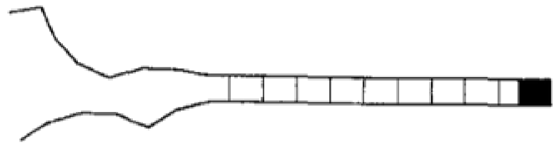
1. Today, we will use statistical mechanics to develop a zipper model commonly used in modeling DNA.



Consider a zipper model with the following properties:

- The zipper is at temperature T and consists of N links.
- Each link can be either closed with energy 0 or open with energy ε.
- When a link is closed, there is only one possible configuration. However, when a link is open, it can rotate freely, resulting in a degeneracy g.
- The zipper can only unzip from one end, meaning that link i can only be open if all preceding links $(0, 1, 2, \ldots, i-1)$ are also open.
- The final link is always closed to prevent the DNA from fully disconnecting.

Show that the average number of open links is given by:

$$\langle i \rangle = \frac{Nx^N}{x^N - 1} - \frac{x}{x-1}$$

where $x \equiv ge^{-\beta\varepsilon}$

Useful formula: The sum of a geometric series is given is:

$$\sum_{a=0}^{N} r^a = \frac{1 - r^{N+1}}{1 - r}, \quad \text{for } r \neq 1$$

We start from our partition function

$$Q = \sum_i e^{-\beta E_s}$$

We sum to $N-1$ since the last link is always closed. Each for a state i, each open link has degeneracy g, so the ith link will have g^i degenerate configurations. The energy E_i has i links open with energy ε each, so $E_i = i\varepsilon$

$$Q = \sum_{i=0}^{N-1} g^i e^{-\beta E_i} = \sum_{i=0}^{N-1} g^i e^{-\beta i \epsilon} = \sum_{i=0}^{N-1} \left[g e^{-\beta\epsilon} \right]^i$$

$$Q = \frac{1 - g e^{-N\beta\epsilon}}{1 - g e^{-\beta\epsilon}}$$

Now we use the definition $x \equiv g e^{-N\beta\epsilon}$

$$Q = \frac{1 - x^N}{1 - x}$$

To relate our partition function to average value of open links, recognize that i is related to energy, $E_i = i\varepsilon$, thus $\langle E_i \rangle = \langle i\varepsilon \rangle = \varepsilon \langle i \rangle$ since ε is a fixed value. Since $\langle E \rangle = -\frac{\partial \ln Q}{\partial \beta}$, we have:

$$\langle i \rangle = -\frac{1}{\epsilon}\frac{\partial}{\partial \beta} ln(Q)$$

Since we have the partition function, we can now solve this expression

$$\begin{aligned}
\langle i \rangle &= -\frac{1}{\epsilon}\frac{\partial}{\partial \beta} \ln(Q) \\
&= -\frac{1}{\epsilon}\frac{\partial}{\partial \beta} \ln\left(\frac{1 - x^N}{1 - x} \right) \\
&= -\frac{1}{\epsilon}\frac{\partial}{\partial \beta} \left[\ln(1 - x^N) - \ln(1 - x) \right] \\
&= -\frac{1}{\epsilon} \left[\frac{\frac{\partial(1-x^N)}{\partial\beta}}{1 - x^N} - \frac{\frac{\partial(1-x)}{\partial\beta}}{1 - x} \right] \\
&= -\frac{1}{\epsilon} \left[\frac{-N x^{N-1} \frac{\partial x}{\partial \beta}}{1 - x^N} - \frac{-\frac{\partial x}{\partial\beta}}{1 - x} \right] \\
&= -\frac{1}{\epsilon} \left[\frac{-N x^{N-1}(-\epsilon x)}{1 - x^N} - \frac{-(-\epsilon x)}{1 - x} \right] \\
&= -\frac{1}{\epsilon} \left[\frac{N\epsilon x^N}{1 - x^N} - \frac{\epsilon x}{1 - x} \right] = \boxed{\frac{N x^N}{x^N - 1} - \frac{x}{x - 1}}
\end{aligned}$$

Homework Problem 6

1. The partition function of a mixture of two ideal gases is given as:

$$Q(N_1, N_2, V, T) = \frac{[q_1(V,T)]^{N_1}}{N_1!} \frac{[q_2(V,T)]^{N_2}}{N_2!}$$

where $q_j(V,T) = \left(\frac{2\pi m_j k_{\mathrm{B}} T}{h^2}\right)^{3/2} V$.
Show that energy is an additive quantity, namely:

$$\langle E \rangle = \frac{3}{2}(N_1 + N_2) k_B T$$