J11T1 - DNA Molecule

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January 6, 2017

Consider a long molecule like DNA that is made out of two polymer strands, with links connecting the monomers between one strand and the other; let the number of links be N. Now imagine that we grab the ends of the two strands and pull them apart with a force F. In order to lengthen the segment that we are pulling on, we have to break links. Each time we break a link the energy of the molecule goes up by an amount Δ, the bond energy of each link. On the other hand each time we break a link, the ends we are pulling on move apart by a distance $2\ell_0$, where ℓ_0 is the distance between the links along one strand. Thus the energy of the molecule with n links broken is $E(n) = n(\Delta - 2F\ell_0)$.

(a) Find an equation that relates the mean number of broken links $\langle n \rangle$ at temperature T to the partition function Z.

Because they just give us an energy E in the problem, it's easy to work in the canonical ensemble, so our partition function Z is constructed the usual way

$$Z = \sum_{\text{all states } n} \exp\left(-\beta E_n\right)$$

The mean energy is,

$$\langle U \rangle = -\frac{\partial}{\partial \beta} \log Z$$

The mean energy can be related to the number of broken links,

$$\langle U \rangle = \langle n \rangle (\Delta - 2F\ell_0), \qquad \Rightarrow \qquad \langle n \rangle = \frac{\langle U \rangle}{\Delta - 2F\ell_0}$$

which means,

$$\boxed{\langle n \rangle = \frac{-1}{\Delta - 2F\ell_0} \frac{\partial \log Z}{\partial \beta}}$$

(b) Define $a = \left(\frac{\Delta - 2F\ell_0}{k_b T}\right)$. Evaluate the partition function Z. Show that in the limit of large N, the behavior of Z is very different depending on whether F is smaller or larger than a critical value F_c. What is value of and the physical meaning of F_c?

Using the substitution $-\beta E_n = -na$. This means that,

$$\begin{aligned} Z &= \sum_{n}^{N} \exp(-na) = 1 + \exp(-a) + \exp(-2a) + \cdots + \exp(-Na) = \frac{1 - \exp(-a(N+1))}{1 - \exp(-a)} \\ &\approx \frac{1}{1 - \exp(-a)} \end{aligned}$$

The approximation was taken as N gets large, and assuming that $F < F_c$ so that a remains positive. The critical force is computed from $a = 0$

$$F_c = \frac{\Delta}{2\ell_0}$$

which makes physical sense because this is when the force is larger than the chemical bond between the links. The partition function would blow up if $F \geq F_c$ because $-a(N+1)$ would be positive.

(c) Use your result for Z to calculate $\langle n \rangle$ in terms of a in the limit of large N.

For this problem $F < F_c$, otherwise all the links would be broken. Using expression in part (a),

$$\begin{aligned} \langle n \rangle &= \frac{1}{\Delta - 2F\ell_0} \frac{1}{1 - \exp(-a)} \left(\frac{\partial a}{\partial \beta} \right) \exp(-a) \\ &= \frac{\exp(-a)}{1 - \exp(-a)} = \boxed{\frac{1}{\exp\left(\frac{\Delta - 2F\ell_0}{k_b T}\right) - 1}} \end{aligned}$$

So in the limit $T \to 0$, we have no broken links. In the limit $T \to \infty$, all our links are broken. For some intermediate temperature, we have more broken links than if $F = 0$.