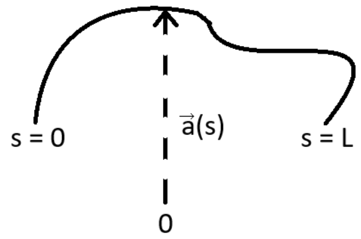
7 Kuhn segment and persistence length

For a polymer of N segments, each segment of length l, the squared end-to-end distance $\langle R^2\rangle$ is related to the persistence length by the equation:

$$\langle R^2\rangle = 2L\xi_p \tag{16}$$

where $L = Nl$ is the total contour length of the chain.

As a matter of fact, the end-to-end vector $\vec{R}$ of the polymer chain can be written as an integral over the chain's tangent vectors:



$$\vec{R} = \int_0^L \frac{\partial \vec{a}(s)}{\partial s} ds \tag{17}$$

So,

$$\begin{aligned}
\langle R^2 \rangle &= \left\langle \left(\int_0^L \frac{\partial \vec{a}(s)}{\partial s} ds \right)^2 \right\rangle \\
&= \int_0^L \int_0^L \left\langle \frac{\partial \vec{a}(s)}{\partial s} \frac{\partial \vec{a}(u)}{\partial u} \right\rangle ds du \\
&= \int_0^L \int_0^L \exp\left(-\frac{|u-s|}{\xi_p} \right) ds du \\
&= 2 \int_0^L \int_0^u \exp\left(-\frac{u-s}{\xi_p} \right) ds du \\
&= 2 \int_0^L \exp\left(-\frac{u}{\xi_p} \right) \xi_p \left(\exp\left(-\frac{u}{\xi_p} \right) - 1 \right) du \\
&= 2\xi_p \int_0^L \left(1 - \exp\left(-\frac{u}{\xi_p} \right) \right) du \\
&= 2\xi_p \left(L + \xi_p \left(\exp\left(-\frac{L}{\xi_p} \right) - 1 \right) \right) \\
&= 2\xi_p^2 \left(\frac{L}{\xi_p} - 1 + \exp\left(-\frac{L}{\xi_p} \right) \right)
\end{aligned} \tag{18}$$

Thus,

$$\langle R^2 \rangle \approx 2\xi_p^2 \frac{L}{\xi_p} = 2\xi_p L \tag{19}$$

And in the case of a freely jointed chain with Kuhn length b the end-to-end distance is given by:

$$\langle R^2 \rangle = N b^2 \tag{20}$$

where $N = \frac{L}{b}$ is the number of Kuhn segments.

Finally,

$$2\xi_p L = N b^2 = L b \tag{21}$$

(If $L \neq 0$)

$$b = 2\xi_p \tag{22}$$