

Explicit solution of extensible worm like chain model for low force regime

Tunc Kayikcioglu

December 9, 2016

DNA can extend to certain extent and act as a spring, an effect that becomes more pronounced if the applied force is very high. Still, an approximate formula for force regime also includes a correction term. For low force regime such as $F < 10\text{pN}$, the following approximation holds (https://en.wikipedia.org/wiki/Worm-like_chain):

$$\frac{FP}{k_B T} = \frac{1}{4} \left(1 - \frac{x}{L} + \frac{F}{S} \right)^{-2} - \frac{1}{4} + \frac{x}{L} - \frac{F}{S} \quad (1)$$

Here, F denotes the applied force, k_B is the Boltzmann constant, P is the persistence length, L is the contour length, S is the stretch modulus governing the extensibility. S is typically cited to be about 1200pN .

We define a new variable u satisfying:

$$\frac{1}{u} = 1 + \frac{F}{S} - \frac{x}{L} \quad (2)$$

using this variable, Eqn. 1 becomes

$$\begin{aligned} \frac{FP}{k_B T} &= \frac{1}{4} \left(\frac{1}{u} \right)^{-2} - \frac{1}{4} + 1 - \frac{1}{u} \\ 0 &= \frac{1}{4} u^2 + \frac{3}{4} - \frac{1}{u} - \frac{FP}{k_B T} \\ 0 &= u^3 + 4u \left(\frac{3}{4} - \frac{FP}{k_B T} \right) - 4 \end{aligned} \quad (3)$$

We note that this equation is of the form $u^3 + Au + B = 0$, which we can analytically solve by noting the Cardano's identity by making a binomial expansion of cubic power:

$$(a - b)^3 = a^3 - 3a^2b + 3ab^2 - b^3 \quad (4)$$

which can be rearranged to give

$$(a - b)^3 + 3ab(a - b) = a^3 - b^3 \quad (5)$$

We note that this is of the same form whose solution we are seeking, which we can achieve by assigning $u = a - b$, $A = 3ab$, $B = b^3 - a^3$. We can solve this latter system easily by the well-known quadratic formula following a simple substitution $b = A/3a$:

$$a^6 + Ba^3 - A^3/27 = 0 \quad (6)$$

$$\begin{aligned} a^3 &= \frac{1}{2} \left(-B \pm \sqrt{B^2 + 4A^3/27} \right) \\ a &= \sqrt[3]{\frac{1}{2} \left(-B \pm \sqrt{B^2 + 4A^3/27} \right)} \\ b &= \sqrt[3]{\frac{1}{2} \left(B \pm \sqrt{B^2 + 4A^3/27} \right)} \end{aligned} \quad (7)$$

Using this, we now can find the analytical expression of the variable u :

$$u(F) = \sqrt[3]{\frac{1}{2} \left(-B \pm \sqrt{B^2 + 4A^3/27} \right)} - \sqrt[3]{\frac{1}{2} \left(B \pm \sqrt{B^2 + 4A^3/27} \right)} \quad (8)$$

which we can directly substitute into Eqn 2 to find the extension as an explicit function of F :

$$x(F) = L \left(1 + \frac{F}{S} - \left[\sqrt[3]{\frac{1}{2} \left(-B \pm \sqrt{B^2 + 4A^3/27} \right)} - \sqrt[3]{\frac{1}{2} \left(B \pm \sqrt{B^2 + 4A^3/27} \right)} \right]^{-1} \right) \quad (9)$$

Note that for our case $B = -4$ and $A = 4(3/4 - FP/k_B T)$. For computational purposes, you can also verify that Eqn 9 is guaranteed to be real and the \pm sign choice is not of importance due to the symmetry.