Zipper problem (Kittel) Masatsugu Sei Suzuki Deaprtment of Physics, SUNY at Binghamton (Date: September 13, 2016)

As far as I know, a problem was first introduced in the exercise in a book of Kittel C. Kittel and H. Kroemer, Thermal physics. (WH Freeman, 1980). Since then this problem is called the zipper problem. We solve this problem using the canonical ensemble method.

A simple statistical physics model of the formation or unraveling of a long double-stranded biomolecule like DNA as a function of temperature is a zipper that has a maximum of N links. The chemistry of the links is such that each link can be closed with energy 0 or open with energy ε (>0) (i.e., it takes energy ε to break a link and open it). The zipper can



unzip only from one side (say from the left as shown in the figure) and the *n*th link from the left can open only if all the links to the left of it (1; 2; ...; n - 1) are already open. The *N*th link on the right is always closed.

(a) Using qualitative reasoning without mathematical calculation (but you need to explain your reasoning briefly), determine the average number of links $\langle n \rangle$ of the biomolecule in the limit of aveilt term embers T corresponding to h_{1}^{T} (1.2)

small temperatures T corresponding to $k_BT \ll \varepsilon$

(b)

Using qualitative reasoning without mathematical calculation (but you need to explain your reasoning briefly), determine the average number of links $\langle n \rangle$ in the limit of large

temperatures T corresponding to $k_B T >> \varepsilon$

((Solution))

We treat a molecular zipper of N parallel links that can be opened from one end. If the links, 1, 2, ..., (s-1) are all open, the energy required to open the *s*-link is ε . However, if all the preceeding links are not open, the energy required to open the *s*-link is infinite.

(a) The partition function is

$$Z_C = \sum_{s} e^{-\beta \varepsilon_s}$$

	Energy required	
No-link	open	0
Link-1	open	Е
Link-1,2	open	2 <i>ɛ</i>
Link-1, 2, 3	open	3ε
Link-1, 2,, s	open	SE

Then we have

$$\begin{split} Z_C &= \sum_{s=0}^{N-1} e^{-\beta \varepsilon_s} \\ &= 1 + e^{-\beta \varepsilon} + e^{-2\beta \varepsilon} + \ldots + e^{-(N-1)\beta \varepsilon} \\ &= \frac{1 - e^{-\beta N \varepsilon}}{1 - e^{-\beta \varepsilon}} \\ &= \frac{1 - x^N}{1 - x} \end{split}$$

Then the average number of open links is

$$\langle s \rangle = \sum_{s=0}^{N-1} \frac{1}{Z_C} s e^{-\beta s \varepsilon}$$
$$= \frac{1}{Z_C} \sum_{s=0}^{N-1} s e^{-\beta s \varepsilon}$$
$$= \frac{1}{Z_C} \sum_{s=0}^{N-1} s x^s$$

where

 $x = e^{-\beta\varepsilon}$. We also note that

$$Z_{C} = \sum_{s=0}^{N-1} e^{-\beta \varepsilon_{s}} = \sum_{s=0}^{N-1} x^{s}$$

$$\frac{\partial Z_C}{\partial x} = \sum_{s=0}^{N-1} s x^{s-1} = x^{-1} \sum_{s=0}^{N-1} s x^s$$

Then $\langle s \rangle$ is rewritten as

$$\langle s \rangle = \frac{x}{Z_C} \frac{\partial Z_C}{\partial x} = x \frac{\partial}{\partial x} \ln Z_C = \frac{x}{1-x} - \frac{Nx^N}{1-x^N}$$

In the limit of $\beta \varepsilon >> 1$ ($x = e^{-\beta \varepsilon} \ll 1$, low temperature limit)

$$\langle s \rangle = \frac{x}{1-x} = \frac{1}{e^{\beta \varepsilon} - 1} \approx e^{-\beta \varepsilon}$$

In the limit of $\beta \varepsilon \ll 1$ ($x = e^{-\beta \varepsilon} >> 1$, high temperature limit



REFERENCES

C. Kittel and H. Kroemer, Thermal physics. (WH Freeman, 1980)